

# IBM SPSS Modeler 17 Algorithms Guide



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# Preface

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# ***Adjusted Propensities Algorithms***

Adjusted propensity scores are calculated as part of the process of building the model, and will not be available otherwise. Once the model is built, it is then scored using data from the test or validation partition, and a new model to deliver adjusted propensity scores is constructed by analyzing the original model's performance on that partition. Depending on the type of model, one of two methods may be used to calculate the adjusted propensity scores.

## ***Model-Dependent Method***

For rule set and tree models, the following method is used:

1. Score the model on the test or validation partition.
2. **Tree models.** Calculate the frequency of each category at each tree node using the test/validation partition, reflecting the distribution of the target value in the records scored to that node.

**Rule set models.** Calculate the support and confidence of each rule using the test/validation partition, reflecting the model performance on the test/validation partition.

This results in a new rule set or tree model which is stored with the original model. Each time the original model is applied to new data, the new model can subsequently be applied to the raw propensity scores to generate the adjusted scores.

## ***General Purpose Method***

For other models, the following method is used:

1. Score the model on the test or validation partition to compute predicted values and predicted raw propensities.
2. Remove all records which have a missing value for the predicted or observed value.
3. Calculate the observed propensities as 1 for true observed values and 0 otherwise.
4. Bin records according to predicted raw propensity using 100 equal-count tiles.
5. Compute the mean predicted raw propensity and mean observed propensity for each bin.
6. Build a neural network with mean observed propensity as the target and predicted raw propensity as a predictor. For the neural network settings:

Use a random seed, value 0

Use the "quick" training method

Stop after 250 cycles

Do not use prevent overtraining option

Use expert mode

Quick Method Expert Options:

Use one hidden layer with 3 neurons and persistence set to 200

Learning Rates Expert Options:

Alpha 0.9

Initial Eta 0.3  
High Eta 0.1  
Eta decay 50  
Low Eta 0.01

The result is a neural network model that attempts to map raw propensity to a more accurate estimate which takes into account the original model's performance on the testing or validation partition. To calculate adjusted propensities at score time, this neural network is applied to the raw propensities obtained from scoring the original model.

# Anomaly Detection Algorithm

## Overview

The Anomaly Detection procedure searches for unusual cases based on deviations from the norms of their cluster groups. The procedure is designed to quickly detect unusual cases for data-auditing purposes in the exploratory data analysis step, prior to any inferential data analysis. This algorithm is designed for generic anomaly detection; that is, the definition of an anomalous case is not specific to any particular application, such as detection of unusual payment patterns in the healthcare industry or detection of money laundering in the finance industry, in which the definition of an anomaly can be well-defined.

## Primary Calculations

### Notation

The following notation is used throughout this chapter unless otherwise stated:

$ID$	The identity variable of each case in the data file.
$n$	The number of cases in the training data $X_{\text{train}}$ .
$X_{ok}, k = 1, \dots, K$	The set of input variables in the training data.
$M_k, k \in \{1, \dots, K\}$	If $X_{ok}$ is a continuous variable, $M_k$ represents the grand mean, or average of the variable across the entire training data.
$SD_k, k \in \{1, \dots, K\}$	If $X_{ok}$ is a continuous variable, $SD_k$ represents the grand standard deviation, or standard deviation of the variable across the entire training data.
$X_{K+1}$	A continuous variable created in the analysis. It represents the percentage of variables ( $k = 1, \dots, K$ ) that have missing values in each case.
$X_k, k = 1, \dots, K$	The set of processed input variables after the missing value handling is applied. For more information, see the topic “Modeling Stage” on p. 4.
$H$ , or the boundaries of $H$ : $[H_{\min}, H_{\max}]$	$H$ is the pre-specified number of cluster groups to create. Alternatively, the bounds $[H_{\min}, H_{\max}]$ can be used to specify the minimum and maximum numbers of cluster groups.
$n_h, h = 1, \dots, H$	The number of cases in cluster $h, h = 1, \dots, H$ , based on the training data.
$p_h, h = 1, \dots, H$	The proportion of cases in cluster $h, h = 1, \dots, H$ , based on the training data. For each $h, p_h = n_h/n$ .
$M_{hk}, k = 1, \dots, K+1, h = 1, \dots, H$	If $X_k$ is a continuous variable, $M_{hk}$ represents the cluster mean, or average of the variable in cluster $h$ based on the training data. If $X_k$ is a categorical variable, it represents the cluster mode, or most popular categorical value of the variable in cluster $h$ based on the training data.
$SD_{hk}, k \in \{1, \dots, K+1\}, h = 1, \dots, H$	If $X_k$ is a continuous variable, $SD_{hk}$ represents the cluster standard deviation, or standard deviation of the variable in cluster $h$ based on the training data.
$\{n_{hkj}\}, k \in \{1, \dots, K\}, h = 1, \dots, H, j = 1, \dots, J_k$	The frequency set $\{n_{hkj}\}$ is defined only when $X_k$ is a categorical variable. If $X_k$ has $J_k$ categories, then $n_{hkj}$ is the number of cases in cluster $h$ that fall into category $j$ .
$m$	An adjustment weight used to balance the influence between continuous and categorical variables. It is a positive value with a default of 6.
$VDI_k, k = 1, \dots, K+1$	The variable deviation index of a case is a measure of the deviation of variable value $X_k$ from its cluster norm.

GDI	The group deviation index GDI of a case is the log-likelihood distance $d(h, s)$ , which is the sum of all of the variable deviation indices $\{VDI_k, k = 1, \dots, K+1\}$ .
anomaly index	The anomaly index of a case is the ratio of the GDI to that of the average GDI for the cluster group to which the case belongs.
variable contribution measure	The variable contribution measure of variable $X_k$ for a case is the ratio of the $VDI_k$ to the case's corresponding GDI.
$pct_{anomaly}$ or $n_{anomaly}$	A pre-specified value $pct_{anomaly}$ determines the percentage of cases to be considered as anomalies. Alternatively, a pre-specified positive integer value $n_{anomaly}$ determines the number of cases to be considered as anomalies.
$cutpoint_{anomaly}$	A pre-specified cutpoint; cases with anomaly index values greater than $cutpoint_{anomaly}$ are considered anomalous.
$k_{anomaly}$	A pre-specified integer threshold $1 \leq k_{anomaly} \leq K+1$ determines the number of variables considered as the reasons that the case is identified as an anomaly.

## Algorithm Steps

This algorithm is divided into three stages:

**Modeling.** Cases are placed into cluster groups based on their similarities on a set of input variables. The clustering model used to determine the cluster group of a case and the sufficient statistics used to calculate the norms of the cluster groups are stored.

**Scoring.** The model is applied to each case to identify its cluster group and some indices are created for each case to measure the unusualness of the case with respect to its cluster group. All cases are sorted by the values of the anomaly indices. The top portion of the case list is identified as the set of anomalies.

**Reasoning.** For each anomalous case, the variables are sorted by its corresponding variable deviation indices. The top variables, their values, and the corresponding norm values are presented as the reasons why a case is identified as an anomaly.

### Modeling Stage

This stage performs the following tasks:

1. **Training Set Formation.** Starting with the specified variables and cases, remove any case with extremely large values (greater than  $1.0E+150$ ) on any continuous variable. If missing value handling is not in effect, also remove cases with a missing value on any variable. Remove variables with all constant nonmissing values or all missing values. The remaining cases and variables are used to create the anomaly detection model. Statistics output to pivot table by the procedure are based on this training set, but variables saved to the dataset are computed for all cases.
2. **Missing Value Handling (Optional).** For each input variable  $X_{ok}$ ,  $k = 1, \dots, K$ , if  $X_{ok}$  is a continuous variable, use all valid values of that variable to compute the grand mean  $M_k$  and grand standard deviation  $SD_k$ . Replace the missing values of the variable by its grand mean. If  $X_{ok}$  is a categorical variable, combine all missing values into a "missing value" category. This category is treated as a valid category. Denote the processed form of  $\{X_{ok}\}$  by  $\{X_k\}$ .

3. **Creation of Missing Value Pct Variable (Optional).** A new continuous variable,  $X_{K+1}$ , is created that represents the percentage of variables (both continuous and categorical) with missing values in each case.
4. **Cluster Group Identification.** The processed input variables  $\{X_k, k = 1, \dots, K+1\}$  are used to create a clustering model. The two-step clustering algorithm is used with noise handling turned on (see the TwoStep Cluster algorithm document for more information).
5. **Sufficient Statistics Storage.** The cluster model and the sufficient statistics for the variables by cluster are stored for the Scoring stage:
  - The grand mean  $M_k$  and standard deviation  $SD_k$  of each continuous variable are stored,  $k \in \{1, \dots, K+1\}$ .
  - For each cluster  $h = 1, \dots, H$ , store the size  $n_h$ . If  $X_k$  is a continuous variable, store the cluster mean  $M_{hk}$  and standard deviation  $SD_{hk}$  of the variable based on the cases in cluster  $h$ . If  $X_k$  is a categorical variable, store the frequency  $n_{hkj}$  of each category  $j$  of the variable based on the cases in cluster  $h$ . Also store the modal category  $M_{hk}$ . These sufficient statistics will be used in calculating the log-likelihood distance  $d(h, s)$  between a cluster  $h$  and a given case  $s$ .

### Scoring Stage

This stage performs the following tasks on scoring (testing or training) data:

1. **New Valid Category Screening.** The scoring data should contain the input variables  $\{X_{ok}, k = 1, \dots, K\}$  in the training data. Moreover, the format of the variables in the scoring data should be the same as those in the training data file during the Modeling Stage.
 

Cases in the scoring data are screened out if they contain a categorical variable with a valid category that does not appear in the training data. For example, if *Region* is a categorical variable with categories IL, MA and CA in the training data, a case in the scoring data that has a valid category FL for *Region* will be excluded from the analysis.
2. **Missing Value Handling (Optional).** For each input variable  $X_{ok}$ , if  $X_{ok}$  is a continuous variable, use all valid values of that variable to compute the grand mean  $M_k$  and grand standard deviation  $SD_k$ . Replace the missing values of the variable by its grand mean. If  $X_{ok}$  is a categorical variable, combine all missing values and put together a missing value category. This category is treated as a valid category.
3. **Creation of Missing Value Pct Variable (Optional depending on Modeling Stage).** If  $X_{K+1}$  is created in the Modeling Stage, it is also computed for the scoring data.
4. **Assign Each Case to its Closest Non-Noise Cluster.** The clustering model from the Modeling Stage is applied to the processed variables of the scoring data file to create a cluster ID for each case. Cases belonging to the noise cluster are reassigned to their closest non-noise cluster. See the TwoStep Cluster algorithm document for more information on the noise cluster.
5. **Calculate Variable Deviation Indices.** Given a case  $s$ , the closest cluster  $h$  is found. The variable deviation index  $VDI_k$  of variable  $X_k$  is defined as the contribution  $d_k(h, s)$  of the variable to its log-likelihood distance  $d(h, s)$ . The corresponding norm value is  $M_{hk}$ , which is the cluster sample mean of  $X_k$  if  $X_k$  is continuous, or the cluster mode of  $X_k$  if  $X_k$  is categorical.

6. **Calculate Group Deviation Index.** The group deviation index GDI of a case is the log-likelihood distance  $d(h, s)$ , which is the sum of all the variable deviation indices  $\{VDI_k, k = 1, \dots, K+1\}$ .
7. **Calculate Anomaly Index and Variable Contribution Measures.** Two additional indices are calculated that are easier to interpret than the group deviation index and the variable deviation index.

The anomaly index of a case is an alternative to the GDI, which is computed as the ratio of the case's GDI to the average GDI of the cluster to which the case belongs. Increasing values of this index correspond to greater deviations from the average and indicate better anomaly candidates.

A variable's variable contribution measure of a case is an alternative to the VDI, which is computed as the ratio of the variable's VDI to the case's GDI. This is the proportional contribution of the variable to the deviation of the case. The larger the value of this measure, the greater the variable's contribution to the deviation.

### **Odd Situations**

#### **Zero Divided by Zero**

The situation in which the GDI of a case is zero and the average GDI of the cluster that the case belongs to is also zero is possible if the cluster is a singleton or is made up of identical cases and the case in question is the same as the identical cases. Whether this case is considered as an anomaly or not depends on whether the number of identical cases that make up the cluster is large or small. For example, suppose that there is a total of 10 cases in the training and two clusters are resulted in which one cluster is a singleton; that is, made up of one case, and the other has nine cases. In this situation, the case in the singleton cluster should be considered as an anomaly as it does not belong to the larger cluster. One way to calculate the anomaly index in this situation is to set it as the ratio of average cluster size to the size of the cluster  $h$ , which is:

$$\frac{n/H}{n_h}$$

Following the 10 cases example, the anomaly index for the case belonging to the singleton cluster would be  $(10/2)/1 = 5$ , which should be large enough for the algorithm to catch it as an anomaly. In this situation, the variable contribution measure is set to  $1/(K+1)$ , where  $(K+1)$  is the number of processed variables in the analysis.

#### **Nonzero Divided by Zero**

The situation in which the GDI of a case is nonzero but the average GDI of the cluster that the case belongs to is 0 is possible if the corresponding cluster is a singleton or is made up of identical cases and the case in question is not the same as the identical cases. Suppose that case  $i$  belongs to cluster  $h$ , which has a zero average GDI; that is,  $\text{average}(GDI)_h = 0$ , but the GDI between case  $i$  and cluster  $h$  is nonzero; that is,  $GDI(i, h) \neq 0$ . One choice for the anomaly index calculation of case  $i$  could be to set the denominator as the weighted average GDI over all other clusters if this value is not 0; else set the calculation as the ratio of average cluster size to the size of cluster  $h$ . That is,

$$\left\{ \begin{array}{ll} \frac{GDI(i,h)}{\frac{1}{(n-n_h)} \sum_{s=1, \neq h}^H n_s \cdot average(GDI)_s} & \text{if } \frac{1}{(n-n_h)} \sum_{s=1, \neq h}^H n_s \cdot average(GDI)_s \neq 0 \\ \frac{n/H}{n_h} & \text{otherwise} \end{array} \right.$$

This situation triggers a warning that the case is assigned to a cluster that is made up of identical cases.

### **Reasoning Stage**

Every case now has a group deviation index and anomaly index and a set of variable deviation indices and variable contribution measures. The purpose of this stage is to rank the likely anomalous cases and provide the reasons to suspect them of being anomalous.

1. **Identify the Most Anomalous Cases.** Sort the cases in descending order on the values of the anomaly index. The top pct<sub>anomaly</sub> % (or alternatively, the top n<sub>anomaly</sub>) gives the anomaly list, subject to the restriction that cases with an anomaly index less than or equal to cutpoint<sub>anomaly</sub> are not considered anomalous.
2. **Provide Reasons for Considering a Case Anomalous.** For each anomalous case, sort the variables by their corresponding VDI<sub>k</sub> values in descending order. The top k<sub>anomaly</sub> variable names, its value (of the corresponding original variable X<sub>ok</sub>), and the norm values are displayed as reasoning.

### **Blank Handling**

Blanks and missing values are handled in model building as described in “Algorithm Steps ” on p. 4, based on user settings.

### **Generated Model/Scoring**

The Anomaly Detection generated model can be used to detect anomalous records in new data based on patterns found in the original training data. For each record scored, an anomaly score is generated and a flag indicating anomaly status and/or the anomaly score are appended as new fields

### **Predicted Values**

For each record, the anomaly score is calculated as described in “Scoring Stage ” on p. 5, based on the cluster model created when the model was built. If anomaly flags were requested, they are determined as described in “Reasoning Stage ” on p. 7.

### **Blank Handling**

In the generated model, blanks are handled according to the setting used in building the model. For more information, see the topic “Scoring Stage ” on p. 5.



# Apriori Algorithms

## Overview

Apriori is an algorithm for extracting association rules from data. It constrains the search space for rules by discovering frequent itemsets and only examining rules that are made up of frequent itemsets (Agrawal and Srikant, 1994).

Apriori deals with items and itemsets that make up transactions. **Items** are flag-type conditions that indicate the presence or absence of a particular thing in a specific transaction. An **itemset** is a group of items which may or may not tend to co-occur within transactions.

IBM® SPSS® Modeler uses Christian Borgelt's Apriori implementation. Full details on this implementation can be obtained at

<http://fuzzy.cs.uni-magdeburg.de/~borgelt/doc/apriori/apriori.html>.

## Deriving Rules

Apriori proceeds in two stages. First it identifies frequent itemsets in the data, and then it generates rules from the table of frequent itemsets.

## Frequent Itemsets

The first step in Apriori is to identify frequent itemsets. A frequent itemset is defined as an itemset with support greater than or equal to the user-specified minimum support threshold  $s_{\min}$ . The support of an itemset is the number of records in which the itemset is found divided by the total number of records.

The algorithm begins by scanning the data and identifying the single-item itemsets (i.e. individual items, or itemsets of length 1) that satisfy this criterion. Any single items that do not satisfy the criterion are not be considered further, because adding an infrequent item to an itemset will always result in an infrequent itemset.

Apriori then generates larger itemsets recursively using the following steps:

- ▶ Generate a candidate set of itemsets of length  $k$  (containing  $k$  items) by combining existing itemsets of length  $(k - 1)$ :

For every possible pair of frequent itemsets  $p$  and  $q$  with length  $(k - 1)$ , compare the first  $(k - 2)$  items (in lexicographic order); if they are the same, and the last item in  $q$  is (lexicographically) greater than the last item in  $p$ , add the last item in  $q$  to the end of  $p$  to create a new candidate itemset with length  $k$ .

- ▶ Prune the candidate set by checking every  $(k - 1)$  length subset of each candidate itemset; all subsets must be frequent itemsets, or the candidate itemset is infrequent and is removed from further consideration.
- ▶ Calculate the support of each itemset in the candidate set, as

$$\text{support} = \frac{N_i}{N}$$

where  $N_i$  is the number of records that match the itemset and  $N$  is the number of records in the training data. (Note that this definition of itemset support is different from the definition used for rule support. )

- ▶ Itemsets with support  $\geq s_{\min}$  are added to the list of frequent itemsets.
- ▶ If any frequent itemsets of length  $k$  were found, and  $k$  is less than the user-specified maximum rule size  $k_{\max}$ , repeat the process to find frequent itemsets of length  $(k + 1)$ .

## Generating Rules

When all frequent itemsets have been identified, the algorithm extracts rules from the frequent itemsets. For each frequent itemset  $L$  with length  $k > 1$ , the following procedure is applied:

- ▶ Calculate all subsets  $A$  of length  $(k - 1)$  of the itemset such that all the fields in  $A$  are input fields and all the other fields in the itemset (those that are *not* in  $A$ ) are output fields. Call the latter subset  $\tilde{A}$ . (In the first iteration this is just one field, but in later iterations it can be multiple fields.)
- ▶ For each subset  $A$ , calculate the evaluation measure (rule confidence by default) for the rule  $A \Rightarrow \tilde{A}$  as described below.
- ▶ If the evaluation measure is greater than the user-specified threshold, add the rule to the rule table, and, if the length  $k'$  of  $A$  is greater than 1, test all possible subsets of  $A$  with length  $(k' - 1)$

## Evaluation Measures

Apriori offers several evaluation measures for determining which rules to retain. The different measures will emphasize different aspects of the rules, as detailed in the *IBM® SPSS® Modeler User's Guide*. Values are calculated based on the prior confidence and the posterior confidence, defined as

$$C_{prior} = \frac{c}{N}$$

and

$$C_{posterior} = \frac{r}{a}$$

where  $c$  is the support of the consequent,  $a$  is the support of the antecedent,  $r$  is the support of the conjunction of the antecedent and the consequent, and  $N$  is the number of records in the training data.

**Rule Confidence.** The default evaluation measure for rules is simply the posterior confidence of the rule,

$$e = C_{posterior}$$

**Confidence Difference (Absolute Confidence Difference to Prior).** This measure is based on the simple difference of the posterior and prior confidence values,

$$e = |C_{posterior} - C_{prior}|$$

**Confidence Ratio (Difference of Confidence Quotient to 1).** This measure is based on the ratio of posterior confidence to prior confidence,

$$e = 1 - \min \left( \frac{C_{posterior}}{C_{prior}}, \frac{C_{prior}}{C_{posterior}} \right)$$

**Information Difference (Information Difference to Prior).** This measure is based on the information gain criterion, similar to that used in building C5.0 trees. The calculation is

$$e = \frac{r \cdot \log \left( \frac{r}{a \cdot c} \right) + (a - r) \log \left( \frac{a-r}{a \cdot \bar{c}} \right) + (c - r) \log \left( \frac{c-r}{\bar{a} \cdot c} \right) + (1 - a - c + r) \log \left( \frac{1-a-c+r}{\bar{a} \cdot \bar{c}} \right)}{\log(2)}$$

where  $r$  is the rule support,  $a$  is the antecedent support,  $c$  is the consequent support,  $\bar{a} = 1 - a$  is the complement of antecedent support, and  $\bar{c} = 1 - c$  is the complement of consequent support.

**Normalized Chi-square (Normalized Chi-squared Measure).** This measure is based on the chi-squared statistical test for independence of categorical data, and is calculated as

$$e = \frac{(a \cdot c - r)^2}{a \cdot \bar{a} \cdot c \cdot \bar{c}}$$

## Blank Handling

Blanks are ignored by the Apriori algorithm. The algorithm will handle records containing blanks for input fields, but such a record will not be considered to match any rule containing one or more of the fields for which it has blank values.

## Effect of Options

**Minimum rule support/confidence.** These values place constraints on which rules may be entered into the table. Only rules whose support and confidence values exceed the specified values can be entered into the rule table.

**Maximum number of antecedents.** This determines the maximum number of antecedents that will be examined for any rule. When the number of conditions in the antecedent part of the rule equals the specified value, the rule will not be specialized further.

**Only true values for flags.** If this option is selected, rules with values of *false* will not be considered for either input or output fields.

**Optimize Speed/Memory.** This option controls the trade-off between speed of processing and memory usage. Selecting Speed will cause Apriori to use condition values directly in the frequent itemset table, and to load the transactions into memory, if possible. Selecting Memory will cause Apriori to use pointers into a value table in the frequent itemset table. Using pointers in

the frequent itemset table reduces the amount of memory required by the algorithm for large problems, but it also involves some additional work to reference and dereference the pointers during model building. The Memory option also causes Apriori to process transactions from the file rather than loading them into memory.

## ***Generated Model/Scoring***

The Apriori algorithm generates an unrefined rule node. To create a model for scoring new data, the unrefined rule node must be refined to generate a ruleset node. Details of scoring for generated ruleset nodes are given below.

### ***Predicted Values***

Predicted values are based on the rules in the ruleset. When a new record is scored, it is compared to the rules in the ruleset. How the prediction is generated depends on the user's setting for Ruleset Evaluation in the stream options.

- **Voting.** This method attempts to combine the predictions of all of the rules that apply to the record. For each record, all rules are examined and each rule that applies to the record is used to generate a prediction. The sum of confidence figures for each predicted value is computed, and the value with the greatest confidence sum is chosen as the final prediction.
- **First hit.** This method simply tests the rules in order, and the first rule that applies to the record is the one used to generate the prediction.

There is a **default rule**, which specifies an output value to be used as the prediction for records that don't trigger any other rules from the ruleset. For rulesets derived from decision trees, the value for the default rule is the modal (most prevalent) output value in the overall training data. For association rulesets, the default value is specified by the user when the ruleset is generated from the unrefined rule node.

### ***Confidence***

Confidence calculations also depend on the user's Ruleset Evaluation stream options setting.

- **Voting.** The confidence for the final prediction is the sum of the confidence values for rules triggered by the current record that give the winning prediction divided by the number of rules that fired for that record.
- **First hit.** The confidence is the confidence value for the first rule in the ruleset triggered by the current record.

If the default rule is the only rule that fires for the record, it's confidence is set to 0.5.

### ***Blank Handling***

Blanks are ignored by the algorithm. The algorithm will handle records containing blanks for input fields, but such a record will not be considered to match any rule containing one or more of the fields for which it has blank values.

# Automated Data Preparation Algorithms

The goal of automated data preparation is to prepare a dataset so as to generally improve the training speed, predictive power, and robustness of models fit to the prepared data.

These algorithms do not assume which models will be trained post-data preparation. At the end of automated data preparation, we output the predictive power of each recommended predictor, which is computed from a linear regression or naïve Bayes model, depending upon whether the target is continuous or categorical.

## Notation

The following notation is used throughout this chapter unless otherwise stated:

$X$	A continuous or categorical variable
$x_i$	Value of the variable $X$ for case $i$ .
$f_i$	Frequency weight for case $i$ . Non-integer positive values are rounded to the nearest integer. If there is no frequency weight variable, then all $f_i = 1$ . If the frequency weight of a case is zero, negative or missing, then this case will be ignored.
$w_i$	Analysis weight for case $i$ . If there is no analysis weight variable, then all $w_i = 1$ . If the analysis weight of a case is zero, negative or missing, then this case will be ignored.
$n$	Number of cases in the dataset
$N_X$	$\sum_{i=1}^n f_i I(x_i \text{ is not missing})$ , where $I(\text{expression})$ is the indicator function taking value 1 when the expression is true, 0 otherwise.
$W_X$	$\sum_{i=1}^n f_i w_i I(x_i \text{ is not missing})$
$N_{XY}$	$\sum_{i=1}^n f_i I(x_i \text{ and } y_i \text{ are not missing})$
$W_{XY}$	$\sum_{i=1}^n f_i w_i I(x_i \text{ and } y_i \text{ are not missing})$
$\bar{x}$	The mean of variable $X$ , $\frac{1}{W_X} \sum_{i=1}^n f_i w_i x_i I(x_i \text{ is not missing})$
$M_X^r$	$\sum_{i=1}^n f_i w_i (x_i - \bar{x})^r$
$\bar{y}$	$\frac{1}{W_{XY}} \sum_{i=1}^n f_i w_i x_i I(x_i \text{ and } y_i \text{ are not missing})$
$M_{XY}$	$\sum_{i=1}^n f_i w_i (x_i - \bar{x}_y) (y_i - \bar{y}_x)$

### A note on missing values

Listwise deletion is used in the following sections:

- “Univariate Statistics Collection ” on p. 15

- “Basic Variable Screening ” on p. 17
- “Measurement Level Recasting ” on p. 17
- “Missing Value Handling ” on p. 19
- “Outlier Identification and Handling ” on p. 18
- “Continuous Predictor Transformations ” on p. 20
- “Target Handling ” on p. 21
- “Reordering Categories ” on p. 25
- “Unsupervised Merge ” on p. 30

Pairwise deletion is used in the following sections:

- “Bivariate Statistics Collection ” on p. 22
- “Supervised Merge ” on p. 26
- “Supervised Binning ” on p. 32
- “Feature Selection and Construction ” on p. 32
- “Predictive Power ” on p. 35

#### ***A note on frequency weight and analysis weight***

The frequency weight variable is treated as a case replication weight. For example if a case has a frequency weight of 2, then this case will count as 2 cases.

The analysis weight would adjust the variance of cases. For example if a case  $x_i$  of a variable  $X$  has an analysis weight  $w_i$ , then we assume that  $x_i \sim N\left(\mu, \frac{\sigma^2}{w_i}\right)$ .

Frequency weights and analysis weights are used in automated preparation of other variables, but are themselves left unchanged in the dataset.

## ***Date/Time Handling***

### ***Date Handling***

If there is a date variable, we extract the date elements (year, month and day) as ordinal variables. If requested, we also calculate the number of elapsed days/months/years since the user-specified reference date (default is the current date). Unless specified by the user, the “best” unit of duration is chosen as follows:

1. If the minimum number of elapsed days is less than 31, then we use days as the best unit.
2. If the minimum number of elapsed days is less than 366 but larger than or equal to 31, we use months as the best unit. The number of months between two dates is calculated based on average number of days in a month (30.4375):  $months = days / 30.4375$ .
3. If the minimum number of elapsed days is larger than or equal to 366, we use years as the best unit. The number of years between two dates is calculated based on average number of days in a year (365.25):  $years = days / 365.25$ .

Once the date elements are extracted and the duration is obtained, then the original date variable will be excluded from the rest of the analysis.

### **Time Handling**

If there is a time variable, we extract the time elements (second, minute and hour) as ordinal variables. If requested, we also calculate the number of elapsed seconds/minutes/hours since the user-specified reference time (default is the current time). Unless specified by the user, the “best” unit of duration is chosen as follows:

1. If the minimum number of elapsed seconds is less than 60, then we use seconds as the best unit.
2. If the minimum number of elapsed seconds is larger than or equal to 60 but less than 3600, we use minutes as the best unit.
3. If the minimum number of elapsed seconds is larger than or equal to 3600, we use hours as the best unit.

Once the elements of time are extracted and time duration is obtained, then original time predictor will be excluded.

## **Univariate Statistics Collection**

### **Continuous Variables**

For each continuous variable, we calculate the following statistics:

- Number of missing values:  $N_X^{missing} = \sum_{i=1}^n f_i I(x_i \text{ is missing})$
- Number of valid values:  $N_X$
- Minimum value:  $\min_i x_i$
- Maximum value:  $\max_i x_i$
- Mean, standard deviation, skewness. (see below)
- The number of distinct values  $I$ .
- The number of cases for each distinct value  $s_i$ :  $c_i = \sum_{j=1}^n f_j I(x_j = s_i)$
- Median: If the distinct values of  $X$  are sorted in ascending order,  $s_1 < s_2 < \dots < s_I$ , then the median can be computed by  $Median(X) = \min \left\{ s_i : \frac{cc_i}{N_X} \geq 0.5 \right\}$ , where  $cc_i = \sum_{j=1}^i c_j$ .

*Note:* If the number of distinct values is larger than a threshold (default is 5), we stop updating the number of distinct values and the number of cases for each distinct value. Also we do not calculate the median.

### **Categorical Numeric Variables**

For each categorical numeric variable, we calculate the following statistics:

- Number of missing values:  $N_X^{missing} = \sum_{i=1}^n f_i I(x_i \text{ is missing})$

- Number of valid values:  $N_X$
- Minimum value:  $\min_i x_i$  (only for ordinal variables)
- Maximum value:  $\max_i x_i$  (only for ordinal variables)
- The number of categories.
- The counts of each category.
- Mean, Standard deviation, Skewness (only for ordinal variables). (see below)
- Mode (only for nominal variables). If several values share the greatest frequency of occurrence, then the mode with the smallest value is used.
- Median (only for ordinal variables): If the distinct values of  $X$  are sorted in ascending order,  $s_1 < s_2 < \dots < s_I$ , then the median can be computed by  $Median(X) = \min \left\{ s_i : \frac{cc_i}{N_X} \geq 0.5 \right\}$ , where  $cc_i = \sum_{j=1}^i c_i$ .

*Notes:*

1. If an ordinal predictor has more categories than a specified threshold (default 10), we stop updating the number of categories and the number of cases for each category. Also we do not calculate mode and median.
2. If a nominal predictor has more categories than a specified threshold (default 100), we stop collecting statistics and just store the information that the variable had more than threshold categories.

### **Categorical String Variables**

For each string variable, we calculate the following statistics:

- Number of missing values:  $N_X^{missing} = \sum_{i=1}^n f_i I(x_i \text{ is missing})$
- Number of valid values:  $N_X$
- The number of categories.
- Counts of each category.
- Mode: If several values share the greatest frequency of occurrence, then the mode with the smallest value is used.

*Note:* If a string predictor has more categories than a specified threshold (default 100), we stop collecting statistics and just store the information that the predictor had more than threshold categories.

### **Mean, Standard Deviation, Skewness**

We calculate mean, standard deviation and skewness by updating moments.

1. Start with  $N_X^{(0)} = W_X^{(0)} = \bar{x}^{(0)} = M_X^{2(0)} = M_X^{3(0)} = 0$ .
2. For  $j=1, \dots, n$  compute:
 
$$N_X^{(j)} = N_X^{(j-1)} + f_j I(x_j \text{ is not missing})$$

$$\begin{aligned}
W_X^{(j)} &= W_X^{(j-1)} + f_j w_j I(x_j \text{ is not missing}) \\
v_j &= \frac{f_j w_j}{W_X^{(j)}} (x_j - \bar{x}^{(j-1)}) \\
\bar{x}^{(j)} &= \bar{x}^{(j-1)} + v_j \\
M_X^{2(j)} &= M_X^{2(j-1)} + \frac{W_X^{(j)} W_X^{(j-1)}}{f_j w_j} v_j^2 \\
M_X^{3(j)} &= M_X^{3(j-1)} - 3v_j M_X^{2(j-1)} + \frac{W_X^{(j)} W_X^{(j-1)}}{(f_j w_j)^2} (W_X^{(j)} - 2f_j w_j) v_j^3
\end{aligned}$$

3. After the last case has been processed, compute:

$$\text{Mean: } \bar{x} = \bar{x}^{(n)}$$

$$\text{Standard deviation: } sd = \sqrt{\frac{M_X^{2(n)}}{N_X - 1}}$$

$$\text{Skewness: } skew = \frac{\frac{N_X}{(N_X - 2)} \frac{1}{(N_X - 1)} M_X^{3(n)}}{sd^3}$$

If  $N_X \leq 2$  or  $sd^2 < 10^{-20}$ , then skewness is not calculated.

## Basic Variable Screening

1. If the percent of missing values is greater than a threshold (default is 50%), then exclude the variable from subsequent analysis.
2. For continuous variables, if the maximum value is equal to minimum value, then exclude the variable from subsequent analysis.
3. For categorical variables, if the mode contains more cases than a specified percentage (default is 95%), then exclude the variable from subsequent analysis.
4. If a string variable has more categories than a specified threshold (default is 100), then exclude the variable from subsequent analysis.

## Checkpoint 1: Exit?

This checkpoint determines whether the algorithm should be terminated. If, after the screening step:

1. The target (if specified) has been removed from subsequent analysis, or
2. All predictors have been removed from subsequent analysis,

then terminate the algorithm and generate an error.

## Measurement Level Recasting

For each continuous variable, if the number of distinct values is less than a threshold (default is 5), then it is recast as an ordinal variable.

For each numeric ordinal variable, if the number of categories is greater than a threshold (default is 10), then it is recast as a continuous variable.

*Note:* The continuous-to-ordinal threshold must be less than the ordinal-to-continuous threshold.

## Outlier Identification and Handling

In this section, we identify outliers in continuous variables and then set the outlying values to a cutoff or to a missing value. The identification is based on the robust mean and robust standard deviation which are estimated by supposing that the percentage of outliers is no more than 5%.

### Identification

1. Compute the mean and standard deviation from the raw data. Split the continuous variable into non-intersecting intervals:  $I_i = (\bar{x} + (i - 1) \times sd_w, \bar{x} + i \times sd_w]$ ,  $i = -3, -2, \dots, 2, 3, 4$ , where  $I_{-3} = (-\infty, \bar{x} - 3sd_w]$ ,  $I_4 = (\bar{x} + 3sd_w, +\infty]$  and  $sd_w = sd \times \sqrt{\frac{N_X - 1}{W_X - 1}}$ .
2. Calculate univariate statistics in each interval:

$$N_{I_i} = \sum_{j=1}^n f_j I(x_j \in I_i), W_{I_i} = \sum_{i=1}^n f_i w_i I(x_j \in I_i)$$

$$\bar{x}_{I_i} = \frac{\sum_{j=1}^n f_j w_j x_j I(x_j \in I_i)}{W_{I_i}}, M_{I_i}^2 = \sum_{j=1}^n f_j w_j (x_j - \bar{x}_{I_i})^2 I(x_j \in I_i)$$

3. Let  $l = -3$ ,  $r = 4$ , and  $p = 0$ .
4. Between two tail intervals  $I_l$  and  $I_r$ , find one interval with the least number of cases.
5. If  $N_{I_l} \leq N_{I_r}$ , then  $p_{current} = \frac{N_{I_l}}{N_X}$ . Check if  $p + p_{current}$  is less than a threshold  $p_{threshold}$  (default is 0.05). If it does, then  $p = p + p_{current}$  and  $l = l + 1$ , go to step 4; otherwise, go to step 6.

Else  $p_{current} = \frac{N_{I_r}}{N_X}$ . Check if  $p + p_{current}$  is less than a threshold,  $p_{threshold}$ . If it is, then  $p = p + p_{current}$  and  $r = r - 1$ , go to step 4; otherwise, go to step 6.

6. Compute the robust mean  $\bar{x}_{robust}$  and robust standard deviation  $sd_{robust}$  within the range  $(\bar{x} + (l - 1) \times sd, \bar{x} + r \times sd]$ . See below for details.
7. If  $x_i$  satisfies the conditions:

$$\sqrt{w_i} (x_i - \bar{x}_{robust}) < -cutoff \times sd_{robust} \text{ or } \sqrt{w_i} (x_i - \bar{x}_{robust}) > cutoff \times sd_{robust}$$

where *cutoff* is positive number (default is 3), then  $x_i$  is detected as an outlier.

### Handling

Outliers will be handled using one of following methods:

- Trim outliers to cutoff values. If  $\sqrt{w_i} (x_i - \bar{x}_{robust}) < -cutoff \times sd_{robust}$  then replace  $x_i$  by  $\bar{x}_{robust} - cutoff \times sd_{robust} / \sqrt{w_i}$ , and if  $\sqrt{w_i} (x_i - \bar{x}_{robust}) > cutoff \times sd_{robust}$  then replace  $x_i$  by  $\bar{x}_{robust} + cutoff \times sd_{robust} / \sqrt{w_i}$ .
- Set outliers to missing values.

### Update Univariate Statistics

After outlier handling, we perform a data pass to calculate univariate statistics for each continuous variable, including the number of missing values, minimum, maximum, mean, standard deviation, skewness, and number of outliers.

### Robust Mean and Standard Deviation

Robust mean and standard deviation within the range  $(\bar{x} + (l - 1) \times sd, \bar{x} + r \times sd]$  are calculated as follows:

$$\bar{x}_{robust} = \frac{\sum_{i=l}^r W_{I_i} \bar{x}_{I_i}}{\sum_{i=l}^r W_{I_i}}$$

and

$$sd_{robust} = \sqrt{\frac{M_{robust}^2}{\sum_{i=l}^r N_{I_i} - 1}}$$

where  $M_{robust}^2 = \sum_{i=l}^r A_{I_i}$  and  $A_{I_i} = M_{I_i}^2 + W_{I_i}(\bar{x}_{robust} - \bar{x}_{I_i})^2$ .

## Missing Value Handling

**Continuous variables.** Missing values are replaced by the mean, and the following statistics are updated:

- Standard deviation:  $sd \times \sqrt{\frac{N_X - 1}{N - 1}}$ , where  $N = N_X + N_X^{missing}$ .
- Skewness:  $skew \times \frac{L_1}{L_2}$ , where  $L_1 = \left(\frac{N}{N-2}\right)\left(\frac{N_X-2}{N_X}\right)$  and  $L_2 = \sqrt{\frac{N_X-1}{N-1}}$
- The number of missing values:  $N_X^{missing} = 0$
- The number of valid values:  $N_X = N$

**Ordinal variables.** Missing values are replaced by the median, and the following statistics are updated:

- The number of cases in the median category:  $c_{median} + N_X^{missing}$ , where  $c_{median}$  is the original number of cases in the median category.
- The number of missing values:  $N_X^{missing} = 0$
- The number of valid values:  $N_X = N$

**Nominal variables.** Missing values are replaced by the mode, and the following statistics are updated:

- The number of cases in the modal category:  $c_{mode} + N_X^{missing}$ , where  $c_{mode}$  is the original number of cases in the modal category.
- The number of missing values:  $N_X^{missing} = 0$
- The number of valid values:  $N_X = N$

## Continuous Predictor Transformations

We transform a continuous predictor so that it has the user-specified mean  $\bar{x}_{user}$  (default 0) and standard deviation  $sd_{user}$  (default 1) using the z-score transformation, or minimum  $\min_{user}$  (default 0) and maximum  $\max_{user}$  (default 100) value using the min-max transformation.

### Z-score Transformation

Suppose a continuous variable has mean  $\bar{x}$  and standard deviation  $sd$ . The z-score transformation is

$$x'_i = \frac{sd_{user}}{sd} \times (x_i - \bar{x}) + \bar{x}_{user}$$

where  $x'_i$  is the transformed value of continuous variable  $X$  for case  $i$ .

Since we do not take into account the analysis weight in the rescaling formula, the rescaled values  $x'_i$  follow a normal distribution  $N\left(\bar{x}_{user}, \frac{sd_{user}^2}{w_i}\right)$ .

#### Update univariate statistics

After a z-score transformation, the following univariate statistics are updated:

- Number of missing values:  $N_{X'}^{missing} = N_X^{missing}$
- Number of valid values:  $N_{X'} = N_X$
- Minimum value:  $\min(x'_i) = \frac{sd_{user}}{sd} \times (\min x_i - \bar{x}) + \bar{x}_{user}$
- Maximum value:  $\max(x'_i) = \frac{sd_{user}}{sd} \times (\max x_i - \bar{x}) + \bar{x}_{user}$
- Mean:  $\bar{x}' = \bar{x}_{user}$
- Standard deviation:  $sd(x') = sd_{user}$
- Skewness:  $skew(x') = skew(x)$

### Min-Max Transformation

Suppose a continuous variable has a minimum value  $\min x_i$  and a maximum value  $\max x_i$ . The min-max transformation is

$$x'_i = \frac{\max_{user} - \min_{user}}{\max x_i - \min x_i} \times (x_i - \min x_i) + \min_{user}$$

where  $x'_i$  is the transformed value of continuous variable  $X$  for case  $i$ .

#### Update univariate statistics

After a min-max transformation, the following univariate statistics are updated:

- The number of missing values:  $N_{X'}^{missing} = N_X^{missing}$

- The number of valid values:  $N_{X'} = N_X$
- Minimum value:  $\min(x'_i) = \min_{user}$
- Maximum value:  $\max(x'_i) = \max_{user}$
- Mean:  $\bar{x}' = \frac{\max_{user} - \min_{user}}{\max x_i - \min x_i} \times (\bar{x} - \min x_i) + \min_{user}$
- Standard deviation:  $sd(x') = \frac{\max_{user} - \min_{user}}{\max x_i - \min x_i} \times sd$
- Skwness:  $skew(x') = skew(x)$

## Target Handling

### Nominal Target

For a nominal target, we rearrange categories from lowest to highest counts. If there is a tie on counts, then ties will be broken by ascending sort or lexical order of the data values.

### Continuous Target

The transformation proposed by Box and Cox (1964) transforms a continuous variable into one that is more normally distributed. We apply the Box-Cox transformation followed by the  $z$  score transformation so that the rescaled target has the user-specified mean and standard deviation.

**Box-Cox transformation.** This transforms a non-normal variable  $Y$  to a more normally distributed variable:

$$g_i(\lambda) = g(y_i, \lambda) = \begin{cases} \frac{(y_i - c)^\lambda - 1}{\lambda} & \lambda \neq 0 \\ \ln(y_i - c) & \lambda = 0 \end{cases}$$

where  $y_i, i = 1, 2, \dots, n$  are observations of variable  $Y$ , and  $c$  is a constant such that all values  $y_i - c$  are positive. Here, we choose  $c = \min(Y) - 1$ .

The parameter  $\lambda$  is selected to maximize the log-likelihood function:

$$L(\lambda) = -\frac{N_Y}{2} \ln \left[ \frac{N_Y - 1}{N_Y} (sd(g(\lambda)))^2 \right] + (\lambda - 1) \sum_{i=1}^n f_i \ln(y_i - c)$$

where  $(sd(g(\lambda)))^2 = \frac{1}{N_Y - 1} \sum_{i=1}^n f_i w_i (g_i(\lambda_j) - \bar{g}(\lambda_j))^2$  and  $\bar{g}(\lambda) = \frac{1}{W_Y} \sum_{i=1}^n f_i w_i g_i(\lambda)$ .

We perform a grid search over a user-specified finite set  $[a, b]$  with increment  $s$ . By default  $a = -3$ ,  $b = 3$ , and  $s = 0.5$ .

The algorithm can be described as follows:

1. Compute  $\lambda_j = a + (j - 1) * s$  where  $j$  is an integer such that  $a \leq \lambda_j \leq b$ .

2. For each  $\lambda_j$ , compute the following statistics:

$$\text{Mean: } \bar{g}(\lambda_j) = \frac{1}{W_Y} \sum_{i=1}^n f_i w_i g_i(\lambda_j)$$

$$\text{Standard deviation: } sd(g(\lambda_j)) = \sqrt{\frac{1}{N_Y - 1} \sum_{i=1}^n f_i w_i (g_i(\lambda_j) - \bar{g}(\lambda_j))^2}$$

$$\text{Skewness: } skew(g(\lambda_j)) = \frac{\frac{N_Y}{(N_Y - 2)} \frac{1}{(N_Y - 1)} \sum_{i=1}^n f_i w_i (g_i(\lambda_j) - \bar{g}(\lambda_j))^3}{sd(g(\lambda_j))^3}$$

$$\text{Sum of logarithm transformation: } \sum_{i=1}^n f_i \ln(y_i - c)$$

3. For each  $\lambda_j$ , compute the log-likelihood function  $L(\lambda_j)$ . Find the value of  $j$  with the largest log-likelihood function, breaking ties by selecting the smallest value of  $\lambda_j$ . Also find the corresponding statistics  $\bar{g}(\lambda^*)$ ,  $sd(g(\lambda^*))$  and  $skew(g(\lambda^*))$ .
4. Transform target to reflect user's mean  $\bar{y}_{user}$  (default is 0) and standard deviation  $sd_{user}$  (default is 1):

$$y'_i = \frac{sd_{user}}{sd(g(\lambda^*))} \times (g_i(\lambda^*) - \bar{g}(\lambda^*)) + \bar{y}_{user}$$

$$\text{where } \bar{g}(\lambda^*) = \frac{1}{W_Y} \sum_{i=1}^n f_i w_i g_i(\lambda^*) \text{ and } sd(g(\lambda^*)) = \sqrt{\frac{1}{N_Y - 1} \sum_{i=1}^n f_i w_i (g_i(\lambda^*) - \bar{g}(\lambda^*))^2}.$$

**Update univariate statistics.** After Box-Cox and Z-score transformations, the following univariate statistics are updated:

- Minimum value:  $\frac{sd_{user}}{sd(g(\lambda^*))} \times (g(\min(y_i) - c, \lambda^*) - \bar{g}(\lambda^*)) + \bar{y}_{user}$
- Maximum value:  $\frac{sd_{user}}{sd(g(\lambda^*))} \times (g(\max(y_i) - c, \lambda^*) - \bar{g}(\lambda^*)) + \bar{y}_{user}$
- Mean:  $\bar{y}_{user}$
- Standard deviation:  $sd_{user}$
- Skewness:  $skew(g(\lambda^*))$

## Bivariate Statistics Collection

For each target/predictor pair, the following statistics are collected according to the measurement levels of the target and predictor.

### **Continuous target or no target and all continuous predictors**

If there is a continuous target and some continuous predictors, then we need to calculate the covariance and correlations between all pairs of continuous variables. If there is no continuous target, then we only calculate the covariance and correlations between all pairs of continuous predictors. We suppose there are there are  $m$  continuous variables, and denote the covariance matrix as  $C_{m \times m}$ , with element  $c_{ij}$ , and the correlation matrix as  $R_{m \times m}$ , with element  $r_{ij}$ .

We define the covariance between two continuous variables  $X$  and  $Y$  as

$$c_{XY} = \frac{1}{N_{XY} - 1} \sum_{i=1}^n f_i w_i (x_i - \bar{x}_y) (y_i - \bar{y}_x)$$

where  $\bar{x}_y = \frac{1}{W_{XY}} \sum_{i=1}^n x_i I(x_i \text{ and } y_i \text{ are not missing})$  and  $\bar{y}_x = \frac{1}{W_{XY}} \sum_{i=1}^n y_i I(x_j \text{ and } y_j \text{ are not missing})$ .

The covariance can be computed by a provisional means algorithm:

1. Start with  $N_{XY}^{(0)} = W_{XY}^{(0)} = \bar{x}_y = \bar{y}_x = M_{XY}^{(0)} = 0$ .

2. For  $j=1, \dots, n$  compute:

$$N_{XY}^{(j)} = N_{XY}^{(j-1)} + f_j I(x_j \text{ and } y_j \text{ are not missing})$$

$$W_{XY}^{(j)} = W_{XY}^{(j-1)} + f_j w_j I(x_j \text{ and } y_j \text{ are not missing})$$

$$v_{xj} = \frac{f_j w_j}{W_{XY}^{(j)}} (x_j - \bar{x}_y)$$

$$\bar{x}_y = \bar{x}_y + v_{xj}$$

$$v_{yj} = \frac{f_j w_j}{W_{XY}^{(j)}} (y_j - \bar{y}_x)$$

$$\bar{y}_x = \bar{y}_x + v_{yj}$$

$$M_{XY}^{(j)} = M_{XY}^{(j-1)} + (x_j - \bar{x}_y) (y_j - \bar{y}_x) \left( f_j w_j - \frac{(f_j w_j)^2}{W_{XY}^{(j)}} \right)$$

After the last case has been processed, we obtain:

$$M_{XY} = M_{XY}^{(n)} = \sum_{i=1}^n f_i w_i (x_i - \bar{x}_y) (y_i - \bar{y}_x)$$

3. Compute bivariate statistics between  $X$  and  $Y$ :

Number of valid cases:  $N_{XY}$

$$\text{Covariance: } c_{XY} = \frac{M_{XY}}{N_{XY} - 1}$$

$$\text{Correlation: } r_{XY} = \frac{c_{XY}}{\sqrt{c_{XX}} \sqrt{c_{YY}}}$$

*Note:* If there are no valid cases when pairwise deletion is used, then we let  $c_{XY} = 0$  and  $r_{XY} = 0$ .

### **Categorical target and all continuous predictors**

For a categorical target  $Y$  with values  $i = 1, 2, \dots, J$  and a continuous predictor  $X$  with values  $x_1, \dots, x_n$ , the bivariate statistics are:

Mean of  $X$  for each  $Y=i, i=1, \dots, J$ :

$$\bar{x}_{\cdot i} = \frac{\sum_{j=1}^n f_j w_j x_j I(y_j = i)}{\sum_{j=1}^n f_j w_j I(y_j = i)}$$

Sum of squared errors of  $X$  for each  $Y=i, i=1, \dots, J$ :

$$M_{.i}^2 = \sum_{j=1}^n f_j w_j (x_j - \bar{x}_{.i})^2 I(y_j = i)$$

Sum of frequency weight for each  $Y=i, i=1, \dots, J$ :

$$N_{.i} = \sum_{j=1}^n f_j I(y_j = i \wedge x_j \text{ is not missing})$$

Number of invalid cases

$$N_{XY} = \sum_{i=1}^J N_{.i}$$

Sum of weights (frequency weight times analysis weight) for each  $Y=i, i=1, \dots, J$ :

$$W_{.i} = \sum_{j=1}^n f_j w_j I(y_j = i \wedge x_j \text{ is not missing})$$

### **Continuous target and all categorical predictors**

For a continuous target  $Y$  and a categorical predictor  $X$  with values  $i=1, \dots, J$ , the bivariate statistics include:

Mean of  $Y$  conditional upon  $X$ :

$$\bar{y}_x = \frac{\sum_{i=1}^J \sum_{j=1}^n f_j w_j y_j I(x_j = i)}{\sum_{i=1}^J \sum_{j=1}^n f_j w_j I(x_j = i)}$$

Sum of squared errors of  $Y$ :

$$M_{X.}^2 = \sum_{j=1}^n f_j w_j (y_j - \bar{y}_x)^2$$

Mean of  $Y$  for each  $X = i, i=1, \dots, J$ :

$$\bar{y}_i = \frac{\sum_{j=1}^n f_j w_j y_j I(x_j = i)}{\sum_{j=1}^n f_j w_j I(x_j = i)}$$

Sum of squared errors of  $Y$  for each  $X = i, i=1, \dots, J$ :

$$M_{i.}^2 = \sum_{j=1}^n f_j w_j (y_j - \bar{y}_{i.})^2 I(x_j = i)$$

Sum of frequency weights for  $X = i, i=1, \dots, J$ :

$$N_{i.} = \sum_{j=1}^n f_j I(x_j = i \wedge y_j \text{ is not missing})$$

Sum of weights (frequency weight times analysis weight) for  $X = i, i=1, \dots, J$ :

$$W_{i.} = \sum_{j=1}^n f_j w_j I(x_j = i \wedge y_j \text{ is not missing})$$

### **Categorical target and all categorical predictors**

For a categorical target  $Y$  with values  $j=1, \dots, J$  and a categorical predictor  $X$  with values  $i=1, \dots, I$ , then bivariate statistics are:

Sum of frequency weights for each combination of  $x_k = i$  and  $y_k = j$ :

$$N_{ij} = \sum_{k=1}^n f_k I(x_k = i \wedge y_k = j)$$

Sum of weights (frequency weight times analysis weight) for each combination of  $x_k = i$  and  $y_k = j$ :

$$W_{ij} = \sum_{k \in 1}^n f_k w_k I(x_k = i \wedge y_k = j)$$

## **Categorical Variable Handling**

In this step, we use univariate or bivariate statistics to handle categorical predictors.

### **Reordering Categories**

For a nominal predictor, we rearrange categories from lowest to highest counts. If there is a tie on counts, then ties will be broken by ascending sort or lexical order of the data values. The new field values start with 0 as the least frequent category. Note that the new field will be numeric even if the original field is a string. For example, if a nominal field's data values are "A", "A", "A", "B", "C", "C", then automated data preparation would recode "B" into 0, "C" into 1, and "A" into 2.

## Identify Highly Associated Categorical Features

If there is a target in the data set, we select a ordinal/nominal predictor if its  $p$ -value is not larger than an alpha-level  $\alpha_{selection}$  (default is 0.05). See “P-value Calculations ” on p. 27 for details of computing these  $p$ -values.

Since we use pairwise deletion to handle missing values when we collect bivariate statistics, we may have some categories with zero cases; that is,  $N_i = 0$  for a category  $i$  of a categorical predictor. When we calculate  $p$ -values, these categories will be excluded.

If there is only one category or no category after excluding categories with zero cases, we set the  $p$ -value to be 1 and this predictor will not be selected.

## Supervised Merge

We merge categories of an ordinal/nominal predictor using a supervised method that is similar to a Chaid Tree with one level of depth.

1. Exclude all categories with zero case count.
2. If  $X$  has 0 categories, merge all excluded categories into one category, then stop.
3. If  $X$  has 1 category, go to step 7.
4. Else, find the allowable pair of categories of  $X$  that is most similar. This is the pair whose test statistic gives the largest  $p$ -value with respect to the target. An allowable pair of categories for an ordinal predictor is two adjacent categories; for a nominal predictor it is any two categories. Note that for an ordinal predictor, if categories between the  $i$ th category and  $j$ th categories are excluded because of zero cases, then the  $i$ th category and  $j$ th categories are two adjacent categories. See “P-value Calculations ” on p. 27 for details of computing these  $p$ -values.
5. For the pair having the largest  $p$ -value, check if its  $p$ -value is larger than a specified alpha-level  $\alpha_{selection}$  (default is 0.05). If it does, this pair is merged into a single compound category and at the same time we calculate the bivariate statistics of this new category. Then a new set of categories of  $X$  is formed. If it does not, then go to step 6.
6. Go to step 3.
7. For an ordinal predictor, find the maximum value in each new category. Sort these maximum values in ascending order. Suppose we have  $r$  new categories, and the maximum values are:  $i_1 < i_2 < \dots < i_r$ , then we get the merge rule as: the first new category will contain all original categories such that  $X \leq i_1$ , the second new category will contain all original categories such that  $i_1 < X \leq i_2, \dots$ , and the last new category will contain all original categories such that  $X > i_{r-1}$ .

For a nominal predictor, all categories excluded at step 1 will be merged into the new category with the lowest count. If there are ties on categories with the lowest counts, then ties are broken by selecting the category with the smallest value by ascending sort or lexical order of the original category values which formed the new categories with the lowest counts.

**Bivariate statistics calculation of new category**

When two categories are merged into a new category, we need to calculate the bivariate statistics of this new category.

**Scale target.** If the categories  $i$  and  $i'$  can be merged based on  $p$ -value, then the bivariate statistics should be calculated as:

$$N_{i,i'} = N_i + N_{i'}$$

$$W_{i,i'} = W_i + W_{i'}$$

$$\bar{y}_{i,i'} = \bar{y}_i + \frac{W_{i'}}{W_{i,i'}} (\bar{y}_{i'} - \bar{y}_i)$$

$$M_{i,i'}^2 = M_i^2 + M_{i'}^2 + W_i (\bar{y}_{i,i'} - \bar{y}_i)^2 + W_{i'} (\bar{y}_{i,i'} - \bar{y}_{i'})^2$$

**Categorical target.** If the categories  $i$  and  $i'$  can be merged based on  $p$ -value, then the bivariate statistics should be calculated as:

$$N_{i,i'j} = N_{ij} + N_{i'j}$$

$$W_{i,i'j} = W_{ij} + W_{i'j}$$

**Update univariate and bivariate statistics**

At the end of the supervised merge step, we calculate the bivariate statistics for each new category. For univariate statistics, the counts for each new category will be sum of the counts of each original categories which formed the new category. Then we update other statistics according to the formulas in “Univariate Statistics Collection” on p. 15, though note that the statistics only need to be updated based on the new categories and the numbers of cases in these categories.

**P-value Calculations**

Each  $p$ -value calculation is based on the appropriate statistical test of association between the predictor and target.

**Scale target**

We calculate an  $F$  statistic:

$$F = \frac{\sum_{i=1}^I W_i (\bar{y}_i - \bar{y}_x)^2 / (I - 1)}{\sum_{i=1}^I M_i^2 / (\sum_{i=1}^I N_i - I)}$$

$$\text{where } \bar{y}_x = \frac{\sum_{i=1}^I W_i \bar{y}_i}{\sum_{i=1}^I W_i}.$$

Based on  $F$  statistics, the  $p$ -value can be derived as

$$p = \Pr \left( F \left( I - 1, \sum_{i=1}^I N_i - I \right) > F \right)$$

where  $F \left( I - 1, \sum_{i=1}^I N_i - I \right)$  is a random variable following a  $F$  distribution with  $I - 1$  and  $\sum_{i=1}^I N_i - I$  degrees of freedom.

At the merge step we calculate the  $F$  statistic and  $p$ -value between two categories  $i$  and  $i'$  of  $X$  as

$$F = \frac{W_i (\bar{y}_i - \bar{y}_{i,i'})^2 + W_{i'} (\bar{y}_{i'} - \bar{y}_{i,i'})^2}{(M_i^2 + M_{i'}^2) / (N_i + N_{i'} - 2)}$$

$$p = \Pr (F (1, N_i + N_{i'} - 2) > F)$$

where  $\bar{y}_{i,i'}$  is the mean of  $Y$  for a new category  $i, i'$  merged by  $i$  and  $i'$ :

$$\bar{y}_{i,i'} = \bar{y}_i + \frac{W_{i'}}{W_i + W_{i'}} (\bar{y}_{i'} - \bar{y}_i)$$

and  $F (I - 1, N_i + N_{i'} - 2)$  is a random variable following a  $F$  distribution with 1 and  $N_i + N_{i'} - 2$  degrees of freedom.

### **Nominal target**

The null hypothesis of independence of  $X$  and  $Y$  is tested. First a contingency (or count) table is formed using classes of  $Y$  as columns and categories of the predictor  $X$  as rows. Then the expected cell frequencies under the null hypothesis are estimated. The observed cell frequencies and the expected cell frequencies are used to calculate the Pearson chi-squared statistic and the  $p$ -value:

$$X^2 = \sum_{j=1}^J \sum_{i=1}^I \frac{(N_{ij} - \hat{m}_{ij})^2}{\hat{m}_{ij}}$$

where  $N_{ij} = \sum_{k \in D} f_k I(x_k = i \wedge y_k = j)$  is the observed cell frequency and  $\hat{m}_{ij}$  is the estimated expected cell frequency for cell  $(x_k = i, y_k = j)$  following the independence model. If  $\hat{m}_{ij} = 0$ , then  $\frac{(N_{ij} - \hat{m}_{ij})^2}{\hat{m}_{ij}} = 0$ . How to estimate  $\hat{m}_{ij}$  is described below.

The corresponding  $p$ -value is given by  $p = \Pr (\chi_d^2 > X^2)$ , where  $\chi_d^2$  follows a chi-squared distribution with  $d = (J - 1)(I - 1)$  degrees of freedom.

When we investigate whether two categories  $i$  and  $i'$  of  $X$  can be merged, the Pearson chi-squared statistic is revised as

$$X^2 = \sum_{j=1}^J \left( \frac{(N_{ij} - \hat{m}_{ij})^2}{\hat{m}_{ij}} + \frac{(N_{i'j} - \hat{m}_{i'j})^2}{\hat{m}_{i'j}} \right)$$

and the  $p$ -value is given by  $p = \Pr(\chi_{J-1}^2 > X^2)$ .

### **Ordinal target**

Suppose there are  $I$  categories of  $X$ , and  $J$  ordinal categories of  $Y$ . Then the null hypothesis of the independence of  $X$  and  $Y$  is tested against the row effects model (with the rows being the categories of  $X$  and columns the classes of  $Y$ ) proposed by Goodman (1979). Two sets of expected cell frequencies,  $\hat{m}_{ij}$  (under the hypothesis of independence) and  $\hat{m}_{ij}$  (under the hypothesis that the data follow a row effects model), are both estimated. The likelihood ratio statistic is

$$H^2 = 2 \sum_{i=1}^I \sum_{j=1}^J H_{ij}^2$$

where

$$H_{ij}^2 = \begin{cases} \hat{m}_{ij} \ln \left( \frac{\hat{m}_{ij}}{\hat{m}_{ij}} \right) \hat{m}_{ij} / \hat{m}_{ij} > 0 \\ 0 & \text{else} \end{cases}$$

The  $p$ -value is given by  $p = \Pr(\chi_{I-1}^2 > H^2)$ .

### **Estimated expected cell frequencies (independence assumption)**

If analysis weights are specified, the expected cell frequency under the null hypothesis of independence is of the form

$$m_{ij} = \bar{w}_{ij}^{-1} \alpha_i \beta_j$$

where  $\alpha_i$  and  $\beta_j$  are parameters to be estimated, and  $\bar{w}_{ij} = \frac{W_{ij}}{N_{ij}}$  if  $N_{ij} > 0$ , otherwise  $\bar{w}_{ij} = 1$ .

Parameter estimates  $\hat{\alpha}_i$ ,  $\hat{\beta}_j$ , and hence  $\hat{m}_{ij}$ , are obtained from the following iterative procedure.

1.  $k = 0$ ,  $\alpha_i^{(0)} = \beta_j^{(0)} = 1$ ,  $m_{ij}^{(0)} = \bar{w}_{ij}^{-1}$
2.  $\alpha_i^{(k+1)} = \frac{N_{i.}}{\sum_j \bar{w}_{ij}^{-1} \beta_j^{(k)}} = \alpha_i^{(k)} \frac{N_{i.}}{\sum_j m_{ij}^{(k)}}$
3.  $\beta_j^{(k+1)} = \frac{N_{.j}}{\sum_i \bar{w}_{ij}^{-1} \alpha_i^{(k+1)}}$
4.  $m_{ij}^{(k+1)} = \bar{w}_{ij}^{-1} \alpha_i^{(k+1)} \beta_j^{(k+1)}$

5. If  $\max_{i,j} \left| m_{ij}^{(k+1)} - m_{ij}^{(k)} \right| < \epsilon$  (default is 0.001) or the number of iterations is larger than a threshold (default is 100), stop and output  $\alpha_i^{(k+1)}, \beta_j^{(k+1)}$  and  $m_{ij}^{(k+1)}$  as the final estimates  $\hat{\alpha}_i, \hat{\beta}_j, \hat{m}_{ij}$ . Otherwise,  $k = k + 1$  and go to step 2.

### **Estimated expected cell frequencies (row effects model)**

In the row effects model, scores for classes of  $Y$  are needed. By default,  $s_j^*$  (the order of a class of  $Y$ ) is used as the class score. These orders will be standardized via the following linear transformation such that the largest score is 100 and the lowest score is 0.

$$s_j = 100 (s_j^* - s_{\min}^*) / (s_{\max}^* - s_{\min}^*)$$

Where  $s_{\min}^*$  and  $s_{\max}^*$  are the smallest and largest order, respectively.

The expected cell frequency under the row effects model is given by

$$m_{ij} = \bar{w}_{ij}^{-1} \alpha_i \beta_j \gamma_i$$

where  $\bar{s} = \sum_{j=1}^J W_{.j} s_j / \sum_{j=1}^J W_{.j}$ , in which  $W_{.j} = \sum_i W_{ij}$ , and  $\alpha_i, \beta_j$ , and  $\gamma_i$  are unknown parameters to be estimated.

Parameter estimates  $\hat{\alpha}_i, \hat{\beta}_j, \hat{\gamma}_i$  and hence  $\hat{m}_{ij}$  are obtained from the following iterative procedure.

1.  $k = 0, \alpha_i^{(0)} = \beta_j^{(0)} = \gamma_i^{(0)} = 1, m_{ij}^{(0)} = \bar{w}_{ij}^{-1}$
2.  $\alpha_i^{(k+1)} = \frac{N_{.j}}{\sum_j \bar{w}_{ij}^{-1} \beta_j^{(k)} (\gamma_i^{(k)})^{(s_j - \bar{s})}} = \alpha_i^{(k)} \frac{N_{.j}}{\sum_j m_{ij}^{(k)}}$
3.  $\beta_j^{(k+1)} = \frac{N_{.j}}{\sum_i \bar{w}_{ij}^{-1} \alpha_i^{(k+1)} (\gamma_i^{(k)})^{(s_j - \bar{s})}}$
4.  $m_{ij}^* = \bar{w}_{ij}^{-1} \alpha_i^{(k+1)} \beta_j^{(k+1)} (\gamma_i^{(k)})^{(s_j - \bar{s})}, G_i = 1 + \frac{\sum_j (s_j - \bar{s})(N_{.j} - m_{ij}^*)}{\sum_j (s_j - \bar{s})^2 m_{ij}^*}$
5.  $\gamma_i^{(k+1)} = \begin{cases} \gamma_i^{(k)} G_i & G_i > 0 \\ \gamma_i^{(k)} & \text{otherwise} \end{cases}$
6.  $m_{ij}^{(k+1)} = \bar{w}_{ij}^{-1} \alpha_i^{(k+1)} \beta_j^{(k+1)} (\gamma_i^{(k+1)})^{(s_j - \bar{s})}$
7. If  $\max_{i,j} \left| m_{ij}^{(k+1)} - m_{ij}^{(k)} \right| < \epsilon$  (default is 0.001) or the number of iterations is larger than a threshold (default is 100), stop and output  $\alpha_i^{(k+1)}, \beta_j^{(k+1)}, \gamma_i^{(k+1)}$  and  $m_{ij}^{(k+1)}$  as the final estimates  $\hat{\alpha}_i, \hat{\beta}_j, \hat{\gamma}_i, \hat{m}_{ij}$ . Otherwise,  $k = k + 1$  and go to step 2.

## **Unsupervised Merge**

If there is no target, we merge categories based on counts. Suppose that  $X$  has  $I$  categories which are sorted in ascending order. For an ordinal predictor, we sort it according to its values, while for nominal predictor we rearrange categories from lowest to highest count, with ties broken

by ascending sort or lexical order of the data values. Let  $c_i$  be the number of cases for the  $i$ th category, and  $N_X$  be the total number of cases for  $X$ . Then we use the equal frequency method to merge sparse categories.

1. Start with  $j_1 = j_2 = 1$  and  $g=1$ .
2. If  $j_1 > I$ , go to step 5.
3. If  $\sum_{i=j_1}^{j_2} c_i < [b\% \times N_X]$ , then  $j_2 = j_2 + 1$ ; otherwise the original categories  $j_1, j_1 + 1, \dots, j_2$  will be merged into the new category  $g$  and let  $j_1 = j_2 + 1, j_2 = j_1$  and  $g = g + 1$ , then go to step 2.
4. If  $j_2 \geq I$ , then merge categories using one of the following rules:
  - i) If  $g = 1$ , then categories  $1, 2, \dots, I - 1$  will be merged into category  $g$  and  $I$  will be left unmerged.
  - ii) If  $g=2$ , then  $j_1, j_1 + 1, \dots, I$  will be merged into category  $g=2$ .
  - iii) If  $g>2$ , then  $j_1, j_1 + 1, \dots, I$  will be merged into category  $g - 1$ .
 If  $j_2 < I$ , then go to step 3.
5. Output the merge rule and merged predictor.

After merging, one of the following rules holds:

- Neither the original category nor any category created during merging has fewer than  $[b\% \times N_X]$  cases, where  $b$  is a user-specified parameter satisfying  $1 < b < 100$  (default is 10) and  $[x]$  denotes the nearest integer of  $x$ .
- The merged predictor has only two categories.

**Update univariate statistics.** When original categories  $j_1, j_1 + 1, \dots, j_2$  are merged into one new category, then the number of cases in this new category will be  $\sum_{i=j_1}^{j_2} c_i$ . At the end of the merge step, we get new categories and the number of cases in each category. Then we update other statistics according to the formulas in “Univariate Statistics Collection” on p. 15, though note that the statistics only need to be updated based on the new categories and the numbers of cases in these categories.

## Continuous Predictor Handling

Continuous predictor handling includes supervised binning when the target is categorical, predictor selection when the target is continuous and predictor construction when the target is continuous or there is no target in the dataset.

After handling continuous predictors, we collect univariate statistics for derived or constructed predictors according to the formulas in “Univariate Statistics Collection” on p. 15. Any derived predictors that are constant, or have all missing values, are excluded from further analysis.

## Supervised Binning

If there is a categorical target, then we will transform each continuous predictor to an ordinal predictor using supervised binning. Suppose that we have already collected the bivariate statistics between the categorical target and a continuous predictor. Using the notations introduced in “Bivariate Statistics Collection” on p. 22, the homogeneous subset will be identified by the Scheffe method as follows:

If  $|\bar{x}_{.i} - \bar{x}_{.j}| \leq c_{critical}$  then  $\bar{x}_{.i}$  and  $\bar{x}_{.j}$  will be a homogeneous subset, where  $c_{critical} = \max(\bar{x}_{.i}) - \min(\bar{x}_{.i})$  if  $N_{XY} = J$ ; otherwise  $c_{critical} = R * C$ , where  $R = \sqrt{2(J-1)F_{1-\alpha}(J-1, N_{XY}-J)}$  and  $C = MS \times \sqrt{\frac{\sum_{i=1}^J 1/W_{.i}}{J}}$ ,  $MS = \sqrt{\frac{\sum_{i=1}^J M_{.i}^2}{N_{XY}-J}}$ .

The supervised algorithm follows:

1. Sort the means  $\bar{x}_{.i}$  in ascending order, denote as  $\bar{x}_{.(1)} \leq \bar{x}_{.(2)} \leq \dots \leq \bar{x}_{.(J)}$ .
2. Start with  $i=1$  and  $q=J$ .
3. If  $|\bar{x}_{.(q)} - \bar{x}_{.(i)}| \leq c_{critical}$ , then  $\{\bar{x}_{.(i)}, \dots, \bar{x}_{.(q)}\}$  can be considered a homogeneous subset. At the same time we compute the mean and standard deviation of this subset:  $\bar{x}_{.(i,q)} = \frac{\sum_{k=i}^q W_{.(k)} \bar{x}_{.(k)}}{\sum_{k=i}^q W_{.(k)}}$  and  $sd_{.(i,q)} = \sqrt{\frac{M_{(i,q)}^2}{\sum_{k=i}^q N_{.(k)} - 1}}$ , where  $M_{(i,q)}^2 = \sum_{k=i}^q A_{.(k)}$  and  $A_{.(k)} = M_{.(k)}^2 + W_{.(k)} (\bar{x}_{.(i,q)} - \bar{x}_{.(k)})^2$ , then set  $i = q + 1$  and  $q = J$ ; Otherwise  $q = q - 1$ .
4. If  $i \leq J$ , go to step 3.
5. Else compute the cut point of bins. Suppose we have  $r \leq J$  homogeneous subsets and we assume that the means of these subsets are  $\bar{x}_{.(1)}^*, \bar{x}_{.(2)}^*, \dots, \bar{x}_{.(r)}^*$ , and standard deviations are  $sd_{.(1)}^*, sd_{.(2)}^*, \dots, sd_{.(r)}^*$ , then the cut points between the  $i$ th and  $(i+1)$ th homogeneous subsets are computed as  $cut_i = \bar{x}_{(i)}^* + \frac{sd_{(i)}^* + \epsilon}{(sd_{(i)}^* + sd_{(i+1)}^* + 2\epsilon)} (\bar{x}_{(i+1)}^* - \bar{x}_{(i)}^*)$ .
6. Output the binning rules. Category 1:  $X \leq cut_1$ ; Category 2:  $cut_1 < X \leq cut_2$ ; ...; Category  $r$ :  $cut_{r-1} < X$ .

## Feature Selection and Construction

If there is a continuous target, we perform predictor selection using  $p$ -values derived from the correlation or partial correlation between the predictors and the target. The selected predictors are grouped if they are highly correlated. In each group, we will derive a new predictor using principal component analysis. However, if there is no target, we will do not implement predictor selection.

To identify highly correlated predictors, we compute the correlation between a scale and a group as follows: suppose that  $X$  is a continuous predictor and continuous predictors  $X_1, X_2, \dots, X_m$  form a group  $G$ . Then the correlation between  $X$  and group  $G$  is defined as:

$$r_{XG} = \min \{|r_{XX_i}|, X_i \in G\}$$

where  $r_{XX_i}$  is correlation between  $X$  and  $X_i$ .

Let  $\alpha_{group}$  be the correlation level at which the predictors are identified as groups. The predictor selection and predictor construction algorithm is as follows:

1. (Target is continuous and predictor selection is in effect ) If the  $p$ -value between a continuous predictor and target is larger than a threshold (default is 0.05), then we remove this predictor from the correlation matrix and covariance matrix. See “Correlation and Partial Correlation ” on p. 34 for details on computing these  $p$ -values.
2. Start with  $\alpha_{group} = 0.9$  and  $i=1$ .
3. If  $\alpha_{group} \leq 0.1$ , stop and output all the derived predictors, their source predictors and coefficient of each source predictor. In addition, output the remaining predictors in the correlation matrix.
4. Find the two most correlated predictors such that their correlation in absolute value is larger than  $\alpha_{group}$ , and put them in group  $i$ . If there are no predictors to be chosen, then go to step 9.
5. Add one predictor to group  $i$  such that the predictor is most correlated with group  $i$  and the correlation is larger than  $\alpha_{group}$ . Repeat this step until the number of predictors in group  $i$  is greater than a threshold (default is 5) or there is no predictor to be chosen.
6. Derive a new predictor from the group  $i$  using principal component analysis. For more information, see the topic “Principal Component Analysis ” on p. 33.
7. (Both predictor selection and predictor construction are in effect) Compute partial correlations between the other continuous predictors and the target, controlling for values of the new predictor. Also compute the  $p$ -values based on partial correlation. See “Correlation and Partial Correlation ” on p. 34 for details on computing these  $p$ -values. If the  $p$ -value based on partial correlation between a continuous predictor and continuous target is larger than a threshold (default is 0.05), then remove this predictor from the correlation and covariance matrices.
8. Remove predictors that are in the group from the correlation matrix. Then let  $i=i+1$  and go to step 4.
9.  $\alpha_{group} = \alpha_{group} - 0.1$ , then go to step 3.

*Notes:*

- If only predictor selection is needed, then only step 1 is implemented. If only predictor construction is needed, then we implement all steps except step 1 and step 7. If both predictor selection and predictor construction are needed, then all steps are implemented.
- If there are ties on correlations when we identify highly correlated predictors, the ties will be broken by selecting the predictor with the smallest index in dataset.

## ***Principal Component Analysis***

Let  $X_1, X_2, \dots, X_m$  be  $m$  continuous predictors. Principal component analysis can be described as follows:

1. Input  $C_{m \times m}$ , the covariance matrix of  $X_1, X_2, \dots, X_m$ .
2. Calculate the eigenvectors and eigenvalues of the covariance matrix. Sort the eigenvalues (and corresponding eigenvectors) in descending order,  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_m$ .

3. Derive new predictors. Suppose the elements of the first component  $v_1$  are  $v_{11}, v_{12}, \dots, v_{1m}$ , then the new derived predictor is  $\frac{v_{11}}{\sqrt{\lambda_1}}X_1 + \frac{v_{12}}{\sqrt{\lambda_1}}X_2 + \dots + \frac{v_{1m}}{\sqrt{\lambda_1}}X_m$ .

## Correlation and Partial Correlation

### Correlation and P-value

Let  $r_{XY}$  be the correlation between continuous predictor  $X$  and continuous target  $Y$ , then the  $p$ -value is derived from the  $t$  test:

$$p = \Pr(|t(N_{XY} - 2)| > t)$$

where  $t(N_{XY} - 2)$  is a random variable with a  $t$  distribution with  $N_{XY} - 2$  degrees of freedom, and  $t = r_{XY} \sqrt{\frac{N_{XY}-2}{1-r_{XY}^2}}$ . If  $r_{XY}^2 = 1$ , then set  $p=0$ ; If  $N_{XY} \leq 2$ , then set  $p=1$ .

### Partial correlation and P-value

For two continuous variables,  $X$  and  $Y$ , we can calculate the partial correlation between them controlling for the values of a new continuous variable  $Z$ :

$$r_{XY|Z} = \frac{r_{XY} - r_{XZ}r_{YZ}}{\sqrt{1 - r_{XZ}^2} \sqrt{1 - r_{YZ}^2}}$$

Since the new variable  $Z$  is always a linear combination of several continuous variables, we compute the correlation of  $Z$  and a continuous variable using a property of the covariance rather than the original dataset. Suppose the new derived predictor  $Z$  is a linear combination of original predictors  $X_1, X_2, \dots, X_m$ :

$$Z = a_1X_1 + a_2X_2 + \dots + a_mX_m$$

Then for any a continuous variable  $X$  (continuous predictor or continuous target), the correlation between  $X$  and  $Z$  is

$$r_{ZX} = \frac{c_{ZX}}{\sqrt{c_{ZZ}c_{XX}}}$$

where  $c_{ZX} = \sum_{i=1}^m a_i c_{X_i X}$ , and  $c_{ZZ} = \sum_{i=1}^m a_i^2 c_{X_i X_i} + 2 \sum_{i \neq j} a_i a_j c_{X_i X_j}$ .

If  $1 - r_{XZ}^2$  or  $1 - r_{YZ}^2$  is less than  $10^{-10}$ , let  $r_{XY|Z} = 0$ . If  $r_{XY|Z}$  is larger than 1, then set it to 1; If  $r_{XY|Z}$  is less than  $-1$ , then set it to  $-1$ . (This may occur with pairwise deletion). Based on partial correlation, the  $p$ -value is derived from the  $t$  test

$$p = \Pr(|t(N_{XY} - 3)| > t)$$

where  $t(N_{XY} - 3)$  is a random variable with a  $t$  distribution with  $N_{XY} - 3$  degrees of freedom, and  $t = r_{XY|Z} \sqrt{\frac{N_{XY}-3}{1-r_{XY|Z}^2}}$ . If  $r_{XY|Z}^2 = 1$ , then set  $p=0$ ; if  $N_{XY} \leq 3$ , then set  $p=1$ .

## ***Discretization of Continuous Predictors***

Discretization is used for calculating predictive power and creating histograms.

### ***Discretization for calculating predictive power***

If the transformed target is categorical, we use the equal width bins method to discretize a continuous predictor into a number of bins equal to the number of categories of the target. Variables considered for discretization include:

- Scale predictors which have been recommended.
- Original continuous variables of recommended predictors.

### ***Discretization for creating histograms***

We use the equal width bins method to discretize a continuous predictor into a maximum of 400 bins. Variables considered for discretization include:

- Recommended continuous variables.
- Excluded continuous variables which have not been used to derive a new variable.
- Original continuous variables of recommended variables.
- Original continuous variables of excluded variables which have not been used to derive a new variable.
- Scale variables used to construct new variables. If their original variables are also continuous, then the original variables will be discretized.
- Date/time variables.

After discretization, the number of cases and mean in each bin are collected to create histograms.

*Note:* If an original predictor has been recast, then this recast version will be regarded as the “original” predictor.

## ***Predictive Power***

### ***Collect bivariate statistics for predictive power***

We collect bivariate statistics between recommended predictors and the (transformed) target. If an original predictor of a recommended predictor exists, then we also collect bivariate statistics between this original predictor and the target; if an original predictor has a recast version, then we use the recast version.

If the target is categorical, but a recommended predictor or its original predictor/recast version is continuous, then we discretize the continuous predictor using the method in “Discretization of Continuous Predictors” on p. 35 and collect bivariate statistics between the categorical target and the categorical predictors.

Bivariate statistics between the predictors and target are same as those described in “Bivariate Statistics Collection ” on p. 22.

### **Computing predictive power**

Predictive power is used to measure the usefulness of a predictor and is computed with respect to the (transformed) target. If an original predictor of a recommended predictor exists, then we also compute predictive power for this original predictor; if an original predictor has a recast version, then we use the recast version.

**Scale target.** When the target is continuous, we fit a linear regression model and predictive power is computed as follows.

- Scale predictor:  $r_{XY}^2 = \left( \frac{c_{XY}}{\sqrt{c_{XX}}\sqrt{c_{YY}}} \right)^2$
- Categorical predictor:  $1 - \frac{S_e}{S_T}$ , where  $S_e = \sum_{i=1}^I M_i^2$  and  $S_T = \sum_{i=1}^n f_i w_i (y_i - \bar{y}_x)^2$ .

**Categorical target.** If the (transformed) target is categorical, then we fit a naïve Bayes model and the classification accuracy will serve as predictive power. We discretize continuous predictors as described in “Discretization of Continuous Predictors ” on p. 35, so we only consider the predictive power of categorical predictors.

If  $N_{ij}$  is the of number cases where  $X = i$  and  $Y = j$ ,  $N_{i.} = \sum_{j=1}^J N_{ij}$ , and  $N_{.j} = \sum_{i=1}^I N_{ij}$ , then the chi-square statistic is calculated as

$$\chi^2 = \sum_{i=1}^I \sum_{j=1}^J \frac{(N_{ij} - \hat{N}_{ij})^2}{\hat{N}_{ij}}$$

where  $\hat{N}_{ij} = \frac{N_{i.} N_{.j}}{N_{XY}}$

and Cramer’s V is defined as

$$V = \left( \frac{\chi^2}{N_{XY} (\min(I, J) - 1)} \right)^{1/2}$$

## **References**

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# Bayesian Networks Algorithms

## Bayesian Networks Algorithm Overview

A Bayesian network provides a succinct way of describing the joint probability distribution for a given set of random variables.

Let  $V$  be a set of categorical random variables and  $G = (V, E)$  be a directed acyclic graph with nodes  $V$  and a set of directed edges  $E$ . A Bayesian network model consists of the graph  $G$  together with a conditional probability table for each node given values of its parent nodes. Given the value of its parents, each node is assumed to be independent of all the nodes that are not its descendants. The joint probability distribution for variables  $V$  can then be computed as a product of conditional probabilities for all nodes, given the values of each node's parents.

Given set of variables  $V$  and a corresponding sample dataset, we are presented with the task of fitting an appropriate Bayesian network model. The task of determining the appropriate edges in the graph  $G$  is called **structure learning**, while the task of estimating the conditional probability tables given parents for each node is called **parameter learning**.

## Primary Calculations

IBM® SPSS® Modeler offers two different methods for building Bayesian network models:

- **Tree Augmented Naïve Bayes.** This algorithm is used mainly for classification. It efficiently creates a simple Bayesian network model. The model is an improvement over the naïve Bayes model as it allows for each predictor to depend on another predictor in addition to the target variable. Its main advantages are its classification accuracy and favorable performance compared with general Bayesian network models. Its disadvantage is also due to its simplicity; it imposes much restriction on the dependency structure uncovered among its nodes.
- **Markov Blanket estimation.** The Markov blanket for the target variable node in a Bayesian network is the set of nodes containing target's parents, its children, and its children's parents. Markov blanket identifies all the variables in the network that are needed to predict the target variable. This can produce more complex networks, but also takes longer to produce. Using feature selection preprocessing can significantly improve performance of this algorithm.

## Notation

The following notation is used throughout this algorithm description:

$G$	A directed acyclic graph representing the Bayesian Network model
$D$	A dataset
$Y$	Categorical target variable
$X_i$	The $i$ th predictor
$\pi_i$	The parent set of the $i$ th predictor besides target $Y$ . For TAN models, its size is $\leq 1$ .
$N$	The number of cases in $D$

$n$	The number of predictors
$N_{ijk}$	Denote the number of records in $D$ for which $(\pi_i, Y)$ take its $j$ th value and for which $X_i$ takes its $k$ th value.
$N_{ij}$	Denote the number of records in $D$ for which $(\pi_i, Y)$ takes its $j$ th value.
$\theta_{ijk}$	$\Pr(X_i = x_i^k   (\pi_i, Y) = (\pi_i, Y)^j)$
$\theta_{Y_i}$	$\Pr(Y = Y_i)$
$K$	The number of non-redundant parameters of TAN
$MB$	The Markov blanket boundary about target $Y$
$S$	A subset of $X$
$S_{X_i X_j}$	A subset of $X \setminus X_i, X_j$ , such that variables $X_i$ and $X_j$ are conditionally independent with respect to $S_{X_i X_j}$
$X_i - X_j$	An undirected arc between variables $X_i, X_j$ in $G$ . $X_i$ and $X_j$ are adjacent to each other.
$X_i \rightarrow X_j$	A directed arc from $X_i$ to $X_j$ in $G$ . $X_i$ is a parent of $X_j$ , and $X_j$ is a child of $X_i$ .
$ADJ_{X_i}$	A variable set which represents all the adjacent variables of variable $X_i$ in $G$ , ignoring the edge directions.
$I(\cdot)$	The conditional independence (CI) test function which returns the $p$ -value of the test.
$\alpha$	The significance level for CI tests between two variables. If the $p$ -value of the test is larger than $\alpha$ then they are independent, and vice-versa.
$r_i$	The cardinality of $X_i$ , $r_i =  X_i $
$q_i$	The cardinality of the parent set $\pi_i$ of $X_i$ .

### Handling of Continuous Predictors

BN models in IBM® SPSS® Modeler can only accommodate discrete variables. Target variables must be discrete (flag or set type). Numeric predictors are discretized into 5 equal-width bins before the BN model is built. If any of the constructed bins is empty (there are no records with a value in the bin's range), that bin is merged to an adjacent non-empty bin.

### Feature Selection via Breadth-First Search

Feature selection preprocessing works as follows:

- ▶ It begins by searching for the direct neighbors of a given target  $Y$ , based on statistical tests of independence. For more information, see the topic “Markov Blanket Conditional Independence Test” on p. 43. These variables are known as the parents or children of  $Y$ , denoted by  $PC(Y)$ .
- ▶ For each  $X \in PC(Y)$ , we look for  $PC(X)$ , or the parents and children of  $X$ .
- ▶ For each  $Z \in PC(X)$ , we add it to  $MB_Y$  if it is not independent of  $Y$ .

The explicit algorithm is given below.

```
RecognizeMB
(
  D : Dataset, eps : threshold
)
{
  // Recognize Y's parents/children
  CanADJ_Y = X \ {Y};
  PC = RecognizePC(Y,CanADJ_Y,D,eps);
  MB = PC;

  // Collect spouse candidates, and remove false
  // positives from PC
  for (each X_i in PC){
    CanADJ_X_i = X \ X_i;
    CanSP_X_i = RecognizePC(X_i,CanADJ_X_i,D,eps);
    if (Y notin CanSP_X_i) // Filter out false positive
      MB = MB \ X_i;
  }
  // Discover true positives among candidates
  for (each X_i in MB)
    for (each Z_i in CanSP_X_i and Z_i notin MB)
      if (I(Y,Z_i){S_Y,Z_i + X_i}) ≤ eps) then
        MB = MB + Z_i;
  return MB;
}
```

```

RecognizePC (
  T      : target to scan,
  ADJ_T  : Candidate adjacency set to search,
  D      : Dataset,
  eps    : threshold,
  maxSetSize : )
{
  NonPC = {empty set};
  cutSetSize = 0;
  repeat
    for (each X_i in ADJ_T){
      for (each subset S of {ADJ_T \ X_i} with |S| = cutSetSize){
        if (I(X_i,T|S) > eps){
          NonPC = NonPC + X_i;
          S_T,X_i = S;
          break;
        }
      }
    }
  }
  if (|NonPC| > 0){
    ADJ_T = ADJ_T \ NonPC;
    cutSetSize +=1;
    NonPC = {empty set};
  } else
    break;
  until (|ADJ_T| ≤ cutSetSize) or (cutSetSize > maxSetSize)
  return ADJ_T;
}

```

### ***Tree Augmented Naïve Bayes Method***

The Bayesian network classifier is a simple classification method, which classifies a case  $d_j = (x_1^j, x_2^j, \dots, x_n^j)$  by determining the probability of it belonging to the  $i$ th target category  $Y_i$ . These probabilities are calculated as

$$\begin{aligned}
& \Pr \left( Y_i | X_1 = x_1^j, X_2 = x_2^j, \dots, X_n = x_n^j \right) \\
&= \frac{\Pr(Y_i) \Pr(X_1 = x_1^j, X_2 = x_2^j, \dots, X_n = x_n^j | Y_i)}{\Pr(X_1 = x_1^j, X_2 = x_2^j, \dots, X_n = x_n^j)} \\
&\propto \Pr(Y_i) \prod_{k=1}^n \Pr \left( X_k = x_k^j | \pi_k^j, Y_i \right)
\end{aligned}$$

where  $\pi_k$  is the parent set of  $X_k$  besides  $Y$ , and it maybe empty.  $\Pr(X_k | \pi_k, Y)$  is the conditional probability table (CPT) associated with each node  $X_k$ . If there are  $n$  independent predictors, then the probability is proportional to

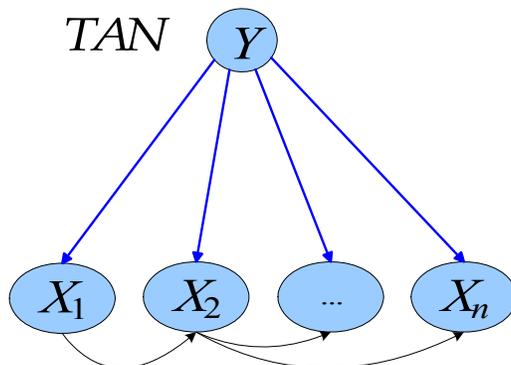
$$\Pr(Y_i) \prod_{k=1}^n \Pr(X_k = x_k^j | Y_i)$$

When this dependence assumption (conditional independence between the predictors given the class) is made, the classifier is called naïve Bayes (NB). Naïve Bayes has been shown to be competitive with more complex, state-of-the-art classifiers. In recent years, a lot of work has focused on improving the naïve Bayes classifier. One important method is to relax independence assumption. We use a tree augmented naïve Bayesian (TAN) classifier (Friedman, Geiger, and Goldszmidt, 1997), and it is defined by the following conditions:

- Each predictor has the target as a parent.
- Predictors may have one other predictor as a parent.

An example of this structure is shown below.

Figure 5-1  
Structure of an simple tree augmented naïve Bayes model.



### **TAN Classifier Learning Procedure**

Let  $\mathbf{X} = (X_1, X_2, \dots, X_n)$  represent a categorical predictor vector. The algorithm for the TAN classifier first learns a tree structure over  $\mathbf{X}$  using mutual information conditioned on  $Y$ . Then it adds a link (or arc) from the target node to each predictor node.

The TAN learning procedure is:

1. Take the training data  $D$ ,  $\mathbf{X}$  and  $Y$  as input.
2. Learn a tree-like network structure over  $\mathbf{X}$  by using the Structure Learning algorithm outlined below.
3. Add  $Y$  as a parent of every  $X_i$  where  $1 \leq i \leq n$ .
4. Learning the parameters of TAN network.

### TAN Structure Learning

We use a maximum weighted spanning tree (MWST) method to construct a tree Bayesian network from data (Chow and Liu, 1968). This method associates a weight to each edge corresponding to the mutual information between the two variables. When the weight matrix is created, the MWST algorithm (Prim, 1957) gives an undirected tree that can be oriented with the choice of a root.

The mutual information of two nodes  $X_i, X_j$  is defined as

$$I(X_i, X_j) = \sum_{x_i, x_j} \Pr(x_i, x_j) \log \left( \frac{\Pr(x_i, x_j)}{\Pr(x_i) \Pr(x_j)} \right)$$

We replace the mutual information between two predictors with the conditional mutual information between two predictors given the target (Friedman et al., 1997). It is defined as

$$I(X_i, X_j|Y) = \sum_{x_i, x_j, y_k} \Pr(x_i, x_j, y_k) \log \left( \frac{\Pr(x_i, x_j|y_k)}{\Pr(x_i|y_k) \Pr(x_j|y_k)} \right)$$

The network over can be constructed using the following steps:

1. Compute  $I(X_i, X_j|Y)$ ,  $i = 1, \dots, n, j = 1, \dots, n, i \neq j$  between each pair of variables.
2. Use Prim's algorithm (Prim et al., 1957) to construct a maximum weighted spanning tree with the weight of an edge connecting  $X_i$  to  $X_j$  by  $I(X_i, X_j|Y)$ .

This algorithm works as follows: it begins with a tree with no edges and marks a variable at a random as input. Then it finds an unmarked variable whose weight with one of the marked variables is maximal, then marks this variable and adds the edge to the tree. This process is repeated until all variables are marked.

3. Transform the resulting undirected tree to directed one by choosing  $X_1$  as a root node and setting the direction of all edges to be outward from it.

### TAN Parameter Learning

Let  $r_i$  be the cardinality of  $X_i$ . Let  $q_i$  denote the cardinality of the parent set  $(\pi_i, Y)$  of  $X_i$ , that is, the number of different values to which the parent of  $X_i$  can be instantiated. So it can be calculated as  $q_i = r_{\pi_i} \times |Y|$ . Note  $\pi_i = \emptyset$  implies  $q_i = |Y|$ . We use  $N_{ij}$  to denote the number of records in  $D$  for which  $(\pi_i, Y)$  takes its  $j$ th value. We use  $N_{ijk}$  to denote the number of records in  $D$  for which  $(\pi_i, Y)$  take its  $j$ th value and for which  $X_i$  takes its  $k$ th value.

#### Maximum Likelihood Estimation

The closed form solution for the parameters  $\theta_{Y_i}$  ( $1 \leq i \leq |Y|$ ) and  $\theta_{ijk}$  ( $1 \leq i \leq n, 1 \leq j \leq q_i, 1 \leq k \leq r_i$ ) that maximize the log likelihood score is

$$\hat{\theta}_{Y_i} = \frac{N_{Y_i}}{N}$$

$$\hat{\theta}_{ijk} = \frac{N_{ijk}}{N_{ij}}$$

where  $N_{Y_i}$  denotes the number of cases with  $Y = Y_i$  in the training data.

Note that if  $N_{ij} = 0$ , then  $\hat{\theta}_{ijk} = 0$ .

The number of parameters  $K$  is

$$K = \sum_{i=1}^n (r_i - 1) \cdot q_i + |Y| - 1$$

### **TAN Posterior Estimation**

Assume that Dirichlet prior distributions are specified for the set of parameters  $\theta_{Y_i}$  ( $1 \leq i \leq |Y|$ ) as well as for each of the sets  $\theta_{ijk}$  ( $1 \leq k \leq r_i$ ),  $1 \leq i \leq n$ , and  $1 \leq j \leq q_i$  (Heckerman, 1999). Let  $N_{Y_i}^0$  and  $N_{ijk}^0$  denote corresponding Dirichlet distribution parameters such that  $N^0 = \sum_i N_{Y_i}^0$  and  $N_{ij}^0 = \sum_k N_{ijk}^0$ . Upon observing the dataset  $D$ , we obtain Dirichlet posterior distributions with the following sets of parameters:

$$\hat{\theta}_{Y_i}^P = \frac{N_{Y_i} + N_{Y_i}^0}{N + N^0}$$

$$\hat{\theta}_{ijk}^P = \frac{N_{ijk} + N_{ijk}^0}{N_{ij} + N_{ij}^0}$$

The posterior estimation is always used for model updating.

### **Adjustment for small cell counts**

To overcome problems caused by zero or very small cell counts, parameters can be estimated as posterior parameters  $\hat{\theta}_{Y_i}^P$  ( $1 \leq i \leq |Y|$ ) and  $\hat{\theta}_{ijk}^P$  ( $1 \leq k \leq r_i$ ),  $1 \leq i \leq n$ ,  $1 \leq j \leq q_i$  using uninformative Dirichlet priors  $N_{Y_i}^0 = \frac{2}{|Y|}$  and  $N_{ijk}^0 = \frac{2}{r_i \cdot q_i}$ .

## **Markov Blanket Algorithms**

The Markov blanket algorithm learns the BN structure by identifying the conditional independence relationships among the variables. Using statistical tests (such as chi-squared test or  $G$  test), this algorithm finds the conditional independence relationships among the nodes and uses these relationships as constraints to construct a BN structure. This algorithm is referred to as a dependency-analysis-based or constraint-based algorithm.

### **Markov Blanket Conditional Independence Test**

The conditional independence (CI) test tests whether two variables are conditionally independent with respect to a conditional variable set. There are two familiar methods to compute the CI test:  $\chi^2$  (Pearson chi-square) test and  $G^2$  (log likelihood ratio) test.

Suppose  $X, Y$  are two variables for testing and  $S$  is a conditional variable set such that  $X, Y \notin S$ . Let  $O(x_i, y_j)$  be the observed count of cases that have  $X = x_i$  and  $Y = y_j$ , and  $E(x_i, y_j)$  is the expect number of cases that have  $X = x_i$  and  $Y = y_j$  under the hypothesis that  $X, Y$  are independent.

### Chi-square Test

We assume the null hypothesis is that  $X, Y$  are independent. The  $\chi^2$  test statistic for this hypothesis is

$$\chi^2(X, Y) = \sum_{i,j} \frac{(O(x_i, y_j) - E(x_i, y_j))^2}{E(x_i, y_j)}$$

Suppose that  $N$  is the total number of cases in  $D$ ,  $N(x_i)$  is the number of cases in  $D$  where  $X_i$  takes its  $i$ th category, and  $N(y_j)$  and  $N(s_k)$  are the corresponding numbers for  $Y$  and  $S$ . So  $N(x_i, y_j)$  is the number of cases in  $D$  where  $X_i$  takes its  $i$ th category and  $Y_j$  takes its  $j$ th category.  $N(x_i, s_k)$ ,  $N(y_j, s_k)$  and  $N(x_i, y_j, s_k)$  are defined similarly. We have:

$$\chi^2(X, Y) = \sum_{i,j} \frac{(N(x_i, y_j) - N(x_i)N(y_j)/N)^2}{N(x_i)N(y_j)/N} = \sum_{i,j} \frac{(N \cdot N(x_i, y_j) - N(x_i)N(y_j))^2}{N(x_i)N(y_j) \cdot N}$$

Because  $\chi^2(X, Y) \sim \chi_v^2$  where  $v = (|X| - 1)(|Y| - 1)$  is the degrees of freedom for the  $\chi^2$  distribution, we get the  $p$ -value for  $\chi^2(X, Y)$  as follows:

$$P(U > \chi^2(X, Y))$$

As we know, the larger  $p$ -value, the less likely we are to reject the null hypothesis. For a given significance level  $\alpha$ , if the  $p$ -value is greater than  $\alpha$  we can not reject the hypothesis that  $X, Y$  are independent.

We can easily generalize this independence test into a conditional independence test:

$$\begin{aligned} \chi^2(X, Y|S) &= \sum_k \chi^2(X, Y|S = s_k) \\ &= \sum_{i,j,k} \frac{(N(x_i, y_j, s_k)N(s_k) - N(x_i, s_k)N(y_j, s_k))^2}{N(x_i, s_k)N(y_j, s_k)N(s_k)} \end{aligned}$$

The degree of freedom for  $\chi^2 \sim \chi_v^2$  is:

$$\nu = (|X| - 1)(|Y| - 1) \cdot |S|$$

### Likelihood Ratio Test

We assume the null hypothesis is that  $X, Y$  are independent. The  $G^2$  test statistic for this hypothesis is

$$G^2(X, Y) = 2 \sum_{i,j} O(x_i, y_j) \ln \left( \frac{O(x_i, y_j)}{E(x_i, y_j)} \right)$$

or equivalently,

$$G^2(X, Y) = 2 \sum_{i,j} N(x_i, y_j) \ln \left( \frac{N(x_i, y_j) N}{N(x_i) N(y_j)} \right)$$

The conditional version of the  $G^2$  independence test is

$$\begin{aligned} G^2(X, Y|S) &= 2 \sum_{i,j,k} O(x_i, y_j|S = s_k) \ln \left( \frac{O(x_i, y_j|S = s_k)}{E(x_i, y_j|S = s_k)} \right) \\ &= 2 \sum_{i,j,k} N(x_i, y_j, s_k) \ln \left( \frac{N(x_i, y_j, s_k) N(s_k)}{N(x_i, s_k) N(y_j, s_k)} \right) \end{aligned}$$

The  $G^2$  test is asymptotically distributed as a  $\chi_v^2$  distribution, where degrees of freedom are the same as in the  $\chi^2$  test. So the  $p$ -value for the  $G^2$  test is

$$P(U > G^2(X, Y))$$

In the following parts of this document, we use  $I(\cdot)$  to uniformly represent the  $p$ -value of whichever test is applied. If  $I(X, Y) > \alpha$ , we say variable  $X$  and  $Y$  are independent, and if  $I(X, Y|S) > \alpha$ , we say variable  $X$  and  $Y$  are conditionally independent given variable set  $S$ .

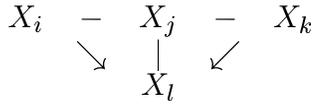
### **Markov Blanket Structure Learning**

This algorithm aims at learning a Bayesian networks structure from a dataset. It starts with a complete graph  $G$ . Let  $X_i, X_j \in \mathbf{X}$ , and compute  $I(X_i, X_j)$  for each variable pair in  $G$ . If  $I(X_i, X_j) > \alpha$ , remove the arc between  $X_i, X_j$ . Then for each arc  $X_i - X_j$  perform an exhaustive search in  $ADJ_{X_i} \setminus \{X_j\}$  to find the smallest conditional variable set  $S$  such that  $I(X_i, X_j|S) > \alpha$ . If such  $S$  exist, delete arc  $X_i - X_j$ . After this, orientation rules are applied to orient the arcs in  $G$ .

### **Markov Blanket Arc Orientation Rules**

Arcs in the derived structure are oriented based on the following rules:

1. All patterns of the of the form  $X_i - X_j - X_k$  or  $X_i \rightarrow X_j - X_k$  are updated to  $X_i \rightarrow X_j \leftarrow X_k$  if  $X_j \notin S_{X_i, X_j}$
2. Patterns of the form  $X_i \rightarrow X_j - X_k$  are updated so that  $X_j \rightarrow X_k$
3. Patterns of the form  $X_i - X_j$  are updated to  $X_i \rightarrow X_j$
4. Patterns of the form



are updated so that  $X_j \rightarrow X_l$

After the last step, if there are still undirected arcs in the graph, return to step 2 and repeat until all arcs are oriented.

### Deriving the Markov Blanket Structure

The Markov Blanket is a local structure of a Bayesian Network. Given a Bayesian Network  $G$  and a target variable  $Y$ , to derive the Markov Blanket of  $Y$ , we should select all the directed parents of  $Y$  in  $G$  denoted as  $\pi_Y$ , all the directed children of  $Y$  in  $G$  denoted as  $X_{Ch}$  and all the directed parents of  $X_{Ch}$  in  $G$  denoted as  $\pi$ .  $\pi_Y \cup Y \cup X_{Ch} \cup \pi$  and their arcs inherited from  $G$  define the Markov Blanket  $MB_Y$ .

### Markov Blanket Parameter Learning

#### Maximum Likelihood Estimation

The closed form solution for the parameters  $\theta_{ijk}$  ( $1 \leq i \leq n, 1 \leq j \leq q_i, 1 \leq k \leq r_i$ ) that maximize the log likelihood score is

$$\hat{\theta}_{ijk} = \frac{N_{ijk}}{N_{ij}}$$

Note that if  $\pi_i = \emptyset$ , then  $\hat{\theta}_{ijk} = \frac{N_k}{N}$ .

The number of parameters  $K$  is

$$K = \sum_{i=1}^n (r_i - 1) \cdot q_i$$

#### Posterior Estimation

Assume that Dirichlet prior distributions are specified for each of the sets  $\theta_{ijk}$  ( $1 \leq k \leq r_i, 1 \leq i \leq n, 1 \leq j \leq q_i$ ) (Heckerman et al., 1999). Let  $N_{ijk}^0$  denote corresponding Dirichlet distributed parameters such that  $N_{ij}^0 = \sum_k N_{ijk}^0$ . Upon observing the dataset  $D$ , we obtain Dirichlet posterior distributions with the following sets of parameters:

$$\hat{\theta}_{ijk}^P = \frac{N_{ijk} + N_{ijk}^0}{N_{ij} + N_{ij}^0}$$

The posterior estimate is always used for model updating.

### Adjustment for Small Cell Counts

To overcome problems caused by zero or very small cell counts, parameters can be estimated as posterior parameters  $\theta_{ijk}$  ( $1 \leq k \leq r_i$ ),  $1 \leq i \leq n$ ,  $1 \leq j \leq q_i$  using uninformative Dirichlet priors specified by  $N_{ijk}^0 = \frac{2}{r_i \cdot q_i}$ .

### Blank Handling

By default, records with missing values for any of the input or output fields are excluded from model building. If the Use only complete records option is deselected, then for each pairwise comparison between fields, all records containing valid values for the two fields in question are used.

### Model Nugget/Scoring

The Bayesian Network Model Nugget produces predicted values and probabilities for scored records.

#### Tree Augmented Naïve Bayes Models

Using the estimated model from training data, for a new case  $\mathbf{x} = (x_1, \dots, x_n)$ , the probability of it belonging to the  $i$ th target category  $Y_i$  is calculated as  $\Pr(Y = Y_i | \mathbf{X} = \mathbf{x})$ . The target category with the highest posterior probability is the predicted category for this case,  $Y(\mathbf{x})$ , is predicted by

$$\begin{aligned} \hat{Y}(\mathbf{x}) &= \arg \max_i \{ \Pr(Y = Y_i | \mathbf{X} = \mathbf{x}) \} \\ &= \arg \max_i \{ \Pr(\mathbf{X} = \mathbf{x} | Y = Y_i) \Pr(Y = Y_i) \} \\ &= \arg \max_i \left\{ \Pr(Y = Y_i) \prod_{i=1}^n \Pr(X_i = x_i | \pi_i = \pi_i, Y = Y_i) \right\} \end{aligned}$$

#### Markov Blanket Models

The scoring function uses the estimated model to compute the probabilities of  $Y$  belongs to each category for a new case  $X_P$ . Suppose  $\pi_Y$  is the parent set of  $Y$ , and  $\pi_{Y|P}$  denotes the configuration of  $\pi_Y$  given case  $X_P$ ,  $X_{Ch} = (X_1, \dots, X_m)$  denotes the direct children set of  $Y$ ,  $\pi_i$  denotes the parent set (excluding  $Y$ ) of the  $i$ th variable in  $X_{Ch}$ . The score for each category of  $Y$  is computed by:

$$\Pr(Y = y_l | X_P = x_P) = \frac{\Pr(Y = y_l, X_P = x_P)}{\sum_{y_l} \Pr(Y = y_l, X_P = x_P)}$$

where the joint probability that  $Y = y_l$  and  $X_P = x_P$  is:

$$\Pr(Y = y_l, X_P = x_P) = c \cdot \Pr(Y = y_l | \pi_Y = \pi_{y|P}) \prod_{i=1}^m \Pr(X_i = x_i | \pi_i = \pi_{i|P}, Y = y_l)$$

where

$$c = \Pr(\pi_Y = \pi_{y|P}) \prod_{i=1}^m \Pr(\pi_i = \pi_{i|P})$$

Note that  $c$  is never actually computed during scoring because its value cancels from the numerator and denominator of the scoring equation given above.

# Binary Classifier Comparison Metrics

The Binary Classifier node generates multiple models for a flag output field. For details on how each model type is built, see the appropriate algorithm documentation for the model type.

The node also reports several comparison metrics for each model, to help you select the optimal model for your application. The following metrics are available:

## **Maximum Profit**

This gives the maximum amount of profit, based on the model and the profit and cost settings. It is calculated as

$$\text{Profit}_{\max} = \sum_{i=1}^j (h(x_i) \cdot r - c)$$

where  $h(x_i)$  is defined as

$$h(x_i) = \begin{cases} 1 & \text{if } x_i \text{ is a hit} \\ 0 & \text{otherwise} \end{cases}$$

$r$  is the user-specified revenue amount per hit, and  $c$  is the user-specified cost per record. The sum is calculated for the  $j$  records with the highest  $\hat{p}_i$ , such that  $(\hat{p}_{j+1} \cdot (r - c)) - ((1 - \hat{p}_{j+1}) \cdot c) \leq 0$

## **Maximum Profit Occurs in %**

This gives the percentage of the training records that provide positive profit based on the predictions of the model,

$$\text{Profit}_{\%} = \frac{j}{n} \cdot 100\%$$

where  $n$  is the overall number of records included in building the model.

## **Lift**

This indicates the response rate for the top  $q\%$  of records (sorted by predicted probability), as a ratio relative to the overall response rate,

$$\text{Lift} = \frac{\sum_{i=1}^k \hat{p}_i / k}{\sum_{i=1}^n h(x_i) / n}$$

where  $k$  is  $q\%$  of  $n$ , the number of training records used to build the model. The default value of  $q$  is 30, but this value can be modified in the binary classifier node options.

## **Overall Accuracy**

This is the percentage of records for which the outcome is correctly predicted,

$$a = \frac{\sum_{i=1}^n m(i)}{n} \cdot 100\%, m(i) = \begin{cases} 1 & \text{if } (\hat{x}_i = x_i) \\ 0 & \text{otherwise} \end{cases}$$

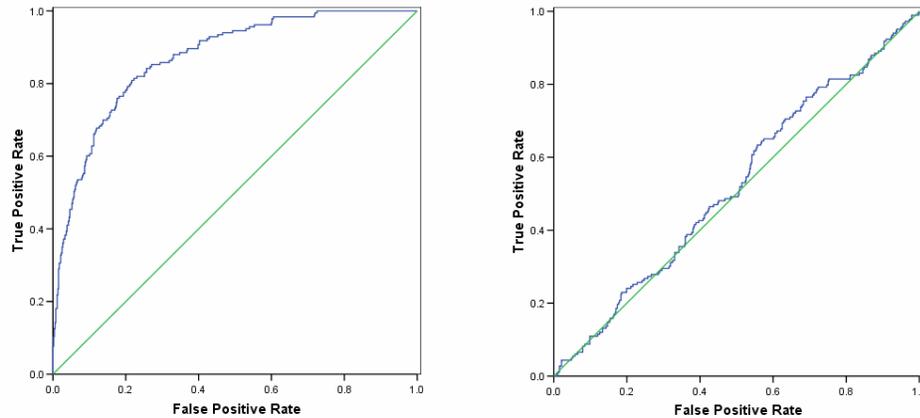
where  $\hat{x}_i$  is the predicted outcome value for record  $i$  and  $x_i$  is the observed value.

### Area Under the Curve (AUC)

This represents the area under the Receiver Operating Characteristic (ROC) curve for the model. The ROC curve plots the true positive rate (where the model predicts the target response and the response is observed) against the false positive rate (where the model predicts the target response but a nonresponse is observed). For a good model, the curve will rise sharply near the left axis and cut across near the top, so that nearly all the area in the unit square falls below the curve. For an uninformative model, the curve will approximate a diagonal line from the lower left to the upper right corner of the graph. Thus, the closer the AUC is to 1.0, the better the model.

Figure 6-1

ROC curves for a good model (left) and an uninformative model (right)



The AUC is computed by identifying segments as unique combinations of predictor values that determine subsets of records which all have the same predicted probability of the target value. The  $s$  segments defined by a given model's predictors are sorted in descending order of predicted probability, and the AUC is calculated as

$$AUC = \sum_{i=1}^s |f_i - f_{i-1}| \cdot \frac{t_i + t_{i-1}}{2}$$

where  $f_i$  is the cumulative number of false positives for segment  $i$ , that is, false positives for segment  $i$  and all preceding segments  $j < i$ ,  $t_i$  is the cumulative number of true positives, and  $f_0 = t_0 = 0$ .

# C5.0 Algorithms

The code for training C5.0 models is licensed from RuleQuest Research Ltd Pty, and the algorithms are proprietary. For more information, see the RuleQuest website at <http://www.rulequest.com/>.

*Note:* Modeler 13 upgraded the C5.0 version from 2.04 to 2.06. See the RuleQuest website for more information.

## Scoring

A record is scored with the class and confidence of the rule that fires for that record.

If a rule set is directly generated from the C5.0 node, then the confidence for the rule is calculated as

$$\frac{(\text{number correct in leaf} + 1)}{(\text{total number of records in leaf} + 2)}$$

If a rule set is generated from a decision tree generated from the C5.0 node, then the confidence is calculated as

$$\frac{(\text{number correct in leaf} + 1)}{(\text{total number of records in leaf} + \text{number of categories in the target})}$$

### **Scores with rule set voting**

When voting occurs between rules within a rule set the final scores assigned to a record are calculated in the following way. For each record, all rules are examined and each rule that applies to the record is used to generate a prediction and an associated confidence. The sum of confidence figures for each output value is computed, and the value with the greatest confidence sum is chosen as the final prediction. The confidence for the final prediction is the confidence sum for that value divided by the number of rules that fired for that record.

### **Scores with boosted C5.0 classifiers (decision trees and rule sets)**

When scoring with a boosted C5.0 rule set the  $n$  rule sets that make up the boosted rule set (one rule set for each boosting trial) vote using their individual scores (as obtained above) to arrive at the final score assigned to the case by the boosted rule set.

The voting for boosted C5 classifiers is as follows. For each record, each composite classifier (rule set or decision tree) assigns a prediction and a confidence. The sum of confidence figures for each output value is computed, and the value with the greatest confidence sum is chosen as the final prediction. The confidence for the final prediction by the boosted classifier is the confidence sum for that value divided by confidence sum for all values.



# Carma Algorithms

## Overview

The **continuous association rule mining algorithm (Carma)** is an alternative to Apriori that reduces I/O costs, time, and space requirements (Hidber, 1999). It uses only two data passes and delivers results for much lower support levels than Apriori. In addition, it allows changes in the support level during execution.

Carma deals with items and itemsets that make up transactions. **Items** are flag-type conditions that indicate the presence or absence of a particular thing in a specific transaction. An **itemset** is a group of items which may or may not tend to co-occur within transactions.

## Deriving Rules

Carma proceeds in two stages. First it identifies frequent itemsets in the data, and then it generates rules from the lattice of frequent itemsets.

## Frequent Itemsets

Carma uses a two-phase method of identifying frequent itemsets.

### Phase I: Estimation

In the estimation phase, Carma uses a single data pass to identify frequent itemset candidates.

A **lattice** is used to store information on itemsets. Each node in the lattice stores the items comprising the itemset, and three values for the associated itemset:

- *count*: number of transactions containing the itemset since the itemset was added to the lattice
- *firstTrans*: the record index of the transaction for which the itemset was added to the lattice
- *maxMissed*: upper bound on the number of occurrences of the itemset before it was added to the lattice

The lattice also encodes information on relationships between itemsets, which are determined by the items in the itemset. An itemset  $Y$  is an **ancestor** of itemset  $X$  if  $X$  contains every item in  $Y$ . More specifically,  $Y$  is a **parent** of  $X$  if  $X$  contains every item in  $Y$  plus one additional item. Conversely,  $Y$  is a **descendant** of  $X$  if  $Y$  contains every item in  $X$ , and  $Y$  is a **child** of  $X$  if  $Y$  contains every item in  $X$  plus one additional item.

For example, if  $X = \{\text{milk, cheese, bread}\}$ , then  $Y = \{\text{milk, cheese}\}$  is a parent of  $X$ , and  $Z = \{\text{milk, cheese, bread, sugar}\}$  is a child of  $X$ .

Initially the lattice contains no itemsets. As each transaction is read, the lattice is updated in three steps:

- **Increment statistics.** For each itemset in the lattice that exists in the current transaction, increment the count value.

- ▶ **Insert new itemsets.** For each itemset  $v$  in the transaction that is not already in the lattice, check all subsets of the itemset in the lattice. If all possible subsets of the itemset are in the lattice with  $maxSupport \geq \sigma_i$ , then add the itemset to the lattice and set its values:

- $count$  is set to 1
- $firstTrans$  is set to the record index of the current transaction
- $maxMissed$  is defined as

$$maxMissed(v) = \min_{w \subset v} \{ (\lfloor (i-1)avg(\lceil \sigma \rceil_{i-1}) \rfloor + |v| - 1), (maxMissed(w) + count(w) - 1) \}$$

where  $w$  is a subset of itemset  $v$ ,  $\lceil \sigma \rceil_{i-1}$  is the ceiling of  $\sigma$  up to transaction  $i$  for varying support (or simply  $\sigma$  for constant support), and  $|v|$  is the number of items in itemset  $v$ .

- ▶ **Prune the lattice.** Every  $k$  transactions (where  $k$  is the **pruning value**, set to 500 by default), the lattice is examined and small itemsets are removed. A small itemset is defined as an itemset for which  $maxSupport < \sigma_i$ , where  $maxSupport = (maxMissed + count)/i$ .

### Phase II: Validation

After the frequent itemset candidates have been identified, a second data pass is made to compute exact frequencies for the candidates, and the final list of frequent itemsets is determined based on these frequencies.

The first step in Phase II is to remove infrequent itemsets from the lattice. The lattice is pruned using the same method described under Phase I, with  $\sigma_n$  as the user-specified support level for the model.

After initial pruning, the training data are processed again and each itemset  $v$  in the lattice is checked and updated for each transaction record with index  $i$ :

- ▶ If  $firstTrans(v) < i$ ,  $v$  is marked as exact and is no longer considered for any updates. (When all nodes in the lattice are marked as exact, phase II terminates.)
- ▶ If  $v$  appears in the current transaction,  $v$  is updated as follows:
  - Increment  $count(v)$
  - Decrement  $maxMissed(v)$
  - If  $firstTrans(v) = i$ , set  $maxMissed(v) = 0$ , and adjust  $maxMissed$  for every superset  $w$  of  $v$  in the lattice for which  $maxSupport(w) > maxSupport(v)$ . For such supersets, set  $maxMissed(w) = count(v) - count(w)$ .
  - If  $maxSupport(v) < \sigma_n$ , remove  $v$  from the lattice.

## Generating Rules

Carma uses a common rule-generating algorithm for extracting rules from the lattice of itemsets that tends to eliminate redundant rules (Aggarwal and Yu, 1998). Rules are generated from the lattice of itemsets (see “Frequent Itemsets” on p. 53) as follows:

- ▶ For each itemset in the lattice, get the set of maximal ancestor itemsets. An itemset  $Y$  is a maximal ancestor of itemset  $X$  if  $\frac{support(Y)}{support(X)} \leq \frac{1}{c}$ , where  $c$  is the specified confidence threshold for rules.

- ▶ Prune the list of maximal ancestors by removing maximal ancestors of all of  $X$ 's child itemsets.
- ▶ For each itemset in the pruned maximal ancestor list, generate a rule  $Y \Rightarrow X - Y$ , where  $X - Y$  is the itemset  $X$  with the items in itemset  $Y$  removed.

For example, if  $X$  the itemset {milk, cheese, bread} and  $Y$  is the itemset {milk, bread}, then the resulting rule would be milk, bread  $\Rightarrow$  cheese

## Blank Handling

Blanks are ignored by the Carma algorithm. The algorithm will handle records containing blanks for input fields, but such a record will not be considered to match any rule containing one or more of the fields for which it has blank values.

## Effect of Options

**Minimum rule support/confidence.** These values place constraints on which rules may be entered into the table. Only rules whose support and confidence values exceed the specified values can be entered into the rule table.

**Maximum rule size.** Sets the limit on the number of items that will be considered as an itemset.

**Exclude rules with multiple consequents.** This option restricts rules in the final rule list to those with a single item as consequent.

**Set pruning value.** Sets the number of transactions to process between pruning passes. For more information, see the topic "Frequent Itemsets" on p. 53.

**Vary support.** Allows support to vary in order to enhance training during the early transactions in the training data. For more information, see "Varying support" below.

**Allow rules without antecedents.** Allows rules that are consequent only, which are simple statements of co-occurring items, along with traditional if-then rules.

## Varying support

If the vary support option is selected, the target support value changes as transactions are processed to provide more efficient training. The support value starts large and decreases in four steps as transactions are processed. The first support value  $s_1$  applies to the first 9 transactions, the second value  $s_2$  applies to the next 90 transactions, the third value  $s_3$  applies to transactions 100-4999, and the fourth value  $s_4$  applies to all remaining transactions. If we call the final support value  $s$ , and the estimated number of transactions  $t$ , then the following constraints are used to determine the support values:

- ▶ If  $s \geq 0.2$  or  $t < 19$ , set  $s_1 = s_2 = s_3 = s_4$ .
- ▶ If  $19 \leq t < 190$ , set  $s_1 = 5s_2$ ,  $s_3 = s_4 = s_2$ , such that  $\frac{(9s_1 + (t-9)s_2)}{t} = s$ .
- ▶ If  $190 \leq t < 7000$ , set  $s_1 = 5s_2$ ,  $s_2 = 2s_3$ ,  $s_4 = s_3$ , such that  $\frac{(9s_1 + 90s_2 + (t-99)s_3)}{t} = s$ .

- If  $t \geq 7000$ , set  $s_1 = 5s_2$ ,  $s_2 = 2s_3$ ,  $s_3 = 5s_4$ , such that  $\frac{(9s_1+90s_2+4900s_3+(t-4999)s_4)}{t} = s$ .

In all cases, if solving the equation yields  $s_1 > 0.5$ ,  $s_1$  is set to 0.5, and the other values adjusted accordingly to preserve the relation  $\frac{\sum_{i=1}^n s(i)}{t} = s$ , where  $s(i)$  is the target support (one of the values  $s_1$ ,  $s_2$ ,  $s_3$ , or  $s_4$ ) for the  $i$ th transaction.

## Generated Model/Scoring

The Carma algorithm generates an unrefined rule node. To create a model for scoring new data, the unrefined rule node must be refined to generate a ruleset node. Details of scoring for generated ruleset nodes are given below.

### Predicted Values

Predicted values are based on the rules in the ruleset. When a new record is scored, it is compared to the rules in the ruleset. How the prediction is generated depends on the user's setting for Ruleset Evaluation in the stream options.

- **Voting.** This method attempts to combine the predictions of all of the rules that apply to the record. For each record, all rules are examined and each rule that applies to the record is used to generate a prediction. The sum of confidence figures for each predicted value is computed, and the value with the greatest confidence sum is chosen as the final prediction.
- **First hit.** This method simply tests the rules in order, and the first rule that applies to the record is the one used to generate the prediction.

There is a **default rule**, which specifies an output value to be used as the prediction for records that don't trigger any other rules from the ruleset. For rulesets derived from decision trees, the value for the default rule is the modal (most prevalent) output value in the overall training data. For association rulesets, the default value is specified by the user when the ruleset is generated from the unrefined rule node.

### Confidence

Confidence calculations also depend on the user's Ruleset Evaluation stream options setting.

- **Voting.** The confidence for the final prediction is the sum of the confidence values for rules triggered by the current record that give the winning prediction divided by the number of rules that fired for that record.
- **First hit.** The confidence is the confidence value for the first rule in the ruleset triggered by the current record.

If the default rule is the only rule that fires for the record, its confidence is set to 0.5.

## ***Blank Handling***

Blanks are ignored by the algorithm. The algorithm will handle records containing blanks for input fields, but such a record will not be considered to match any rule containing one or more of the fields for which it has blank values.

There is an exception to this: when a numeric field is examined based on a split point, user-defined missing values are included in the comparison. For example, if you define -999 as a missing value for a field, Carma will still compare it to the split point for that field, and may return a match if the rule is of the form  $(X < 50)$ . You may need to preprocess specially coded numeric missing values (replacing them with `$null$`, for example) before scoring data with Carma.



# C&RT Algorithms

## Overview of C&RT

C&RT stands for **Classification and Regression Trees**, originally described in the book by the same name (Breiman, Friedman, Olshen, and Stone, 1984). C&RT partitions the data into two subsets so that the records within each subset are more homogeneous than in the previous subset. It is a **recursive** process—each of those two subsets is then split again, and the process repeats until the homogeneity criterion is reached or until some other stopping criterion is satisfied (as do all of the tree-growing methods). The same predictor field may be used several times at different levels in the tree. It uses surrogate splitting to make the best use of data with missing values.

C&RT is quite flexible. It allows unequal misclassification costs to be considered in the tree growing process. It also allows you to specify the prior probability distribution in a classification problem. You can apply automatic cost-complexity pruning to a C&RT tree to obtain a more generalizable tree.

## Primary Calculations

The calculations directly involved in building the model are described below.

## Frequency and Case Weight Fields

Frequency and case weight fields are useful for reducing the size of your dataset. Each has a distinct function, though. If a case weight field is mistakenly specified to be a frequency field, or vice versa, the resulting analysis will be incorrect.

For the calculations described below, if no frequency or case weight fields are specified, assume that frequency and case weights for all records are equal to 1.0.

### Frequency Fields

A **frequency field** represents the total number of observations represented by each record. It is useful for analyzing aggregate data, in which a record represents more than one individual. The sum of the values for a frequency field should always be equal to the total number of observations in the sample. Note that output and statistics are the same whether you use a frequency field or case-by-case data. The table below shows a hypothetical example, with the predictor fields *sex* and *employment* and the target field *response*. The frequency field tells us, for example, that 10 employed men responded *yes* to the target question, and 19 unemployed women responded *no*.

Table 9-1  
Dataset with frequency field

Sex	Employment	Response	Frequency
M	Y	Y	10
M	Y	N	17
M	N	Y	12
M	N	N	21
F	Y	Y	11
F	Y	N	15

Sex	Employment	Response	Frequency
F	N	Y	15
F	N	N	19

The use of a frequency field in this case allows us to process a table of 8 records instead of case-by-case data, which would require 120 records.

### **Case weights**

The use of a case weight field gives unequal treatment to the records in a dataset. When a **case weight field** is used, the contribution of a record in the analysis is weighted in proportion to the population units that the record represents in the sample. For example, suppose that in a direct marketing promotion, 10,000 households respond and 1,000,000 households do not respond. To reduce the size of the data file, you might include all of the responders but only a 1% sample (10,000) of the nonresponders. You can do this if you define a case weight equal to 1 for responders and 100 for nonresponders.

## **Model Parameters**

C&RT works by choosing a split at each node such that each child node created by the split is more pure than its parent node. Here **purity** refers to similarity of values of the target field. In a completely pure node, all of the records have the same value for the target field. C&RT measures the impurity of a split at a node by defining an **impurity measure**. For more information, see the topic “Impurity Measures” on p. 62.

The following steps are used to build a C&RT tree (starting with the root node containing all records):

**Find each predictor’s best split.** For each predictor field, find the best possible split for that field, as follows:

- **Range (numeric) fields.** Sort the field values for records in the node from smallest to largest. Choose each point in turn as a split point, and compute the impurity statistic for the resulting child nodes of the split. Select the best split point for the field as the one that yields the largest decrease in impurity relative to the impurity of the node being split.
- **Symbolic (categorical) fields.** Examine each possible combination of values as two subsets. For each combination, calculate the impurity of the child nodes for the split based on that combination. Select the best split point for the field as the one that yields the largest decrease in impurity relative to the impurity of the node being split.

**Find the best split for the node.** Identify the field whose best split gives the greatest decrease in impurity for the node, and select that field’s best split as the best overall split for the node.

**Check stopping rules, and recurse.** If no stopping rules are triggered by the split or by the parent node, apply the split to create two child nodes. (For more information, see the topic “Stopping Rules” on p. 64.) Apply the algorithm again to each child node.

## Blank Handling

Records with missing values for the target field are ignored in building the tree model.

**Surrogate splitting** is used to handle blanks for predictor fields. If the best predictor field to be used for a split has a blank or missing value at a particular node, another field that yields a split similar to the predictor field in the context of that node is used as a surrogate for the predictor field, and its value is used to assign the record to one of the child nodes.

For example, suppose that  $X^*$  is the predictor field that defines the best split  $s^*$  at node  $t$ . The surrogate-splitting process finds another split  $s$ , the surrogate, based on another predictor field  $X$  such that this split is most similar to  $s^*$  at node  $t$  (for records with valid values for both predictors). If a new record is to be predicted and it has a missing value on  $X^*$  at node  $t$ , the surrogate split  $s$  is applied instead. (Unless, of course, this record also has a missing value on  $X$ . In such a situation, the next best surrogate is used, and so on, up to the limit of number of surrogates specified.)

In the interest of speed and memory conservation, only a limited number of surrogates is identified for each split in the tree. If a record has missing values for the split field and all surrogate fields, it is assigned to the child node with the higher weighted probability, calculated as

$$\frac{N_{f,j}(t)}{N_f(t)}$$

where  $N_{f,j}(t)$  is the sum of frequency weights for records in category  $j$  for node  $t$ , and  $N_f(t)$  is the sum of frequency weights for all records in node  $t$ .

If the model was built using equal or user-specified priors, the priors are incorporated into the calculation:

$$\frac{\pi(j)}{p_f(t)} \times \frac{N_{f,j}(t)}{N_f(t)}$$

where  $\pi(j)$  is the prior probability for category  $j$ , and  $p_f(t)$  is the weighted probability of a record being assigned to the node,

$$p_f(t) = \sum_j \frac{\pi(j)N_{f,j}(t)}{N_{f,j}}$$

where  $N_{f,j}(t)$  is the sum of the frequency weights (or the number of records if no frequency weights are defined) in node  $t$  belonging to category  $j$ , and  $N_{f,j}$  is the sum of frequency weights for records belonging to category  $j$  in the entire training sample.

### Predictive measure of association

Let  $\tilde{n}_{X^* \cap X}$  (resp.  $\tilde{n}_{X^* \cap X}(t)$ ) be the set of learning cases (resp. learning cases in node  $t$ ) that has non-missing values of both  $X^*$  and  $X$ . Let  $p(s^* \approx s_X | t)$  be the probability of sending a case in  $\tilde{n}_{X^* \cap X}(t)$  to the same child by both  $s^*$  and  $s_X$ , and  $\tilde{s}_X$  be the split with maximized probability  $p(s^* \approx \tilde{s}_X | t) = \max_{s_X} (p(s^* \approx s_X | t))$ .

The predictive measure of association  $\lambda(s^* \approx \tilde{s}_X|t)$  between  $s^*$  and  $\tilde{s}_X$  at node  $t$  is

$$\lambda(s^* \approx \tilde{s}_X|t) = \frac{\min(p_L, p_R) - (1 - p(s^* \approx \tilde{s}_X|t))}{\min(p_L, p_R)}$$

where  $p_L$  (resp.  $p_R$ ) is the relative probability that the best split  $s^*$  at node  $t$  sends a case with non-missing value of  $X^*$  to the left (resp. right) child node. And where

$$p(s^* \approx s_X|t) = \begin{cases} \sum_j \frac{\pi(j) N_{w,j}(s^* \approx s_X, t)}{N_{w,j}(X^* \cap X)} & \text{if } Y \text{ is categorical} \\ \frac{N_w(s^* \approx s_X, t)}{N_w(X^* \cap X)} & \text{if } Y \text{ is continuous} \end{cases}$$

with

$$N_w(X^* \cap X) = \sum_{n \in \tilde{h}_{X^* \cap X}} w_n f_n, \quad N_w(X^* \cap X, t) = \sum_{n \in \tilde{h}_{X^* \cap X}(t)} w_n f_n$$

$$N_w(s^* \approx s_X, t) = \sum_{n \in \tilde{h}_{X^* \cap X}(t)} w_n f_n I(n : s^* \approx s_X)$$

$$N_{w,j}(X^* \cap X) = \sum_{n \in \tilde{h}_{X^* \cap X}} w_n f_n I(y_n = j), \quad N_{w,j}(X^* \cap X, t) = \sum_{n \in \tilde{h}_{X^* \cap X}(t)} w_n f_n I(y_n = j)$$

$$N_{w,j}(s^* \approx s_X, t) = \sum_{n \in \tilde{h}_{X^* \cap X}(t)} w_n f_n I(y_n = j) I(n : s^* \approx s_X)$$

and  $I(n : s^* \approx s_X)$  being the indicator function taking value 1 when both splits  $s^*$  and  $s_X$  send the case  $n$  to the same child, 0 otherwise.

## Effect of Options

### Impurity Measures

There are three different impurity measures used to find splits for C&RT models, depending on the type of the target field. For symbolic target fields, you can choose Gini or twining. For continuous targets, the least-squared deviation (LSD) method is automatically selected.

### Gini

The Gini index  $g(t)$  at a node  $t$  in a C&RT tree, is defined as

$$g(t) = \sum_{j \neq i} p(j|t)p(i|t)$$

where  $i$  and  $j$  are categories of the target field, and

$$p(j|t) = \frac{p(j, t)}{p(t)}$$

$$p(j, t) = \frac{\pi(j)N_j(t)}{N_j}$$

$$p(t) = \sum_j p(j, t)$$

where  $\pi(j)$  is the prior probability value for category  $j$ ,  $N_j(t)$  is the number of records in category  $j$  of node  $t$ , and  $N_j$  is the number of records of category  $j$  in the root node. Note that when the Gini index is used to find the improvement for a split during tree growth, only those records in node  $t$  and the root node with valid values for the split-predictor are used to compute  $N_j(t)$  and  $N_j$ , respectively.

The equation for the Gini index can also be written as

$$g(t) = 1 - \sum_j p^2(j|t)$$

Thus, when the records in a node are evenly distributed across the categories, the Gini index takes its maximum value of  $1 - 1/k$ , where  $k$  is the number of categories for the target field. When all records in the node belong to the same category, the Gini index equals 0.

The Gini criterion function  $\Phi(s, t)$  for split  $s$  at node  $t$  is defined as

$$\Phi(s, t) = g(t) - p_L g(t_L) - p_R g(t_R)$$

where  $p_L$  is the proportion of records in  $t$  sent to the left child node, and  $p_R$  is the proportion sent to the right child node. The proportions  $p_L$  and  $p_R$  are defined as

$$p_L = \frac{p(t_L)}{p(t)}$$

and

$$p_R = \frac{p(t_R)}{p(t)}$$

The split  $s$  is chosen to maximize the value of  $\Phi(s, t)$ .

### **Twoing**

The twoing index is based on splitting the target categories into two superclasses, and then finding the best split on the predictor field based on those two superclasses. The superclasses  $C_1$  and  $C_2$  are defined as

$$C_1 = \{j : p(j|t_L) \geq p(j|t_R)\}$$

and

$$C_2 = C - C_1$$

where  $C$  is the set of categories of the target field, and  $p(j|t_R)$  and  $p(j|t_L)$  are  $p(j|t)$ , as defined as in the Gini formulas, for the right and left child nodes, respectively. For more information, see the topic “Gini” on p. 62.

The twofing criterion function for split  $s$  at node  $t$  is defined as

$$\Phi(s, t) = p_L p_R \left[ \sum_j |p(j|t_L) - p(j|t_R)| \right]^2$$

where  $t_L$  and  $t_R$  are the nodes created by the split  $s$ . The split  $s$  is chosen as the split that maximizes this criterion.

### **Least Squared Deviation**

For continuous target fields, the **least squared deviation** (LSD) impurity measure is used. The LSD measure  $R(t)$  is simply the weighted within-node variance for node  $t$ , and it is equal to the resubstitution estimate of risk for the node. It is defined as

$$R(t) = \frac{1}{N_W(t)} \sum_{i \in t} w_i f_i (y_i - \bar{y}(t))^2$$

where  $N_W(t)$  is the weighted number of records in node  $t$ ,  $w_i$  is the value of the weighting field for record  $i$  (if any),  $f_i$  is the value of the frequency field (if any),  $y_i$  is the value of the target field, and  $\bar{y}(t)$  is the (weighted) mean for node  $t$ . The LSD criterion function for split  $s$  at node  $t$  is defined as

$$\Phi(s, t) = R(t) - p_L R(t_L) - p_R R(t_R)$$

The split  $s$  is chosen to maximize the value of  $\Phi(s, t)$ .

### **Stopping Rules**

Stopping rules control how the algorithm decides when to stop splitting nodes in the tree. Tree growth proceeds until every leaf node in the tree triggers at least one stopping rule. Any of the following conditions will prevent a node from being split:

- The node is pure (all records have the same value for the target field)
- All records in the node have the same value for all predictor fields used by the model
- The tree depth for the current node (the number of recursive node splits defining the current node) is the *maximum tree depth* (default or user-specified).
- The number of records in the node is less than the *minimum parent node size* (default or user-specified)

- The number of records in any of the child nodes resulting from the node's best split is less than the *minimum child node size* (default or user-specified)
- The best split for the node yields a decrease in impurity that is less than the *minimum change in impurity* (default or user-specified).

### Profits

**Profits** are numeric values associated with categories of a (symbolic) target field that can be used to estimate the gain or loss associated with a segment. They define the relative value of each value of the target field. Values are used in computing gains but not in tree growing.

Profit for each node in the tree is calculated as

$$\sum_j f_j(t)P_j$$

where  $j$  is the target field category,  $f_j(t)$  is the sum of frequency field values for all records in node  $t$  with category  $j$  for the target field, and  $P_j$  is the user-defined profit value for category  $j$ .

### Priors

**Prior probabilities** are numeric values that influence the misclassification rates for categories of the target field. They specify the proportion of records expected to belong to each category of the target field prior to the analysis. The values are involved both in tree growing and risk estimation.

There are three ways to derive prior probabilities.

#### Empirical Priors

By default, priors are calculated based on the training data. The prior probability assigned to each target category is the weighted proportion of records in the training data belonging to that category,

$$\pi(j) = \frac{N_{w,j}}{N_w}$$

In tree-growing and class assignment, the  $N$ s take both case weights and frequency weights into account (if defined); in risk estimation, only frequency weights are included in calculating empirical priors.

#### Equal Priors

Selecting equal priors sets the prior probability for each of the  $J$  categories to the same value,

$$\pi(j) = \frac{1}{J}$$

### **User-Specified Priors**

When user-specified priors are given, the specified values are used in the calculations involving priors. The values specified for the priors must conform to the probability constraint: the sum of priors for all categories must equal 1.0. If user-specified priors do not conform to this constraint, adjusted priors are derived which preserve the proportions of the original priors but conform to the constraint, using the formula

$$\pi'(j) = \frac{\pi(j)}{\sum_J \pi(j)}$$

where  $\pi'(j)$  is the adjusted prior for category  $j$ , and  $\pi(j)$  is the original user-specified prior for category  $j$ .

### **Costs**

**Gini.** If costs are specified, the Gini index is computed as

$$g(t) = \sum_{j \neq i} C(i|j)p(j|t)p(i|t)$$

where  $C(i|j)$  specifies the cost of misclassifying a category  $j$  record as category  $i$ .

**Twoing.** Costs, if specified, are not taken into account in splitting nodes using the twoing criterion. However, costs will be incorporated into node assignment and risk estimation, as described in Predicted Values and Risk Estimates, below.

**LSD.** Costs do not apply to regression trees.

### **Pruning**

**Pruning** refers to the process of examining a fully grown tree and removing bottom-level splits that do not contribute significantly to the accuracy of the tree. In pruning the tree, the software tries to create the smallest tree whose misclassification risk is not too much greater than that of the largest tree possible. It removes a tree branch if the cost associated with having a more complex tree exceeds the gain associated with having another level of nodes (branch).

It uses an index that measures both the misclassification risk and the complexity of the tree, since we want to minimize both of these things. This cost-complexity measure is defined as follows:

$$R_\alpha(T) = R(T) + \alpha |\tilde{T}|$$

$R(T)$  is the misclassification risk of tree  $T$ , and  $|\tilde{T}|$  is the number of terminal nodes for tree  $T$ . The term  $\alpha$  represents the complexity cost *per terminal node* for the tree. (Note that the value of  $\alpha$  is calculated by the algorithm during pruning.)

Any tree you might generate has a maximum size ( $T_{\max}$ ), in which each terminal node contains only one record. With no complexity cost ( $\alpha = 0$ ), the maximum tree has the lowest risk, since every record is perfectly predicted. Thus, the larger the value of  $\alpha$ , the fewer the number of terminal nodes in  $T(\alpha)$ , where  $T(\alpha)$  is the tree with the lowest complexity cost for the given  $\alpha$ . As  $\alpha$  increases from 0, it produces a finite sequence of subtrees ( $T_1, T_2, T_3$ ), each with progressively fewer terminal nodes. Cost-complexity pruning works by removing the weakest split.

The following equations represent the cost complexity for  $\{t\}$ , which is any single node, and for  $T_t$ , the subbranch of  $\{t\}$ .

$$R_\alpha(\{t\}) = R(t) + \alpha$$

$$R_\alpha(T_t) = R(T_t) + \alpha \left| \tilde{T}_t \right|$$

If  $R_\alpha(T_t)$  is less than  $R_\alpha(\{t\})$ , then the branch  $T_t$  has a smaller cost complexity than the single node  $\{t\}$ .

The tree-growing process ensures that  $R_\alpha(\{t\}) \geq R_\alpha(T_t)$  for ( $\alpha = 0$ ). As  $\alpha$  increases from 0, both  $R_\alpha(\{t\})$  and  $R_\alpha(T_t)$  grow linearly, with the latter growing at a faster rate. Eventually, you will reach a threshold  $\alpha'$ , such that  $R_\alpha(\{t\}) < R_\alpha(T_t)$  for all  $\alpha > \alpha'$ . This means that when  $\alpha$  grows larger than  $\alpha'$ , the cost complexity of the tree can be reduced if we cut the subbranch  $T_t$  under  $\{t\}$ . Determining the threshold is a simple computation. You can solve this first inequality,  $R_\alpha(\{t\}) \geq R_\alpha(T_t)$ , to find the largest value of  $\alpha$  for which the inequality holds, which is also represented by  $g(t)$ . You end up with

$$\alpha \leq g(t) = \frac{R(t) - R(T_t)}{\left| \tilde{T}_t \right| - 1}$$

You can define the weakest link ( $t$ ) in tree  $T$  as the node that has the smallest value of  $g(t)$ :

$$g(\bar{t}) = \min_{t \in T} g(t)$$

Therefore, as  $\alpha$  increases,  $\bar{t}$  is the first node for which  $R_\alpha(\{t\}) = R_\alpha(T_t)$ . At that point,  $\{\bar{t}\}$  becomes preferable to  $T_{\bar{t}}$ , and the subbranch is pruned.

With that background established, the pruning algorithm follows these steps:

- ▶ Set  $\alpha_1 = 0$  and start with the tree  $T_1 = T(0)$ , the fully grown tree.
- ▶ Increase  $\alpha$  until a branch is pruned. Prune the branch from the tree, and calculate the risk estimate of the pruned tree.
- ▶ Repeat the previous step until only the root node is left, yielding a series of trees,  $T_1, T_2, \dots, T_k$ .
- ▶ If the standard error rule option is selected, choose the smallest tree  $T_{\text{opt}}$  for which

$$R(T_{\text{opt}}) \leq \min_k R(T_k) + m \times SE(R(T))$$

- ▶ If the standard error rule option is not selected, then the tree with the smallest risk estimate  $R(T)$  is selected.

## Secondary Calculations

Secondary calculations are not directly related to building the model, but give you information about the model and its performance.

### Risk Estimates

**Risk estimates** describe the risk of error in predicted values for specific nodes of the tree and for the tree as a whole.

#### Risk Estimates for Symbolic Target Field

For classification trees (with a symbolic target field), the risk estimate  $r(t)$  of a node  $t$  is computed as

$$r(t) = \frac{1}{N_f} \sum_j N_{f,j}(t) C(j^*(t)|j)$$

where  $C(j^*(t)|j)$  is the misclassification cost of classifying a record with target value  $j$  as  $j^*(t)$ ,  $N_{f,j}(t)$  is the sum of the frequency weights for records in node  $t$  in category  $j$  (or the number of records if no frequency weights are defined), and  $N_f$  is the sum of frequency weights for all records in the training data.

If the model uses user-specified priors, the risk estimate is calculated as

$$\sum_j \frac{\pi(j) N_{f,j}(t)}{N_{f,j}} C(j^*(t)|j)$$

Note that case weights are not considered in calculating risk estimates.

#### Risk Estimates for numeric target field

For regression trees (with a numeric target field), the risk estimate  $r(t)$  of a node  $t$  is computed as

$$r(t) = \frac{1}{N_f(t)} \sum_{i \in t} f_i (y_i - \bar{y}(t))^2$$

where  $f_i$  is the frequency weight for record  $i$  (a record assigned to node  $t$ ),  $y_i$  is the value of the target field for record  $i$ , and  $\bar{y}(t)$  is the weighted mean of the target field for all records in node  $t$ .

**Tree Risk Estimate**

For both classification trees and regression trees, the risk estimate  $R(T)$  for the tree ( $T$ ) is calculated by taking the sum of the risk estimates for the terminal nodes  $r(t)$ :

$$R(T) = \sum_{t \in T'} r(t)$$

where  $T'$  is the set of terminal nodes in the tree.

**Gain Summary**

The **gain summary** provides descriptive statistics for the terminal nodes of a tree.

If your target field is continuous (scale), the gain summary shows the weighted mean of the target value for each terminal node,

$$g(t) = \sum_{i \in t} w_i f_i x_i$$

If your target field is symbolic (categorical), the gain summary shows the weighted percentage of records in a selected target category,

$$g(t, j) = \frac{\sum_{i \in t} f_i x_i(j)}{\sum_{i \in t} f_i}$$

where  $x_i(j) = 1$  if record  $x_i$  is in target category  $j$ , and 0 otherwise. If profits are defined for the tree, the gain is the average profit value for each terminal node,

$$g(t) = \sum_{i \in t} f_i P(x_i)$$

where  $P(x_i)$  is the profit value assigned to the target value observed in record  $x_i$ .

**Generated Model/Scoring**

Calculations done by the C&RT generated model are described below

**Predicted Values**

New records are scored by following the tree splits to a terminal node of the tree. Each terminal node has a particular predicted value associated with it, determined as follows:

**Classification Trees**

For trees with a symbolic target field, each terminal node's predicted category is the category with the lowest weighted cost for the node. This weighted cost is calculated as

$$\min_i \sum_j C(i|j)p(j|t)$$

where  $C(i|j)$  is the user-specified misclassification cost for classifying a record as category  $i$  when it is actually category  $j$ , and  $p(j|t)$  is the conditional weighted probability of a record being in category  $j$  given that it is in node  $t$ , defined as

$$p(j|t) = \frac{p(j, t)}{\sum_j p(j, t)}, p(j, t) = \pi(j) \frac{N_{w,j}(t)}{N_{w,j}}$$

where  $\pi(j)$  is the prior probability for category  $j$ ,  $N_{w,j}(t)$  is the weighted number of records in node  $t$  with category  $j$  (or the number of records if no frequency or case weights are defined),

$$N_{w,j}(t) = \sum_{i \in t} w_i f_{ij}(i)$$

and  $N_{w,j}$  is the weighted number records in category  $j$  (any node),

$$N_{w,j} = \sum_{i \in T} w_i f_{ij}(i)$$

### **Regression Trees**

For trees with a numeric target field, each terminal node's predicted category is the weighted mean of the target values for records in the node. This weighted mean is calculated as

$$\bar{y}(t) = \frac{1}{N_w(t)} \sum_{i \in t} w_i f_{iy_i}$$

where  $N_w(t)$  is defined as

$$N_w(t) = \sum_{i \in t} w_i f_i$$

### **Confidence**

For classification trees, confidence values for records passed through the generated model are calculated as follows. For regression trees, no confidence value is assigned.

**Classification Trees**

Confidence for a scored record is the proportion of weighted records in the training data in the scored record's assigned terminal node that belong to the predicted category, modified by the Laplace correction:

$$\frac{N_{f,j}(t) + 1}{N_f(t) + k}$$

**Blank Handling**

In classification of new records, blanks are handled as they are during tree growth, using surrogates where possible, and splitting based on weighted probabilities where necessary. For more information, see the topic "Blank Handling" on p. 61.



# CHAID Algorithms

## Overview of CHAID

CHAID stands for Chi-squared Automatic Interaction Detector. It is a highly efficient statistical technique for segmentation, or tree growing, developed by (Kass, 1980). Using the significance of a statistical test as a criterion, CHAID evaluates all of the values of a potential predictor field. It merges values that are judged to be statistically homogeneous (similar) with respect to the target variable and maintains all other values that are heterogeneous (dissimilar).

It then selects the best predictor to form the first branch in the decision tree, such that each child node is made of a group of homogeneous values of the selected field. This process continues recursively until the tree is fully grown. The statistical test used depends upon the measurement level of the target field. If the target field is continuous, an  $F$  test is used. If the target field is categorical, a chi-squared test is used.

CHAID is not a binary tree method; that is, it can produce *more* than two categories at any particular level in the tree. Therefore, it tends to create a wider tree than do the binary growing methods. It works for all types of variables, and it accepts both case weights and frequency variables. It handles missing values by treating them all as a single valid category.

### **Exhaustive CHAID**

Exhaustive CHAID is a modification of CHAID developed to address some of the weaknesses of the CHAID method (Biggs, de Ville, and Suen, 1991). In particular, sometimes CHAID may not find the optimal split for a variable, since it stops merging categories as soon as it finds that all remaining categories are statistically different. Exhaustive CHAID remedies this by continuing to merge categories of the predictor variable until only two supercategories are left. It then examines the series of merges for the predictor and finds the set of categories that gives the strongest association with the target variable, and computes an adjusted  $p$ -value for that association. Thus, Exhaustive CHAID can find the best split for each predictor, and then choose which predictor to split on by comparing the adjusted  $p$ -values.

Exhaustive CHAID is identical to CHAID in the statistical tests it uses and in the way it treats missing values. Because its method of combining categories of variables is more thorough than that of CHAID, it takes longer to compute. However, if you have the time to spare, Exhaustive CHAID is generally safer to use than CHAID. It often finds more useful splits, though depending on your data, you may find no difference between Exhaustive CHAID and CHAID results.

## Primary Calculations

The calculations directly involved in building the model are described below.

### **Frequency and Case Weight Fields**

Frequency and case weight fields are useful for reducing the size of your dataset. Each has a distinct function, though. If a case weight field is mistakenly specified to be a frequency field, or vice versa, the resulting analysis will be incorrect.

For the calculations described below, if no frequency or case weight fields are specified, assume that frequency and case weights for all records are equal to 1.0.

### **Frequency Fields**

A **frequency field** represents the total number of observations represented by each record. It is useful for analyzing aggregate data, in which a record represents more than one individual. The sum of the values for a frequency field should always be equal to the total number of observations in the sample. Note that output and statistics are the same whether you use a frequency field or case-by-case data. The table below shows a hypothetical example, with the predictor fields *sex* and *employment* and the target field *response*. The frequency field tells us, for example, that 10 employed men responded *yes* to the target question, and 19 unemployed women responded *no*.

Table 10-1  
Dataset with frequency field

<b>Sex</b>	<b>Employment</b>	<b>Response</b>	<b>Frequency</b>
M	Y	Y	10
M	Y	N	17
M	N	Y	12
M	N	N	21
F	Y	Y	11
F	Y	N	15
F	N	Y	15
F	N	N	19

The use of a frequency field in this case allows us to process a table of 8 records instead of case-by-case data, which would require 120 records.

### **Case weights**

The use of a case weight field gives unequal treatment to the records in a dataset. When a **case weight field** is used, the contribution of a record in the analysis is weighted in proportion to the population units that the record represents in the sample. For example, suppose that in a direct marketing promotion, 10,000 households respond and 1,000,000 households do not respond. To reduce the size of the data file, you might include all of the responders but only a 1% sample (10,000) of the nonresponders. You can do this if you define a case weight equal to 1 for responders and 100 for nonresponders.

## **Binning of Scale-Level Predictors**

Scale level (continuous) *predictor* fields are automatically discretized or **binned** into a set of ordinal categories. This process is performed once for each scale-level predictor in the model, prior to applying the CHAID (or Exhaustive CHAID) algorithm. The binned categories are determined as follows:

1. The data values  $y_i$  are sorted.

- For each unique value, starting with the smallest, calculate the relative (weighted) frequency of values less than or equal to the current value  $y_i$ :

$$cf_i = \sum_{y_k < y_i} w_k$$

where  $w_k$  is the weight for record  $k$  (or 1.0 if no weights are defined).

- Determine the bin to which the value belongs by comparing the relative frequency with the ideal bin percentile cutpoints of 0.10, 0.20, 0.30, etc.

$$binindex = \frac{g}{W + 1} \times 10$$

where  $W$  is the total weighted frequency for all records in the training data,  $\sum_i w_i$ , and

$$g = \begin{cases} cf_{i-1} + \frac{w_i + 1}{2}, & w_i \geq 1 \\ cf_{i-1} + \frac{w_i}{2}, & w_i < 1 \end{cases}$$

- If the bin index for this value is different from the bin index for the previous data value, add a new bin to the bin list and set its cutpoint to the current data value.
- If the bin index is the same as the bin index for the previous value, update the cut point for that bin to the current data value.

Normally, CHAID will try to create  $k = 10$  bins by default. However, when the number of records having a single value is large (or a set of records with the same value has a large combined weighted frequency), the binning may result in fewer bins. This will happen if the weighted frequency for records with the same value is greater than the expected weighted frequency in a bin ( $1/k$ th of the total weighted frequency). This will also happen if there are fewer than  $k$  distinct values for the binned field for records in the training data.

## Model Parameters

CHAID works with all types of continuous or categorical fields. However, continuous *predictor* fields are automatically categorized for the purpose of the analysis. For more information, see the topic “Binning of Scale-Level Predictors” on p. 74.

Note that you can set some of the options mentioned below using the Expert Options for CHAID. These include the choice of the Pearson chi-squared or likelihood-ratio test, the level of  $\alpha_{merge}$ , the level of  $\alpha_{split}$ , score values, and details of stopping rules.

The CHAID algorithm proceeds as follows:

### **Merging Categories for Predictors (CHAID)**

To determine each split, all predictor fields are merged to combine categories that are not statistically different with respect to the target field. Each final category of a predictor field  $X$  will represent a child node if  $X$  is used to split the node. The following steps are applied to each predictor field  $X$ :

1. If  $X$  has one or two categories, no more categories are merged, so proceed to node splitting below.
2. Find the eligible pair of categories of  $X$  that is least significantly different (most similar) as determined by the  $p$ -value of the appropriate statistical test of association with the target field. For more information, see the topic “Statistical Tests Used” on p. 77.

For ordinal fields, only adjacent categories are eligible for merging; for nominal fields, all pairs are eligible.

3. For the pair having the largest  $p$ -value, if the  $p$ -value is greater than  $\alpha_{\text{merge}}$ , then merge the pair of categories into a single category. Otherwise, skip to step 6.
4. If the user has selected the Allow splitting of merged categories option, and the newly formed compound category contains three or more original categories, then find the best binary split within the compound category (that for which the  $p$ -value of the statistical test is smallest). If that  $p$ -value is less than or equal to  $\alpha_{\text{split-merge}}$ , perform the split to create two categories from the compound category.
5. Continue merging categories from step 1 for this predictor field.
6. Any category with fewer than the user-specified minimum segment size records is merged with the most similar other category (that which gives the largest  $p$ -value when compared with the small category).

### **Merging Categories for Predictors (Exhaustive CHAID)**

Exhaustive CHAID works much the same as CHAID, except that the category merging is more thoroughly tested to find the ideal set of categories for each predictor field. As with regular CHAID, each final category of a predictor field  $X$  will represent a child node if  $X$  is used to split the node. The following steps are applied to each predictor field  $X$ :

1. For each predictor variable  $X$ , find the pair of categories of  $X$  that is least significantly different (that is, has the largest  $p$ -value) with respect to the target variable  $Y$ . The method used to calculate the  $p$ -value depends on the measurement level of  $Y$ . For more information, see the topic “Statistical Tests Used” on p. 77.
2. Merge into a compound category the pair that gives the largest  $p$ -value.
3. Calculate the  $p$ -value based on the new set of categories of  $X$ . This represents one set of categories for  $X$ . Remember the  $p$ -value and its corresponding set of categories.

4. Repeat steps 1, 2, and 3 until only two categories remain. Then, compare the sets of categories of  $X$  generated during each step of the merge sequence, and find the one for which the  $p$ -value in step 3 is the smallest. That set is the set of merged categories for  $X$  to be used in determining the split at the current node.

### **Splitting Nodes**

When categories have been merged for all predictor fields, each field is evaluated for its association with the target field, based on the adjusted  $p$ -value of the statistical test of association, as described below.

The predictor with the strongest association, indicated by the smallest adjusted  $p$ -value, is compared to the split threshold,  $\alpha_{\text{split}}$ . If the  $p$ -value is less than or equal to  $\alpha_{\text{split}}$ , that field is selected as the split field for the current node. Each of the merged categories of the split field defines a child node of the split.

After the split is applied to the current node, the child nodes are examined to see if they warrant splitting by applying the merge/split process to each in turn. Processing proceeds recursively until one or more stopping rules are triggered for every unsplit node, and no further splits can be made.

### **Statistical Tests Used**

Calculations of the unadjusted  $p$ -values depend on the type of the target field. During the merge step, categories are compared pairwise, that is, one (possibly compound) category is compared against another (possibly compound) category. For such comparisons, only records belonging to one of the comparison categories in the current node are considered. During the split step, all categories are considered in calculating the  $p$ -value, thus all records in the current node are used.

### **Scale Target Field ( $F$ Test).**

For models with a scale-level target field, the  $p$ -value is calculated based on a standard ANOVA  $F$ -test comparing the target field means across categories of the predictor field under consideration. The  $F$  statistic is calculated as

$$F = \frac{\sum_{i=1}^I \sum_{n \in D} w_n f_n I(x_n = i) (\bar{y}_i - \bar{y})^2 / (I - 1)}{\sum_{i=1}^I \sum_{n \in D} w_n f_n I(x_n = i) (y_n - \bar{y}_i)^2 / (N_f - I)}$$

and the  $p$ -value is

$$p = \Pr(F(I - 1, N_f - I) > F)$$

where

$$\bar{y}_i = \frac{\sum_{n \in D} w_n f_n y_n I(x_n = i)}{\sum_{n \in D} w_n f_n I(x_n = i)}, \bar{y} = \frac{\sum_{n \in D} w_n f_n y_n}{\sum_{n \in D} w_n f_n}, N_f = \sum_{n \in D} f_n$$

and  $F(I-1, N_f-I)$  is a random variable following an  $F$ -distribution with  $(I-1)$  and  $(N_f-I)$  degrees of freedom.

### **Nominal Target Field (Chi-Squared Test)**

If the target field  $Y$  is a set (categorical) field, the null hypothesis of independence of  $X$  and  $Y$  is tested. To do the test, a contingency (count) table is formed using classes of  $Y$  as columns and categories of the predictor  $X$  as rows. The expected cell frequencies under the null hypothesis of independence are estimated. The observed cell frequencies and the expected cell frequencies are used to calculate the chi-squared statistic, and the  $p$ -value is based on the calculated statistic.

#### **Pearson Chi-squared test**

The Pearson chi-square statistic is calculated as

$$X^2 = \sum_{j=1}^J \sum_{i=1}^I \frac{(n_{ij} - \hat{m}_{ij})^2}{\hat{m}_{ij}}$$

where  $n_{ij} = \sum_n f_n I(x_n = i \wedge y_n = j)$  is the observed cell frequency and  $\hat{m}_{ij}$  is the expected cell frequency for cell  $(x_n = i, y_n = j)$  from the independence model as described below. The corresponding  $p$  value is calculated as  $p = \Pr(\chi_d^2 > X^2)$ , where  $\chi_d^2$  follows a chi-square distribution with  $d = (J-1)(I-1)$  degrees of freedom.

#### **Expected Frequencies for Chi-Square Test**

#### **Likelihood-ratio Chi-squared test**

The likelihood-ratio chi-square is calculated based on the expected and observed frequencies, as described above. The likelihood ratio chi-square is calculated as

$$G^2 = 2 \sum_{j=1}^J \sum_{i=1}^I n_{ij} \ln(n_{ij} / \hat{m}_{ij})$$

and the  $p$ -value is calculated as  $p = \Pr(\chi_d^2 > G^2)$

#### **Expected frequencies for chi-squared tests**

For models with no case weights, expected frequencies are calculated as

$$\hat{m}_{ij} = \frac{n_{i.} n_{.j}}{n_{..}}$$

where

$$n_{i.} = \sum_{j=1}^J n_{ij}, \quad n_{.j} = \sum_{i=1}^I n_{ij}, \quad n_{..} = \sum_{j=1}^J \sum_{i=1}^I n_{ij}.$$

If case weights are specified, the expected cell frequency under the null hypothesis of independence takes the form

$$m_{ij} = \bar{w}_{ij}^{-1} \alpha_i \beta_j$$

where  $\alpha_i$  and  $\beta_j$  are parameters to be estimated, and

$$\bar{w}_{ij} = \frac{w_{ij}}{n_{ij}}, \quad w_{ij} = \sum_{n \in D} w_n f_n I(x = i \wedge y_n = j).$$

The parameter estimates  $\hat{\alpha}_i$ ,  $\hat{\beta}_j$ , and hence  $\hat{m}_{ij}$ , are calculated based on the following iterative procedure:

1. Initially,  $k = 0$ ,  $\alpha_i^{(0)} = \beta_j^{(0)} = 1$ ,  $m_{ij}^{(0)} = \bar{w}_{ij}^{-1}$ .
2.  $\alpha_i^{(k+1)} = \frac{n_{i.}}{\sum_j \bar{w}_{ij}^{-1} \beta_j^{(k)}} = \alpha_i^{(k)} \frac{n_{i.}}{\sum_j m_{ij}^{(k)}}$ .
3.  $\beta_j^{(k+1)} = \frac{n_{.j}}{\sum_i \bar{w}_{ij}^{-1} \alpha_i^{(k+1)}}$ .
4.  $m_{ij}^{(k+1)} = \bar{w}_{ij}^{-1} \alpha_i^{(k+1)} \beta_j^{(k+1)}$ .
5. If  $\max_{i,j} |m_{ij}^{(k+1)} - m_{ij}^{(k)}| < \epsilon$ , stop and output  $\alpha_i^{(k+1)}$ ,  $\beta_j^{(k+1)}$ , and  $m_{ij}^{(k+1)}$  as the final estimates of  $\hat{\alpha}_i$ ,  $\hat{\beta}_j$ , and  $\hat{m}_{ij}$ . Otherwise, increment  $k$  and repeat from step 2.

### **Ordinal Target Field (Row Effects Model)**

If the target field  $Y$  is ordinal, the null hypothesis of independence of  $X$  and  $Y$  is tested against the row effects model, with the rows being the categories of  $X$  and the columns the categories of  $Y$  (Goodman, 1979). Two sets of expected cell frequencies,  $\hat{m}_{ij}$  (under the hypothesis of independence) and  $\hat{\hat{m}}_{ij}$  (under the hypothesis that the data follow the row effects model), are both estimated. The likelihood ratio statistic is computed as

$$H^2 = 2 \sum_{i=1}^I \sum_{j=1}^J \hat{\hat{m}}_{ij} \ln \left( \hat{\hat{m}}_{ij} / \hat{m}_{ij} \right)$$

and the  $p$ -value is calculated as

$$p = \Pr \left( \chi_{I-1}^2 > H^2 \right)$$

### Expected Cell Frequencies for the Row Effects Model

For the row effects model, scores for categories of  $Y$  are needed. By default, the order of each category is used as the category score. Users can specify their own set of scores. The expected cell frequency under the row effects model is

$$m_{ij} = \bar{w}_{ij}^{-1} \alpha_i \beta_j \gamma_i^{(s_j - \bar{s})}$$

where  $s_j$  is the score for category  $j$  of  $Y$ , and

$$\bar{s} = \frac{\sum_{j=1}^J w_{.j} s_j}{\sum_{j=1}^J w_{.j}}$$

in which  $w_{.j} = \sum_i w_{ij}$ ,  $\alpha_i$ ,  $\beta_j$  and  $\gamma_i$  are unknown parameters to be estimated.

Parameter estimates  $\hat{\alpha}_i$ ,  $\hat{\beta}_j$ ,  $\hat{\gamma}_i$ , and hence  $\hat{m}_{ij}$  are calculated using the following iterative procedure:

1.  $k = 0, \alpha_i^{(0)} = \beta_j^{(0)} = \gamma_i^{(0)} = 1, m_{ij}^{(0)} = \bar{w}_{ij}^{-1}$
2.  $\alpha_i^{(k+1)} = \frac{n_{.j}}{\sum_j \bar{w}_{ij}^{-1} \beta_j^{(k)} (\gamma_i^{(k)})^{(s_j - \bar{s})}} = \alpha_i^{(k)} \frac{n_{.j}}{\sum_j m_{ij}^{(k)}}$
3.  $\beta_j^{(k+1)} = \frac{n_{.j}}{\sum_i \bar{w}_{ij}^{-1} \alpha_i^{(k)} (\gamma_i^{(k)})^{(s_j - \bar{s})}}$
4.  $m_{ij}^* = \bar{w}_{ij}^{-1} \alpha_i^{(k+1)} \beta_j^{(k+1)} (\gamma_i^{(k)})^{(s_j - \bar{s})}$ ,  $G_i = 1 + \frac{\sum_j (s_j - \bar{s})(n_{ij} - m_{ij}^*)}{\sum_j (s_j - \bar{s})^2 m_{ij}^*}$
5.  $\gamma_i^{(k+1)} = \begin{cases} \gamma_i^{(k)} G_i & G_i > 0 \\ \gamma_i^{(k)} & \text{otherwise} \end{cases}$
6.  $m_{ij}^{(k+1)} = \bar{w}_{ij}^{-1} \alpha_i^{(k+1)} \beta_j^{(k+1)} (\gamma_i^{(k+1)})^{(s_j - \bar{s})}$
7. If  $\max_{i,j} |m_{ij}^{(k+1)} - m_{ij}^{(k)}| < \epsilon$ , stop and set  $\alpha_i^{(k+1)}$ ,  $\beta_j^{(k+1)}$ ,  $\gamma_i^{(k+1)}$ , and  $m_{ij}^{(k+1)}$  as the final estimates of  $\hat{\alpha}_i$ ,  $\hat{\beta}_j$ ,  $\hat{\gamma}_i$ , and  $\hat{m}_{ij}$ . Otherwise, increment  $k$  and repeat from step 2.

### Bonferroni Adjustment

The **adjusted  $p$ -value** is calculated as the  $p$ -value times a Bonferroni multiplier. The Bonferroni multiplier controls the overall  $p$ -value across multiple statistical tests.

Suppose that a predictor field originally has  $I$  categories, and it is reduced to  $r$  categories after the merging step. The Bonferroni multiplier  $B$  is the number of possible ways that  $I$  categories can be merged into  $r$  categories. For  $r = I$ ,  $B = 1$ . For  $2 \leq r < I$ ,

$$B = \begin{cases} \binom{I-1}{r-1} & \text{Ordinal predictor} \\ \sum_{v=0}^{r-1} (-1)^v \frac{(r-v)^I}{v!(r-v)!} & \text{Nominal predictor} \\ \binom{I-2}{r-2} + r \binom{I-2}{r-1} & \text{Ordinal with a missing value} \end{cases}$$

## Blank Handling

If the target field for a record is blank, or all the predictor fields are blank, the record is ignored in model building. If case weights are specified and the case weight for a record is blank, zero, or negative, the record is ignored, and likewise for frequency weights.

For other records, blanks in predictor fields are treated as an additional category for the field.

### Ordinal Predictors

The algorithm first generates the best set of categories using all non-blank information. Then the algorithm identifies the category that is most similar to the blank category. Finally, two  $p$ -values are calculated: one for the set of categories formed by merging the blank category with its most similar category, and the other for the set of categories formed by adding the blank category as a separate category. The set of categories with the smallest  $p$ -value is used.

### Nominal Predictors

The missing category is treated the same as other categories in the analysis.

## Effect of Options

### Stopping Rules

Stopping rules control how the algorithm decides when to stop splitting nodes in the tree. Tree growth proceeds until every leaf node in the tree triggers at least one stopping rule. Any of the following conditions will prevent a node from being split:

- The node is pure (all records have the same value for the target field)
- All records in the node have the same value for all predictor fields used by the model
- The tree depth for the current node (the number of recursive node splits defining the current node) is the *maximum tree depth* (default or user-specified).
- The number of records in the node is less than the *minimum parent node size* (default or user-specified)
- The number of records in any of the child nodes resulting from the node's best split is less than the *minimum child node size* (default or user-specified)
- The best split for the node yields a  $p$ -value that is greater than the  $\alpha_{\text{split}}$  (default or user-specified).

**Profits**

**Profits** are numeric values associated with categories of a (symbolic) target field that can be used to estimate the gain or loss associated with a segment. They define the relative value of each value of the target field. Values are used in computing gains but not in tree growing.

Profit for each node in the tree is calculated as

$$\sum_j f_j(t)P_j$$

where  $j$  is the target field category,  $f_j(t)$  is the sum of frequency field values for all records in node  $t$  with category  $j$  for the target field, and  $P_j$  is the user-defined profit value for category  $j$ .

**Score Values**

**Scores** are available in CHAID and Exhaustive CHAID. They define the order and distance between categories of an ordinal categorical target field. In other words, the scores define the field's scale. Values of scores are involved in tree growing.

If user-specified scores are provided, they are used in calculation of expected cell frequencies, as described above.

**Costs**

Costs, if specified, are not taken into account in growing a CHAID tree. However, costs will be incorporated into node assignment and risk estimation, as described in Predicted Values and Risk Estimates, below.

**Secondary Calculations**

Secondary calculations are not directly related to building the model, but give you information about the model and its performance.

**Risk Estimates**

**Risk estimates** describe the risk of error in predicted values for specific nodes of the tree and for the tree as a whole.

**Risk Estimates for Symbolic Target Field**

For classification trees (with a symbolic target field), the risk estimate  $r(t)$  of a node  $t$  is computed as

$$r(t) = \frac{1}{N_f} \sum_j N_{f,j}(t)C(j^*(t)|j)$$

where  $C(j^*(t)|j)$  is the misclassification cost of classifying a record with target value  $j$  as  $j^*(t)$ ,  $N_{f_j}(t)$  is the sum of the frequency weights for records in node  $t$  in category  $j$  (or the number of records if no frequency weights are defined), and  $N_f$  is the sum of frequency weights for all records in the training data.

Note that case weights are not considered in calculating risk estimates.

### **Risk Estimates for numeric target field**

For regression trees (with a numeric target field), the risk estimate  $r(t)$  of a node  $t$  is computed as

$$r(t) = \frac{1}{N_f(t)} \sum_{i \in t} f_i (y_i - \bar{y}(t))^2$$

where  $f_i$  is the frequency weight for record  $i$  (a record assigned to node  $t$ ),  $y_i$  is the value of the target field for record  $i$ , and  $\bar{y}(t)$  is the weighted mean of the target field for all records in node  $t$ .

### **Tree Risk Estimate**

For both classification trees and regression trees, the risk estimate  $R(T)$  for the tree ( $T$ ) is calculated by taking the sum of the risk estimates for the terminal nodes  $r(t)$ :

$$R(T) = \sum_{t \in T'} r(t)$$

where  $T'$  is the set of terminal nodes in the tree.

## **Gain Summary**

The **gain summary** provides descriptive statistics for the terminal nodes of a tree.

If your target field is continuous (scale), the gain summary shows the weighted mean of the target value for each terminal node,

$$g(t) = \sum_{i \in t} w_i f_i x_i$$

If your target field is symbolic (categorical), the gain summary shows the weighted percentage of records in a selected target category,

$$g(t, j) = \frac{\sum_{i \in t} f_i x_i(j)}{\sum_{i \in t} f_i}$$

where  $x_i(j) = 1$  if record  $x_i$  is in target category  $j$ , and 0 otherwise. If profits are defined for the tree, the gain is the average profit value for each terminal node,

$$g(t) = \sum_{i \in t} f_i P(x_i)$$

where  $P(x_i)$  is the profit value assigned to the target value observed in record  $x_i$ .

## Generated Model/Scoring

Calculations done by the CHAID generated model are described below

### Predicted Values

New records are scored by following the tree splits to a terminal node of the tree. Each terminal node has a particular predicted value associated with it, determined as follows:

#### Classification Trees

For trees with a symbolic target field, each terminal node's predicted category is the category with the lowest weighted cost for the node. This weighted cost is calculated as

$$\min_i \sum_j C(i|j)p(j|t)$$

where  $C(i|j)$  is the user-specified misclassification cost for classifying a record as category  $i$  when it is actually category  $j$ , and  $p(j|t)$  is the conditional weighted probability of a record being in category  $j$  given that it is in node  $t$ , defined as

$$p(j|t) = \frac{p(j, t)}{\sum_j p(j, t)}, p(j, t) = \pi(j) \frac{N_{w,j}(t)}{N_{w,j}}$$

where  $\pi(j)$  is the prior probability for category  $j$ ,  $N_{w,j}(t)$  is the weighted number of records in node  $t$  with category  $j$  (or the number of records if no frequency or case weights are defined),

$$N_{w,j}(t) = \sum_{i \in t} w_i f_{ij}(i)$$

and  $N_{w,j}$  is the weighted number records in category  $j$  (any node),

$$N_{w,j} = \sum_{i \in T} w_i f_{ij}(i)$$

#### Regression Trees

For trees with a numeric target field, each terminal node's predicted category is the weighted mean of the target values for records in the node. This weighted mean is calculated as

$$\bar{y}(t) = \frac{1}{N_w(t)} \sum_{i \in t} w_i f_{ij} y_i$$

where  $N_w(t)$  is defined as

$$N_w(t) = \sum_{i \in t} w_i f_i$$

## **Confidence**

For classification trees, confidence values for records passed through the generated model are calculated as follows. For regression trees, no confidence value is assigned.

### **Classification Trees**

Confidence for a scored record is the proportion of weighted records in the training data in the scored record's assigned terminal node that belong to the predicted category, modified by the Laplace correction:

$$\frac{N_{f,j}(t) + 1}{N_f(t) + k}$$

## **Blank Handling**

In classification of new records, blanks are handled as they are during tree growth, being treated as an additional category (possibly merged with other non-blank categories). For more information, see the topic "Blank Handling" on p. 81.

For nodes where there were no blanks in the training data, a blank category will not exist for the split of that node. In that case, records with a blank value for the split field are assigned a null value.



# Cluster Evaluation Algorithms

This document describes measures used for evaluating clustering models.

- The **Silhouette coefficient** combines the concepts of cluster cohesion (favoring models which contain tightly cohesive clusters) and cluster separation (favoring models which contain highly separated clusters). It can be used to evaluate individual objects, clusters, and models.
- The **sum of squares error (SSE)** is a measure of prototype-based cohesion, while **sum of squares between (SSB)** is a measure of prototype-based separation.
- **Predictor importance** indicates how well the variable can differentiate different clusters. For both range (numeric) and discrete variables, the higher the importance measure, the less likely the variation for a variable between clusters is due to chance and more likely due to some underlying difference.

## Notation

The following notation is used throughout this chapter unless otherwise stated:

$x_{ik}$	Continuous variable $k$ in case $i$ (standardized).
$x_{iks}$	The $s$ th category of variable $k$ in case $i$ (one-of- $c$ coding).
$N$	Total number of valid cases.
$N_j$	The number of cases in cluster $j$ .
$Y$	Variable with $J$ cluster labels.
$\mu_{jk}$	The centroid of cluster $j$ for variable $k$ .
$D_{ij}$	The distance between case $i$ and the centroid of cluster $j$ .
$D_j$	The distance between the overall mean $u$ and the centroid of cluster $j$ .

## Goodness Measures

The average Silhouette coefficient is simply the average over all cases of the following calculation for each individual case:

$$(B - A) / \max(A, B)$$

where  $A$  is the average distance from the case to every other case assigned to the same cluster and  $B$  is the minimal average distance from the case to cases of a different cluster across all clusters.

Unfortunately, this coefficient is computationally expensive. In order to ease this burden, we use the following definitions of  $A$  and  $B$ :

- $A$  is the distance from the case to the centroid of the cluster which the case belongs to;
- $B$  is the minimal distance from the case to the centroid of every other cluster.

Distances may be calculated using Euclidean distances. The Silhouette coefficient and its average range between  $-1$ , indicating a very poor model, and  $1$ , indicating an excellent model. As found by Kaufman and Rousseeuw (1990), an average silhouette greater than  $0.5$  indicates reasonable partitioning of data; less than  $0.2$  means that the data do not exhibit cluster structure.

## Data Preparation

Before calculating Silhouette coefficient, we need to transform cases as follows:

1. **Recode categorical variables using one-of-c coding.** If a variable has  $c$  categories, then it is stored as  $c$  vectors, with the first category denoted  $(1,0,\dots,0)$ , the next category  $(0,1,0,\dots,0)$ , ..., and the final category  $(0,0,\dots,0,1)$ . The order of the categories is based on the ascending sort or lexical order of the data values.
2. **Rescale continuous variables.** Continuous variables are normalized to the interval  $[-1, 1]$  using the transformation  $[2*(x-\min)/(\max-\min)]-1$ . This normalization tries to equalize the contributions of continuous and categorical features to the distance computations.

## Basic Statistics

The following statistics are collected in order to compute the goodness measures: the centroid  $\mu_{jk}$  of variable  $k$  for cluster  $j$ , the distance between a case and the centroid, and the overall mean  $u$ .

For  $\mu_{jk}$  with an ordinal or continuous variable  $k$ , we average all standardized values of variable  $k$  within cluster  $j$ . For nominal variables,  $\mu_{jk}$  is a vector  $\{\varphi_{jks}\}$  of probabilities of occurrence for each state  $s$  of variable  $k$  for cluster  $j$ . Note that in counting, we do not consider cases with missing values in variable  $k$ . If the value of variable  $k$  is missing for all cases within cluster  $j$ ,  $\mu_{jk}$  is marked as missing.

The distance  $D_{ij}^2$  between case  $i$  and the centroid of cluster  $j$  can be calculated in terms of the weighted sum of the distance components  $d_{ijk}^2$  across all variables; that is

$$D_{ij}^2 = \frac{\sum_k w_{ijk} d_{ijk}^2}{\sum_k w_{ijk}}$$

where  $w_{ijk}$  denotes a weight. At this point, we do not consider differential weights, thus  $w_{ijk}$  equals  $1$  if the variable  $k$  in case  $i$  is valid,  $0$  if not. If all  $w_{ijk}$  equal  $0$ , set  $D_{ij}^2 = 0$ .

The distance component  $d_{ijk}^2$  is calculated as follows for ordinal and continuous variables

$$d_{ijk}^2 = (x_{ik} - \mu_{jk})^2$$

For binary or nominal variables, it is

$$d_{ijk}^2 = \frac{1}{S_k} \sum_{s=1}^{S_k} (x_{iks} - \varphi_{jks})^2$$

where variable  $k$  uses one-of- $c$  coding, and  $S_k$  is the number of its states.

The calculation of  $D_j$  is the same as that of  $D_{ij}$ , but the overall mean  $u$  is used in place of  $\mu_{jk}$  and  $\mu_{jk}$  is used in place of  $x_{ik}$ .

### **Silhouette Coefficient**

The Silhouette coefficient of case  $i$  is

$$\frac{\min \{D_{ij}, j \in C_{-i}\} - D_{ic_i}}{\max (\min \{D_{ij}, j \in C_{-i}\}, D_{ic_i})}$$

where  $C_{-i}$  denotes cluster labels which do not include case  $i$  as a member, while  $c_i$  is the cluster label which includes case  $i$ . If  $\max (\min \{D_{ij}, j \in C_{-i}\}, D_{ic_i})$  equals 0, the Silhouette of case  $i$  is not used in the average operations.

Based on these individual data, the total average Silhouette coefficient is:

$$SC = \frac{1}{N} \sum_{i=1}^N \frac{\min \{D_{ij}, j \in C_{-i}\} - D_{ic_i}}{\max (\min \{D_{ij}, j \in C_{-i}\}, D_{ic_i})}$$

### **Sum of Squares Error (SSE)**

SSE is a prototype-based cohesion measure where the squared Euclidean distance is used. In order to compare between models, we will use the averaged form, defined as:

$$\text{Average SSE} = \frac{1}{N} \sum_{j \in C} \sum_{i \in j} D_{ij}^2$$

### **Sum of Squares Between (SSB)**

SSB is a prototype-based separation measure where the squared Euclidean distance is used. In order to compare between models, we will use the averaged form, defined as:

$$\text{Average SSB} = \frac{1}{N} \sum_{j \in C} N_j D_j^2$$

### **Predictor Importance**

The importance of field  $i$  is defined as

$$VI_i = \frac{-\log_{10} (sig_i)}{\max_{j \in \Omega} (-\log_{10} (sig_j))}$$

where  $\Omega$  denotes the set of predictor and evaluation fields,  $sig_i$  is the significance or  $p$ -value computed from applying a certain test, as described below. If  $sig_i$  equals zero, set  $sig_i = MinDouble$ , where  $MinDouble$  is the minimal double value.

### Across Clusters

The  $p$ -value for **categorical** fields is based on Pearson's chi-square. It is calculated by

$$p\text{-value} = \text{Prob}(\chi_d^2 > X^2),$$

where

$$X^2 = \sum_{i=1}^I \sum_{j=1}^J \left( N_{ij} - \hat{N}_{ij} \right)^2 / \hat{N}_{ij}$$

where  $\hat{N}_{ij} = N_i \cdot N_{.j} / N(X)$ .

- If  $N(X) = 0$ , the importance is set to be undefined or unknown;
- If  $N_i = 0$ , subtract one from  $I$  for each such category to obtain  $I'$ ;
- If  $N_{.j} = 0$ , subtract one from  $J$  for each such cluster to obtain  $J'$ ;
- If  $J' \leq 1$  or  $I' \leq 1$ , the importance is set to be undefined or unknown.

The degrees of freedom are  $(I' - 1)(J' - 1)$ .

The  $p$ -value for **continuous** fields is based on an  $F$  test. It is calculated by

$$p\text{-value} = \text{Prob}\{F(J - 1, N - J) > F\},$$

where

$$F = \frac{\sum_{j=1}^J N_j (\bar{x}_j - \bar{\bar{x}})^2 / (J - 1)}{\sum_{j=1}^J (N_j - 1) s_j / (N - J)}$$

- If  $N=0$ , the importance is set to be undefined or unknown;
- If  $N_j = 0$ , subtract one from  $J$  for each such cluster to obtain  $J'$ ;
- If  $J' \leq 1$  or  $N \leq J'$ , the importance is set to be undefined or unknown;
- If the denominator in the formula for the  $F$  statistic is zero, the importance is set to be undefined or unknown;
- If the numerator in the formula for the  $F$  statistic is zero, set  $p$ -value = 1;

The degrees of freedom are  $(J' - 1, N - J')$ .

**Within Clusters**

The null hypothesis for **categorical** fields is that the proportion of cases in the categories in cluster  $j$  is the same as the overall proportion.

The chi-square statistic for cluster  $j$  is computed as follows

$$X^2 = \sum_{i=1}^I \frac{(N_{ij} - N_j p_i)^2}{N_j p_i}$$

If  $N_j = 0$ , the importance is set to be undefined or unknown;

If  $p_i = 0$ , subtract one from  $I$  for each such category to obtain  $I'$ ;

If  $I' \leq 1$ , the importance is set to be undefined or unknown.

The degrees of freedom are  $d = I' - 1$ .

The null hypothesis for **continuous** fields is that the mean in cluster  $j$  is the same as the overall mean.

The Student's  $t$  statistic for cluster  $j$  is computed as follows

$$t = \frac{(\bar{x}_j - \bar{x})}{s_j / \sqrt{N_j}}$$

with  $d = N_j - 1$  degrees of freedom.

If  $N_j \leq 1$  or  $s_j = 0$ , the importance is set to be undefined or unknown;

If the numerator is zero, set  $p$ -value = 1;

Here, the  $p$ -value based on Student's  $t$  distribution is calculated as

$$p\text{-value} = 1 - \text{Prob}\{|T(d)| \leq |t|\}.$$

**References**

Kaufman, L., and P. J. Rousseeuw. 1990. *Finding groups in data: An introduction to cluster analysis*. New York: John Wiley and Sons.

Tan, P., M. Steinbach, and V. Kumar. 2006. *Introduction to Data Mining*. : Addison-Wesley.



# COXREG Algorithms

## Cox Regression Algorithms

Cox (1972) first suggested the models in which factors related to lifetime have a multiplicative effect on the hazard function. These models are called proportional hazards models. Under the proportional hazards assumption, the hazard function  $h$  of  $t$  given  $X$  is of the form

$$h(t|\mathbf{x}) = h_0(t)e^{\mathbf{x}'\beta}$$

where  $\mathbf{x}$  is a known vector of regressor variables associated with the individual,  $\beta$  is a vector of unknown parameters, and  $h_0(t)$  is the baseline hazard function for an individual with  $\mathbf{x} = 0$ . Hence, for any two covariates sets  $\mathbf{x}_1$  and  $\mathbf{x}_2$ , the log hazard functions  $h(t|\mathbf{x}_1)$  and  $h(t|\mathbf{x}_2)$  should be parallel across time.

When a factor does not affect the hazard function multiplicatively, stratification may be useful in model building. Suppose that individuals can be assigned to one of  $m$  different strata, defined by the levels of one or more factors. The hazard function for an individual in the  $j$ th stratum is defined as

$$h_j(t|\mathbf{x}) = h_{0j}(t)e^{\mathbf{x}'\beta}$$

There are two unknown components in the model: the regression parameter  $\beta$  and the baseline hazard function  $h_{0j}(t)$ . The estimation for the parameters is described below.

## Estimation

We begin by considering a nonnegative random variable  $T$  representing the lifetimes of individuals in some population. Let  $f(t|\mathbf{x})$  denote the probability density function (pdf) of  $T$  given a regressor  $x$  and let  $S(t|\mathbf{x})$  be the survivor function (the probability of an individual surviving until time  $t$ ). Hence

$$S(t|\mathbf{x}) = \int_t^{\infty} f(u|\mathbf{x})du$$

The hazard  $h(t|\mathbf{x})$  is then defined by

$$h(t|\mathbf{x}) = \frac{f(t|\mathbf{x})}{S(t|\mathbf{x})}$$

Another useful expression for  $S(t|\mathbf{x})$  in terms of  $h(t|\mathbf{x})$  is

$$S(t|\mathbf{x}) = \exp\left(-\int_0^t h(u|\mathbf{x})du\right)$$

Thus,

$$\ln S(t|\mathbf{x}) = -\int_0^t h(u|\mathbf{x})du$$

For some purposes, it is also useful to define the cumulative hazard function

$$H(t|\mathbf{x}) = \int_0^t h(u|\mathbf{x})du = -\ln S(t|\mathbf{x})$$

Under the proportional hazard assumption, the survivor function can be written as

$$S(t|\mathbf{x}) = [S_0(t)]^{\exp(\mathbf{x}'\beta)}$$

where  $S_0(t)$  is the baseline survivor function defined by

$$S_0(t) = \exp(-H_0(t))$$

and

$$H_0(t) = \int_0^t h_0(u)du$$

Some relationships between  $S(t|\mathbf{x})$ ,  $H(t|\mathbf{x})$  and  $H_0(t)$ ,  $S_0(t)$  and  $h_0(t)$  which will be used later are

$$\ln S(t|\mathbf{x}) = -H(t|\mathbf{x}) = -\exp(\mathbf{x}'\beta)H_0(t)$$

$$\ln(-\ln S(t|\mathbf{x})) = \mathbf{x}'\beta + \ln H_0(t)$$

To estimate the survivor function  $S(t|\mathbf{x})$ , we can see from the equation for the survivor function that there are two components,  $\beta$  and  $S_0(t)$ , which need to be estimated. The approach we use here is to estimate  $\beta$  from the partial likelihood function and then to maximize the full likelihood for  $S_0(t)$ .

## Estimation of Beta

Assume that

- There are  $m$  levels for the stratification variable.
- Individuals in the same stratum have proportional hazard functions.
- The relative effect of the regressor variables is the same in each stratum.

Let  $t_{j1} < \dots < t_{jk_j}$  be the observed uncensored failure time of the  $n_j$  individuals in the  $j$ th stratum and  $x_{j1}, \dots, x_{jk_j}$  be the corresponding covariates. Then the partial likelihood function is defined by

$$L(\beta) = \prod_{j=1}^m \prod_{i=1}^{k_j} \frac{e^{\mathbf{S}'_{ji}\beta}}{\left( \sum_{l \in R_{ji}} w_l e^{\mathbf{x}'_l \beta} \right)^{d_{ji}}}$$

where  $d_{ji}$  is the sum of case weights of individuals whose lifetime is equal to  $t_{ji}$  and  $\mathbf{S}_{ji}$  is the weighted sum of the regression vector  $\mathbf{x}$  for those  $d_{ji}$  individuals,  $w_l$  is the case weight of individual  $l$ , and  $R_{ji}$  is the set of individuals alive and uncensored just prior to  $t_{ji}$  in the  $j$ th stratum. Thus the log-likelihood arising from the partial likelihood function is

$$l = \ln L(\beta) = \sum_{j=1}^m \sum_{i=1}^{k_j} \mathbf{S}'_{ji} \beta - \sum_{j=1}^m \sum_{i=1}^{k_j} d_{ji} \ln \left( \sum_{l \in R_{ji}} w_l e^{\mathbf{x}'_l \beta} \right)$$

and the first derivatives of  $l$  are

$$D_{\beta_r} = \frac{\partial l}{\partial \beta_r} = \sum_{j=1}^m \sum_{i=1}^{k_j} \left( S_{ji}^{(r)} - d_{ji} \frac{\sum_{l \in R_{ji}} w_l x_{lr} e^{\mathbf{x}'_l \beta}}{\sum_{l \in R_{ji}} w_l e^{\mathbf{x}'_l \beta}} \right), \quad r = 1, \dots, p$$

$S_{ji}^{(r)}$  is the  $r$ th component of  $\mathbf{S}_{ji} = (S_{ji}^{(1)}, \dots, S_{ji}^{(p)})'$ . The maximum partial likelihood estimate (MPLE) of  $\beta$  is obtained by setting  $\frac{\partial l}{\partial \beta_r}$  equal to zero for  $r = 1, \dots, p$ , where  $p$  is the number of independent variables in the model. The equations  $\frac{\partial l}{\partial \beta_r} = 0$  ( $r = 1, \dots, p$ ) can usually be solved by using the Newton-Raphson method.

Note that from its equation that the partial likelihood function  $L(\beta)$  is invariant under translation. All the covariates are centered by their corresponding overall mean. The overall mean of a covariate is defined as the sum of the product of weight and covariate for all the censored and uncensored cases in each stratum. For notational simplicity,  $\mathbf{x}_l$  used in the Estimation Section denotes centered covariates.

Three convergence criteria for the Newton-Raphson method are available:

- Absolute value of the largest difference in parameter estimates between iterations ( $\delta$ ) divided by the value of the parameter estimate for the previous iteration; that is,

$$\text{BCON} = \left| \frac{\delta}{\text{parameter estimate for previous iteration}} \right|$$

- Absolute difference of the log-likelihood function between iterations divided by the log-likelihood function for previous iteration.
- Maximum number of iterations.

The asymptotic covariance matrix for the MPLE  $\hat{\beta} = (\hat{\beta}_1, \dots, \hat{\beta}_p)'$  is estimated by  $\mathbf{I}^{-1}$  where  $\mathbf{I}$  is the information matrix containing minus the second partial derivatives of  $\ln L$ . The  $(r, s)$ -th element of  $\mathbf{I}$  is defined by

$$\begin{aligned} \mathbf{I}_{rs} &= -E \frac{\partial^2}{\partial \beta_r \partial \beta_s} \ln L \\ &= \sum_{j=1}^m \sum_{i=1}^{k_j} d_{ji} \left[ \frac{\sum_{l \in R_{ji}} w_l x_{ls} x_{lr} e^{\mathbf{x}'_l \beta}}{\sum_{l \in R_{ji}} w_l e^{\mathbf{x}'_l \beta}} - \frac{\left( \sum_{l \in R_{ji}} w_l x_{lr} e^{\mathbf{x}'_l \beta} \right) \left( \sum_{l \in R_{ji}} w_l x_{ls} e^{\mathbf{x}'_l \beta} \right)}{\left( \sum_{l \in R_{ji}} w_l e^{\mathbf{x}'_l \beta} \right)^2} \right] \end{aligned}$$

We can also write  $\mathbf{I}$  in a matrix form as

$$I_{rs} = \sum_{j=1}^m \sum_{i=1}^{k_j} d_{ji} \left( \mathbf{x}'(t_{ji}) \right) V(t_{ji}) (\mathbf{x}(t_{ji}))$$

where  $\mathbf{x}(t_{ji})$  is a  $n_{ji} \times p$  matrix which represents the  $p$  covariate variables in the model evaluated at time  $t_{ji}$ ,  $n_{ji}$  is the number of distinct individuals in  $R_{ji}$ , and  $\mathbf{V}(t_{ji})$  is a  $n_{ji} \times n_{ji}$  matrix with the  $l$ th diagonal element  $v_{ll}(t_{ji})$  defined by

$$v_{ll}(t_{ji}) = p_l(t_{ji})w_l - (w_l p_l(t_{ji}))^2$$

$$p_l(t_{ji}) = \frac{\exp(\mathbf{x}'_l \hat{\beta})}{\sum_{h \in R_{ji}} w_h \exp(\mathbf{x}'_h \hat{\beta})}$$

and the  $(l, k)$  element  $v_{lk}(t_{ji})$  defined by

$$v_{lk}(t_{ji}) = w_l p_l(t_{ji}) \times w_k p_k(t_{ji})$$

## Estimation of the Baseline Function

After the MPLE  $\hat{\beta}$  of  $\beta$  is found, the baseline survivor function  $S_{0j}(t)$  is estimated separately for each stratum. Assume that, for a stratum,  $t_1 < \dots < t_k$  are observed lifetimes in the sample. There are  $n_i$  at risk and  $d_i$  deaths at  $t_i$ , and in the interval  $[t_{i-1}, t_i)$  there are  $\lambda_i$  censored times. Since  $S_0(t)$  is a survivor function, it is non-increasing and left continuous, and thus  $\hat{S}_0(t)$  must be constant except for jumps at the observed lifetimes  $t_1, \dots, t_k$ .

Further, it follows that

$$\hat{S}_0(t_1) = 1$$

and

$$\hat{S}_0(t_i+) = \hat{S}_0(t_{i+1})$$

Writing  $\hat{S}_0(t_i+) = p_i (i = 1, \dots, k)$ , the observed likelihood function is of the form

$$L_1 = \prod_{i=1}^k \left\{ \prod_{l \in D_i} \left( p_{i-1}^{\exp(\mathbf{x}'_l \beta)} - p_i^{\exp(\mathbf{x}'_l \beta)} \right)^{w_l} \prod_{l \in C_i} \left( p_{i-1}^{\exp(\mathbf{x}'_l \beta)} \right)^{w_l} \right\} \prod_{l \in C_{k+1}} \left( p_k^{\exp(\mathbf{x}'_l \beta)} \right)^{w_l}$$

where  $D_i$  is the set of individuals dying at  $t_i$  and  $C_i$  is the set of individuals with censored times in  $[t_{i-1}, t_i)$ . (Note that if the last observation is uncensored,  $C_{k+1}$  is empty and  $p_k = 0$ )

If we let  $\alpha_i = p_i/p_{i-1} (i = 1, \dots, k)$ ,  $L_1$  can be written as

$$L_1 = \prod_{i=1}^k \prod_{l \in D_i} \left( 1 - \alpha_i^{\exp(\mathbf{x}'_l \beta)} \right)^{w_l} \prod_{l \in R_i - D_i} \alpha_i^{w_l \exp(\mathbf{x}'_l \beta)}$$

Differentiating  $\ln L_1$  with respect to  $\alpha_1, \dots, \alpha_k$  and setting the equations equal to zero, we get

$$\sum_{l \in D_i} \frac{w_l \exp(\mathbf{x}'_l \beta)}{1 - \alpha_i^{\exp(\mathbf{x}'_l \beta)}} = \sum_{l \in R_i} w_l \exp(\mathbf{x}'_l \beta) \quad i = 1, \dots, k$$

We then plug the MPLE  $\hat{\beta}$  of  $\beta$  into this equation and solve these  $k$  equations separately.

There are two things worth noting:

- If any  $|D_i| = 1$ ,  $\hat{\alpha}_i$  can be solved explicitly.

$$\hat{\alpha}_i = \left[ 1 - \frac{w_i \exp(\mathbf{x}'_i \hat{\beta})}{\sum_{l \in R_i} w_l \exp(\mathbf{x}'_l \hat{\beta})} \right]^{\exp(-\mathbf{x}'_i \bar{\beta})}$$

- If  $|D_i| > 1$ , the equation for the cumulative hazard function must be solved iteratively for  $\hat{\alpha}_i$ . A good initial value for  $\hat{\alpha}_i$  is

$$\hat{\alpha}_i = \exp\left(\frac{-d_i}{\sum_{l \in R_i} w_l \exp(\mathbf{x}'_l \hat{\beta})}\right)$$

where  $d_i = \sum_{l \in D_i} w_l$  is the weight sum for set  $D_i$ . (See Lawless, 1982, p. 361.)

Once the  $\hat{\alpha}_i$ ,  $i = 1, \dots, k$  are found,  $S_0(t)$  is estimated by

$$\hat{S}_0(t) = \prod_{i: (t_i < t)} \hat{\alpha}_i$$

Since the above estimate of  $S_0(t)$  requires some iterative calculations when ties exist, Breslow (1974) suggests using the equation for  $\alpha_i$  when  $|D_i| > 1$  as an estimate; however, we will use this as an initial estimate.

The asymptotic variance for  $-\ln \hat{S}_0(t)$  can be found in Chapter 4 of Kalbfleisch and Prentice (1980). At a specified time  $t$ , it is consistently estimated by

$$\text{var}(-\ln \hat{S}_0(t)) = \sum_{t_i < t} |D_i| \left( \sum_{l \in R_i} w_l \exp(\mathbf{x}'_l \hat{\beta}) \right)^{-2} + \mathbf{a}' \mathbf{I}^{-1} \mathbf{a}$$

where  $\mathbf{a}$  is a  $p \times 1$  vector with the  $j$ th element defined by

$$\sum_{t_i < t} |D_i| \frac{\sum_{l \in R_i} w_l x_{lj} \exp(\mathbf{x}'_l \hat{\beta})}{\left( \sum_{l \in R_i} w_l \exp(\mathbf{x}'_l \hat{\beta}) \right)^2}$$

and  $\mathbf{I}$  is the information matrix. The asymptotic variance of  $\hat{S}(t|x)$  is estimated by

$$e^{2\mathbf{x}' \hat{\beta}} \left( \hat{S}(t|x) \right)^2 \text{var}(-\ln \hat{S}_0(t))$$

## Selection Statistics for Stepwise Methods

The same methods for variable selection are offered as in binary logistic regression. For more information, see the topic “Stepwise Variable Selection” on p. 253. Here we will only define the three removal statistics—Wald, LR, and Conditional—and the Score entry statistic.

### Score Statistic

The score statistic is calculated for every variable not in the model to decide which variable should be added to the model. First we compute the information matrix  $\mathbf{I}$  for all eligible variables based on the parameter estimates for the variables in the model and zero parameter estimates for the variables not in the model. Then we partition the resulting  $\mathbf{I}$  into four submatrices as follows:

$$\begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}$$

where  $\mathbf{A}_{11}$  and  $\mathbf{A}_{22}$  are square matrices for variables in the model and variables not in the model, respectively, and  $\mathbf{A}_{12}$  is the cross-product matrix for variables in and out. The score statistic for variable  $\mathbf{x}_i$  is defined by

$$\mathbf{D}'_{x_i} \mathbf{B}_{22,i} \mathbf{D}_{x_i}$$

where  $\mathbf{D}_{x_i}$  is the first derivative of the log-likelihood with respect to all the parameters associated with  $\mathbf{x}_i$  and  $\mathbf{B}_{22,i}$  is equal to  $(\mathbf{A}_{22,i} - \mathbf{A}_{21,i} \mathbf{A}_{11}^{-1} \mathbf{A}_{12,i})^{-1}$ , and  $\mathbf{A}_{22,i}$  and  $\mathbf{A}_{12,i}$  are the submatrices in  $\mathbf{A}_{22}$  and  $\mathbf{A}_{12}$  associated with variable  $\mathbf{x}_i$ .

### Wald Statistic

The Wald statistic is calculated for the variables in the model to select variables for removal. The Wald statistic for variable  $\mathbf{x}_j$  is defined by

$$\hat{\beta}'_j \mathbf{B}_{11,j} \hat{\beta}_j$$

where  $\hat{\beta}_j$  is the parameter estimate associated with  $\mathbf{x}_j$  and  $\mathbf{B}_{11,j}$  is the submatrix of  $\mathbf{A}_{11}^{-1}$  associated with  $\mathbf{x}_j$ .

### LR (Likelihood Ratio) Statistic

The LR statistic is defined as twice the log of the ratio of the likelihood functions of two models evaluated at their own MPLES. Assume that  $r$  variables are in the current model and let us call the current model the full model. Based on the MPLES of parameters for the full model,  $l(full)$  is defined in "Estimation of Beta". For each of  $r$  variables deleted from the full model, MPLES are found and the reduced log-likelihood function,  $l(reduced)$ , is calculated. Then LR statistic is defined as

$$-2(l(reduced) - l(full))$$

### Conditional Statistic

The conditional statistic is also computed for every variable in the model. The formula for conditional statistic is the same as LR statistic except that the parameter estimates for each reduced model are conditional estimates, not MPLES. The conditional estimates are defined as

follows. Let  $\hat{\beta} = (\hat{\beta}_1, \dots, \hat{\beta}_r)'$  be the MPLES for the  $r$  variables (blocks) and  $C$  be the asymptotic covariance for the parameters left in the model given  $\hat{\beta}_i$  is

$$\tilde{\beta}_{(i)} = \hat{\beta}_{(i)} - \mathbf{C}_{12}^{(i)} \left( \mathbf{C}_{22}^{(i)} \right)^{-1} \hat{\beta}_i$$

where  $\hat{\beta}_i$  is the MPLE for the parameter(s) associated with  $\mathbf{x}_i$  and  $\hat{\beta}_{(i)}$  is  $\hat{\beta}$  without  $\hat{\beta}_i$ ,  $\mathbf{C}_{12}^{(i)}$  is the covariance between the parameter estimates left in the model  $\hat{\beta}_{(i)}$  and  $\hat{\beta}_i$ , and  $\mathbf{C}_{22}^{(i)}$  is the covariance of  $\hat{\beta}_i$ . Then the conditional statistic for variable  $\mathbf{x}_i$  is defined by

$$-2(l(\mathbf{b}_{(i)}) - l(\mathit{full}))$$

where  $l(\tilde{\beta}_{(i)})$  is the log-likelihood function evaluated at  $\tilde{\beta}_{(i)}$ .

Note that all these four statistics have a chi-square distribution with degrees of freedom equal to the number of parameters the corresponding model has.

## Statistics

The following output statistics are available.

### Initial Model Information

The initial model for the first method is for a model that does not include covariates. The log-likelihood function  $l$  is equal to

$$l(0) = - \sum_{j=1}^m \sum_{i=1}^{k_j} d_{ji} \ln(n_{ji}^*)$$

where  $n_{ji}^*$  is the sum of weights of individuals in set  $R_{ji}$ .

### Model Information

When a stepwise method is requested, at each step, the  $-2$  log-likelihood function and three chi-square statistics (model chi-square, improvement chi-square, and overall chi-square) and their corresponding degrees of freedom and significance are printed.

#### **-2 Log-Likelihood**

$$-2 \sum_{j=1}^m \sum_{i=1}^{k_j} \left( \mathbf{s}'_{ji} \hat{\beta} - d_{ji} \ln \left( \sum_{l \in R_{ji}} w_l \exp(\mathbf{x}'_l \hat{\beta}) \right) \right)$$

where  $\hat{\beta}$  is the MPLE of  $\beta$  for the current model.

**Improvement Chi-Square**

$(-2 \log\text{-likelihood function for previous model}) - (-2 \log\text{-likelihood function for current model}).$

The previous model is the model from the last step. The degrees of freedom are equal to the absolute value of the difference between the number of parameters estimated in these two models.

**Model Chi-Square**

$(-2 \log\text{-likelihood function for initial model}) - (-2 \log\text{-likelihood function for current model}).$

The initial model is the final model from the previous method. The degrees of freedom are equal to the absolute value of the difference between the number of parameters estimated in these two model.

*Note:* The values of the model chi-square and improvement chi-square can be less than or equal to zero. If the degrees of freedom are equal to zero, the chi-square is not printed.

**Overall Chi-Square**

The overall chi-square statistic tests the hypothesis that all regression coefficients for the variables in the model are identically zero. This statistic is defined as

$$\mathbf{u}'(0)\mathbf{I}^{-1}\mathbf{u}(0)$$

where  $\mathbf{u}(0)$  represents the vector of first derivatives of the partial log-likelihood function evaluated at  $\beta = 0$ . The elements of  $\mathbf{u}$  and  $\mathbf{I}$  are defined in "Estimation of Beta".

**Information for Variables in the Equation**

For each of the single variables in the equation, MPLE, SE for MPLE, Wald statistic, and its corresponding  $df$ , significance, and partial  $R$  are given. For a single variable,  $R$  is defined by

$$R = \left[ \frac{\text{Wald}_{-2}}{-2 \log\text{-likelihood for the intial model}} \right]^{1/2} \times \text{sign of MPLE}$$

if  $\text{Wald} > 2$ . Otherwise  $R$  is set to zero. For a multiple category variable, only the Wald statistic,  $df$ , significance, and partial  $R$  are printed, where  $R$  is defined by

$$R = \left[ \frac{\text{Wald}_{-2*df}}{-2 \log\text{-likelihood for the intial model}} \right]^{1/2}$$

if  $\text{Wald} > 2df$ . Otherwise  $R$  is set to zero.

### **Information for the Variables Not in the Equation**

For each of the variables not in the equation, the Score statistic is calculated and its corresponding degrees of freedom, significance, and partial  $R$  are printed. The partial  $R$  for variables not in the equation is defined similarly to the  $R$  for the variables in the equation by changing the Wald statistic to the Score statistic.

There is one overall statistic called the residual chi-square. This statistic tests if all regression coefficients for the variables not in the equation are zero. It is defined by

$$\mathbf{u}'(\hat{\beta})\mathbf{B}_{22}\mathbf{u}(\hat{\beta})$$

where  $\mathbf{u}(\hat{\beta})$  is the vector of first derivatives of the partial log-likelihood function with respect to all the parameters not in the equation evaluated at MPLE  $\hat{\beta}$  and  $\mathbf{B}_{22}$  is equal to  $(\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12})^{-1}$  and  $\mathbf{A}$  is defined in "Score Statistic".

### **Survival Table**

For each stratum, the estimates of the baseline cumulative survival ( $S_0$ ) and hazard ( $H_0$ ) function and their standard errors are computed.  $H_0(t)$  is estimated by

$$\hat{H}_0(t) = -\ln \hat{S}_0(t)$$

and the asymptotic variance of  $\hat{H}_0(t)$  is defined in "Estimation of the Baseline Function". Finally, the cumulative hazard function  $H(t|\mathbf{x})$  and survival function  $S(t|\mathbf{x})$  are estimated by

$$\hat{H}(t|\mathbf{x}) = \exp(\mathbf{x}'\hat{\beta})\hat{H}_0(t)$$

and, for a given  $\mathbf{x}$ ,

$$\hat{S}(t|\mathbf{x}) = [\hat{S}_0(t)]^{\exp(\mathbf{x}'\hat{\beta})}$$

The asymptotic variances are

$$\text{var}(\hat{H}(t|\mathbf{x})) = \exp(2\mathbf{x}'\hat{\beta})\text{var}(\hat{H}_0(t))$$

and

$$\text{var}(\hat{S}(t|\mathbf{x})) = \exp(2\mathbf{x}'\hat{\beta})(\hat{S}(t|\mathbf{x}))^2\text{var}(\hat{H}_0(t))$$

### **Plots**

For a specified pattern, the covariate values  $\mathbf{x}_c$  are determined and  $\mathbf{x}_c$  is computed. There are three plots available for Cox regression.

### Survival Plot

For stratum  $j$ ,  $(t_i, \hat{S}_0(t_i|\mathbf{x}_c))$ ,  $i = 1, \dots, k_j$  are plotted where

$$\hat{S}(t_i|\mathbf{x}_c) = (\hat{S}_0(t_i))^{\exp(\mathbf{x}'_c \hat{\beta})}$$

### Hazard Plot

For stratum  $j$ ,  $(t_i, \hat{H}(t_i|\mathbf{x}_c))$ ,  $i = 1, \dots, k_j$  are plotted where

$$\hat{H}(t_i|\mathbf{x}_c) = \exp(\mathbf{x}'_c \hat{\beta}) \hat{H}_0(t_i)$$

### LML Plot

The log-minus-log plot is used to see whether the stratification variable should be included as a covariate. For stratum  $j$ ,  $(t_i, \mathbf{x}'_c \hat{\beta} + \ln \hat{H}_0(t_i))$ ,  $i = 1, \dots, k_j$  are plotted. If the plot shows parallelism among strata, then the stratum variable should be a covariate.

### Blank Handling

All records with missing values for any input or output field are excluded from the estimation of the model.

### Scoring

Survival and cumulative hazard estimates are given in “Survival Table” on p. 101.

Conditional upon survival until time  $t_0$ , the probability of survival until time  $t$  is

$$\hat{S}(t + t_0|t_0) = \frac{\hat{S}(t + t_0)}{\hat{S}(t_0)}$$

### Blank Handling

Records with missing values for any input field in the final model cannot be scored, and are assigned a predicted value of \$null\$.

Additionally, records with “total” survival time (past + future) greater than the record with the longest observed uncensored survival time are also assigned a predicted value of \$null\$.

### References

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# Decision List Algorithms

The objective of decision lists is to find a group of individuals with a distinct behavior pattern; for example, a high probability of buying a product. A decision list model consists of a set of decision rules. A decision rule is an if-then rule, which has two parts: antecedent and consequent. The **antecedent** is a Boolean expression of predictors, and the **consequent** is the predicted value of the target field when the antecedent is true. The simplest construct of a decision rule is a segment based on one predictor; for example,  $\text{Gender} = \text{'Male'}$  or  $10 < \text{Age} \leq 20$ .

A record is **covered** by a rule if the rule antecedent is true. If a case is covered by one of the rules in a decision list, then it is considered to be covered by the list.

In a decision list, order of rules is significant; if a case is covered by a rule, it will be ignored by subsequent rules.

## Algorithm Overview

The decision list algorithm can be summarized as follows:

- ▶ Candidate rules are found from the original dataset.
- ▶ The best rules are appended to the decision list.
- ▶ Records covered by the decision list are removed from the dataset.
- ▶ New rules are found based on the reduced dataset.

The process repeats until one or more of the stopping criteria are met.

## Terminology of Decision List Algorithm

The following terms are used in describing the decision list algorithm:

**Model.** A decision list model.

**Cycle.** In every rule discovery cycle, a set of candidate rules will be found. They will then be added to the model under construction. The resulting models will be inputs to the next cycle.

**Attribute.** Another name for a variable or field in the dataset.

**Source attribute.** Another name for predictor field.

**Extending the model.** Adding decision rules to a decision list or adding segments to a decision rule.

**Group.** A subset of records in the dataset.

**Segment.** Another name for group.

## Main Calculations

### Notation

The following notations are used in describing the decision list algorithm:

$X$	Data matrix. Columns are fields (attributes), and rows are records (cases).
$L$	A collection of list models.
$L_i$	The $i$ th list model of $L$ .
$L_{null}$	A list model that contains no rules.
$\hat{P}_{L_i}$	The estimated response probability of list $L_i$ .
$N$	Total population size
$X_{m,n}$	The value of the $m$ th field (column) for the $n$ th record (row) of $X$ .
$X_{L_i}$	The subset of records in $X$ that are covered by list model $L_i$ .
$Y$	The target field in $X$ .
$Y_n$	The value of the target field for the $n$ th record.
$A$	Collection of all attributes (fields) of $X$ .
$A_j$	The $j$ th attribute of $X$ .
$R$	A collection of rules to extend a preceding rule list.
$R_k$	The $k$ th rule in rule collection $R$ .
$T$	A set of candidate list models.
ResultSet	A collection of decision list models.

### Primary Algorithm

The primary algorithm for creating a decision list model is as follows:

1. Initialize the model.
  - ▶ Let  $d$  = Search depth, and  $w$  = Search width.
  - ▶ If  $L = \emptyset$ , add  $L_{null}$  to  $L$ .
  - ▶  $T = \emptyset$ .
2. Loop over all elements  $L_i$  of  $L$ .
  - ▶ Select the records  $X_{\bar{L}_i}$  not covered by rules of  $L_i$ :
 
$$X_{\bar{L}_i} = X - X_{L_i}$$
  - ▶ Call the decision rule algorithm to create an alternative rule set  $R$  on  $X_{\bar{L}_i}$ . For more information, see the topic “Decision Rule Algorithm” on p. 107.

- ▶ Construct a set of new candidate models by appending each rule in  $R$  to  $L_i$ .
  - ▶ Save extended list(s) to  $T$ .
3. Select list models from  $T$ .

- ▶ Calculate the estimated response probability  $\hat{P}_{L_i}$  of each list model in  $T$  as

$$\hat{P}_{L_i} = \frac{N(Y_n = 1, X_n \in X_{L_i})}{N(X_n \in X_{L_i})}$$

- ▶ Select the  $w$  lists in  $T$  with the highest  $\hat{P}_{L_i}$  as  $L^*$ .
4. Add  $L^*$  to ResultSet.
5. If  $d = 1$  or  $L^* = \emptyset$ , return ResultSet and terminate; otherwise, reduce  $d$  by one and repeat from step 2.

### Decision Rule Algorithm

Each rule is extended in decision rule cycles. With decision rules, groups are searched for significantly increased occurrence of the target value. Decision rules will search for groups with a higher or lower probability as required.

#### Notation

The following notations are used in describing the decision list algorithm:

$X$	Data matrix. Columns are fields (attributes), and rows are records (cases).
$R$	A collection of rules to extend a preceding rule list.
$R_i$	The $i$ th rule in rule collection $R$ .
$R_{all}$	A special rule that covers all the cases in $X$ .
$\hat{P}_{R_i}$	The estimated response probability of $R_i$ .
$N$	Total population size.
$X_{m,n}$	The value of the $m$ th field (column) for the $n$ th record (row) of $X$ .
$X_{R_i}$	The subset of records in $X$ that are covered by rule $R_i$ .
$Y$	The target field in $X$ .
$Y_n$	The value of the target field for the $n$ th record.
$A$	Collection of all attributes (fields) of $X$ .
$A_j$	The $j$ th attribute of $X$ . If Allow attribute re-use is false, $A$ excludes attributes existing in the preceding rule.
SplitRule( $X, A_j$ )	The rule split algorithm for deriving rules about $A_j$ and records in $X$ . For more information, see the topic "Decision Rule Split Algorithm" on p. 108.
$T$	A set of candidate list models.
ResultSet	A collection of decision list models.

**Algorithm Steps**

The decision rule algorithm proceeds as follows:

1. Initialize the rule set.
  - ▶ Let  $d = \text{Search depth}$ , and  $w = \text{Search width}$ .
  - ▶ If  $R = \emptyset$ , add  $R_{all}$  to  $R$ .
  - ▶  $T = \emptyset$ .
2. Loop over all rules  $R_i$  in  $R$ .
  - ▶ Select records  $X_{R_i}$  covered by rule  $R_i$ .
  - ▶ Create an empty set  $S$  of new segments.
  - ▶ Loop over attributes  $A_j$  in  $A$ .
    - Generate new segments based on attribute  $A_j$ :
 
$$\text{SplitRule}(X_{R_i}, A_j)$$
      - Add new segments to  $S$ .
  - ▶ Construct a set of new candidate rules by extending  $R_i$  with each segment in  $S$ .
  - ▶ Save extended rules to  $T$ . If  $S = \emptyset$ , add  $R_i$  to ResultSet.
3. Select rules from  $T$ .
  - ▶ Calculate the estimated response probability  $\hat{P}_{R_i}$  for each extended rule in  $T$  as
 
$$\hat{P}_{R_i} = \frac{N(Y_n = 1, X_n \in X_{R_i})}{N(X_n \in X_{R_i})}$$
  - ▶ Select the  $w$  rules with the highest  $\hat{P}_{R_i}$  as  $R^*$ .
    - Add  $R^*$  to ResultSet.
  - ▶ If  $d = 1$ , return ResultSet and terminate. Otherwise, set  $R = R^*$ ,  $T = \emptyset$ , reduce  $d$  by one, and repeat from step 2.

**Decision Rule Split Algorithm**

The decision rule split algorithm is used to generate high response segments from a single attribute (field). The records and the attribute from which to generate segments should be given. This algorithm is applicable to all ordinal attributes, and the ordinal attribute should have values that are unambiguously ordered. The segments generated by the algorithm can be used to expand an  $n$ -dimensional rule to an  $(n + 1)$ -dimensional rule. This decision rule split algorithm is sometimes referred to as the sea-level method.

### Notation

The following notations are used in describing the decision rule split algorithm:

$X$	Data matrix. Columns are fields (attributes), and rows are records (cases).
$C$	A sorted list of attribute values (categories) to split. Values are sorted in ascending order.
$C_i$	The $i$ th category in the list of categories $C$ .
$X_{n,c}$	The value of the split field (attribute) for the $n$ th record (row) of $X$ .
$Y$	The target field in $X$ .
$Y_n$	The value of the target field for the $n$ th record.
$N$	Total population size.
$M$	Number of categories in $C$ .
$P_i$	Observed response probability of category $C_i$ .
$S_{L,R}$	A segment of categories, $S_{L,R} = \{C_i   C_i \in C, 1 \leq L \leq i \leq R \leq M\}$ .
$(p_{S_{L,R}}^-, p_{S_{L,R}}^+)$	The confidence interval (CI) for the response probability of $S_{L,R}$ .
$\max_p(C_i, C_j)$	The category with the higher response probability from $\{C_i, C_j\}$ .
$\max_n(C_i, C_j)$	The category with the larger number of records from $\{C_i, C_j\}$ .

### Algorithm Steps

The decision rule split algorithm proceeds as follows:

1. Compute  $P_i$  of each category  $C_i$ .

$$P_i = \frac{N(Y_n = 1, X_{n,c} \in C_i)}{N(X_{n,c} \in C_i)}, P_0 = P_{(M+1)} = 0$$

If  $N(X_{n,c} \in C_i) = 0$ ,  $C_i$  will be skipped.

2. Find local maxima of  $P_i$  to create a segment set.

$$PeakSet = \{C_i | C_i \in C, 0 \leq i = I \leq M\}$$

where  $I$  is a positive integer satisfying the conditions

$$P_I > P_{(I-1)}$$

$$P_I = P_{(I+l)}, 0 \leq l \leq L - I$$

$$P_L > P_{(L+1)}$$

The segment set is the ordered segments based on  $P_{S_i}$

$$SegmentSet = \{S_{L,R} | C_i \in PeakSet, L = R = i, P_{S_i} \geq P_{S_{i+1}}\}$$

3. Select a segment in *SegmentSet*.
  - ▶ If *SegmentSet* is empty, return *ResultSet* and terminate.
  - ▶ Select the segment  $S_{L,R}$  with the highest response probability  $P_{S_{L,R}}$ .
  - ▶ If  $R - L + 1 = M$  or  $P_{S_{L,R}} \leq P_{S_{1,M}}$ , remove the segment from *SegmentSet* and choose another.
4. Validate the segment.

- ▶ If the following conditions are satisfied:

- The size of the segment exceeds the minimum segment size criterion

$$Size(S_{L,R}) > Max(gs_{\min}, d, Max(g \cdot Size(parent)))$$

where

$$parent \in ResultSet, L_{parent} \geq L, R_{parent} \leq R$$

- Response probability for the segment is significantly higher than that for the overall sample, as indicated by non-overlapping confidence intervals

$$p_{S_{L,R}}^- > p_{Pop}^+$$

For more information, see the topic “Confidence Intervals” on p. 110.

- Extending the segment would lower the response probability

$$P_{S_{L-1,R}} < P_{S_{L,R}} \text{ and } P_{S_{L,R+1}} < P_{S_{L,R}}$$

then add the segment  $S_{L,R}$  to *ResultSet*, and remove any segments  $S'_{L,R}$  from *ResultSet* that have  $S_{L,R}$  as parent and for which  $Size(S'_{L,R}) \leq g \cdot Size(S_{L,R})$ .

5. Extend the segment.

- ▶ Add  $C_{adjacent}$  to  $S_{L,R}$ , where

$$C_{adjacent} = \begin{cases} Max_p(C_{L-1}, C_{R+1}) & \text{if } P_{L-1} \neq P_{R+1} \\ Max_n(C_{L-1}, C_{R+1}) & \text{if } P_{L-1} = P_{R+1} \text{ and } N(C_{L-1}) \neq N(C_{R+1}) \\ C_{R+1} & \text{otherwise} \end{cases}$$

- ▶ Adjust R or L accordingly, i.e. if  $C_{adjacent} = C_{L-1}$ , set  $L = L - 1$ ; if  $C_{adjacent} = C_{R+1}$ , set  $R = R + 1$ .
- ▶ Return  $S_{L,R}$  to *SegmentSet*, and repeat from step 3.

### Confidence Intervals

The confidence limits ( $p^-, p^+$ ) for  $\hat{p}$  are calculated as

$$p^- = \begin{cases} \frac{x}{x+(n-x+1)F_{2(n-x+1),2x;1-\alpha/2}} & \text{if } x \neq 0 \\ 0 & \text{if } x = 0 \end{cases}$$

$$p^+ = \begin{cases} \frac{(x+1)F_{2(x+1),2(n-x);1-\alpha/2}}{n-x+(x+1)F_{2(x+1),2(n-x);1-\alpha/2}} & \text{if } x \neq n \\ 1 & \text{if } x = n \end{cases}$$

where  $n$  is the coverage of the rule or list,  $x$  is the response frequency of the rule or list,  $\alpha$  is the desired confidence level, and  $F_{a,b;c}$  is the inverse cumulative distribution function for  $F$  with  $a$  and  $b$  degrees of freedom, for percentile  $100c$ .

## Secondary Measures

For each segment, the following measures are reported:

**Coverage.** The number of records in the segment,  $N(S)$ .

**Frequency.** The number of records in the segment for which the response is true,  $N(Y_n = 1, X_n \in S)$ .

**Probability.** The proportion of records in the segment for which the response is true,  $\frac{N(Y_n=1, X_n \in S)}{N(S)}$ ,  
or  $\frac{\text{Frequency}}{\text{Coverage}}$ .

## Blank Handling

In decision list models, blank values for input fields can be treated as a separate category that can be used to define segments, or can be excluded from the model, depending on the expert model option. The default is to use blanks as a category for defining segments. Records with blank values for the target field are excluded from model building.

## Generated Model/Scoring

The decision list generated model consists of a set of segments. When scoring new data, each record is evaluated for membership in each segment, in order. The first segment in model order that describes the record based on the predictor fields claims the record and determines the predicted value and the probability. Records where the predicted value is not the response value will have a value of \$null. Probabilities are calculated as described above.

## Blank Handling

In scoring data with a decision list generated model, blanks are considered valid values for defining segments. If the model was built with the expert option Allow missing values in conditions disabled, a record with a missing value for one of the input fields will not match any segment that depends on that field for its definition.



# DISCRIMINANT Algorithms

No analysis is done for any subfile group for which the number of non-empty groups is less than two or the number of cases or sum of weights fails to exceed the number of non-empty groups. An analysis may be stopped if no variables are selected during variable selection or the eigenanalysis fails.

## Notation

The following notation is used throughout this chapter unless otherwise stated:

Table 14-1

Notation

Notation	Description
$g$	Number of groups
$p$	Number of variables
$q$	Number of variables selected
$X_{ijk}$	Value of variable $i$ for case $k$ in group $j$
$f_{jk}$	Case weights for case $k$ in group $j$
$m_j$	Number of cases in group $j$
$n_j$	Sum of case weights in group $j$
$n$	Total sum of weights

## Basic Statistics

The procedure calculates the following basic statistics.

### Mean

$$\bar{X}_{ij} = \left( \sum_{k=1}^{m_j} f_{jk} X_{ijk} \right) / n_j \quad (\text{variable } i \text{ in group } j)$$

$$\bar{X}_{i\bullet} = \left( \sum_{j=1}^g \sum_{k=1}^{m_j} f_{jk} X_{ijk} \right) / n \quad (\text{variable } i)$$

### Variances

$$S_{ij}^2 = \frac{\left( \sum_{k=1}^{m_j} f_{jk} X_{ijk}^2 - n_j \bar{X}_{ij}^2 \right)}{(n_j - 1)} \quad (\text{variable } i \text{ in group } j)$$

$$S_{i\bullet}^2 = \frac{\left( \sum_{j=1}^g \sum_{k=1}^{m_j} f_{jk} X_{ijk}^2 - n \bar{X}_{i\bullet}^2 \right)}{(n - 1)} \quad (\text{variable } i)$$

**Within-Groups Sums of Squares and Cross-Product Matrix (W)**

$$w_{il} = \sum_{j=1}^g \sum_{k=1}^{m_j} f_{jk} X_{ijk} X_{ljk} - \sum_{j=1}^g \left( \sum_{k=1}^{m_j} f_{jk} X_{ijk} \right) \left( \sum_{k=1}^{m_j} f_{jk} X_{ljk} \right) / n_j \quad i, l = 1, \dots, p$$

**Total Sums of Squares and Cross-Product Matrix (T)**

$$t_{il} = \sum_{j=1}^g \sum_{k=1}^{m_j} f_{jk} X_{ijk} X_{ljk} - \left( \sum_{j=1}^g \sum_{k=1}^{m_j} f_{jk} X_{ijk} \right) \left( \sum_{j=1}^g \sum_{k=1}^{m_j} f_{jk} X_{ljk} \right) / n$$

**Within-Groups Covariance Matrix**

$$C = \frac{W}{(n-g)} \quad n > g$$

**Individual Group Covariance Matrices**

$$c_{il}^{(j)} = \frac{\left( \sum_{k=1}^{m_j} f_{jk} X_{ijk} X_{ljk} - \bar{X}_{ij} \bar{X}_{lj} n_j \right)}{(n_j - 1)}$$

**Within-Groups Correlation Matrix (R)**

$$r_{il} = \begin{cases} \frac{w_{il}}{\sqrt{w_{ii} w_{ll}}} & \text{if } w_{ii} w_{ll} > 0 \\ \text{SYSMIS} & \text{otherwise} \end{cases}$$

**Total Covariance Matrix**

$$T' = \frac{T}{n-1}$$

**Univariate F and  $\Lambda$  for Variable I**

$$F_i = \frac{(t_{ii} - w_{ii})(n-g)}{w_{ii}(g-1)}$$

with  $g-1$  and  $n-g$  degrees of freedom

$$\Lambda_i = \frac{w_{ii}}{t_{ii}}$$

with 1,  $g-1$  and  $n-g$  degrees of freedom

**Rules of Variable Selection**

Both direct and stepwise variable entry are possible. Multiple inclusion levels may also be specified.

### **Method = Direct**

For direct variable selection, variables are considered for inclusion in the order in which they are passed from the upstream node. A variable is included in the analysis if, when it is included, no variable in the analysis will have a tolerance less than the specified tolerance limit (default = 0.001).

### **Stepwise Variable Selection**

At each step, the following rules control variable selection:

- Eligible variables with higher inclusion levels are entered before eligible variables with lower inclusion levels.
- The order of entry of eligible variables with the same even inclusion level is determined by their order in the upstream node.
- The order of entry of eligible variables with the same odd level of inclusion is determined by their value on the entry criterion. The variable with the “best” value for the criterion statistic is entered first.
- When level-one processing is reached, prior to inclusion of any eligible variables, all already-entered variables which have level one inclusion numbers are examined for removal. A variable is considered eligible for removal if its  $F$ -to-remove is less than the  $F$  value for variable removal, or, if probability criteria are used, the significance of its  $F$ -to-remove exceeds the specified probability level. If more than one variable is eligible for removal, that variable is removed that leaves the “best” value for the criterion statistic for the remaining variables. Variable removal continues until no more variables are eligible for removal. Sequential entry of variables then proceeds as described previously, except that after each step, variables with inclusion numbers of one are also considered for exclusion as described before.
- A variable with a zero inclusion level is never entered, although some statistics for it are printed.

### **Ineligibility for Inclusion**

A variable with an odd inclusion number is considered ineligible for inclusion if:

- The tolerance of any variable in the analysis (including its own) drops below the specified tolerance limit if it is entered, or
- Its  $F$ -to-enter is less than the  $F$ -value for a variable to enter value, or
- If probability criteria are used, the significance level associated with its  $F$ -to-enter exceeds the probability to enter.

A variable with an even inclusion number is ineligible for inclusion if the first condition above is met.

## Computations During Variable Selection

During variable selection, the matrix  $\mathbf{W}$  is replaced at each step by a new matrix  $\mathbf{W}^*$  using the symmetric sweep operator described by Dempster (1969). If the first  $q$  variables have been included in the analysis,  $\mathbf{W}$  may be partitioned as:

$$\begin{bmatrix} \mathbf{W}_{11} & \mathbf{W}_{12} \\ \mathbf{W}_{21} & \mathbf{W}_{22} \end{bmatrix}$$

where  $\mathbf{W}_{11}$  is  $q \times q$ . At this stage, the matrix  $\mathbf{W}^*$  is defined by

$$\mathbf{W}^* = \begin{bmatrix} -\mathbf{W}_{11}^{-1} & \mathbf{W}_{11}^{-1}\mathbf{W}_{12} \\ \mathbf{W}_{21}\mathbf{W}_{11}^{-1} & \mathbf{W}_{22} - \mathbf{W}_{21}\mathbf{W}_{11}^{-1}\mathbf{W}_{12} \end{bmatrix} = \begin{bmatrix} \mathbf{W}_{11}^* & \mathbf{W}_{12}^* \\ \mathbf{W}_{21}^* & \mathbf{W}_{22}^* \end{bmatrix}$$

In addition, when stepwise variable selection is used,  $T$  is replaced by the matrix  $T^*$ , defined similarly.

The following statistics are computed.

### Tolerance

$$\text{TOL}_i = \begin{cases} 0 & \text{if } w_{ii} = 0 \\ w_{ii}^*/w_{ii} & \text{if variable } i \text{ is not in the analysis and } w_{ii} \neq 0 \\ -1/(w_{ii}^*w_{ii}) & \text{if variable } i \text{ is in the analysis and } w_{ii} \neq 0. \end{cases}$$

If a variable's tolerance is less than or equal to the specified tolerance limit, or its inclusion in the analysis would reduce the tolerance of another variable in the equation to or below the limit, the following statistics are not computed for it or any set including it.

### F-to-Remove

$$F_i = \frac{(w_{ii}^* - t_{ii}^*)(n - q - g + 1)}{t_{ii}^*(g - 1)}$$

with degrees of freedom  $g-1$  and  $n-q-g+1$ .

### F-to-Enter

$$F_i = \frac{(t_{ii}^* - w_{ii}^*)(n - q - g)}{w_{ii}^*(g - 1)}$$

with degrees of freedom  $g-1$  and  $n-q-g$ .

### Wilks' Lambda for Testing the Equality of Group Means

$$\Lambda = |\mathbf{W}_{11}|/|\mathbf{T}_{11}|$$

with degrees of freedom  $q$ ,  $g-1$  and  $n-g$ .

**The Approximate F Test for Lambda (the “overall F”), also known as Rao’s R (Tatsuoka, 1971)**

$$F = \frac{(1-\Lambda^s)(r/s+1-qh/2)}{\Lambda^s qh}$$

where

$$s = \begin{cases} \sqrt{\frac{q^2+h^2-5}{q^2h^2-4}} & \text{if } q^2 + h^2 \neq 5 \\ 1 & \text{otherwise} \end{cases}$$

$$r = n - 1 - (q + g)/2$$

$$h = g - 1$$

with degrees of freedom  $qh$  and  $r/s+1-qh/2$ . The approximation is exact if  $q$  or  $h$  is 1 or 2.

**Rao’s V (Lawley-Hotelling Trace) (Rao, 1952; Morrison, 1976)**

$$V = -(n-g) \sum_{i=1}^q \sum_{l=1}^q w_{il}^* (t_{il} - w_{il})$$

When  $n-g$  is large,  $V$ , under the null hypothesis, is approximately distributed as  $\chi^2$  with  $q(g-1)$  degrees of freedom. When an additional variable is entered, the change in  $V$ , if positive, has approximately a  $\chi^2$  distribution with  $g-1$  degrees of freedom.

**The Squared Mahalanobis Distance (Morrison, 1976) between groups a and b**

$$D_{ab}^2 = -(n-g) \sum_{i=1}^q \sum_{l=1}^q w_{il}^* (\bar{X}_{ia} - \bar{X}_{ib})(\bar{X}_{la} - \bar{X}_{lb})$$

**The F Value for Testing the Equality of Means of Groups a and b (Smallest F ratio)**

$$F_{ab} = \frac{(n-q-g+1)n_a n_b}{q(n-g)(n_a+n_b)} D_{ab}^2$$

**The Sum of Unexplained Variations (Dixon, 1973)**

$$R = \sum_{a=1}^{g-1} \sum_{b=a+1}^g 4/(4 + D_{ab}^2)$$

**Classification Functions**

Once a set of  $q$  variables has been selected, the classification functions (also known as Fisher’s linear discriminant functions) can be computed using

$$b_{ij} = (n-g) \sum_{l=1}^q w_{il}^* \bar{X}_{lj} \quad i = 1, 2, \dots, q, j = 1, 2, \dots, g$$

for the coefficients, and

$$a_j = \log p_j - \frac{1}{2} \sum_{i=1}^q b_{ij} \bar{X}_{ij} \quad j = 1, 2, \dots, q$$

for the constant, where  $p_j$  is the prior probability of group  $j$ .

## Canonical Discriminant Functions

The canonical discriminant function coefficients are determined by solving the general eigenvalue problem

$$(\mathbf{T} - \mathbf{W})\mathbf{V} = \lambda\mathbf{W}\mathbf{V}$$

where  $\mathbf{V}$  is the unscaled matrix of discriminant function coefficients and  $\lambda$  is a diagonal matrix of eigenvalues. The eigensystem is solved as follows:

The Cholesky decomposition

$$\mathbf{W} = \mathbf{L}\mathbf{U}$$

is formed, where  $\mathbf{L}$  is a lower triangular matrix, and  $\mathbf{U} = \mathbf{L}'$ .

The symmetric matrix  $\mathbf{L}^{-1}\mathbf{B}\mathbf{U}^{-1}$  is formed and the system

$$(\mathbf{L}^{-1}(\mathbf{T} - \mathbf{W})\mathbf{U}^{-1} - \lambda\mathbf{I})(\mathbf{U}\mathbf{V}) = 0$$

is solved using tridiagonalization and the QL method. The result is  $m$  eigenvalues, where  $m = \min(q, g - 1)$  and corresponding orthonormal eigenvectors,  $\mathbf{U}\mathbf{V}$ . The eigenvectors of the original system are obtained as

$$\mathbf{V} = \mathbf{U}^{-1}(\mathbf{U}\mathbf{V})$$

For each of the eigenvalues, which are ordered in descending magnitude, the following statistics are calculated.

### Percentage of Between-Groups Variance Accounted for

$$\frac{100\lambda_k}{m} \sum_{k=1}^m \lambda_k$$

### Canonical Correlation

$$\sqrt{\lambda_k / (1 + \lambda_k)}$$

### **Wilks' Lambda**

Testing the significance of all the discriminating functions after the first  $k$ :

$$\Lambda_k = \prod_{i=k+1}^m 1/(1 + \lambda_i) \quad k = 0, 1, \dots, m - 1$$

The significance level is based on

$$\chi^2 = -(n - (q + g)/2 - 1) \ln \Lambda_k$$

which is distributed as a  $\chi^2$  with  $(q-k)(g-k-1)$  degrees of freedom.

### **The Standardized Canonical Discriminant Coefficient Matrix D**

The standard canonical discriminant coefficient matrix **D** is computed as

$$\mathbf{D} = \mathbf{S}_{11} \mathbf{V}$$

where

$$\mathbf{S} = \text{diag}(\sqrt{w_{11}}, \sqrt{w_{22}}, \dots, \sqrt{w_{pp}})$$

$\mathbf{S}_{11}$  = partition containing the first  $q$  rows and columns of **S**

**V** is a matrix of eigenvectors such that  $\mathbf{V}' \mathbf{W}_{11} \mathbf{V} = \mathbf{I}$

### **The Correlations Between the Canonical Discriminant Functions and the Discriminating Variables**

The correlations between the canonical discriminant functions and the discriminating variables are given by

$$\mathbf{R} = \mathbf{S}_{11}^{-1} \mathbf{W}_{11} \mathbf{V}$$

If some variables were not selected for inclusion in the analysis ( $q < p$ ), the eigenvectors are implicitly extended with zeroes to include the nonselected variables in the correlation matrix. Variables for which  $W_{ii} = 0$  are excluded from **S** and **W** for this calculation;  $p$  then represents the number of variables with non-zero within-groups variance.

### **The Unstandardized Coefficients**

The unstandardized coefficients are calculated from the standardized ones using

$$\mathbf{B} = \sqrt{(n - g)} \mathbf{S}_{11}^{-1} \mathbf{D}$$

The associated constants are:

$$a_k = -\sum_{i=1}^q b_{ik} \bar{X}_i$$

The group centroids are the canonical discriminant functions evaluated at the group means:

$$\bar{f}_{kj} = a_k + \sum_{i=1}^q b_{ik} \bar{X}_{ij}$$

### Tests For Equality Of Variance

Box's  $M$  is used to test for equality of the group covariance matrices.

$$M = (n - g) \log |\mathbf{C}'| - \sum_{j=1}^g (n_j - 1) \log |\mathbf{C}^{(j)}|$$

where

$\mathbf{C}'$  = pooled within-groups covariance matrix excluding groups with singular covariance matrices

$\mathbf{C}^{(j)}$  = covariance matrix for group  $j$ .

Determinants of  $\mathbf{C}'$  and  $\mathbf{C}^{(j)}$  are obtained from the Cholesky decomposition. If any diagonal element of the decomposition is less than  $10^{-11}$ , the matrix is considered singular and excluded from the analysis.

$$\log |\mathbf{C}^{(j)}| = 2 \sum_{i=1}^p \log l_{ii} - p \log (n_j - 1)$$

where  $l_{ii}$  is the  $i$ th diagonal entry of  $\mathbf{L}$  such that  $(n_j - 1)\mathbf{C}^{(j)} = \mathbf{L}'\mathbf{L}$ . Similarly,

$$\log |\mathbf{C}'| = 2 \sum_{i=1}^p \log l_{ii} - p \log (n' - g)$$

where

$$(n' - g)\mathbf{C}' = \mathbf{L}'\mathbf{L}$$

$n'$  = sum of weights of cases in all groups with nonsingular covariance matrices

The significance level is obtained from the  $F$  distribution with  $t_1$  and  $t_2$  degrees of freedom using (Cooley and Lohnes, 1971):

$$F = \begin{cases} M/b & \text{if } e_2 > e_1^2 \\ \frac{t_2 M}{t_1(b-M)} & \text{if } e_2 < e_1^2 \end{cases}$$

where

$$e_1 = \left( \sum_{j=1}^g \frac{1}{n_j - 1} - \frac{1}{n - g} \right) \frac{2p^2 + 3p - 1}{6(g-1)(p+1)}$$

$$e_2 = \left( \sum_{j=1}^g \frac{1}{(n_j - 1)^2} - \frac{1}{(n - g)^2} \right) \frac{(p-1)(p+2)}{6(g-1)}$$

$$t_1 = (g - 1)p(p + 1)/2$$

$$t_2 = (t_1 + 2)/|e_2 - e_1^2|$$

$$b = \begin{cases} \frac{t_1}{1 - e_1 - t_1/t_2} & \text{if } e_2 > e_1^2 \\ \frac{t_2}{1 - e_1 - 2/t_2} & \text{if } e_2 < e_1^2 \end{cases}$$

If  $e_1^2 - e_2$  is zero, or much smaller than  $e_2$ ,  $t_2$  cannot be computed or cannot be computed accurately. If

$$e_2 = e_2 + 0.0001(e_2 - e_1^2)$$

the program uses Bartlett's  $\chi^2$  statistic rather than the  $F$  statistic:

$$\chi^2 = M(1 - e_1)$$

with  $t_1$  degrees of freedom.

For testing the group covariance matrix of the canonical discriminant functions, the procedure is similar. The covariance matrices  $\mathbf{C}'$  and  $\mathbf{C}^{(j)}$  are replaced by  $\mathbf{D}_j$  and  $\mathbf{D}'$ , where

$$\mathbf{D}_j = \mathbf{B}' \mathbf{C}^{(j)} \mathbf{B}$$

is the group covariance matrix of the discriminant functions.

The pooled covariance matrix in this case is an identity, so that

$$\mathbf{D}' = (n - g)\mathbf{I}_m - \sum_j (n_j - 1)\mathbf{D}_j$$

where the summation is only over groups with singular  $\mathbf{D}_j$ .

## Blank Handling

All records with missing values for any input or output field are excluded from the estimation of the model.

## Generated model/scoring

The basic procedure for classifying a case is as follows:

- If  $\mathbf{X}$  is the  $1 \times q$  vector of discriminating variables for the case, the  $1 \times m$  vector of canonical discriminant function values is

$$\mathbf{f} = \mathbf{XB} + \mathbf{a}$$

- A chi-square distance from each centroid is computed

$$\chi_j^2 = (\mathbf{f} - \bar{\mathbf{f}}_j) \mathbf{D}_j^{-1} (\mathbf{f} - \bar{\mathbf{f}}_j)'$$

where  $\mathbf{D}_j$  is the covariance matrix of canonical discriminant functions for group  $j$  and  $\bar{\mathbf{f}}_j$  is the group centroid vector. If the case is a member of group  $j$ ,  $\chi_j^2$  has a  $\chi^2$  distribution with  $m$  degrees of freedom.  $P(\mathbf{X}|\mathbf{G})$ , labeled as  $P(\mathbf{D}>d|\mathbf{G}=g)$  in the output, is the significance level of such a  $\chi_j^2$ .

- The classification, or posterior probability, is

$$P(\mathbf{G}_j|\mathbf{X}) = \frac{P_j |\mathbf{D}_j|^{-1/2} e^{-\chi_j^2/2}}{\sum_{j=1}^g P_j |\mathbf{D}_j|^{-1/2} e^{-\chi_j^2/2}}$$

where  $p_j$  is the prior probability for group  $j$ . A case is classified into the group for which  $P(\mathbf{G}_j|\mathbf{X})$  is highest.

The actual calculation of  $P(\mathbf{G}_j|\mathbf{X})$  is

$$g_j = \log P_j - \frac{1}{2} (\log |\mathbf{D}_j| + \chi_j^2)$$

$$P(\mathbf{G}_j|\mathbf{X}) = \begin{cases} \frac{\exp(g_j - \max_j g_j)}{\sum_{j=1}^g \exp(g_j - \max_j g_j)} & \text{if } g_j - \max_j g_j > -46 \\ 0 & \text{otherwise} \end{cases}$$

If individual group covariances are not used in classification, the pooled within-groups covariance matrix of the discriminant functions (an identity matrix) is substituted for  $\mathbf{D}_j$  in the above calculation, resulting in considerable simplification.

If any  $\mathbf{D}_j$  is singular, a pseudo-inverse of the form

$$\begin{bmatrix} \mathbf{D}_{j11}^{-1} & 0 \\ 0 & 0 \end{bmatrix}$$

replaces  $\mathbf{D}_j^{-1}$  and  $|\mathbf{D}_{j11}|$  replaces  $|\mathbf{D}_j|$ .  $\mathbf{D}_{j11}$  is a submatrix of  $\mathbf{D}_j$  whose rows and columns correspond to functions not dependent on preceding functions. That is, function 1 will be excluded only if the rank of  $\mathbf{D}_j = 0$ , function 2 will be excluded only if it is dependent on function 1, and so on. This choice of the pseudo-inverse is not optimal for the numerical stability of  $\mathbf{D}_{j11}^{-1}$ , but maximizes the discrimination power of the remaining functions.

### ***Cross-Validation (Leave-one-out classification)***

The following notation is used in this section:

Table 14-2

Notation

Notation	Description
$\underset{\sim}{X}_{jk}$	$(X_{1jk}, \dots, X_{qjk})^T$

Notation	Description
$M_{\tilde{j}}$	Sample mean of $j$ th group
	$M_{\tilde{j}} = \frac{1}{n_j} \sum_{k=1}^{m_j} f_{jk} X_{jk}$
$M_{\tilde{j}k}$	Sample mean of $j$ th group excluding point $X_{jk}$
	$M_{\tilde{j}k} = \frac{1}{n_j - f_{jk}} \sum_{\substack{l=1 \\ l \neq k}}^{m_j} f_{jl} X_{jl}$
$\Sigma$	Polled sample covariance matrix
$\Sigma_j$	Sample covariance matrix of $j$ th group
$\Sigma_{jk}$	Polled sample covariance matrix without point $X_{jk}$
$\Sigma_{jk}^{-1}$	$= \frac{n-g-f_{jk}}{n-g} \left( \Sigma^{-1} + \frac{n_j \Sigma_j^{-1} \begin{pmatrix} X_{jk} - M_j \\ \tilde{\phantom{X}} \end{pmatrix} \begin{pmatrix} X_{jk} - M_j \\ \tilde{\phantom{X}} \end{pmatrix}^T \Sigma_j^{-1}}{(n_j - f_{jk})(n_j - g) - n_j \begin{pmatrix} X_{jk} - M_j \\ \tilde{\phantom{X}} \end{pmatrix}^T \Sigma_j^{-1} \begin{pmatrix} X_{jk} - M_j \\ \tilde{\phantom{X}} \end{pmatrix}} \right)$
$d_0^2 \left( \begin{matrix} a \\ \tilde{\phantom{a}} \end{matrix}, \begin{matrix} b \\ \tilde{\phantom{b}} \end{matrix} \right)$	$\begin{pmatrix} a - b \\ \tilde{\phantom{a}} \tilde{\phantom{b}} \end{pmatrix}^T \Sigma_{jk}^{-1} \begin{pmatrix} a - b \\ \tilde{\phantom{a}} \tilde{\phantom{b}} \end{pmatrix}$

Cross-validation applies only to linear discriminant analysis (not quadratic). During cross-validation, all cases in the dataset are looped over. Each case, say  $X_{jk}$ , is extracted once and treated as test data. The remaining cases are treated as a new dataset.

Here we compute  $d_0^2 \left( X_{jk}, M_{jk} \right)$  and  $d_0^2 \left( X_{jk}, M_i \right)$  ( $i = 1, \dots, g, i \neq j$ ). If there is an  $i$  ( $i \neq j$ ) that satisfies  $(\log(P_i) - d_0^2 \left( X_{jk}, M_i \right) / 2) > (\log(P_j) - d_0^2 \left( X_{jk}, M_{jk} \right) / 2)$ , then the extracted point  $X_{jk}$  is misclassified. The estimate of prediction error rate is the ratio of the sum of misclassified case weights and the sum of all case weights.

To reduce computation time, the linear discriminant method is used instead of the canonical discriminant method. The theoretical solution is exactly the same for both methods.

### **Blank Handling (discriminant analysis algorithms scoring)**

Records with missing values for any input field in the final model cannot be scored, and are assigned a predicted value of \$null\$.

### **References**

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# Ensembles Algorithms

Ensembles are used to enhance model accuracy (boosting), enhance model stability (bagging), build models for very large datasets (pass, stream, merge), and generally combine scores from different models.

- For more information, see the topic “Very large datasets (pass, stream, merge) algorithms” on p. 130.
- For more information, see the topic “Bagging and Boosting Algorithms” on p. 125.
- For more information, see the topic “Ensembling model scores algorithms” on p. 136.

## Bagging and Boosting Algorithms

Bootstrap aggregating (Bagging) and boosting are algorithms used to improve model stability and accuracy. Bagging works well for unstable base models and can reduce variance in predictions. Boosting can be used with any type of model and can reduce variance and bias in predictions.

### Notation

The following notation is used for bagging and boosting unless otherwise stated:

$K$	The number of distinct records in the training set.
$X_k$	Predictor values for the $k$ th record.
$y_k$	Target value for the $k$ th record.
$f_k$	Frequency weight for the $k$ th record.
$w_k$	Analysis weight for the $k$ th record.
$N$	The total number of records; $N = \sum_{k=1}^K f_k$ .
$M$	The number of base models to build; for bagging, this is the number of bootstrap samples.
$T^m(\cdot)$	The model built on the $m$ th bootstrap sample.
$f_k^m$	Simulated frequency weight for the $k$ th record of the $m$ th bootstrap sample.
$w_k^m$	Updated analysis weight for the $k$ th record of the $m$ th bootstrap sample.
$\hat{y}_k^m = T^m(X_k)$	Predicted target value of the $k$ th record by the $m$ th model.
$P_{l_i}^m(X_k)$	For a categorical target, the probability that the $k$ th record belongs to category $l_i$ , $i=1, \dots, C$ , in model $m$ .
$II(\pi)$	For any condition $\pi$ , $II(\pi)$ is 1 if $\pi$ holds and 0 otherwise.

## Bootstrap Aggregation

Bootstrap aggregation (bagging) produces replicates of the training dataset by sampling with replacement from the original dataset. This creates bootstrap samples of equal size to the original dataset. The algorithm is performed iteratively over  $k=1, \dots, K$  and  $m=1, \dots, M$  to generate frequency weights:

$$f_{mk}^* = \begin{cases} rv.binom\left(N, \frac{f_k}{N}\right) & k = 1 \\ rv.binom\left(N - \sum_{i=1}^{k-1} f_{mi}^*, \frac{f_k}{N - \sum_{i=1}^{k-1} f_i}\right) & \text{otherwise} \end{cases}$$

Then a model is built on each replicate. Together these models form an ensemble model. The ensemble model scores new records using one of the following methods; the available methods depend upon the measurement level of the target.

### Scoring a Continuous Target

- Mean

$$\hat{y}_k = \frac{1}{M} \sum_{m=1}^M \hat{y}_k^m$$

- Median

Sort  $\hat{y}_k^m$  and relabel them  $\hat{y}_{(1)} \leq \dots \leq \hat{y}_{(M)}$

$$\hat{y}_k = \begin{cases} \hat{y}_{(\frac{M+1}{2})} & \text{if } M \text{ is odd} \\ \frac{1}{2} \left( \hat{y}_{(\frac{M}{2})} + \hat{y}_{(\frac{M}{2}+1)} \right) & \text{if } M \text{ is even} \end{cases}$$

### Scoring a Categorical Target

- Voting

$$\hat{y}_k = \arg \max_{l_i \in \Omega} \frac{1}{|M_{l_i}|} \sum_{m \in M_{l_i}} P_{l_i}^m(X_k)$$

$$\hat{p}_{\hat{y}_k} = \frac{1}{|M_{\hat{y}_k}|} \sum_{m \in M_{\hat{y}_k}} P_{\hat{y}_k}^m(X_k)$$

where  $\Omega = \{\arg \max_{l_i} |M_{l_i}|\}$

- Highest probability

$$\hat{y}_k = \arg \max_{l_i} \left( \max_m (P_{l_i}^m(X_k)) \right)$$

$$\hat{p}_{\hat{y}_k} = \max_m \left( P_{\hat{y}_k}^m(X_k) \right)$$

- Highest mean probability

$$\hat{y}_k = \arg \max_{l_i} \frac{1}{M} \sum_{m=1}^M P_{l_i}^m(X_k)$$

$$\hat{p}_{\hat{y}_k} = \frac{1}{M} \sum_{m=1}^M P_{\hat{y}_k}^m(X_k)$$

## Bagging Model Measures

### Accuracy

Accuracy is computed for the naive model, reference (simple) model, ensemble model (associated with each ensemble method), and base models.

For categorical targets, the classification accuracy is

$$\frac{1}{N} \sum_{k=1}^K f_k II(y_k == \hat{y}_k)$$

For continuous targets, it is

$$R^2 = 1 - \frac{\sum_{k=1}^K f_k (y_k - \hat{y}_k)^2}{\sum_{k=1}^K f_k (y_k - \bar{y})^2}$$

where  $\bar{y} = \frac{1}{N} \sum_{k=1}^K f_k y_k$

Note that  $R^2$  can never be greater than one, but can be less than zero.

For the naïve model,  $\hat{y}_k$  is the modal category for categorical targets and the mean for continuous targets.

### Diversity

Diversity is a range measure between 0 and 1 in the larger-is-more-diverse form. It shows how much predictions vary across base models.

For categorical targets, diversity is

$$\frac{1}{N \cdot M^2} \sum_{k=1}^K f_k L(y_k) [M - L(y_k)]$$

where  $L(y_k) = \sum_{m=1}^M II(y_k = \hat{y}_k^m)$ .

For continuous targets, diversity is

$$D = \frac{\sum_{k=1}^K f_k \left[ \frac{1}{M(M-1)} \sum_{m=1}^M \sum_{n=1, n \neq m}^M (y_k - \hat{y}_k^m) (\hat{y}_k^n - y_k) \right]}{\sum_{k=1}^K f_k (y_k - \bar{y}_k)^2}$$

## Adaptive Boosting

Adaptive boosting (AdaBoost) is an algorithm used to boost models with continuous targets (Freund and Schapire 1996, Drucker 1997).

1. Initialize values.

$$\text{Set } w_k = \begin{cases} \frac{w_k}{\sum_{i=1}^K w_i f_i} & \text{if analysis weights specified} \\ 1/N & \text{otherwise} \end{cases}$$

Set  $m=1$ ,  $w_k^m = w_k$ , and  $f_k^m = f_k$ . Note that analysis weights are initialized even if the method used to build base models does not support analysis weights.

2. Build base model  $m$ ,  $T^m(\cdot)$ , using the training set and score the training set.

$$\text{Set the model weight for base model } m, \omega^m = \log \left( \frac{1 - \sum_{k=1}^K L_k w_k^m f_k}{\sum_{k=1}^K L_k w_k^m f_k} \right)$$

$$\text{where } L_k = \frac{\text{abs}(\hat{y}_k^m - y_k)}{\max_k (\text{abs}(\hat{y}_k^m - y_k))}.$$

3. Set weights for the next base model .

$$w_k^{m+1} = \frac{a_k^{m+1}}{\sum_{i=1}^K a_i^{m+1} f_i}$$

$$\text{where } a_k^{m+1} = w_k^m \left( \frac{\sum_{k=1}^K L_k w_k^m f_k}{1 - \sum_{k=1}^K L_k w_k^m f_k} \right)^{1-L_k}. \text{ Note that analysis weights are always updated. If}$$

the method used to build base models does not support analysis weights, the frequency weights are updated for the next base model as follows:

$$f_k^{m+1} = \begin{cases} rv.binom(N, w_k^{m+1} f_k) & k = 1 \\ rv.binom\left(N - \sum_{i=1}^{k-1} f_i^{m+1}, \frac{w_k^{m+1} f_k}{1 - \sum_{i=1}^{k-1} w_i^{m+1} f_i}\right) & \text{otherwise} \end{cases}$$

If  $m < M$ , set  $m=m+1$  and go to step 2. Otherwise, the ensemble model is complete.

*Note:* base models where  $\sum_{k=1}^K L_k w_k^m f_k \geq 0.5$  or  $\max_k (\text{abs}(\hat{y}_k^m - y_k))$  are removed from the ensemble.

### Scoring

AdaBoost uses the weighted median method to score the ensemble model.

Sort  $\hat{y}_k^m$  and relabel them  $\hat{y}_{(1)} \leq \dots \leq \hat{y}_{(M)}$ , retaining the association of the model weights,  $\omega^m$ , and relabeling them  $\omega_{(1)}, \dots, \omega_{(M)}$

The ensemble predicted value is then  $\hat{y}_k = \hat{y}_{(i)}$ , where  $i$  is the value such that

$$\sum_{m=1}^{i-1} \omega^m < \frac{1}{2} \sum_{m=1}^M \omega^m \leq \sum_{m=1}^i \omega^m$$

### Stagewise Additive Modeling using Multiclass Exponential loss

Stagewise Additive Modeling using a Multiclass Exponential loss function (SAMME) is an algorithm that extends the original AdaBoost algorithm to categorical targets.

1. Initialize values.

$$\text{Set } w_k = \begin{cases} \frac{w_k}{\sum_{i=1}^K w_i f_i} & \text{if analysis weights specified} \\ 1/N & \text{otherwise} \end{cases}$$

Set  $m=1$ ,  $w_k^m = w_k$ , and  $f_k^m = f_k$ . Note that analysis weights are initialized even if the method used to build base models does not support analysis weights.

2. Build base model  $m$ ,  $T^m(\cdot)$ , using the training set and score the training set.

Set the model weight for base model  $m$ ,  $\omega^m = \log \frac{1 - \text{err}_m}{\text{err}_m} + \log(C - 1)$

$$\text{where } \text{err}_m = \sum_{k=1}^K w_k^m f_k II(y_k \neq \hat{y}_k^m).$$

3. Set weights for the next base model.

$$w_k^{m+1} = \frac{a_k^{m+1}}{\sum_{i=1}^K a_i^{m+1} f_i}$$

where  $a_k^{m+1} = w_k^m \exp(\omega^m II(y_k \neq \hat{y}_k^m))$ . Note that analysis weights are always updated. If the method used to build base models does not support analysis weights, the frequency weights are updated for the next base model as follows:

$$f_k^{m+1} = \begin{cases} rv.binom(N, w_k^{m+1} f_k) & k = 1 \\ rv.binom\left(N - \sum_{i=1}^{k-1} f_i^{m+1}, \frac{w_k^{m+1} f_k}{1 - \sum_{i=1}^{k-1} w_i^{m+1} f_i}\right) & \text{otherwise} \end{cases}$$

If  $m < M$ , set  $m=m+1$  and go to step 2. Otherwise, the ensemble model is complete.

*Note:* base models where  $\text{err}_m = 0$  or  $\omega^m \leq 0$  are removed from the ensemble.

#### Scoring

SAMME uses the weighted majority vote method to score the ensemble model.

The predicted value of the  $k$ th record for the  $m$ th base model is  $\hat{y}_k^m = \arg \max_{l_i} P_{l_i}^m(X_k)$ .

The ensemble predicted value is then  $\hat{y}_k = \arg \max_{l_i} \sum_{m=1}^M \omega^m II(\hat{y}_k^m == l_i)$ . Ties are resolved at random.

The ensemble predicted probability is  $\hat{p}_{\hat{y}_k} = \sum_{m \in M_{\hat{y}_k}} \frac{\omega^m}{\sum_{i \in M_{\hat{y}_k}} \omega^i} P_{\hat{y}_k}^m(X_k)$ .

## Boosting Model Measures

### Accuracy

Accuracy is computed for the naive model, reference (simple) model, ensemble model (associated with each ensemble method), and base models.

For categorical targets, the classification accuracy is

$$\frac{1}{N} \sum_{k=1}^K f_k II(y_k == \hat{y}_k)$$

For continuous targets, it is

$$R^2 = 1 - \frac{\sum_{k=1}^K f_k (y_k - \hat{y}_k)^2}{\sum_{k=1}^K f_k (y_k - \bar{y})^2}$$

where  $\bar{y} = \frac{1}{N} \sum_{k=1}^K f_k y_k$

Note that  $R^2$  can never be greater than one, but can be less than zero.

For the naïve model,  $\hat{y}_k$  is the modal category for categorical targets and the mean for continuous targets.

## References

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Freund, Y., and R. E. Schapire. 1995. A decision theoretic generalization of on-line learning and an application to boosting. In: *Computational Learning Theory: 7 Second European Conference, EuroCOLT '95*, , 23–37.

## Very large datasets (pass, stream, merge) algorithms

We implement the PSM features PASS, STREAM, and MERGE through ensemble modeling. PASS builds models on very large data sets with only one data pass; STREAM updates the existing model with new cases without the need to store or recall the old training data; MERGE builds models in a distributed environment and merges the built models into one model.

In an ensemble model, the training set will be divided into subsets called blocks, and a model will be built on each block. Because the blocks may be dispatched to different threads (here one process contains one thread) and even different machines, models in different processes can be built at the same time. As new data blocks arrive, the algorithm simply repeats this procedure. Therefore it can easily handle the data stream and perform incremental learning for ensemble modeling.

## Pass

The PASS operation includes following steps:

1. Split the data into training blocks, a testing set and a holdout set. Note that the frequency weight, if specified, is ignored when splitting the training set into blocks (to prevent blocks from being entirely represented by a single case) but is accounted for when creating the testing and holdout sets.
2. Build base models on training blocks and build a reference model on the testing set. A single model is built on the testing set and each training block.
3. Evaluate each base model by computing the accuracy based on the testing set. Select a subset of base models as ensemble elements according to accuracy.
4. Evaluate the ensemble model and the reference model by computing the accuracy based on the holdout set. If the ensemble model's performance is not better than the reference model's performance on the holdout set, we use the reference model to score the new cases.

### Computing Model Accuracy

The accuracy of a base model is assessed on the testing set. For each vector of predictors  $x_i$  and the corresponding label  $c_i$  observed in the testing set  $T$ , let  $\hat{c}(x_i)$  be the label predicted by the given model. Then the testing error is estimated as:

$$\text{Categorical target. } E = \frac{1}{\sum_{i=1}^{|T|} f_i} \sum_{i=1}^{|T|} (f_i \cdot I(c_i \neq \hat{c}(x_i)))$$

$$\text{Continuous target. } E = \frac{1}{\sum_{i=1}^{|T|} f_i} \sum_{i=1}^{|T|} (f_i \cdot |y_i - \hat{y}_i|)$$

Where  $I(c_i \neq \hat{c}(x_i))$  is 1 if  $c_i \neq \hat{c}(x_i)$  and 0 otherwise.

The accuracy for the given model is computed by  $A=1-E$ . The accuracy for the whole ensemble model and the reference model is assessed on the holdout set.

## **Stream**

When new cases arrive and the user wants to update the existing ensemble model with these cases, the algorithm will:

1. Start a PASS operation to build an ensemble model on the new data, then
2. MERGE the newly created ensemble model and the existing ensemble model.

## **Merge**

The MERGE operation has the following steps:

1. Merge the holdout sets into a single holdout set and, if necessary, reduce this set to a reasonable size.
2. Merge the testing sets into a single testing set and, if necessary, reduce this set to a reasonable size.
3. Build a merged reference model on the merged testing set.
4. Evaluate every base model by computing the accuracy based on the merged testing set. Select a subset of base models as elements of the merged ensemble model according to accuracy.
5. Evaluate the merged ensemble model and the merged reference model by computing the accuracy based on the merged holdout set.

## **Adaptive Predictor Selection**

There are two methods, depending upon whether the method used to build base models has an internal predictor selection algorithm.

### ***Method has predictor selection algorithm***

The first base model is built with all predictors available to the method's predictor selection algorithm. Base model  $j$  ( $j > 1$ ) makes the  $i$ th predictor available with probability

$$p_i = \max \left( \frac{n'_i + C}{n_i + C}, \beta \right)$$

where  $n'_i$  is the number of times the  $i$ th predictor was selected by the method's predictor selection algorithm in the previous  $j-1$  base models,  $n_i$  is the number of times the  $i$ th predictor was made available to the method's predictor selection algorithm in the previous  $j-1$  base models,  $C$  is a constant to smooth the value of  $p_i$ , and  $\beta$  is a lower limit on  $p_i$ .

### ***Method does not have predictor selection algorithm***

Each base model makes the  $i$ th predictor available with probability

$$p_i = \begin{cases} (1 - \rho_i)^2 & \text{if } \rho_i < 0.05 \\ \beta & \text{otherwise} \end{cases}$$

where  $\rho_i$  is the  $p$ -value of a test for the  $i$ th predictor, as defined below.

- For a categorical target and categorical predictor,  $\rho$  is a chi-square test of

$$G^2 = 2 \sum_{i=1}^I \sum_{j=1}^J G_{ij}^2 \text{ where } G_{ij}^2 = \begin{cases} N_{ij} \ln \left( \frac{N_{ij}}{\hat{N}_{ij}} \right) & N_{ij} > 0 \\ 0 & \text{else} \end{cases} \text{ and with degrees of}$$

freedom  $(I - 1)(J - 1)$ .  $N_{ij}$  is the number of cases with  $X=i$  and  $Y=j$ ,  $N_{i\cdot} = \sum_{j=1}^J N_{ij}$ ,  $N_{\cdot j} = \sum_{i=1}^I N_{ij}$ , and  $\hat{N}_{ij} = N_{i\cdot} N_{\cdot j} / N$ .

- For a categorical target and continuous predictor,  $\rho$  is an  $F$  test of

$$F = \frac{\sum_{j=1}^J N_j (\bar{x}_j - \bar{x})^2 / (J-1)}{\sum_{j=1}^J (N_j - 1) s_j^2 / (N - J)} \text{ with degrees of freedom } J - 1, N - J. N_j \text{ is the}$$

number of cases with  $Y=j$ ,  $\bar{x}_j$  and  $s_j^2$  are the sample mean and sample variance of  $X$  given  $Y=j$ , and  $\bar{x} = \sum_{j=1}^J N_j \bar{x}_j / N$

- For a continuous target and categorical predictor,  $\rho$  is an  $F$  test of

$$F = \frac{\sum_{i=1}^I N_i (\bar{y}_i - \bar{y})^2 / (I-1)}{\sum_{i=1}^I (N_i - 1) s(y)_i^2 / (N - I)} \text{ with degrees of freedom } I - 1, N - I. N_i \text{ is the}$$

number of cases with  $X=i$ ,  $\bar{y}_i$  and  $s(y)_i^2$  are the sample mean and sample variance of  $Y$  given  $X=i$ , and  $\bar{y} = \sum_{i=1}^I N_i \bar{y}_i / N$ .

- For a continuous target and continuous predictor,  $\rho$  is a two-sided  $t$  test of  $t = r \sqrt{\frac{N-2}{1-r^2}}$  where  $r = \frac{\sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y}) / (N-1)}{\sqrt{s(x)^2 s(y)^2}}$  and with degrees of freedom  $N - 2$ .  $s(x)^2$  is the sample variance of  $X$  and  $s(y)^2$  is the sample variance of  $Y$ .

## Automatic Category Balancing

When a target category occurs relatively infrequently, many models do a poor job of predicting members of that rarely occurring category, even if the overall prediction rate of the model is fairly good. Automatic category balancing should improve the model's accuracy when predicting infrequently occurring values.

As records arrive, they are added to a training block until it is full. Then the proportion of records in each category is computed:  $C_i = \frac{w_i}{w}$ , where  $w_i$  is the weighted number of records taking category  $i$  and  $w$  is the total weighted number of records.

- ▶ If there is any category such that  $C_i < \alpha / (10 \cdot |C|)$ , where  $|C|$  is the number of target categories and  $\alpha = 0.3$ , then randomly remove each record from the training block with probability

$$\text{Min} \left\{ (1 - \text{Min}(C) / C_i), \left( 1 - \frac{\alpha}{|C|} \right) \right\}$$

This operation will tend to remove records from frequently-occurring categories. Add new records to the training block until it is full again, and repeat this step until the condition is not satisfied.

- ▶ If there is any category such that  $C_i < \alpha / |C|$ , then recompute the frequency weight for record  $k$  as  $f_k = f_k \max(10, \alpha \max(C) / C_{i(k)})$ , where  $i(k)$  is the category of the  $k$ th record. This operation gives greater weight to infrequently occurring categories.

## Model Measures

The following notation applies.

$N$	Total number of records
$M$	Total number of base models
$f_k$	The frequency weight of record $k$
$y_k$	The observed target value of record $k$
$\hat{y}_k$	The predicted target value of record $k$ by the ensemble model
$\hat{y}_k^m$	The predicted target value of record $k$ by base model $m$

### Accuracy

Accuracy is computed for the naive model, reference (simple) model, ensemble model (associated with each ensemble method), and base models.

For categorical targets, the classification accuracy is

$$\frac{1}{N} \sum_{k=1}^K f_k II(y_k == \hat{y}_k)$$

where

$$II(y_k = \hat{y}_k) = \begin{cases} 1, & \text{if } (y_k = \hat{y}_k) \\ 0, & \text{otherwise} \end{cases}$$

For continuous targets, it is

$$R^2 = 1 - \frac{\sum_{k=1}^K f_k (y_k - \hat{y}_k)^2}{\sum_{k=1}^K f_k (y_k - \bar{y})^2}$$

where  $\bar{y} = \frac{1}{N} \sum_{k=1}^K f_k y_k$

Note that  $R^2$  can never be greater than one, but can be less than zero.

For the naïve model,  $\hat{y}_k$  is the modal category for categorical targets and the mean for continuous targets.

### Diversity

Diversity is a range measure between 0 and 1 in the larger-is-more-diverse form. It shows how much predictions vary across base models.

For categorical targets, diversity is

$$\frac{1}{N \cdot M^2} \sum_{k=1}^K f_k L(y_k) [M - L(y_k)]$$

where  $L(y_k) = \sum_{m=1}^M II(y_k = \hat{y}_k^m)$  and  $II(y_k = \hat{y}_k^m)$  is defined as above.

Diversity is not available for continuous targets.

## Scoring

There are several strategies for scoring using the ensemble models.

### Continuous Target

$$\text{Mean. } \hat{y}_{i,PSM} = \frac{1}{M} \sum_{m=1}^M \hat{y}_{i,m}$$

$$\text{Median. } \hat{y}_{i,PSM} = \text{Median}_1^M(\hat{y}_{i,m})$$

where  $\hat{y}_{i,PSM}$  is the final predicted value of case  $i$ , and  $\hat{y}_{i,m}$  is the  $m$ th base model's predicted value of case  $i$ .

### Categorical Target

**Voting.** Assume that  $d_{m,k}$  represents the label output of the  $m$ th base model for a given vector of predictor values.  $d_{m,k} = 1$  if the label assigned by the  $m$ th base model is the  $k$ th target category and 0 otherwise. There are total of  $M$  base models and  $K$  target categories. The majority vote method selects the  $j$ th category if it is assigned by the plurality of base models. It satisfies the following equation:

$$\sum_{m=1}^M d_{m,j} = \max_{k=1}^K \left( \sum_{m=1}^M d_{m,k} \right)$$

Let  $E_m$  be the testing error estimated for the  $m$ th base model. Weights for the weighted majority vote are then computed according to the following expression:

$$w_m = \max \left( \log \frac{1 - E_m}{E_m}, 0 \right) / \sum_{i=1}^M \max \left( \log \frac{1 - E_i}{E_i}, 0 \right)$$

**Probability voting.** Assume that  $p_{m,k}$  is the posterior probability estimated for the  $k$ th target category by the  $m$ th base model for a given vector of predictor values. The following rules combine the probabilities computed by the base models. The  $j$ th category is selected such that it satisfies the corresponding equation.

- Highest probability.  $\max_{m=1}^M (p_{m,j}) = \max_{k=1}^K (\max_{m=1}^M (p_{m,k}))$
- Highest mean probability.  $\frac{1}{M} \sum_{m=1}^M p_{m,j} = \max_{k=1}^K \left( \frac{1}{M} \sum_{m=1}^M p_{m,k} \right)$

Ties are resolved at random.

**Softmax smoothing.** The softmax function can be used for smoothing the probabilities:

$$p_i^S = \frac{\text{Exp}(p_i)}{\sum_{i=1}^K \text{Exp}(p_i)}$$

where  $p_i$  is the rule-based confidence for category  $i$  and  $p_i^S$  is the smoothed value.

## Ensembling model scores algorithms

Ensembling scores from individual models can give more accurate predictions. By combining scores from multiple models, limitations in individual models may be avoided, resulting in a higher overall accuracy. Models combined in this manner typically perform at least as well as the best of the individual models and often better.

Note that while the options for general ensembling of scores are similar to those for boosting, bagging, and very large datasets, the specific options for combining scoring are slightly different.

### Notation

The following notation applies.

$N$	Total number of records
$M$	Total number of base models
$y_i$	The observed target value of record $i$
$\hat{y}_i$	The predicted target value of record $i$ by the ensemble model
$\hat{y}_i^m$	The predicted target value of record $i$ by base model $m$

### Scoring

There are several strategies for scoring using the ensemble models.

#### Continuous Target

**Mean.**  $\hat{y}_{i,M} = \frac{1}{M} \sum_{m=1}^M \hat{y}_{i,m}$

where  $\hat{y}_{i,M}$  is the final predicted value of case  $i$ , and  $\hat{y}_{i,m}$  is the  $m$ th base model's predicted value of case  $i$ .

**Standard error.**  $\hat{SE}_{i,M} = \frac{1}{\sqrt{M}} \sqrt{\frac{1}{M-1} \sum_{m=1}^M (\hat{y}_{i,m} - \hat{y}_{i,M})^2}$

### **Categorical Target**

**Voting.** Assume that  $d_{m,k}$  represents the label output of the  $m$ th base model for a given vector of predictor values.  $d_{m,k} = 1$  if the label assigned by the  $m$ th base model is the  $k$ th target category and 0 otherwise. There are total of  $M$  base models and  $K$  target categories. The majority vote method selects the  $j$ th category if it is assigned by the plurality of base models. It satisfies the following equation:

$$\sum_{m=1}^M d_{m,j} = \max_{k=1}^K \left( \sum_{m=1}^M d_{m,k} \right)$$

**Confidence-weighted (probability) voting.** Assume that  $p_{m,k}$  is the posterior probability estimated for the  $k$ th target category by the  $m$ th base model for a given vector of predictor values. The following rules combine the probabilities computed by the base models. The  $j$ th category is selected such that it satisfies the corresponding equation.

$$\sum_{m=1}^M p_{m,j} d_{m,j} = \max_{k=1}^K p_{m,k} \left( \sum_{m=1}^M d_{m,k} \right)$$

**Highest confidence (probability) wins.**

$$\max_{m=1}^M (p_{m,j}) = \max_{k=1}^K (\max_{m=1}^M (p_{m,k}))$$

**Raw propensity-weighted voting.** This is equivalent to confidence-weighted voting for a flag target, where the weights for *true* are the propensities and the weights for *false* are 1-propensity.

**Adjusted propensity-weighted voting.** This is similar to raw propensity-weighted voting for a flag target, where the weights for *true* are the adjusted propensities and the weights for *false* are 1-adjusted propensity.

**Average raw propensity.** The raw propensities scores are averaged across the base models. If the average is  $> 0.5$ , then the record is scored as *true*.

**Average adjusted propensity.** The adjusted propensities scores are averaged across the base models. If the average is  $> 0.5$ , then the record is scored as *true*.



# Factor Analysis/PCA Algorithms

## Overview

The Factor/PCA node performs principal components analysis and six types of factor analysis.

## Primary Calculations

### Factor Extraction

#### Principal Components Analysis

The matrix of factor loadings based on factor  $m$  is

$$\Lambda_m = \Omega_m \Gamma_m^{\frac{1}{2}}$$

where

$$\Omega_m = (\omega_1, \omega_2, \dots, \omega_m)$$

$$\Gamma_m = \text{diag}(|\gamma_1|, |\gamma_2|, \dots, |\gamma_m|)$$

The communality of variable  $i$  is given by

$$h_i = \sum_{j=1}^m |\gamma_j| \omega_{ij}^2$$

#### Analyzing a Correlation Matrix

$\gamma_1 \geq \gamma_2 \geq \dots \geq \gamma_m$  are the eigenvalues and  $\omega_i$  are the corresponding eigenvectors of  $\mathbf{R}$ , where  $\mathbf{R}$  is the correlation matrix.

#### Analyzing a Covariance Matrix

$\gamma_1 \geq \gamma_2 \geq \dots \geq \gamma_m$  are the eigenvalues and  $\omega_i$  are the corresponding eigenvectors of  $\mathbf{\Sigma}$ , where  $\mathbf{\Sigma} = (\sigma_{ij})_{n \times n}$  is the covariance matrix.

The rescaled loadings matrix is  $\Lambda_{mR} = [\text{diag}(\mathbf{\Sigma})]^{-\frac{1}{2}} \Lambda_m$ .

The rescaled communality of variable  $i$  is  $h_{iR} = \sigma_{ii}^{-1} h_i$ .

### Principal Axis Factoring

#### Analyzing a Correlation Matrix

An iterative solution for communalities and factor loadings is sought. At iteration  $i$ , the communalities from the preceding iteration are placed on the diagonal of  $\mathbf{R}$ , and the resulting  $\mathbf{R}$  is denoted by  $\mathbf{R}_i$ . The eigenanalysis is performed on  $\mathbf{R}_i$ , and the new communality of variable  $j$  is estimated by

$$h_{j(i)} = \sum_{k=1}^m |\gamma_{k(i)}| \omega_{jk(i)}^2$$

The factor loadings are obtained by

$$\Lambda_{m(i)} = \Omega_{m(i)} \Gamma_{m(i)}^{\frac{1}{2}}$$

Iterations continue until the maximum number (default 25) is reached or until the maximum change in the communality estimates is less than the convergence criterion (default 0.001).

#### Analyzing a Covariance Matrix

This analysis is the same as analyzing a correlation matrix, except  $\Sigma$  is used instead of the correlation matrix  $\mathbf{R}$ . Convergence is dependent on the maximum change of rescaled communality estimates.

At iteration  $i$ , the rescaled loadings matrix is  $\Lambda_{m(i)R} = [\text{diag}(\Sigma)]^{-\frac{1}{2}} \Lambda_{m(i)}$ . The rescaled communality of variable  $i$  is  $h_{j(i)R} = \sigma_{ii}^{-1} h_{j(i)}$ .

### Maximum Likelihood

The maximum likelihood solutions of  $\Lambda$  and  $\psi^2$  are obtained by minimizing

$$F = \text{tr} \left[ (\Lambda \Lambda' + \psi^2)^{-1} \mathbf{R} \right] - \log \left| (\Lambda \Lambda' + \psi^2)^{-1} \mathbf{R} \right| - p$$

with respect to  $\Lambda$  and  $\psi$ , where  $p$  is the number of variables,  $\Lambda$  is the factor loading matrix, and  $\psi^2$  is the diagonal matrix of unique variances.

The minimization of  $F$  is performed by way of a two-step algorithm. First, the conditional minimum of  $F$  for a given  $\psi$  is found. This gives the function  $f(\psi)$ , which is minimized numerically using the Newton-Raphson procedure. Let  $\mathbf{x}^{(s)}$  be the column vector containing the logarithm of the diagonal elements of  $\psi$  at the  $s$ th iteration. Then

$$\mathbf{x}^{(s+1)} = \mathbf{x}^{(s)} - \mathbf{d}^{(s)}$$

where  $\mathbf{d}^{(s)}$  is the solution to the system of linear equations

$$\mathbf{H}^{(s)} \mathbf{d}^{(s)} = \mathbf{h}^{(s)}$$

and where

$$\mathbf{H}^{(s)} = \frac{\partial^2 f(\psi)}{\partial x_i \partial x_j}$$

and  $\mathbf{h}^{(s)}$  is the column vector containing  $\frac{\partial f(\psi)}{\partial x_i}$ . The starting point  $\mathbf{x}^{(1)}$  is

$$\mathbf{x}_i^1 = \begin{cases} \log \left[ \left(1 - \frac{m}{2p}\right) / r^{ii} \right] & \text{for ML and GLS} \\ \left[ \left(1 - \frac{m}{2p}\right) / r^{ii} \right]^{\frac{1}{2}} & \text{for ULS} \end{cases}$$

where  $m$  is the number of factors and  $r^{ii}$  is the  $i$ th diagonal element of  $\mathbf{R}^{-1}$ .

The values of  $f(\psi)$ ,  $\frac{\partial f}{\partial x_i}$ , and  $\frac{\partial^2 f}{\partial x_i \partial x_j}$  can be expressed in terms of the eigenvalues  $\gamma_1 \leq \gamma_2 \leq \dots \leq \gamma_p$  and corresponding eigenvectors  $\omega_1, \omega_2, \dots, \omega_p$  of matrix  $\psi \mathbf{R}^{-1} \psi$ . That is,

$$\begin{aligned} f(\psi) &= \sum_{k=m+1}^p (\log \gamma_k + \gamma_k^{-1} - 1) \\ \frac{\partial f}{\partial x_i} &= \sum_{k=m+1}^p (1 - \gamma_k^{-1}) \omega_{ik}^2 \\ \frac{\partial^2 f}{\partial x_i \partial x_j} &= -\delta_{ij} \frac{\partial f}{\partial x_i} + \sum_{k=m+1}^p \omega_{ik} \omega_{jk} \left( \sum_{n=1}^m \frac{\gamma_k + \gamma_n - 2}{\gamma_k - \gamma_n} \omega_{in} \omega_{jn} + \delta_{ij} \right) \end{aligned}$$

where

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

The approximate second-order derivatives

$$\frac{\partial^2 f}{\partial x_i \partial x_j} \cong \left( \sum_{k=m+1}^p \omega_{ik} \omega_{jk} \right)^2$$

are used in the initial step and when the matrix of the exact second-order derivatives is not positive definite or when all elements of the vector  $\mathbf{d}$  are greater than 0.1. If  $\frac{\partial^2 f}{\partial x_i^2} < 0.05$  (Heywood variables), the diagonal element is replaced by 1 and the rest of the elements of that column and row are set to 0. If the value of  $f(\psi)$  is not decreased by step  $\mathbf{d}$ , the step is halved and halved again until the value of  $f(\psi)$  decreases or 25 halvings fail to produce a decrease. (In this case, the computations are terminated.) Stepping continues until the largest absolute value of the elements of  $\mathbf{d}$  is less than the criterion value (default 0.001) or until the maximum number of iterations (default 25) is reached. Using the converged value of  $\psi$  (denoted by  $\hat{\psi}$ ), the eigenanalysis is performed on the matrix  $\hat{\psi} \mathbf{R}^{-1} \hat{\psi}$ . The factor loadings are computed as

$$\hat{\Lambda}_m = \hat{\psi} \Omega_m (\Gamma_m^{-1} - \mathbf{I}_m)^{\frac{1}{2}}$$

where

$$\Gamma_m = \text{diag}(\gamma_1, \gamma_2, \dots, \gamma_m)$$

$$\Omega_m = (\omega_1, \omega_2, \dots, \omega_m)$$

### Unweighted and Generalized Least Squares

The same basic algorithm is used in ULS and GLS as in maximum likelihood, except that

$$f(\psi) = \begin{cases} \sum_{k=m+1}^p \frac{\gamma_k^2}{2} & \text{for ULS} \\ \sum_{k=m+1}^p \frac{(\gamma_k - 1)^2}{2} & \text{for GLS} \end{cases}$$

for the ULS method, the eigenanalysis is performed on the matrix  $\mathbf{R} - \psi^2$ , where  $\gamma_1 \geq \gamma_2 \geq \dots \geq \gamma_p$  are the eigenvalues. In terms of the derivatives, for ULS,

$$\frac{\partial f}{\partial x_i} = 2x_i \sum_{k=m+1}^p \gamma_k \omega_{ik}^2$$

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = 4 \left[ x_i x_j \sum_{k=m+1}^p \omega_{ik} \omega_{jk} \sum_{n=1}^m \frac{\gamma_k + \gamma_n}{\gamma_k - \gamma_n} \omega_{ik} \omega_{jk} + \delta_{ij} \sum_{k=m+1}^p \left( x_i^2 - \frac{\gamma_k}{2} \right) \omega_{ik}^2 \right]$$

and

$$\frac{\partial^2 f}{\partial x_i \partial x_j} \cong 4x_i x_j \left( \sum_{k=m+1}^p \omega_{ik} \omega_{jk} \right)^2$$

For GLS,

$$\frac{\partial f}{\partial x_i} = \sum_{k=m+1}^p (\gamma_k^2 - \gamma_k) \omega_{ik}^2$$

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \delta_{ij} \frac{\partial f}{\partial x_i} + \sum_{k=m+1}^p \gamma_k \omega_{ik} \omega_{jk} \left( \sum_{n=1}^m \gamma_n \frac{\gamma_k + \gamma_n - 2}{\gamma_k - \gamma_n} \omega_{in} \omega_{jn} + r^{ii} \exp \left( \frac{x_i + x_j}{2} \right) \right)$$

and

$$\frac{\partial^2 f}{\partial x_i \partial x_j} \cong \left( \sum_{k=m+1}^p \omega_{ik} \omega_{jk} \right)^2$$

Also, the factor loadings of the ULS method are obtained by

$$\hat{\Lambda}_m = \Omega_m \Gamma_m^{\frac{1}{2}}$$

The chi-square statistic for  $m$  factors for the ML and GLS methods is given by

$$\chi_m^2 = \left( W - 1 - \frac{2p + 5}{6} - \frac{2m}{3} \right) f(\hat{\psi})$$

with  $\left( (p - m)^2 - p - m \right) / 2$  degrees of freedom.

### Alpha Factoring

Alpha factoring involves an iterative procedure, where at each iteration  $i$ :

The eigenvalues  $(\gamma_{(i)})$  and eigenvectors  $(\omega_{(i)})$  of

$$\mathbf{H}_{(i-1)}^{\frac{1}{2}} (\mathbf{R} - \mathbf{I}) \mathbf{H}_{(i-1)}^{\frac{1}{2}} + \mathbf{I}$$

are computed.

The new communalities are

$$h_{k(i)} \left( \sum_{j=1}^m |\gamma_{j(i)}| \omega_{kj(i)}^2 \right) h_{k(i-1)}$$

The initial values of the communalities,  $\mathbf{H}_0$ , are

$$h_{io} = \begin{cases} 1 - \frac{1}{r^{ii}} & |\mathbf{R}| \geq 10^{-8} \text{ and all } 0 \leq h_{io} \leq 1 \\ \max_j |r_{ij}| & \text{otherwise} \end{cases}$$

where  $r^{ii}$  is the  $i$ th diagonal entry of  $\mathbf{R}^{-1}$ .

If  $|R| \geq 10^{-8}$  and all  $r^{ii}$  are equal to one, the procedure is terminated. If for some  $i$ ,  $\max_j |r_{ij}| > 1$ , the procedure is terminated.

Iteration stops if any of the following are true:

$$\max_k |h_{k(i)} - h_{k(i-1)}| < \epsilon$$

$$i = MAX$$

$$h_{k(i)} = 0 \text{ for any } k$$

The communalities are the values when iteration stops, unless the last termination criterion is true, in which case the procedure terminates. The factor pattern matrix is

$$F_m = H_{(f)}^{\frac{1}{2}} \Omega_{m(f)} \Gamma_{m(f)}^{\frac{1}{2}}$$

where  $f$  is the final iteration.

### **Image Factoring**

#### **Analyzing a Correlation Matrix**

Eigenvalues and eigenvectors of  $\mathbf{S}^{-1}\mathbf{R}\mathbf{S}^{-1}$  are found.

$$\mathbf{S}^2 = \text{diag} \left( \frac{1}{r^{11}}, \dots, \frac{1}{r^{nn}} \right)$$

where  $r^{ii}$  is the  $i$ th diagonal element of  $\mathbf{R}^{-1}$

The factor pattern matrix is

$$\mathbf{F}_m = \mathbf{S}\Omega_m(\Lambda_m - \mathbf{I}_m)\Lambda_m^{-\frac{1}{2}}$$

where  $\Lambda_m$  and  $\Omega_m$  correspond to the  $m$  eigenvalues greater than 1 (and the associated eigenvectors). If  $m = 0$ , the procedure is terminated.

The communalities are

$$h_i = \sum_{j=1}^m \frac{(\gamma_j - 1)^2 \omega_{ij}^2}{(\gamma_j r^{ii})}$$

The image covariance matrix is

$$\mathbf{R} + \mathbf{S}^2\mathbf{R}^{-1}\mathbf{S}^2 - 2\mathbf{S}^2$$

The anti-image covariance matrix is

$$\mathbf{S}^2\mathbf{R}^{-1}\mathbf{S}^2$$

#### **Analyzing a Covariance Matrix**

When analyzing a covariance matrix, the covariance matrix  $\Sigma$  is used instead of the correlation matrix  $\mathbf{R}$ . The calculation is similar to the correlation matrix case.

The rescaled factor pattern matrix is

$$\mathbf{F}_{mR} = [\text{diag}(\Sigma)]^{\frac{1}{2}}\mathbf{F}_m$$

and the rescaled communality of variable  $i$  is  $h_{iR} = \sigma_{ii}^{-1}h_i$ .

## Factor Rotation

### Orthogonal Rotations

Rotations are done cyclically on pairs of factors until the maximum number of iterations is reached or the convergence criterion is met. The algorithm is the same for all orthogonal rotations, differing only in computations of the tangent values of the rotation angles.

The factor pattern matrix is normalized by the square root of communalities:

$$\Lambda_m^* = \mathbf{H}^{\frac{1}{2}} \Lambda_m$$

where

$\Lambda_m = (\lambda_1, \dots, \lambda_m)$  is the factor pattern matrix

$$\mathbf{H} = \text{diag}(h_1, \dots, h_n)$$

The transformation matrix  $\mathbf{T}$  is initialized to  $\mathbf{I}_m$ .

At each iteration  $i$ :

- The convergence criterion is

$$SV_{(i)} = \sum_{j=1}^m \left( n \sum_{k=1}^n \lambda_{kj(i)}^{*4} - \left( \sum_{k=1}^n \lambda_{kj(i)}^{*2} \right)^2 \right) / n^2$$

where the initial value of  $\Lambda_{m(1)}^*$  is the original factor pattern matrix. For subsequent iterations, the initial value is the final value of  $\Lambda_{m(i-1)}^*$  when all factor pairs have been rotated.

For all pairs of factors  $(\lambda_j, \lambda_k)$  where  $k > j$ , the following are computed:

- The angle of rotation is

$$P = \frac{1}{4} \tan^{-1} \left( \frac{X}{Y} \right)$$

where

$$X = \begin{cases} D - \frac{2AB}{n} & \text{Varimax} \\ D - \frac{mAB}{n} & \text{Equamax} \\ D & \text{Quartimax} \end{cases}$$

$$Y = \begin{cases} C - \left( \frac{A^2 - B^2}{n} \right) & \text{Varimax} \\ C - \frac{m(A^2 - B^2)}{2n} & \text{Equamax} \\ C & \text{Quartimax} \end{cases}$$

$$u_{p(i)} = f_{pj(i)}^{*2} - f_{pk(i)}^{*2} \quad v_{p(i)} = 2f_{pj(i)}^* f_{pk(i)}^* \quad p = 1, \dots, n$$

$$A = \sum_{p=1}^n u_{p(i)} \quad B = \sum_{p=1}^n v_{p(i)}$$

$$C = \sum_{p=1}^n \left[ u_{p(i)}^2 - v_{p(i)}^2 \right] \quad D = \sum_{p=1}^n 2u_{p(i)}v_{p(i)}$$

If  $|\sin(P)| \leq 10^{-15}$ , no rotation is done on the pair of factors.

- The new rotated factors are

$$\left( \tilde{\lambda}_{j(i)}, \tilde{\lambda}_{k(i)} \right) = \left( \lambda_{j(i)}^*, \lambda_{k(i)}^* \right) \begin{vmatrix} \cos(P) & -\sin(P) \\ \sin(P) & \cos(P) \end{vmatrix}$$

where  $\lambda_{j(i)}^*$  are the last values for factor  $j$  calculated in this iteration.

- The accrued rotation transformation matrix is

$$\left( \tilde{t}_j, \tilde{t}_k \right) = \left( t_j, t_k \right) \begin{vmatrix} \cos(P) & -\sin(P) \\ \sin(P) & \cos(P) \end{vmatrix}$$

where  $t_j$  and  $t_k$  are the last calculated values of the  $j$ th and  $k$ th columns of  $\mathbf{T}$ .

- Iteration is terminated when

$$|SV_{(i)} - SV_{(i-1)}| \leq 10^{-5}$$

or the maximum number of iterations is reached.

Final rotated factor pattern matrix

$$\hat{\Lambda}_m = H^{\frac{1}{2}} \Lambda_{m(f)}^*$$

where  $\Lambda_{m(f)}^*$  is the value of the last iteration.

Reflect factors with negative sums. If

$$\sum_{i=1}^n \tilde{\lambda}_{ij(f)} < 0$$

then

$$\tilde{\lambda}_j = -\tilde{\lambda}_{j(f)}$$

Rearrange the rotated factors such that

$$\sum_{j=1}^n \tilde{\lambda}_{j1}^2 \geq \dots \geq \sum_{j=1}^n \tilde{\lambda}_{jm}^2$$

The communalities are

$$h_j = \sum_{i=1}^m \tilde{\lambda}_{ji}^2$$

### **Direct Oblimin Rotation**

The direct oblimin method (Jennrich and Sampson, 1966) is used for oblique rotation. The user can choose the parameter  $\delta$ . The default value is  $\delta = 0$ .

The factor pattern matrix is normalized by the square root of the communalities

$$\Omega_m^* = H^{\frac{1}{2}} \Lambda_m$$

where

$$h_j = \sum_{k=1}^m \lambda_{jk}^2$$

If no Kaiser is specified, this normalization is not done.

Initializations

The factor correlation matrix  $\mathbf{C}$  is initialized to  $\mathbf{I}_m$ . The following are also computed:

$$s_k = \begin{cases} 1 & \text{if Kaiser} \\ h_k & \text{if no Kaiser} \end{cases} \quad k = 1, \dots, n$$

$$u_i = \sum_{j=1}^n \lambda_{ji}^{*2} \quad i = 1, \dots, m$$

$$v_i = \sum_{j=1}^n \lambda_{ji}^{*4}$$

$$x_i = v_i - \left(\frac{\delta}{n}\right) u_i^2$$

$$D = \sum_{i=1}^m u_i$$

$$G = \sum_{i=1}^m x_i$$

$$H = \sum_{k=1}^n s_k^2 - \left(\frac{\delta}{n}\right) D^2$$

$$FO = H - G$$

At each iteration, all possible factor pairs are rotated. For a pair of factors  $\underline{\lambda}_p^*$  and  $\underline{\lambda}_q^*$  ( $p \neq q$ ), the following are computed:

$$D_{pq} = D - u_p - u_q$$

$$G_{pq} = G - x_p - x_q$$

$$s_{pq,i} = s_i - \lambda_{ip}^{*2} - \lambda_{iq}^{*2}$$

$$y_{pq} = \sum_{i=1}^n \lambda_{ip}^* \lambda_{iq}^*$$

$$z_{pq} = \sum_{i=1}^n \lambda_{ip}^{*2} \lambda_{iq}^{*2}$$

$$T = \sum_{i=1}^n s_{pq,i} \lambda_{ip}^{*2} - \left(\frac{\delta}{n}\right) u_p D_{pq}$$

$$Z = \sum_{i=1}^n s_{pq,i} \lambda_{ip}^* \lambda_{iq}^* - \left(\frac{\delta}{n}\right) y_{pq} D_{pq}$$

$$P = \sum_{i=1}^n \lambda_{ip}^{*3} \lambda_{iq}^* - \left(\frac{\delta}{n}\right) u_p y_{pq}$$

$$R = z_{pq} - \left(\frac{\delta}{n}\right) u_p u_q$$

$$P' = \frac{3}{2} \left( c_{pq} - \frac{P}{x_p} \right)$$

$$Q' = \frac{1}{2} (x_p - 4c_{pq}P + R + 2T) / x_p$$

$$R' = \frac{1}{2} (c_{pq}(T + R) - P - Z) / x_p$$

A root  $a$  of the equation  $b^3 + P'b^2 + Q'b + R = 0$  is computed, as well as

$$A = 1 + 2c_{pq}a + a^2$$

$$t_1 = |A|^{\frac{1}{2}}$$

$$t_2 = \frac{a}{t_1}$$

The rotated pair of factors is

$$\left( \tilde{\lambda}_p^*, \tilde{\lambda}_q^* \right) = \left( \lambda_p^*, \lambda_q^* \right) \begin{vmatrix} t_1 & -a \\ 0 & 1 \end{vmatrix}$$

These replace the previous factor values.

New values are computed for

$$\tilde{u}_p = |A|u_p$$

$$\tilde{x}_p = A^2 x_p$$

$$\tilde{v}_q = \sum_{i=1}^n \tilde{\lambda}_{iq}^{*4}$$

$$\tilde{u}_q = \sum_{i=1}^n \tilde{\lambda}_{iq}^{*2}$$

$$\tilde{x}_q = \tilde{v}_q - \left( \frac{\delta}{n} \right) \tilde{u}_q^2$$

$$\tilde{S}_k = S_{pq,k} + \tilde{\lambda}_{kp}^{*2} + \tilde{\lambda}_{kq}^{*2}$$

$$\tilde{D} = D_{pq} + \tilde{u}_p + \tilde{u}_q$$

$$\tilde{G} = G_{pq} + \tilde{x}_p + \tilde{x}_q$$

All values designated with a tilde (~) replace the original values and are used in subsequent calculations.

The new factor correlations with factor  $p$  are

$$\tilde{c}_{ip} = t_1^{-1}c_{ip} + t_2c_{iq} \quad (i \neq p)$$

$$\tilde{c}_{pi} = \tilde{c}_{ip}$$

$$\tilde{c}_{pp} = 1$$

After all factor pairs have been rotated, iteration is terminated if:

MAX iterations have been done, *or*

$$\left| F1_{(i)} - F1_{(i-1)} \right| < (FO)(EPS)$$

where

$$F1_{(i)} = \tilde{H} - \tilde{G}$$

$$\tilde{H} = \sum_{i=1}^n \tilde{s}_k^2 - \left(\frac{\delta}{n}\right) \tilde{D}^2$$

$$F1_{(0)} = FO$$

Otherwise, the factor pairs are rotated again.

The final rotated factor pattern matrix is

$$\tilde{\lambda}_m = \mathbf{H}^{\frac{1}{2}} \tilde{\lambda}_m^*$$

where  $\tilde{\lambda}_m$  is the value in the final iteration.

The factor structure matrix is

$$\mathbf{S} = \tilde{\Lambda}_m \tilde{\mathbf{C}}_m$$

where  $\tilde{\mathbf{C}}_m$  is the factor correlation matrix in the final iteration.

### **Promax Rotation**

The promax rotation is a computationally fast rotation (Hendrickson and White, 1964). The speed is achieved by first rotating to an orthogonal varimax solution and then relaxing the orthogonality of the factors to better fit the simple structure.

Varimax rotation is used to get an orthogonal rotated matrix  $\Lambda_R = \{\lambda_{ij}\}$ .

The matrix  $\mathbf{P} = (p_{ij})_{p \times m}$  is calculated, where

$$p_{ij} = \left| \frac{\lambda_{ij}}{\left(\sum_{j=1}^m \lambda_{ij}^2\right)^{\frac{1}{2}}} \right|^{k+1} \frac{\left(\sum_{j=1}^m \lambda_{ij}^2\right)^{\frac{1}{2}}}{\lambda_{ij}}$$

Here,  $k$  is the power of promax rotation ( $k > 1$ ).

The matrix  $\mathbf{L}$  is calculated.

$$\mathbf{L} = (\Lambda'_R \Lambda_R)^{-1} \Lambda'_R \mathbf{P}$$

The matrix  $\mathbf{L}$  is normalized by column to a transformation matrix

$$\mathbf{Q} = \mathbf{L}\mathbf{D}$$

where  $\mathbf{D} = (\text{diag}(\mathbf{L}'\mathbf{L}))^{\frac{1}{2}}$  is the diagonal matrix that normalizes the columns of  $\mathbf{L}$ .

At this stage, the rotated factors are

$$f_{promax\_temp} = \mathbf{Q}^{-1} f_{varimax}$$

Because  $\text{var}(f_{promax\_temp}) = (\mathbf{Q}'\mathbf{Q})^{-1}$ , and the diagonal elements do not equal 1, we must modify the rotated factor to

$$f_{promax} = \mathbf{C}f_{promax\_temp}$$

$$\text{where } \mathbf{C} = \left\{ \text{diag} \left( (\mathbf{Q}'\mathbf{Q})^{-1} \right) \right\}^{-\frac{1}{2}}$$

The rotated factor pattern is

$$\Lambda_{promax} = \Lambda_{varimax} \mathbf{Q} \mathbf{C}^{-1}$$

The correlation matrix of the factors is

$$\mathbf{R}_{ff} = \mathbf{C}(\mathbf{Q}'\mathbf{Q})^{-1}\mathbf{C}'$$

The factor structure matrix is

$$\Lambda_S = \Lambda_{promax} \mathbf{R}_{ff}$$

### Factor Score Coefficients

IBM® SPSS® Modeler uses the regression method of computing factor score coefficients (Harman, 1976).

$$\mathbf{W} = \begin{cases} \Lambda_m \Gamma_m^{-1} & \text{PCA without rotation} \\ \Lambda_m (\Lambda_m' \Lambda_m)^{-1} & \text{PCA with rotation} \\ \mathbf{R}^{-1} \mathbf{S}_m & \text{otherwise} \end{cases}$$

where  $\mathbf{S}_m$  is the factor structure matrix. For orthogonal rotations  $\mathbf{S}_m = \Lambda_m$ .

For principal components analysis without rotation, if any  $|\gamma_i| \leq 10^{-8}$ , factor score coefficients are not computed. For principal components with rotation, if the determinant of  $\Lambda_m' \Lambda_m$  is less than  $10^{-8}$ , the coefficients are not computed. Otherwise, if  $\mathbf{R}$  is singular, factor score coefficients are not computed.

### Blank Handling

By default, a case that has a missing value for any input or output field is deleted from the computation of the correlation matrix on which all consequent computations are based. If the Only use complete records option is deselected, each correlation in the correlation matrix  $\mathbf{R}$  is computed based on records with complete data for the two fields associated with the correlation, regardless of missing values on other fields. For some datasets, this approach can lead to a nonpositive definite  $\mathbf{R}$  matrix, so that the model cannot be estimated.

## **Secondary Calculations**

### **Field Statistics and Other Calculations**

The statistics shown in the advanced output for the regression equation node are calculated in the same manner as in the FACTOR procedure in IBM® SPSS® Statistics. For more details, see the SPSS Statistics Factor algorithm document, available at <http://www.ibm.com/support>.

## **Generated Model/Scoring**

### **Factor Scores**

Factor scores are assigned to scored records by applying the factor score coefficients to the input field value for the record,

$$f s_k = \sum_{i=1}^n w_{ki} f_i$$

where  $f s_k$  is the factor score for the  $k$ th factor,  $w_{ki}$  is the factor score coefficient for the  $i$ th input field (from the **W** matrix) and the  $k$ th factor, and  $f_i$  is the value of the  $i$ th input field for the record being scored. For more information, see the topic “Factor Score Coefficients” on p. 151.

### **Blank Handling**

Records with missing values for any input field in the final model cannot be scored and are assigned factor/component score values of \$NULL\$.

# ***Feature Selection Algorithm***

## ***Introduction***

Data mining problems often involve hundreds, or even thousands, of variables. As a result, the majority of time and effort spent in the model-building process involves examining which variables to include in the model. Fitting a neural network or a decision tree to a set of variables this large may require more time than is practical.

Feature selection allows the variable set to be reduced in size, creating a more manageable set of attributes for modeling. Adding feature selection to the analytical process has several benefits:

- Simplifies and narrows the scope of the features that is essential in building a predictive model.
- Minimizes the computational time and memory requirements for building a predictive model because focus can be directed to the subset of predictors that is most essential.
- Leads to more accurate and/or more parsimonious models.
- Reduces the time for generating scores because the predictive model is based upon only a subset of predictors.

## ***Primary Calculations***

Feature selection consists of three steps:

- **Screening.** Removes unimportant and problematic predictors and cases.
- **Ranking.** Sorts remaining predictors and assigns ranks.
- **Selecting.** Identifies the important subset of features to use in subsequent models.

The algorithm described here is limited to the supervised learning situation in which a set of predictor variables is used to predict a target variable. Any variables in the analysis can be either categorical or continuous. Common target variables include whether or not a customer churns, whether or not a person will buy, and whether or not a disease is present.

The terms **features**, **variables**, and **attributes** are often used interchangeably. Within this document, we use variables and predictors when discussing input to the feature selection algorithm, with features referring to the predictors that actually get selected by the algorithm for use in a subsequent modeling process.

## ***Screening***

This step removes variables and cases that do not provide useful information for prediction and issues warnings about variables that may not be useful.

The following variables are removed:

- Variables that have all missing values.
- Variables that have all constant values.
- Variables that represent case ID.

The following cases are removed:

- Cases that have missing target values.
- Cases that have missing values in all its predictors.

The following variables are removed based on user settings:

- Variables that have more than  $m_1\%$  missing values.
- Categorical variables that have a single category counting for more than  $m_2\%$  cases.
- Continuous variables that have standard deviation  $< m_3\%$ .
- Continuous variables that have a coefficient of variation  $|CV| < m_4\%$ .  $CV = \text{standard deviation} / \text{mean}$ .
- Categorical variables that have a number of categories greater than  $m_5\%$  of the cases.

Values  $m_1$ ,  $m_2$ ,  $m_3$ ,  $m_4$ , and  $m_5$  are user-controlled parameters.

## Ranking Predictors

This step considers one predictor at a time to see how well each predictor alone predicts the target variable. The predictors are ranked according to a user-specified criterion. Available criteria depend on the measurement levels of the target and predictor.

The **importance** value of each variable is calculated as  $(1 - p)$ , where  $p$  is the  $p$  value of the appropriate statistical test of association between the candidate predictor and the target variable, as described below.

### Categorical Target

This section describes ranking of predictors for a categorical target under the following scenarios:

- All predictors categorical
- All predictors continuous
- Some predictors categorical, some continuous

### All Categorical Predictors

The following notation applies:

Table 17-1  
Notation

Notation	Description
$X$	The predictor under consideration with $I$ categories.
$Y$	Target variable with $J$ categories.
$N$	Total number of cases.
$N_{ij}$	The number of cases with $X = i$ and $Y = j$ .

Notation	Description
$N_{i.}$	The number of cases with $X = i$ . $N_{i.} = \sum_{j=1}^J N_{ij}$
$N_{.j}$	The number of cases with $Y = j$ . $N_{.j} = \sum_{i=1}^I N_{ij}$

The above notations are based on nonmissing pairs of  $(X, Y)$ . Hence  $J$ ,  $N$ , and  $N_{.j}$  may be different for different predictors.

#### P Value Based on Pearson's Chi-square

Pearson's chi-square is a test of independence between  $X$  and  $Y$  that involves the difference between the observed and expected frequencies. The expected cell frequencies under the null hypothesis of independence are estimated by  $\hat{N}_{ij} = N_{i.}N_{.j}/N$ . Under the null hypothesis, Pearson's chi-square converges asymptotically to a chi-square distribution  $\chi_d^2$  with degrees of freedom  $d = (I-1)(J-1)$ .

The  $p$  value based on Pearson's chi-square  $X^2$  is calculated by  $p$  value =  $\text{Prob}(\chi_d^2 > X^2)$ , where

$$X^2 = \sum_{i=1}^I \sum_{j=1}^J \frac{(N_{ij} - \hat{N}_{ij})^2}{\hat{N}_{ij}}$$

Predictors are ranked by the following rules.

1. Sort the predictors by  $p$  value in the ascending order
2. If ties occur, sort by chi-square in descending order.
3. If ties still occur, sort by degree of freedom  $d$  in ascending order.
4. If ties still occur, sort by the data file order.

#### P Value Based on Likelihood Ratio Chi-square

The likelihood ratio chi-square is a test of independence between  $X$  and  $Y$  that involves the ratio between the observed and expected frequencies. The expected cell frequencies under the null hypothesis of independence are estimated by  $\hat{N}_{ij} = N_{i.}N_{.j}/N$ . Under the null hypothesis, the likelihood ratio chi-square converges asymptotically to a chi-square distribution  $\chi_d^2$  with degrees of freedom  $d = (I-1)(J-1)$ .

The  $p$  value based on likelihood ratio chi-square  $G^2$  is calculated by  $p$  value =  $\text{Prob}(\chi_d^2 > G^2)$ , where

$$G^2 = 2 \sum_{i=1}^I \sum_{j=1}^J G_{ij}^2, \text{ with } G_{ij}^2 = \begin{cases} N_{ij} \ln \left( N_{ij} / \hat{N}_{ij} \right) & N_{ij} > 0, \\ 0 & \text{else.} \end{cases}$$

Predictors are ranked according to the same rules as those for the  $p$  value based on Pearson's chi-square.

#### Cramer's V

Cramer's  $V$  is a measure of association, between 0 and 1, based upon Pearson's chi-square. It is defined as

$$V = \left( \frac{X^2}{N(\min\{I, J\} - 1)} \right)^{1/2}.$$

Predictors are ranked by the following rules:

1. Sort predictors by Cramer's  $V$  in descending order.
2. If ties occur, sort by chi-square in descending order.
3. If ties still occur, sort by data file order.

Lambda

Lambda is a measure of association that reflects the proportional reduction in error when values of the independent variable are used to predict values of the dependent variable. A value of 1 means that the independent variable perfectly predicts the dependent variable. A value of 0 means that the independent variable is no help in predicting the dependent variable. It is computed as

$$\lambda(Y|X) = \frac{\sum_i \max_j (N_{ij}) - \max_j (N_{.j})}{N - \max_j (N_{.j})}.$$

Predictors are ranked by the following rules:

1. Sort predictors by lambda in descending order.
2. If ties occur, sort by  $I$  in ascending order.
3. If ties still occur, sort by data file order.

### All Continuous Predictors

If all predictors are continuous,  $p$  values based on the  $F$  statistic are used. The idea is to perform a one-way ANOVA  $F$  test for each continuous predictor; this tests if all the different classes of  $Y$  have the same mean as  $X$ .

The following notation applies:

Table 17-2

Notation

Notation	Description
$N_j$	The number of cases with $Y = j$ .
$\bar{x}_j$	The sample mean of predictor $X$ for target class $Y = j$ .
$s_j^2$	The sample variance of predictor $X$ for target class $Y = j$ .
	$s_j^2 = \sum_{i=1}^{N_j} (x_{ij} - \bar{x}_j)^2 / (N_j - 1)$
$\bar{\bar{x}}$	The grand mean of predictor $X$ . $\bar{\bar{x}} = \sum_{j=1}^J N_j \bar{x}_j / N$

The above notations are based on nonmissing pairs of  $(X, Y)$ .

P Value Based on the F Statistic

The  $p$  value based on the  $F$  statistic is calculated by  $p$  value =  $\text{Prob}\{F(J-1, N-J) > F\}$ , where

$$F = \frac{\sum_{j=1}^J N_j (\bar{x}_j - \bar{x})^2 / (J-1)}{\sum_{j=1}^J (N_j - 1) s_j^2 / (N-J)},$$

and  $F(J-1, N-J)$  is a random variable that follows an  $F$  distribution with degrees of freedom  $J-1$  and  $N-J$ . If the denominator for a predictor is zero, set the  $p$  value = 0 for the predictor.

Predictors are ranked by the following rules:

1. Sort predictors by  $p$  value in ascending order.
2. If ties occur, sort by  $F$  in descending order.
3. If ties still occur, sort by  $N$  in descending order.
4. If ties still occur, sort by the data file order.

### **Mixed Type Predictors**

If some predictors are continuous and some are categorical, the criterion for continuous predictors is still the  $p$  value based on the  $F$  statistic, while the available criteria for categorical predictors are restricted to the  $p$  value based on Pearson's chi-square or the  $p$  value based on the likelihood ratio chi-square. These  $p$  values are comparable and therefore can be used to rank the predictors.

Predictors are ranked by the following rules:

1. Sort predictors by  $p$  value in ascending order.
2. If ties occur, follow the rules for breaking ties among all categorical and all continuous predictors separately, then sort these two groups (categorical predictor group and continuous predictor group) by the data file order of their first predictors.

### **Continuous Target**

This section describes ranking of predictors for a continuous target under the following scenarios:

- All predictors categorical
- All predictors continuous
- Some predictors categorical, some continuous

### All Categorical Predictors

If all predictors are categorical and the target is continuous,  $p$  values based on the  $F$  statistic are used. The idea is to perform a one-way ANOVA  $F$  test for the continuous target using each categorical predictor as a factor; this tests if all different classes of  $X$  have the same mean as  $Y$ .

The following notation applies:

Table 17-3

Notation

Notation	Description
$X$	The categorical predictor under consideration with $I$ categories.
$Y$	The continuous target variable. $y_{ij}$ represents the value of the continuous target for the $j^{\text{th}}$ case with $X = i$ .
$N_i$	The number of cases with $X = i$ .
$\bar{y}_i$	The sample mean of target $Y$ in predictor category $X = i$ .
$s(y)_i^2$	The sample variance of target $Y$ for predictor category $X = i$ . $s(y)_i^2 = \sum_{j=1}^{N_i} (y_{ij} - \bar{y}_i)^2 / (N_i - 1)$
$\bar{y}$	The grand mean of target $Y$ . $\bar{y} = \sum_{i=1}^I N_i \bar{y}_i / N$

The above notations are based on nonmissing pairs of  $(X, Y)$ .

The  $p$  value based on the  $F$  statistic is  $p \text{ value} = \text{Prob}\{F(I-1, N-I) > F\}$ , where

$$F = \frac{\sum_{i=1}^I N_i (\bar{y}_i - \bar{y})^2 / (I-1)}{\sum_{i=1}^I (N_i - 1) s(y)_i^2 / (N-I)},$$

in which  $F(I-1, N-I)$  is a random variable that follows a  $F$  distribution with degrees of freedom  $I-1$  and  $N-I$ . When the denominator of the above formula is zero for a given categorical predictor  $X$ , set the  $p$  value = 0 for that predictor.

Predictors are ranked by the following rules:

1. Sort predictors by  $p$  value in ascending order.
2. If ties occur, sort by  $F$  in descending order.
3. If ties still occur, sort by  $N$  in descending order.
4. If ties still occur, sort by the data file order.

### All Continuous Predictors

If all predictors are continuous and the target is continuous, the  $p$  value is based on the asymptotic  $t$  distribution of a transformation  $t$  on the Pearson correlation coefficient  $r$ .

The following notation applies:

**Table 17-4**

*Notation*

<b>Notation</b>	<b>Description</b>
$X$	The continuous predictor under consideration.
$Y$	The continuous target variable.
$\bar{x} = \sum_{i=1}^N x_i / N$	The sample mean of predictor variable $X$ .
$\bar{y} = \sum_{i=1}^N y_i / N$	The sample mean of target $Y$ .
$s(x)^2$	The sample variance of predictor variable $X$ .
$s(y)^2$	The sample variance of target variable $Y$ .

The above notations are based on nonmissing pairs of  $(X, Y)$ .

The Pearson correlation coefficient  $r$  is

$$r = \frac{\sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y}) / (N-1)}{\sqrt{s(x)^2 s(y)^2}}.$$

The transformation  $t$  on  $r$  is given by

$$t = r \sqrt{\frac{N-2}{1-r^2}}.$$

Under the null hypothesis that the population Pearson correlation coefficient  $\rho = 0$ , the  $p$  value is calculated as

$$p \text{ value} = \begin{cases} 0 & \text{if } r^2 = 1, \\ 2 \text{ Prob}\{T > |t|\} & \text{else.} \end{cases}$$

$T$  is a random variable that follows a  $t$  distribution with  $N-2$  degrees of freedom. The  $p$  value based on the Pearson correlation coefficient is a test of a linear relationship between  $X$  and  $Y$ . If there is some nonlinear relationship between  $X$  and  $Y$ , the test may fail to catch it.

Predictors are ranked by the following rules:

1. Sort predictors by  $p$  value in ascending order.
2. If ties occur in, sort by  $r^2$  in descending order.
3. If ties still occur, sort by  $N$  in descending order.
4. If ties still occur, sort by the data file order.

### **Mixed Type Predictors**

If some predictors are continuous and some are categorical in the dataset, the criterion for continuous predictors is still based on the  $p$  value from a transformation and that for categorical predictors from the  $F$  statistic.

Predictors are ranked by the following rules:

1. Sort predictors by  $p$  value in ascending order.
2. If ties occur, follow the rules for breaking ties among all categorical and all continuous predictors separately, then sort these two groups (categorical predictor group and continuous predictor group) by the data file order of their first predictors.

### Selecting Predictors

If the length of the predictor list has not been prespecified, the following formula provides an automatic approach to determine the length of the list.

Let  $L_0$  be the total number of predictors under study. The length of the list  $L$  may be determined by

$$L = \lceil \min(\max(30, 2\sqrt{L_0}), L_0) \rceil,$$

where  $\lceil x \rceil$  is the closest integer of  $x$ . The following table illustrates the length  $L$  of the list for different values of the total number of predictors  $L_0$ .

$L_0$	$L$	$L/L_0(\%)$
10	10	100.00%
15	15	100.00%
20	20	100.00%
25	25	100.00%
30	30	100.00%
40	30	75.00%
50	30	60.00%
60	30	50.00%
100	30	30.00%
500	45	9.00%
1000	63	6.30%
1500	77	5.13%
2000	89	4.45%
5000	141	2.82%
10,000	200	2.00%
20,000	283	1.42%
50,000	447	0.89%

### Generated Model

The feature selection generated model is different from most other generated models in that it does not add predictors or other derived fields to the data stream. Instead, it acts as a filter, removing unwanted fields from the data stream based on generated model settings.

The set of fields filtered from the stream is controlled by one of the following criteria:

- Field importance categories (**Important**, **Marginal**, or **Unimportant**). Fields assigned to any of the selected categories are preserved; others are filtered.
- Top  $k$  fields. The  $k$  fields with the highest importance values are preserved; others are filtered.
- Importance value. Fields with importance value greater than the specified value are preserved; others are filtered.
- Manual selection. The user can select specific fields to be preserved or filtered.



# GENLIN Algorithms

Generalized linear models (GZLM) are commonly used analytical tools for different types of data. Generalized linear models cover not only widely used statistical models, such as linear regression for normally distributed responses, logistic models for binary data, and log linear model for count data, but also many useful statistical models via its very general model formulation.

## Generalized Linear Models

Generalized linear models were first introduced by Nelder and Wedderburn (1972) and later expanded by McCullagh and Nelder (1989). The following discussion is based on their works.

### Notation

The following notation is used throughout this section unless otherwise stated:

Table 18-1

Notation

Notation	Description
$n$	Number of complete cases in the dataset. It is an integer and $n \geq 1$ .
$p$	Number of parameters (including the intercept, if exists) in the model. It is an integer and $p \geq 1$ .
$p_x$	Number of non-redundant columns in the design matrix. It is an integer and $p_x \geq 1$ .
$\mathbf{y}$	$n \times 1$ dependent variable vector. The rows are the cases.
$\mathbf{r}$	$n \times 1$ vector of events for the binomial distribution; it usually represents the number of "successes." All elements are non-negative integers.
$\mathbf{m}$	$n \times 1$ vector of trials for the binomial distribution. All elements are positive integers and $m_i \geq r_i, i=1, \dots, n$ .
$\boldsymbol{\mu}$	$n \times 1$ vector of expectations of the dependent variable.
$\boldsymbol{\eta}$	$n \times 1$ vector of linear predictors.
$\mathbf{X}$	$n \times p$ design matrix. The rows represent the cases and the columns represent the parameters. The $i$ th row is $x_i = (x_{i1}, \dots, x_{ip})^T, i=1, \dots, n$ with $x_{i1} = 1$ if the model has an intercept.
$\mathbf{O}$	$n \times 1$ vector of scale offsets. This variable can't be the dependent variable ( $\mathbf{y}$ ) or one of the predictor variables ( $\mathbf{X}$ ).
$\boldsymbol{\beta}$	$p \times 1$ vector of unknown parameters. The first element in $\boldsymbol{\beta}$ is the intercept, if there is one.
$\boldsymbol{\omega}$	$n \times 1$ vector of scale weights. If an element is less than or equal to 0 or missing, the corresponding case is not used.
$\mathbf{f}$	$n \times 1$ vector of frequency counts. Non-integer elements are treated by rounding the value to the nearest integer. For values less than 0.5 or missing, the corresponding cases are not used.
$N$	Effective sample size. $N = \sum_{i=1}^n f_i$ . If frequency count variable $\mathbf{f}$ is not used, $N = n$ .

### Model

A GZLM of  $\mathbf{y}$  with predictor variables  $\mathbf{X}$  has the form

$$\eta = g(E(\mathbf{y})) = \mathbf{X}\beta + \mathbf{O}, \quad \mathbf{y} \sim F$$

where  $\boldsymbol{\eta}$  is the linear predictor;  $\mathbf{O}$  is an offset variable with a constant coefficient of 1 for each observation;  $g(\cdot)$  is the monotonic differentiable link function which states how the mean of  $\mathbf{y}$ ,  $E(\mathbf{y}) = \boldsymbol{\mu}$ , is related to the linear predictor  $\boldsymbol{\eta}$ ;  $F$  is the response probability distribution. Choosing different combinations of a proper probability distribution and a link function can result in different models.

In addition, GZLM also assumes  $y_i$  are independent for  $i=1, \dots, n$ . Then for each observation, the model becomes

$$\eta_i = g(\mu_i) = \mathbf{x}_i^T \boldsymbol{\beta} + o_i, \quad y_i \sim F$$

#### Notes

- $\mathbf{X}$  can be any combination of scale variables (covariates), categorical variables (factors), and interactions. The parameterization of  $\mathbf{X}$  is the same as in the GLM procedure. Due to use of the over-parameterized model where there is a separate parameter for every factor effect level occurring in the data, the columns of the design matrix  $\mathbf{X}$  are often dependent. Collinearity between scale variables in the data can also occur. To establish the dependencies in the design matrix, columns of  $\mathbf{X}^T \boldsymbol{\Psi} \mathbf{X}$ , where  $\boldsymbol{\Psi} = \text{diag}(f_1 \omega_1, \dots, f_n \omega_n)$ , are examined by using the sweep operator. When a column is found to be dependent on previous columns, the corresponding parameter is treated as redundant. The solution for redundant parameters is fixed at zero.
- When  $\mathbf{y}$  is a binary dependent variable which can be character or numeric, such as “male”/“female” or 1/2, its values will be transformed to 0 and 1 with 1 typically representing a success or some other positive result. In this document, we assume to be modeling the probability of success. In this document, we assume that  $\mathbf{y}$  has been transformed to 0/1 values and we always model the probability of success; that is,  $\text{Prob}(\mathbf{y} = 1)$ . Which original value should be transformed to 0 or 1 depends on what the reference category is. If the reference category is the last value, then the first category represents a success and we are modeling the probability of it. For example, if the reference category is the last value, “male” in “male”/“female” and 2 in 1/2 are the last values (since “male” comes later in the dictionary than “female”) and would be transformed to 0, and “female” and 1 would be transformed to 1 as we model the probability of them, respectively. However, one way to change to model the probability of “male” and 2 instead is to specify the reference category as the first value. Note if original binary format is 0/1 and the reference category is the last value, then 0 would be transformed to 1 and 1 to 0.
- When  $\mathbf{r}$ , representing the number of successes (or number of 1s) and  $\mathbf{m}$ , representing the number of trials, are used for the binomial distribution, the response is the binomial proportion  $\mathbf{y} = \mathbf{r}/\mathbf{m}$ .

### **Probability Distribution**

GZLMs are usually formulated within the framework of the exponential family of distributions. The probability density function of the response  $Y$  for the exponential family can be presented as

$$f(y) = \exp \left\{ \frac{y\theta - b(\theta)}{\phi/\omega} + c(y, \phi/\omega) \right\}$$

where  $\theta$  is the canonical (natural) parameter,  $\phi$  is the scale parameter related to the variance of  $y$  and  $\omega$  is a known prior weight which varies from case to case. Different forms of  $b(\theta)$  and  $c(y, \phi/\omega)$  will give specific distributions. In fact, the exponential family provides a notation that allows us to model both continuous and discrete (count, binary, and proportional) outcomes. Several are available including continuous ones: normal, inverse Gaussian, gamma; discrete ones: negative binomial, Poisson, binomial.

The mean and variance of  $y$  can be expressed as follows

$$E(y) = b'(\theta) = \mu$$

$$\text{Var}(y) = b''(\theta) \frac{\phi}{\omega} = V(\mu) \frac{\phi}{\omega}$$

where  $b'(\theta)$  and  $b''(\theta)$  denote the first and second derivatives of  $b$  with respect to  $\theta$ , respectively;  $V(\mu)$  is the variance function which is a function of  $\mu$ .

In GZLM, the distribution of  $y$  is parameterized in terms of the mean ( $\mu$ ) and a scale parameter ( $\phi$ ) instead of the canonical parameter ( $\theta$ ). The following table lists the distribution of  $y$ , corresponding range of  $y$ , variance function ( $V(\mu)$ ), the variance of  $y$  ( $\text{Var}(y)$ ), and the first derivative of the variance function ( $V'(\mu)$ ), which will be used later.

**Table 18-2**  
*Distribution, range and variance of the response, variance function, and its first derivative*

Distribution	Range of $y$	$V(\mu)$	$\text{Var}(y)$	$V'(\mu)$
Normal	$(-\infty, \infty)$	1	$\phi$	0
Inverse Gaussian	$(0, \infty)$	$\mu^3$	$\phi\mu^3$	$3\mu^2$
Gamma	$(0, \infty)$	$\mu^2$	$\phi\mu^2$	$2\mu$
Negative binomial	$0(1)\infty$	$\mu+k\mu^2$	$\mu+k\mu^2$	$1+2k\mu$
Poisson	$0(1)\infty$	$\mu$	$\mu$	1
Binomial( $m$ )	$0(1)m/m$	$\mu(1-\mu)$	$\mu(1-\mu)/m$	$1-2\mu$

#### Notes

- $0(1)z$  means the range is from 0 to  $z$  with increments of 1; that is, 0, 1, 2, ...,  $z$ .
- For the binomial distribution, the binomial trial variable  $m$  is considered as a part of the weight variable  $\omega$ .
- If a weight variable  $\omega$  is presented,  $\phi$  is replaced by  $\phi/\omega$ .
- For the negative binomial distribution, the ancillary parameter ( $k$ ) can be user-specified. When  $k = 0$ , the negative binomial distribution reduces to the Poisson distribution. When  $k = 1$ , the negative binomial is the geometric distribution.

**Scale parameter handling.** The expressions for  $V(\mu)$  and  $\text{Var}(y)$  for continuous distributions include the scale parameter  $\phi$  which can be used to scale the relationship of the variance and mean ( $\text{Var}(y)$  and  $\mu$ ). Since it is usually unknown, there are three ways to fit the scale parameter:

1. It can be estimated with  $\beta$  jointly by maximum likelihood method.
2. It can be set to a fixed positive value.
3. It can be specified by the deviance or Pearson chi-square. For more information, see the topic “Goodness-of-Fit Statistics ” on p. 178.

On the other hand, discrete distributions do not have this extra parameter (it is theoretically equal to one). Because of it, the variance of  $y$  might not be equal to the nominal variance in practice (especially for Poisson and binomial because the negative binomial has an ancillary parameter  $k$ ). A simple way to adjust this situation is to allow the variance of  $y$  for discrete distributions to have the scale parameter as well, but unlike continuous distributions, it can't be estimated by the ML method. So for discrete distributions, there are two ways to obtain the value of  $\phi$ :

1. It can be specified by the deviance or Pearson chi-square.
2. It can be set to a fixed positive value.

To ensure the data fit the range of response for the specified distribution, we follow the rules:

- For the gamma or inverse Gaussian distributions, values of  $y$  must be real and greater than zero. If a value of  $y$  is less than or equal to 0 or missing, the corresponding case is not used.
- For the negative binomial and Poisson distributions, values of  $y$  must be integer and non-negative. If a value of  $y$  is non-integer, less than 0 or missing, the corresponding case is not used.
- For the binomial distribution and if the response is in the form of a single variable,  $y$  must have only two distinct values. If  $y$  has more than two distinct values, the algorithm terminates in an error.
- For the binomial distribution and the response is in the form of ratio of two variables denoted events/trials, values of  $\mathbf{r}$  (the number of events) must be nonnegative integers, values of  $\mathbf{m}$  (the number of trials) must be positive integers and  $m_i \geq r_i, \forall i$ . If a value of  $\mathbf{r}$  is not integer, less than 0, or missing, the corresponding case is not used. If a value of  $\mathbf{m}$  is not integer, less than or equal to 0, less than the corresponding value of  $\mathbf{r}$ , or missing, the corresponding case is not used.

The ML method will be used to estimate  $\beta$  and possibly  $\phi$ . The kernels of the log-likelihood function ( $\ell_k$ ) and the full log-likelihood function ( $\ell$ ), which will be used as the objective function for parameter estimation, are listed for each distribution in the following table. Using  $\ell$  or  $\ell_k$  won't affect the parameter estimation, but the selection will affect the calculation of information criteria. For more information, see the topic “Goodness-of-Fit Statistics ” on p. 178.

Table 18-3  
The log-likelihood function for probability distribution

Distribution	$\ell_k$ and $\ell$
Normal	$\ell_k = \sum_{i=1}^n -\frac{f_i}{2} \left\{ \frac{\omega_i(y_i - \mu_i)^2}{\phi} + \ln \left( \frac{\phi}{\omega_i} \right) \right\}$ $\ell = \ell_k + \sum_{i=1}^n -\frac{f_i}{2} \{\ln(2\pi)\}$
Inverse Gaussian	$\ell_k = \sum_{i=1}^n -\frac{f_i}{2} \left\{ \frac{\omega_i(y_i - \mu_i)^2}{\phi y_i \mu_i^2} + \ln \left( \frac{\phi y_i^3}{\omega_i} \right) \right\}$ $\ell = \ell_k + \sum_{i=1}^n -\frac{f_i}{2} \{\ln(2\pi)\}$
Gamma	$\ell_k = \sum_{i=1}^n f_i \left\{ \frac{\omega_i}{\phi} \ln \left( \frac{\omega_i y_i}{\phi \mu_i} \right) - \frac{\omega_i y_i}{\phi \mu_i} - \ln \left( \Gamma \left( \frac{\omega_i}{\phi} \right) \right) \right\}$ $\ell = \ell_k + \sum_{i=1}^n f_i \{-\ln(y_i)\}$
Negative binomial	$\ell_k = \sum_{i=1}^n f_i \frac{\omega_i}{\phi} \{y_i \ln(k\mu_i) - (y_i + 1/k) \ln(1 + k\mu_i) + \ln(\Gamma(y_i + 1/k)) - \ln(\Gamma(1/k))\}$ $\ell = \ell_k + \sum_{i=1}^n f_i \frac{\omega_i}{\phi} \{-\ln(\Gamma(y_i + 1))\}$
Poisson	$\ell_k = \sum_{i=1}^n f_i \frac{\omega_i}{\phi} \{y_i \ln(\mu_i) - \mu_i\}$ $\ell = \ell_k + \sum_{i=1}^n f_i \frac{\omega_i}{\phi} \{-\ln(y_i!)\}$
Binomial( $m$ )	$\ell_k = \sum_{i=1}^n f_i \frac{\omega_i^*}{\phi} \{y_i \ln(\mu_i) + (1 - y_i) \ln(1 - \mu_i)\}$ $\ell = \ell_k + \sum_{i=1}^n f_i \frac{\omega_i}{\phi} \left\{ \ln \binom{m_i}{r_i} \right\}, \text{ where } \binom{m_i}{r_i} = \frac{m_i!}{r_i!(m_i - r_i)!}$

When an individual  $y = 0$  for the negative binomial or Poisson distributions and  $y = 0$  or 1 for the binomial distribution, a separate value of the log-likelihood is given. Let  $\ell_{k,i}$  be the log-likelihood value for individual case  $i$  when  $y_i = 0$  for the negative binomial and Poisson and 0/1 for the binomial. The full log-likelihood for  $i$  is equal to the kernel of the log-likelihood for  $i$ ; that is,  $\ell_i = \ell_{k,i}$ .

Table 18-4  
Log-likelihood

Distribution	$\ell_{k,i}$
Negative binomial	$\ell_{k,i} = -f_i \frac{\omega_i}{\phi} \frac{\ln(1+k\mu_i)}{k}$ if $y_i = 0$

Distribution	$\ell_{k,i}$
Poisson	$\ell_{k,i} = -f_i \frac{\omega_i}{\phi} \mu_i$ if $y_i = 0$
Binomial( $m$ )	$\ell_{k,i} = \begin{cases} f_i \frac{\omega_i}{\phi} \ln(1 - \mu_i) & \text{if } y_i = 0 \\ f_i \frac{\omega_i}{\phi} \ln(\mu_i) & \text{if } y_i = 1 \end{cases}$

- $\Gamma(z)$  is the gamma function and  $\ln(\Gamma(z))$  is the log-gamma function (the logarithm of the gamma function), evaluated at  $z$ .
- For the negative binomial distribution, the scale parameter is still included in  $\ell_k$  for flexibility, although it is usually set to 1.
- For the binomial distribution ( $\mathbf{r}/\mathbf{m}$ ), the scale weight variable becomes  $\omega_i^* = \omega_i m_i$  in  $\ell_k$ ; that is, the binomial trials variable  $\mathbf{m}$  is regarded as a part of the weight. However, the scale weight in the extra term of  $\ell$  is still  $\omega_i$ .

### Link Function

The following tables list the form, inverse form, range of  $\hat{\mu}$ , and first and second derivatives for each link function.

Table 18-5

Link function name, form, inverse of link function, and range of the predicted mean

Link function	$\eta=g(\mu)$	Inverse $\mu=g^{-1}(\eta)$	Range of $\hat{\mu}$
Identity	$\mu$	$\eta$	$\hat{\mu} \in R$
Log	$\ln(\mu)$	$\exp(\eta)$	$\hat{\mu} \geq 0$
Logit	$\ln\left(\frac{\mu}{1-\mu}\right)$	$\frac{\exp(\eta)}{1+\exp(\eta)}$	$\hat{\mu} \in [0, 1]$
Probit	$\Phi^{-1}(\mu)$ , where $\Phi(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\xi} e^{-z^2/2} dz$	$\Phi(\eta)$	$\hat{\mu} \in [0, 1]$
Complementary log-log	$\ln(-\ln(1-\mu))$	$1-\exp(-\exp(\eta))$	$\hat{\mu} \in [0, 1]$
Power( $\alpha$ ) $\begin{cases} \alpha \neq 0 \\ \alpha = 0 \end{cases}$	$\begin{cases} \mu^\alpha \\ \ln(\mu) \end{cases}$	$\begin{cases} \eta^{1/\alpha} \\ \exp(\eta) \end{cases}$	$\begin{cases} \hat{\mu} \in R \text{ if } \alpha \text{ or } 1/\alpha \text{ is odd integer} \\ \hat{\mu} \geq 0 \text{ otherwise} \end{cases}$
Log-complement	$\ln(1-\mu)$	$1-\exp(\eta)$	$\hat{\mu} \leq 1$
Negative log-log	$-\ln(-\ln(\mu))$	$\exp(-\exp(-\eta))$	$\hat{\mu} \in [0, 1]$
Negative binomial	$\ln\left(\frac{\mu}{\mu+\frac{1}{k}}\right)$	$\frac{\exp(\eta)}{k(1-\exp(\eta))}$	$\hat{\mu} \geq 0$
Odds power( $\alpha$ ) $\begin{cases} \alpha \neq 0 \\ \alpha = 0 \end{cases}$	$\begin{cases} \frac{(\mu/(1-\mu))^\alpha - 1}{\alpha} \\ \ln\left(\frac{\mu}{1-\mu}\right) \end{cases}$	$\begin{cases} \frac{(1+\alpha\eta)^{1/\alpha}}{1+(1+\alpha\eta)^{1/\alpha}} \\ \frac{\exp(\eta)}{1+\exp(\eta)} \end{cases}$	$\hat{\mu} \in [0, 1]$

Note: In the power link function, if  $|\alpha| < 2.2\text{e-}16$ ,  $\alpha$  is treated as 0.

Table 18-6

The first and second derivatives of link function

Link function	First derivative $g'(\mu) = \frac{\partial \eta}{\partial \mu} = \Delta$	Second derivative $g''(\mu) = \frac{\partial^2 \eta}{\partial \mu^2}$
Identity	1	0

Link function	First derivative $g'(\mu) = \frac{\partial \eta}{\partial \mu} = \Delta$	Second derivative $g''(\mu) = \frac{\partial^2 \eta}{\partial \mu^2}$
Log	$\frac{1}{\mu}$	$-\Delta^2$
Logit	$\frac{1}{\mu(1-\mu)}$	$\Delta^2(2\mu - 1)$
Probit	$\frac{1}{\phi(\Phi^{-1}(\mu))}$ , where $\phi(z) = \frac{1}{\sqrt{2\pi}} e^{-z^2/2}$	$\Delta^2 \Phi^{-1}(\mu)$
Complementary log-log	$\frac{1}{(\mu-1) \ln(1-\mu)}$	$-\Delta^2(1 + \ln(1-\mu))$
Power( $\alpha$ ) $\begin{cases} \alpha \neq 0 \\ \alpha = 0 \end{cases}$	$\begin{cases} \alpha \mu^{\alpha-1} \\ \frac{1}{\mu} \end{cases}$	$\begin{cases} \Delta \frac{\alpha-1}{\mu} \\ -\Delta^2 \end{cases}$
Log-complement	$\frac{-1}{1-\mu}$	$-\Delta^2$
Negative log-log	$\frac{-1}{\mu \ln(\mu)}$	$\Delta^2(1 + \ln(\mu))$
Negative binomial	$\frac{1}{\mu+k\mu^2}$	$-\Delta^2(1 + 2k\mu)$
Odds power( $\alpha$ ) $\begin{cases} \alpha \neq 0 \\ \alpha = 0 \end{cases}$	$\begin{cases} \frac{\mu^{\alpha-1}}{(1-\mu)^{\alpha+1}} \\ \frac{1}{\mu(1-\mu)} \end{cases}$	$\begin{cases} \Delta \left( \frac{\alpha-1}{\mu} + \frac{\alpha+1}{1-\mu} \right) \\ \Delta^2(2\mu - 1) \end{cases}$

When the canonical parameter is equal to the linear predictor,  $\theta = \eta$ , then the link function is called the **canonical link function**. Although the canonical links lead to desirable statistical properties of the model, particularly in small samples, there is in general no a priori reason why the systematic effects in a model should be additive on the scale given by that link. The canonical link functions for probability distributions are given in the following table.

Table 18-7  
Canonical and default link functions for probability distributions

Distribution	Canonical link function
Normal	Identity
Inverse Gaussian	Power(-2)
Gamma	Power(-1)
Negative binomial	Negative binomial
Poisson	Log
Binomial	Logit

## Estimation

Having selected a particular model, it is required to estimate the parameters and to assess the precision of the estimates.

### Parameter estimation

The parameters are estimated by maximizing the log-likelihood function (or the kernel of the log-likelihood function) from the observed data. Let  $\mathbf{s}$  be the first derivative (gradient) vector of the log-likelihood with respect to each parameter, then we wish to solve

$$\mathbf{s} = \left[ \frac{\partial \ell}{\partial \beta} \right]_{p \times 1} = 0$$

In general, there is no closed form solution except for a normal distribution with identity link function, so estimates are obtained numerically via an iterative process. A Newton-Raphson and/or Fisher scoring algorithm is used and it is based on a linear Taylor series approximation of the first derivative of the log-likelihood.

#### First Derivatives

If the scale parameter  $\phi$  is not estimated by the ML method,  $\mathbf{s}$  is a  $p \times 1$  vector with the form:

$$\mathbf{s} = \sum_{i=1}^n \frac{f_i \omega_i (y_i - \mu_i)}{\phi V(\mu_i) g'(\mu_i)} \cdot x_i = \frac{1}{\phi} \sum_{i=1}^n \frac{f_i \omega_i (y_i - \mu_i)}{V(\mu_i) g'(\mu_i)} \cdot x_i$$

where  $\mu_i$ ,  $V(\mu_i)$  and  $g'(\mu_i)$  are defined in Table 18-5“Link function name, form, inverse of link function, and range of the predicted mean” on p. 168, Table 18-2“Distribution, range and variance of the response, variance function, and its first derivative” on p. 165 and Table 18-6“the first and second derivatives of link function” on p. 168, respectively.

If the scale parameter  $\phi$  is estimated by the ML method, it is handled by searching for  $\ln(\phi)$  since  $\phi$  is required to be greater than zero.

Let  $\tau = \ln(\phi)$  so  $\phi = \exp(\tau)$ , then  $\mathbf{s}$  is a  $(p+1) \times 1$  vector with the following form

$$\mathbf{s} = \left[ \begin{array}{c} \frac{\partial \ell}{\partial \beta} \\ \frac{\partial \ell}{\partial \tau} \end{array} \right]_{(p+1) \times 1} = \left[ \begin{array}{c} \frac{1}{\exp(\tau)} \sum_{i=1}^n \frac{f_i \omega_i (y_i - \mu_i)}{V(\mu_i) g'(\mu_i)} \cdot x_i \\ \frac{\partial \ell}{\partial \tau} \end{array} \right]$$

where  $\partial \ell / \partial \beta$  is the same as the above with  $\phi$  is replaced with  $\exp(\tau)$ ,  $\partial \ell / \partial \tau$  has a different form depending on the distribution as follows:

**Table 18-8**

*The 1st derivative functions w.r.t. the scale parameter for probability distributions*

Distribution	$\frac{\partial \ell}{\partial \tau}$
Normal	$\sum_{i=1}^n \frac{f_i}{2} \left\{ \frac{\omega_i (y_i - \mu_i)^2}{\exp(\tau)} - 1 \right\}$
Inverse Gaussian	$\sum_{i=1}^n \frac{f_i}{2} \left\{ \frac{\omega_i (y_i - \mu_i)^2}{\exp(\tau) y_i \mu_i^2} - 1 \right\}$
Gamma	$\sum_{i=1}^n -\frac{f_i \omega_i}{\exp(\tau)} \left\{ \ln \left( \frac{\omega_i y_i}{\exp(\tau) \mu_i} \right) + \left( 1 - \frac{y_i}{\mu_i} \right) - \psi \left( \frac{\omega_i}{\exp(\tau)} \right) \right\}$

*Note:*  $\psi(z)$  is a digamma function, which is the derivative of logarithm of a gamma function, evaluated at  $z$ ; that is,  $\psi(z) = \frac{\partial \ln(\Gamma(z))}{\partial z} = \frac{\Gamma'(z)}{\Gamma(z)}$ .

As mentioned above, for normal distribution with identity link function which is a classical linear regression model, there is a closed form solution for both  $\beta$  and  $\tau$ , so no iterative process is needed. The solution for  $\beta$ , after applying the SWEEP operation in GLM procedure, is

$$\hat{\beta} = \left( \sum_{i=1}^n f_i \omega_i \mathbf{x}_i^T \mathbf{x}_i \right)^{-1} \left( \sum_{i=1}^n f_i \omega_i \mathbf{x}_i^T (y_i - o_i) \right) = \left( \mathbf{X}^T \Psi \mathbf{X} \right)^{-1} \left( \mathbf{X}^T \Psi (\mathbf{y} - \mathbf{o}) \right),$$

where  $\Psi = \text{diag}(f_1 \omega_1, \dots, f_n \omega_n)$  and  $(\mathbf{Z})^{-}$  is the generalized inverse of a matrix  $\mathbf{Z}$ . If the scale parameter  $\phi$  is also estimated by the ML method, the estimate of  $\tau$  is

$$\hat{\tau} = \ln(\hat{\phi}) = \ln \left( \frac{1}{N} \sum_{i=1}^n f_i \omega_i (y_i - \mathbf{x}_i^T \hat{\beta} - o_i)^2 \right).$$

### Second Derivatives

Let  $\mathbf{H}$  be the second derivative (Hessian) matrix. If the scale parameter is not estimated by the ML method,  $\mathbf{H}$  is a  $p \times p$  matrix with the following form

$$\mathbf{H} = \left[ \frac{\partial^2 \ell}{\partial \beta \partial \beta^T} \right]_{p \times p} = -\mathbf{X}^T \mathbf{W} \mathbf{X}$$

where  $\mathbf{W}$  is an  $n \times n$  diagonal matrix. There are two definitions for  $\mathbf{W}$  depending on which algorithm is used:  $\mathbf{W}_e$  for Fisher scoring and  $\mathbf{W}_o$  for Newton-Raphson. The  $i$ th diagonal element for  $\mathbf{W}_e$  is

$$w_{e,i} = \frac{f_i \omega_i}{\phi} \cdot \frac{1}{V(\mu_i) (g'(\mu_i))^2},$$

and the  $i$ th diagonal element for  $\mathbf{W}_o$  is

$$w_{o,i} = w_{e,i} + \frac{f_i \omega_i}{\phi} (y_i - \mu_i) \cdot \frac{V(\mu_i) g''(\mu_i) + V'(\mu_i) g'(\mu_i)}{(V(\mu_i))^2 (g'(\mu_i))^3},$$

where  $V'(\mu_i)$  and  $g''(\mu_i)$  are defined in Table 18-2 "Distribution, range and variance of the response, variance function, and its first derivative" on p. 165 and Table 18-6 "The first and second derivatives of link function" on p. 168, respectively. Note the expected value of  $\mathbf{W}_o$  is  $\mathbf{W}_e$  and when the canonical link is used for the specified distribution, then  $\mathbf{W}_o = \mathbf{W}_e$ .

If the scale parameter is estimated by the ML method,  $\mathbf{H}$  becomes a  $(p+1) \times (p+1)$  matrix with the form

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 \ell}{\partial \beta \partial \beta^T} & \frac{\partial^2 \ell}{\partial \beta \partial \tau} \\ \frac{\partial^2 \ell}{\partial \tau \partial \beta^T} & \frac{\partial^2 \ell}{\partial \tau^2} \end{bmatrix}_{(p+1) \times (p+1)}$$

where  $\partial^2 \ell / \partial \beta \partial \tau$  is a  $p \times 1$  vector and  $\partial^2 \ell / \partial \tau \partial \beta^T$  is a  $1 \times p$  vector and the transpose of  $\partial^2 \ell / \partial \beta \partial \tau$ . For all three continuous distributions:

$$\frac{\partial^2 \ell}{\partial \beta \partial \tau} = \sum_{i=1}^n -\frac{f_i \omega_i (y_i - \mu_i)}{\exp(\tau) V(\mu_i) g'(\mu_i)} \cdot \mathbf{x}_i = -\frac{\partial \ell}{\partial \beta}.$$

The forms of  $\partial^2 \ell / \partial \tau^2$  are listed in the following table.

**Table 18-9**

*The second derivative functions w.r.t. the scale parameter for probability distributions*

Distribution	$\frac{\partial^2 \ell}{\partial \tau^2}$
Normal	$\sum_{i=1}^n -\frac{f_i \omega_i}{2 \exp(\tau)} (y_i - \mu_i)^2$
Inverse Gaussian	$\sum_{i=1}^n -\frac{f_i \omega_i}{2 \exp(\tau) y_i \mu_i^2} (y_i - \mu_i)^2$
Gamma	$\sum_{i=1}^n \frac{f_i \omega_i}{\exp(\tau)} \left\{ \ln \left( \frac{\omega_i y_i}{\exp(\tau) \mu_i} \right) + \left( 2 - \frac{y_i}{\mu_i} \right) - \psi \left( \frac{\omega_i}{\exp(\tau)} \right) - \frac{\omega_i}{\exp(\tau)} \psi' \left( \frac{\omega_i}{\exp(\tau)} \right) \right\}$

*Note:*  $\psi'(z)$  is a trigamma function, which is the derivative of  $\psi(z)$ , evaluated at  $z$ .

### Iterations

An iterative process to find the solution for  $\beta$  (which might include  $\phi$ ) is based on Newton-Raphson (for all iterations), Fisher scoring (for all iterations) or a hybrid method. The hybrid method consists of applying Fisher scoring steps for a specified number of iterations before switching to Newton-Raphson steps. Newton-Raphson performs well if the initial values are close to the solution, but the hybrid method can be used to improve the algorithm's robustness from bad initial values. Apart from improved robustness, Fisher scoring is faster due to the simpler form of the Hessian matrix.

The following notation applies to the iterative process:

**Table 18-10**

*Notation*

Notation	Description
$I$	Starting iteration for checking complete separation and quasi-complete separation. It must be 0 or a positive integer. This criterion is not used if the value is 0.
$J$	The maximum number of steps in step-halving method. It must be a positive integer.
$K$	The first number of iterations using Fisher scoring, then switching to Newton-Raphson. It must be 0 or a positive integer. A value of 0 means using Newton-Raphson for all iterations and a value greater or equal to $M$ means using Fisher scoring for all iterations.
$M$	The maximum number of iterations. It must be a non-negative integer. If the value is 0, then initial parameter values become final estimates.
$\epsilon_\ell, \epsilon_p, \epsilon_H$	Tolerance levels for three types of convergence criteria.
$Abs$	A 0/1 binary variable; $Abs = 1$ if absolute change is used for convergence criteria and $Abs = 0$ if relative change is used.

And the iterative process is outlined as follows:

1. Input values for  $I, J, K, M, \epsilon_\ell, \epsilon_p, \epsilon_H$  and  $Abs$  for each type of three convergence criteria.
2. For  $\beta^{(0)}$  compute initial values (see below), then calculate log-likelihood  $\ell^{(0)}$ , gradient vector  $\mathbf{s}^{(0)}$  and Hessian matrix  $\mathbf{H}^{(0)}$  based on  $\beta^{(0)}$ .
3. Let  $\xi=1$ .
4. Compute estimates of  $i$ th iteration:  

$$\beta^{(i)} = \beta^{(i-1)} - \xi \left( \mathbf{H}^{(i-1)} \right)^- \mathbf{s}^{(i-1)},$$
 where  $(\mathbf{H})^-$  is a generalized inverse of  $\mathbf{H}$ . Then compute the log-likelihood based on  $\beta^{(i)}$ .
5. Use step-halving method if  $\ell^{(i)} < \ell^{(i-1)}$ : reduce  $\xi$  by half and repeat step (4). The set of values of  $\xi$  is  $\{0.5^j : j = 0, \dots, J-1\}$ . If  $J$  is reached but the log-likelihood is not improved, issue a warning message, then stop.
6. Compute gradient vector  $\mathbf{s}^{(i)}$  and Hessian matrix  $\mathbf{H}^{(i)}$  based on  $\beta^{(i)}$ . Note that  $\mathbf{W}_e$  is used to calculate  $\mathbf{H}^{(i)}$  if  $i \leq K$ ;  $\mathbf{W}_o$  is used to calculate  $\mathbf{H}^{(i)}$  if  $i > K$ .
7. Check if complete or quasi-complete separation of the data is established (see below) if distribution is binomial and the current iteration  $i \geq I$ . If either complete or quasi-complete separation is detected, issue a warning message, then stop.
8. Check if all three convergence criteria (see below) are met. If they are not but  $M$  is reached, issue a warning message, then stop.
9. If all three convergence criteria are met, check if complete or quasi-complete separation of the data is established if distribution is binomial and  $i < I$  (because checking for complete or quasi-complete separation has not started yet). If complete or quasi-complete separation is detected, issue a warning message, then stop, otherwise, stop (the process converges for binomial successfully). If all three convergence criteria are met for the distributions other than binomial, stop (the process converges for other distributions successfully). The final vector of estimates is denoted by  $\hat{\beta}$  (and  $\hat{\tau}$ ). Otherwise, go back to step (3).

#### Initial Values

Initial values are calculated as follows:

1. Set the initial fitted values  $\tilde{\mu}_i = (y_i m_i + 0.5)/(m_i + 1)$  for a binomial distribution ( $y_i$  can be a proportion or 0/1 value) and  $\tilde{\mu}_i = y_i$  for a non-binomial distribution. From these derive  $\tilde{\eta}_i = g(\tilde{\mu}_i), g'(\tilde{\mu}_i)$  and  $V(\tilde{\mu}_i)$ . If  $\tilde{\eta}_i$  becomes undefined, set  $\tilde{\eta}_i = 1$ .
2. Calculate the weight matrix  $\tilde{W}_e$  with the diagonal element  $\tilde{w}_{ei} = \frac{f_i \omega_i}{\phi} \cdot \frac{1}{V(\tilde{\mu}_i) (g'(\tilde{\mu}_i))^2}$ , where  $\phi$  is set to 1 or a fixed positive value. If the denominator of  $\tilde{w}_{ei}$  becomes 0, set  $\tilde{w}_{ei} = 0$ .
3. Assign the adjusted dependent variable  $z$  with the  $i$ th observation  $z_i = (\tilde{\eta}_i - o_i) + (y_i - \tilde{\mu}_i) g'(\tilde{\mu}_i)$  for a binomial distribution and  $z_i = (\tilde{\eta}_i - o_i)$  for a non-binomial distribution.

4. Calculate the initial parameter values

$$\beta^{(0)} = \left( \mathbf{X}^T \tilde{W}_e \mathbf{X} \right)^{-1} \mathbf{X}^T \tilde{W}_e \mathbf{z}$$

and

$$\phi^{(0)} = \left( \mathbf{z} - \mathbf{X}\beta^{(0)} \right)^T \tilde{W}_e \left( \mathbf{z} - \mathbf{X}\beta^{(0)} \right).$$

if the scale parameter is estimated by the ML method.

#### Scale Parameter Handling

1. For normal, inverse Gaussian, and gamma response, if the scale parameter is estimated by the ML method, then it will be estimated jointly with the regression parameters; that is, the last element of the gradient vector  $\mathbf{s}$  is with respect to  $\tau$ .
2. If the scale parameter is set to be a fixed positive value, then it will be held fixed at that value for in each iteration of the above process.
3. If the scale parameter is specified by the deviance or Pearson chi-square divided by degrees of freedom, then it will be fixed at 1 to obtain the regression estimates through the whole iterative process. Based on the regression estimates, calculate the deviance and Pearson chi-square values and obtain the scale parameter estimate.

#### Checking for Separation

For each iteration after the user-specified number of iterations; that is, if  $i > I$ , calculate (note here  $v$  refers to cases in the dataset)

$$p_{\min} = \min_v p_v$$

$$p_{\max} = \max_v p_v,$$

$$p_{\min}^* = \min_v \left( \min(\mu_v, 1 - \mu_v) \right),$$

where

$$p_v = \begin{cases} \mu_v & \text{if } y_v = \text{success } (= 1) \\ 1 - \mu_v & \text{if } y_v = \text{failure } (= 0) \end{cases}$$

( $p_v$  is the probability of the observed response for case  $v$ ) and  $\mu_v = g^{-1} \left( \mathbf{x}_v^T \beta + o_v \right)$ .

If  $\min(p_{\min}, p_{\max}) = p_{\min} > 0.99$  we consider there to be complete separation. Otherwise, if  $p_{\max} > 0.99$  or  $p_{\min}^* < 0.001$  and if there are very small diagonal elements (absolute value  $< \sqrt{10^{-7}} \approx 3.16 \times 10^{-4}$ ) in the non-redundant parameter locations in the lower triangular matrix in Cholesky decomposition of  $-\mathbf{H}$ , where  $\mathbf{H}$  is the Hessian matrix, then there is a quasi-complete separation.

### Convergence Criteria

The following convergence criteria are considered:

$$\text{Log-likelihood convergence: } \begin{cases} \frac{|\ell^{(i)} - \ell^{(i-1)}|}{|\ell^{(i-1)}| + 10^{-6}} < \epsilon_\ell \text{ if relative change} \\ |\ell^{(i)} - \ell^{(i-1)}| < \epsilon_\ell \text{ if absolute change} \end{cases}$$

$$\text{Parameter convergence: } \begin{cases} \max_j \left( \frac{|\beta_j^{(i)} - \beta_j^{(i-1)}|}{|\beta_j^{(i-1)}| + 10^{-6}} \right) < \epsilon_p \text{ if relative change} \\ \max_j (|\beta_j^{(i)} - \beta_j^{(i-1)}|) < \epsilon_p \text{ if absolute change} \end{cases}$$

$$\text{Hessian convergence: } \begin{cases} \frac{(\mathbf{s}^{(i)})^T (\mathbf{H}^{(i)})^{-1} (\mathbf{s}^{(i)})}{|\ell^{(v)}| + 10^{-6}} < \epsilon_H \text{ if relative change} \\ (\mathbf{s}^{(i)})^T (\mathbf{H}^{(i)})^{-1} (\mathbf{s}^{(i)}) < \epsilon_H \text{ if absolute change} \end{cases}$$

where  $\epsilon_\ell$ ,  $\epsilon_p$  and  $\epsilon_H$  are the given tolerance levels for each type.

If the Hessian convergence criterion is not user-specified, it is checked based on absolute change with  $\epsilon_H = 1\text{E-}4$  after the log-likelihood or parameter convergence criterion has been satisfied. If Hessian convergence is not met, a warning is displayed.

### **Parameter Estimate Covariance Matrix, Correlation Matrix and Standard Errors**

The parameter estimate covariance matrix, correlation matrix and standard errors can be obtained easily with parameter estimates. Whether or not the scale parameter is estimated by ML, parameter estimate covariance and correlation matrices are listed for  $\hat{\beta}$  only because the covariance between  $\hat{\beta}$  and  $\hat{\tau}$  should be zero.

#### Model-Based Parameter Estimate Covariance

The model-based parameter estimate covariance matrix is given by

$$\Sigma_m = -\mathbf{H}^- = -(-\mathbf{X}\mathbf{W}\mathbf{X})^-$$

where  $\mathbf{H}^-$  is the generalized inverse of the Hessian matrix evaluated at the parameter estimates. The corresponding rows and columns for redundant parameter estimates should be set to zero.

#### Robust Parameter Estimate Covariance

The validity of the parameter estimate covariance matrix based on the Hessian depends on the correct specification of the variance function of the response in addition to the correct specification of the mean regression function of the response. The robust parameter estimate covariance provides a consistent estimate even when the specification of the variance function of the response is incorrect. The robust estimator is also called Huber's estimator because Huber (1967) was

the first to describe this variance estimate; White's estimator or HCCM (heteroskedasticity consistent covariance matrix) estimator because White (1980) independently showed that this variance estimate is consistent under a linear regression model including heteroskedasticity; or the sandwich estimator because it includes three terms. The robust (or Huber/White/sandwich) estimator is defined as follows

$$\Sigma_{\mathbf{r}} = \Sigma_{\mathbf{m}} \left( \sum_{i=1}^n \begin{bmatrix} \frac{\partial \ell_i}{\partial \beta} \\ \frac{\partial \ell_i}{\partial \beta} \end{bmatrix} \begin{bmatrix} \frac{\partial \ell_i}{\partial \beta} \\ \frac{\partial \ell_i}{\partial \beta} \end{bmatrix}^{\mathbf{T}} \right) \Sigma_{\mathbf{m}} = \Sigma_{\mathbf{m}} \left( \sum_{i=1}^n f_i \left( \frac{\omega_i (y_i - \mu_i)}{\phi V(\mu_i) g'(\mu_i)} \right)^2 \cdot x_i \cdot x_i^{\mathbf{T}} \right) \Sigma_{\mathbf{m}}$$

#### Parameter Estimate Correlation

The correlation matrix is calculated from the covariance matrix as usual. Let  $\sigma_{ij}$  be an element of  $\Sigma_{\mathbf{m}}$  or  $\Sigma_{\mathbf{r}}$ , then the corresponding element of the correlation matrix is  $\frac{\sigma_{ij}}{\sqrt{\sigma_{ii}}\sqrt{\sigma_{jj}}}$ . The corresponding rows and columns for redundant parameter estimates should be set to system missing values.

#### Parameter Estimate Standard Error

Let  $\hat{\beta}_i$  denote a non-redundant parameter estimate. Its standard error is the square root of the  $i$ th diagonal element of  $\Sigma_{\mathbf{m}}$  or  $\Sigma_{\mathbf{r}}$ :

$$\hat{\sigma}_{\beta_i} = \sqrt{\sigma_{ii}}$$

The standard error for redundant parameter estimates is set to a system missing value. If the scale parameter is estimated by the ML method, we obtain  $\hat{\tau}$  and its standard error estimate  $\hat{\sigma}_{\tau} = \sqrt{-\frac{1}{\frac{\partial^2 \ell}{\partial \tau^2}}}$ , where  $\frac{\partial^2 \ell}{\partial \tau^2}$  can be found in Table 18-9 "The second derivative functions w.r.t. the scale parameter for probability distributions" on p. 172. Then the estimate of the scale parameter is  $\exp(\hat{\tau})$  and the standard error estimate is  $(\exp(\hat{\tau}) \cdot \hat{\sigma}_{\tau})$

### **Wald Confidence Intervals**

Wald confidence intervals are based on the asymptotic normal distribution of the parameter estimates. The  $100(1 - \alpha)\%$  Wald confidence interval for  $\beta_j$  is given by

$$\left( \hat{\beta}_j - z_{1-\alpha/2} \hat{\sigma}_{\beta_j}, \hat{\beta}_j + z_{1-\alpha/2} \hat{\sigma}_{\beta_j} \right),$$

where  $z_p$  is the 100 $p$ th percentile of the standard normal distribution.

If exponentiated parameter estimates are requested for logistic regression or log-linear models, then using the delta method, the estimate of  $\exp(\beta_j)$  is  $\exp(\hat{\beta}_j)$ , the standard error estimate of  $\exp(\hat{\beta}_j)$  is  $(\exp(\hat{\beta}_j) \cdot \hat{\sigma}_{\beta_j})$  and the corresponding  $100(1 - \alpha)\%$  Wald confidence interval for  $\exp(\beta_j)$  is

$$\left( \exp\left(\hat{\beta}_j - z_{1-\alpha/2} \hat{\sigma}_{\beta_j}\right), \exp\left(\hat{\beta}_j + z_{1-\alpha/2} \hat{\sigma}_{\beta_j}\right) \right).$$

Wald confidence intervals for redundant parameter estimates are set to system missing values.

Similarly, the  $100(1 - \alpha)\%$  Wald confidence interval for  $\phi$  is

$$\left( \exp(\hat{\tau} - z_{1-\alpha/2} \hat{\sigma}_{\tau}), \exp(\hat{\tau} + z_{1-\alpha/2} \hat{\sigma}_{\tau}) \right)$$

### **Chi-Square Statistics**

The hypothesis  $H_{0i} : \beta_i = 0$  is tested for each non-redundant parameter using the chi-square statistic:

$$c_i = \left( \frac{\hat{\beta}_i}{\hat{\sigma}_{\beta_i}} \right)^2$$

which has an asymptotic chi-square distribution with 1 degree of freedom.

Chi-square statistics and their corresponding  $p$ -values are set to system missing values for redundant parameter estimates.

The chi-square statistic is not calculated for the scale parameter, even if it is estimated by ML method.

### **P Values**

Given a test statistic  $T$  and a corresponding cumulative distribution function  $G$  as specified above, the  $p$ -value is defined as  $p = 1 - G(T)$ . For example, the  $p$ -value for the chi-square test of  $H_{0i} : \beta_i = 0$  is  $p_i = 1 - \text{prob}(\chi_1^2 \leq c_i)$ .

## **Model Testing**

After estimating parameters and calculating relevant statistics, several tests for the given model are performed.

### **Lagrange Multiplier Test**

If the scale parameter for normal, inverse Gaussian and gamma distributions is set to a fixed value or specified by the deviance or Pearson chi-square divided by the degrees of freedom (when the scale parameter is specified by the deviance or Pearson chi-square divided by the degrees of freedom, it can be considered as a fixed value), or an ancillary parameter  $k$  for the negative binomial is set to a fixed value other than 0, the Lagrange Multiplier (LM) test assesses the validity of the value. For a fixed  $\phi$  or  $k$ , the test statistic is defined as

$$T_{LM} = \frac{s^2}{A}$$

where  $s = \partial \ell / \partial \tau$  and  $A = -\left(\frac{\partial^2 \ell}{\partial \tau^2}\right) - \left(-\frac{\partial^2 \ell}{\partial \tau \partial \beta \mathbf{T}}\right) \left(-\frac{\partial^2 \ell}{\partial \beta \partial \beta \mathbf{T}}\right)^{-1} \left(-\frac{\partial^2 \ell}{\partial \beta \partial \tau}\right)$  evaluated at the parameter estimates and fixed  $\phi$  or  $k$  value.  $T_{LM}$  has an asymptotic chi-square distribution with 1 degree of freedom, and the  $p$ -values are calculated accordingly.

For testing  $\phi$ , see Table 18-8 “The 1st derivative functions w.r.t. the scale parameter for probability distributions” on p. 170 and see Table 18-9 “The second derivative functions w.r.t. the scale parameter for probability distributions” on p. 172 for the elements of  $s$  and  $A$ , respectively.

If  $k$  is set to 0, then the above statistic can't be applied. According to Cameron and Trivedi (1998), the LM test statistic should now be based on the following auxiliary OLS regression (without constant)

$$\frac{(y_i - \hat{\mu}_i)^2 - y_i}{\hat{\mu}_i} = \alpha \hat{\mu}_i + \epsilon_i$$

where  $\hat{\mu}_i = g^{-1}(x_i^T \hat{\beta})$  and  $\epsilon_i$  is an error term. Let the response of the above OLS regression  $\left[\frac{(y_i - \hat{\mu}_i)^2 - y_i}{\hat{\mu}_i}\right]$  be  $z_i$  and the explanatory variable  $\hat{\mu}_i$  be  $w_i$ . The estimate of the above regression parameter  $\alpha$  and the standard error of the estimate of  $\alpha$  are

$$\hat{\alpha} = \frac{\sum_{i=1}^n f_i w_i z_i}{\sum_{i=1}^n f_i w_i^2} \quad \text{and} \quad \hat{\sigma}_\alpha = \sqrt{\frac{s_e^2}{\sum_{i=1}^n f_i w_i^2}},$$

where  $s_e^2 = \frac{1}{N-1} \sum_{i=1}^n f_i e_i^2$  and  $e_i = z_i - \hat{\alpha} w_i$ . Then the LM test statistic is a  $z$  statistic

$$z = \frac{\hat{\alpha}}{\hat{\sigma}_\alpha},$$

and it has an asymptotic standard normal distribution under the null hypothesis of equidispersion in a Poisson model ( $H_0 : k = 0$ ). Three  $p$ -values are provided. The alternative hypothesis can be one-sided overdispersion ( $H_a : k > 0$ ), underdispersion ( $H_a : k < 0$ ) or two-sided non-directional ( $H_a : k \neq 0$ ) with the variance function of  $V(\mu) = \mu + k\mu^2$ . The calculation of  $p$ -values depends on the alternative. For  $H_a : k > 0$ ,  $p$ -value =  $1 - \Phi(z)$ , where  $\Phi(\cdot)$  is the cumulative probability of a standard normal distribution; for  $H_a : k < 0$ ,  $p$ -value =  $\Phi(z)$ ; and for  $H_a : k \neq 0$ ,  $p$ -value =  $2(1 - \Phi(|z|))$ .

### Goodness-of-Fit Statistics

Several statistics are calculated to assess goodness of fit of a given generalized linear model.

#### Deviance

The theoretical definition of deviance is:

$$D = 2\phi(\ell(\mathbf{y}; \mathbf{y}) - \ell(\hat{\mu}; \mathbf{y})),$$

where  $\ell(\hat{\mu}; \mathbf{y})$  is the log-likelihood function expressed as the function of the predicted mean values  $\hat{\mu}$  (calculated based on the parameter estimates) given the response variable, and  $\ell(\mathbf{y}; \mathbf{y})$  is the log-likelihood function computed by replacing  $\hat{\mu}$  with  $\mathbf{y}$ . The formula used for the deviance is  $\sum_{i=1}^n f_i d_i$ , where the form of  $d_i$  for the distributions are given in the following table:

Table 18-11  
Deviance for individual case

Distribution	$d_i$
Normal	$\omega_i (y_i - \mu_i)^2$
Inverse Gaussian	$\frac{\omega_i}{y_i \mu_i^2} (y_i - \mu_i)^2$
Gamma	$2\omega_i \left\{ -\ln \left( \frac{y_i}{\mu_i} \right) + \frac{y_i - \mu_i}{\mu_i} \right\}$
Negative Binomial	$2\omega_i \left\{ y_i \ln \left( \frac{y_i}{\mu_i} \right) - (y_i + 1/k) \ln \left( \frac{y_i + 1/k}{\mu_i + 1/k} \right) \right\}$
Poisson	$2\omega_i \left\{ y_i \ln \left( \frac{y_i}{\mu_i} \right) - (y_i - \mu_i) \right\}$
Binomial( $m$ )	$2\omega_i^* \left\{ y_i \ln \left( \frac{y_i}{\mu_i} \right) + (1 - y_i) \ln \left( \frac{1 - y_i}{1 - \mu_i} \right) \right\}$

Note

- When  $\mathbf{y}$  is a binary dependent variable with 0/1 values (binomial distribution), the deviance and Pearson chi-square are calculated based on the subpopulations; see below.
- When  $y = 0$  for negative binomial and Poisson distributions and  $y = 0$  (for  $r = 0$ ) or 1 (for  $r = m$ ) for binomial distribution with  $\mathbf{r}/\mathbf{m}$  format, separate values are given for the deviance. Let  $d_i$  be the deviance value for individual case  $i$  when  $y_i = 0$  for negative binomial and Poisson and 0/1 for binomial.

Table 18-12  
Deviance for individual case

Distribution	$d_i$
Negative Binomial	$2\omega_i \frac{\ln(1+k\mu_i)}{k}$ if $y_i = 0$
Poisson	$2\omega_i \mu_i$ if $y_i = 0$
Binomial( $m$ )	$\begin{cases} -2\omega_i^* \ln(1 - \mu_i) & \text{if } y_i = 0 \text{ or } r_i = 0 \\ -2\omega_i^* \ln(\mu_i) & \text{if } y_i = 1 \text{ or } r_i = m_i \end{cases}$

Pearson Chi-Square

$$\chi^2 = \sum_{i=1}^n f_i \gamma_i$$

where  $\gamma_i = \frac{\omega_i^* (y_i - \mu_i)^2}{V(\mu_i)}$  for the binomial distribution and  $\gamma_i = \frac{\omega_i (y_i - \mu_i)^2}{V(\mu_i)}$  for other distributions.

Scaled Deviance and Scaled Pearson Chi-Square

The scaled deviance is  $D^* = D/\phi$  and the scaled Pearson chi-square is  $\chi^{2*} = \chi^2/\phi$ .

Since the scaled deviance and Pearson chi-square statistics have a limiting chi-square distribution with  $N - p_x$  degrees of freedom, the deviance or Pearson chi-square divided by its degrees of freedom can be used as an estimate of the scale parameter for both continuous and discrete distributions.

$$\hat{\phi} = \frac{D}{N - p_x} \text{ or } \hat{\phi} = \frac{\chi^2}{N - p_x}.$$

If the scale parameter is measured by the deviance or Pearson chi-square, first we assume  $\phi = 1$ , then estimate the regression parameters, calculate the deviance and Pearson chi-square values and obtain the scale parameter estimate from the above formula. Then the scaled version of both statistics is obtained by dividing the deviance and Pearson chi-square by  $\hat{\phi}$ . In the meantime, some statistics need to be revised. The gradient vector and the Hessian matrix are divided by  $\hat{\phi}$  and the covariance matrix is multiplied by  $\hat{\phi}$ . Accordingly the estimated standard errors are also adjusted, the Wald confidence intervals and significance tests will be affected even the parameter estimates are not affected by  $\hat{\phi}$ .

Note that the log-likelihood is not revised; that is, the log-likelihood is based on  $\phi = 1$  because the scale parameter should be kept the same in the log-likelihood for fair comparison in information criteria and model fitting omnibus test.

#### Overdispersion

For the Poisson and binomial distributions, if the estimated scale parameter is not near the assumed value of one, then the data may be overdispersed if the value is greater than one or underdispersed if the value is less than one. Overdispersion is more common in practice. The problem with overdispersion is that it may cause standard errors of the estimated parameters to be underestimated. A variable may appear to be a significant predictor, when in fact it is not.

#### Deviance and Pearson Chi-Square for Binomial Distribution with 0/1 Binary Response Variable

When **r** and **m** (event/trial) variables are used for the binomial distribution, each case represents **m** Bernoulli trials. When **y** is a binary dependent variable with 0/1 values, each case represents a single trial. The trial can be repeated for several times with the same setting (i.e. the same values for all predictor variables). For example, suppose the first 10 **y** values are 2 1s and 8 0s and **x** values are the same (if recorded in events/trials format, these 10 cases is recorded as 1 case with **r** = 2 and **m** = 10), then these 10 cases should be considered from the same subpopulation. Cases with common values in the variable list that includes all predictor variables are regarded as coming from the same subpopulation. When the binomial distribution with binary response is used, we should calculate the deviance and Pearson chi-square based on the subpopulations. If we calculate them based on the cases, the results might not be useful.

If subpopulations are specified for the binomial distribution with 0/1 binary response variable, the data should be reconstructed from the single trial format to the events/trials format. Assume the following notation for formatted data:

Table 18-13

Notation

Notation	Description
$n_s$	Number of subpopulations.

<b>Notation</b>	<b>Description</b>
$r_{j1}$	Sum of the product of the frequencies and the scale weights associated with $y = 1$ in the $j$ th subpopulation. So $r_{j0}$ is that with $y = 0$ in the $j$ th subpopulation.
$m_j$	Total weighted observations; $m_j = r_{j1} + r_{j0}$ .
$y_{j1}$	The proportion of 1s in the $j$ th subpopulation; $y_{j1} = r_{j1}/m_j$ .
$\mu_j$	The fitted probability in the $j$ th subpopulation ( $\hat{\mu}_j$ would be the same for each case in the $j$ th subpopulation because values for all predictor variables are the same for each case.)

The deviance and Pearson chi-square are defined as follows:

$$D = 2 \sum_{j=1}^{n_s} m_j \left\{ y_{j1} \ln \left( \frac{y_{j1}}{\mu_j} \right) + (1 - y_{j1}) \ln \left( \frac{1 - y_{j1}}{1 - \mu_j} \right) \right\} \text{ and } \chi^2 = \sum_{j=1}^{n_s} \frac{m_j (y_{j1} - \mu_j)^2}{\mu_j (1 - \mu_j)},$$

then the corresponding estimate of the scale parameter will be

$$\hat{\phi} = \frac{D}{n_s - p_x} \text{ and } \hat{\phi} = \frac{\chi^2}{n_s - p_x}.$$

The full log likelihood, based on subpopulations, is defined as follows:

$$\ell = \ell_k + \sum_{j=1}^{n_s} \frac{1}{\phi} \left\{ \ln \left( \frac{m_j}{r_{j1}} \right) \right\} = \ell_k + \sum_{j=1}^{n_s} \frac{1}{\phi} \left\{ \ln \frac{m_j!}{r_{j1}! r_{j0}!} \right\},$$

where  $\ell_k$  is the kernel log likelihood; it should be the same as the kernel log-likelihood computed based on cases before, there is no need to compute again.

#### Information Criteria

Information criteria are used when comparing different models for the same data. The formulas for various criteria are as follows.

**Akaike information criteria (AIC).**  $-2\ell + 2d$

**Finite sample corrected (AICC).**  $-2\ell + \frac{2d \cdot N}{(N - d - 1)}$

**Bayesian information criteria (BIC).**  $-2\ell + d \ln(N)$

**Consistent AIC (CAIC).**  $-2\ell + d(\ln(N) + 1)$ .

where  $\ell$  is the log-likelihood evaluated at the parameter estimates. Notice that  $d = p_x$  if only  $\beta$  is included;  $d = p_x + 1$  if the scale parameter is included for normal, inverse Gaussian, or gamma.

#### Notes

- $\ell$  (the full log-likelihood) can be replaced with  $\ell_k$  (the kernel of the log-likelihood) depending on the user's choice.
- When  $\mathbf{r}$  and  $\mathbf{m}$  (event/trial) variables are used for the binomial distribution, then the  $N$  used here would be the sum of the trials frequencies;  $N = \sum_{i=1}^n f_i m_i$ . In this way, the same value results whether the data are in raw, binary form or in summarized, binomial form.

### **Test of Model Fit**

The model fitting omnibus test is based on  $-2$  log-likelihood values for the model under consideration and the initial model. For the model under consideration, the value of the  $-2$  log-likelihood is

$$-2\ell(\hat{\beta})$$

Let the initial model be the intercept-only model if intercept is in the considered model or the empty model otherwise. For the intercept-only model, the value of the  $-2$  log-likelihood is

$$-2\ell(\hat{\beta}_0)$$

For the empty model, the value of the  $-2$  log-likelihood is

$$-2\ell(0)$$

Then the omnibus (or global) test statistic is

$$S = 2\left(\ell(\hat{\beta}) - \ell(\beta_0)\right) \text{ for the intercept-only model or}$$

$$S = 2\left(\ell(\hat{\beta}) - \ell(0)\right) \text{ for the empty model.}$$

$S$  has an asymptotic chi-square distribution with  $r$  degrees of freedom, equal to the difference in the number of valid parameters between the model under consideration and the initial model.  $r = p_x - 1$  for the intercept-only model,;  $r = p_x$  for the empty model. The  $p$ -values then can be calculated accordingly.

Note if the scale parameter is estimated by the ML method in the model under consideration, then it will also be estimated by the ML method in the initial model.

### **Default Tests of Model Effects**

For each regression effect specified in the model, type I and III analyses can be conducted.

#### Type I Analysis

Type I analysis consists of fitting a sequence of models, starting with a model with only an intercept term (if there is one), and adding one additional effect, which can be covariates, factors and interactions, of the model on each step. So it depends on the order of effects specified in the model. On the other hand, type III analysis won't depend on the order of effects.

**Wald Statistics.** For each effect specified in the model, type I test matrix  $\mathbf{L}_i$  is constructed and  $H_0: \mathbf{L}_i\beta = \mathbf{0}$  is tested. Construction of matrix  $\mathbf{L}_i$  is based on the generating matrix  $\mathbf{H}_\omega = \left(\mathbf{X}^T \boldsymbol{\Omega} \mathbf{X}\right)^{-1} \mathbf{X}^T \boldsymbol{\Omega} \mathbf{X}$ , where  $\boldsymbol{\Omega}$  is the scale weight matrix with  $i$ th diagonal element  $\omega_i$  and such that  $\mathbf{L}_i\beta$  is estimable. It involves parameters only for the given effect and the effects containing the given effect. If such a matrix cannot be constructed, the effect is not testable.

Since Wald statistics can be applied to type I and III analysis and custom tests, we express Wald statistics in a more general form. The Wald statistic for testing  $\mathbf{L}_i\beta = \mathbf{K}$ , where  $\mathbf{L}_i$  is a  $r \times p$  full row rank hypothesis matrix and  $\mathbf{K}$  is a  $r \times 1$  resulting vector, is defined by

$$S = \left( \mathbf{L}_i \hat{\beta} - \mathbf{K} \right)^T \left( \mathbf{L}_i \boldsymbol{\Sigma} \mathbf{L}_i^T \right)^- \left( \mathbf{L}_i \hat{\beta} - \mathbf{K} \right)$$

where  $\hat{\beta}$  is the maximum likelihood estimate and  $\boldsymbol{\Sigma}$  is the parameter estimates covariance matrix.  $S$  has an asymptotic chi-square distribution with  $r_C$  degrees of freedom, where  $r_C = \text{rank}(\mathbf{L}_i \boldsymbol{\Sigma} \mathbf{L}_i^T)$ .

If  $r_C < r$ , then  $(\mathbf{L}_i \boldsymbol{\Sigma} \mathbf{L}_i^T)^-$  is a generalized inverse such that Wald tests are effective for a restricted set of hypotheses  $\mathbf{L}_{iC}\beta - \mathbf{K}_C$  containing a particular subset  $C$  of independent rows from  $H_0$ .

For type I and III analysis, calculate the Wald statistic for each effect  $i$  according to the corresponding hypothesis matrix  $\mathbf{L}_i$  and  $\mathbf{K}=\mathbf{0}$ .

Type III Analysis

**Wald statistics.** See the discussion of Wald statistics for Type I analysis above.  $\mathbf{L}_i$  is the type III test matrix for the  $i$ th effect.

## Blank handling

All records with missing values for any input or output field are excluded from the estimation of the model.

## Scoring

Scoring is defined as assigning one or more values to a case in a data set.

### Predicted Values

Due to the non-linear link functions, the predicted values will be computed for the linear predictor and the mean of the response separately. Also, since estimated standard errors of predicted values of linear predictor are calculated, the confidence intervals for the mean are obtained easily.

Predicted values are still computed as long all the predictor variables have non-missing values in the given model.

Predicted Values of the Linear Predictors

$$\hat{\eta}_i = x_i^T \hat{\beta} + o_i$$

Estimated Standard Errors of Predicted Values of the Linear Predictors

$$\hat{\sigma}_{\eta} = \sqrt{x_i^T \boldsymbol{\Sigma} x_i}$$

Predicted Values of the Means

$$\hat{\mu}_i = g^{-1}(x_i^T \hat{\beta} + o_i)$$

where  $g^{-1}$  is the inverse of the link function. For binomial response with 0/1 binary response variable, this is the predicted probability of category 1.

Confidence Intervals for the Means

Approximate  $100(1-\alpha)\%$  confidence intervals for the mean can be computed as follows

$$g^{-1}(x_i^T \hat{\beta} + o_i \pm z_{1-\alpha/2} \hat{\sigma}_\eta)$$

If either endpoint in the argument is outside the valid range for the inverse link function, the corresponding confidence interval endpoint is set to a system missing value.

### **Blank handling**

Records with missing values for any input field in the final model cannot be scored, and are assigned a predicted value of \$null\$.

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# Generalized linear mixed models algorithms

Generalized linear mixed models extend the linear model so that:

- The target is linearly related to the factors and covariates via a specified link function.
- The target can have a non-normal distribution.
- The observations can be correlated.

Generalized linear mixed models cover a wide variety of models, from simple linear regression to complex multilevel models for non-normal longitudinal data.

## Notation

The following notation is used throughout this chapter unless otherwise stated:

$n$	Number of complete cases in the dataset. It is an integer and $n \geq 1$ .
$p$	Number of parameters (including the constant, if it exists) in the model. It is an integer and $p \geq 1$ .
$p_x$	Number of non-redundant columns in the design matrix of fixed effects. It is an integer and $p_x \geq 1$ .
$K$	Number of random effects.
$y$	$n \times 1$ target vector. The rows are records.
$r$	$n \times 1$ events vector for the binomial distribution representing the number of “successes” within a number of trials. All elements are non-negative integers.
$m$	$n \times 1$ trials vector for the binomial distribution. All elements are positive integers and $m_i \geq r_i, i=1, \dots, n$ .
$\mu$	$n \times 1$ expected target value vector.
$\eta$	$n \times 1$ linear predictor vector.
$X$	$n \times p$ design matrix. The rows represent the records and the columns represent the parameters. The $i$ th row is $x_i^T = (x_{i1}, \dots, x_{ip})$ , where the superscript $T$ means transpose of a matrix or vector, $i = 1, \dots, n$ with $x_{i1} = 1$ if the model has an intercept.
$Z$	$n \times r$ design matrix of random effects.
$O$	$n \times 1$ offset vector. This can't be the target or one of the predictors. Also this can't be a categorical field.
$\beta$	$p \times 1$ parameter vector. The first element is the intercept, if there is one.
$\gamma$	$r \times 1$ random effect vector.
$\omega$	$n \times 1$ scale weight vector. If an element is less than or equal to 0 or missing, the corresponding record is not used.
$f$	$n \times 1$ frequency weight vector. Non-integer elements are treated by rounding the value to the nearest integer. For values less than 0.5 or missing, the corresponding records are not used.
$N$	Effective sample size, $N = \sum_{i=1}^n f_i$ . If frequency weights are not used, $N = n$ .
$\theta_k$	covariance parameters of the $k$ th random effect
$\theta_G$	covariance parameters of the random effects, $\theta_G = [\theta_1^T, \dots, \theta_K^T]^T$

$\theta_R$	covariance parameters of the residuals
$\theta$	$\theta = [\theta_G^T, \theta_R^T]^T = [\theta_1^T, \dots, \theta_K^T, \theta_R^T]^T$
$V_{Y \gamma}$	Covariance matrix of $\mathbf{y}$ , conditional on the random effects

## Model

The form of a generalized linear mixed model for the target  $\mathbf{y}$  with the random effects  $\gamma$  is

$$\eta = g(E(y|\gamma)) = \mathbf{X}\beta + \mathbf{Z}\gamma + \mathbf{O}, y|\gamma \sim F,$$

where  $\eta$  is the linear predictor;  $g(\cdot)$  is the monotonic differentiable link function;  $\gamma$  is a  $(r \times 1)$  vector of random effects which are assumed to be normally distributed with mean 0 and variance matrix  $\mathbf{G}$ ,  $\mathbf{X}$  is a  $(n \times p)$  design matrix for the fixed effects;  $\mathbf{Z}$  is a  $(n \times r)$  design matrix for the random effects;  $\mathbf{O}$  is an offset with a constant coefficient of 1 for each observation;  $F$  is the conditional target probability distribution. Note that if there are no random effects, the model reduces to a generalized linear model (GZLM).

The probability distributions without random effects offered (except multinomial) are listed in Table 19-1 on p. 188. The link functions offered are listed in Table 19-3 on p. 189. Different combinations of probability distribution and link function can result in different models.

See “Nominal multinomial distribution” on p. 206 for more information on the nominal multinomial distribution.

See “Ordinal multinomial distribution” on p. 213 for more information on the ordinal multinomial distribution.

Note that the available distributions depend on the measurement level of the target:

- A continuous target can have any distribution except multinomial. The binomial distribution is allowed because the target could be an “events” field. The default distribution for a continuous target is the normal distribution.
- A nominal target can have the multinomial or binomial distribution. The default is multinomial.
- An ordinal target can have the multinomial or binomial distribution. The default is multinomial.

Table 19-1

*Distribution, range and variance of the response, variance function, and its first derivative*

Distribution	Range of $y$	$V(\mu)$	$\text{Var}(y)$	$V'(\mu)$
Normal	$(-\infty, \infty)$	1	$\phi$	0
Inverse Gaussian	$(0, \infty)$	$\mu^3$	$\phi\mu^3$	$3\mu^2$
Gamma	$(0, \infty)$	$\mu^2$	$\phi\mu^2$	$2\mu$
Negative binomial	$0(1)\infty$	$\mu+k\mu^2$	$\mu+k\mu^2$	$1+2k\mu$
Poisson	$0(1)\infty$	$\mu$	$\mu$	1
Binomial( $m$ )	$0(1)m/m$	$\mu(1-\mu)$	$\mu(1-\mu)/m$	$1-2\mu$

**Notes**

- $0(1)z$  means the range is from 0 to  $z$  with increments of 1; that is, 0, 1, 2, ...,  $z$ .
- For the binomial distribution, the binomial trial variable  $m$  is considered as a part of the weight variable  $\omega$ .
- If a scale weight variable  $\omega$  is presented,  $\phi$  is replaced by  $\phi/\omega$ .
- For the negative binomial distribution, the ancillary parameter ( $k$ ) is estimated by the maximum likelihood (ML) method. When  $k = 0$ , the negative binomial distribution reduces to the Poisson distribution. When  $k = 1$ , the negative binomial is the geometric distribution.

The full log-likelihood function ( $\ell$ ), which will be used as the objective function for parameter estimation, is listed for each distribution in the following table.

**Table 19-2**  
The log-likelihood function for probability distribution

Distribution	$\ell$
Normal	$\ell = \ell_k + \sum_{i=1}^n -\frac{f_i}{2} \{\ln(2\pi)\}$
Inverse Gaussian	$\ell = \ell_k + \sum_{i=1}^n -\frac{f_i}{2} \{\ln(2\pi)\}$
Gamma	$\ell = \ell_k + \sum_{i=1}^n f_i \{-\ln(y_i)\}$
Negative binomial	$\ell = \ell_k + \sum_{i=1}^n f_i \frac{\omega_i}{\phi} \{-\ln(\Gamma(y_i + 1))\}$
Poisson	$\ell = \ell_k + \sum_{i=1}^n f_i \frac{\omega_i}{\phi} \{-\ln(y_i!)\}$
Binomial( $m$ )	$\ell = \ell_k + \sum_{i=1}^n f_i \frac{\omega_i}{\phi} \left\{ \ln \binom{m_i}{r_i} \right\}$ , where $\binom{m_i}{r_i} = \frac{m_i!}{r_i!(m_i - r_i)!}$

The following tables list the form, inverse form, range of  $\hat{\mu}$ , and first and second derivatives for each link function.

**Table 19-3**  
Link function name, form, inverse of link function, and range of the predicted mean

Link function	$\eta = g(\mu)$	Inverse $\mu = g^{-1}(\eta)$	Range of $\hat{\mu}$
Identity	$\mu$	$\eta$	$\hat{\mu} \in R$
Log	$\ln(\mu)$	$\exp(\eta)$	$\hat{\mu} \geq 0$
Logit	$\ln\left(\frac{\mu}{1-\mu}\right)$	$\frac{\exp(\eta)}{1+\exp(\eta)}$	$\hat{\mu} \in [0, 1]$
Probit	$\Phi^{-1}(\mu)$ , where $\Phi(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\xi} e^{-z^2/2} dz$	$\Phi(\eta)$	$\hat{\mu} \in [0, 1]$
Complementary log-log	$\ln(-\ln(1-\mu))$	$1 - \exp(-\exp(\eta))$	$\hat{\mu} \in [0, 1]$

Link function	$\eta=g(\mu)$	Inverse $\mu=g^{-1}(\eta)$	Range of $\hat{\mu}$
Power( $\alpha$ ) $\begin{cases} \alpha \neq 0 \\ \alpha = 0 \end{cases}$	$\begin{cases} \mu^\alpha \\ \ln(\mu) \end{cases}$	$\begin{cases} \eta^{1/\alpha} \\ \exp(\eta) \end{cases}$	$\begin{cases} \hat{\mu} \in R \text{ if } \alpha \text{ or } 1/\alpha \text{ is odd integer} \\ \hat{\mu} \geq 0 \text{ otherwise} \end{cases}$
Log-complement	$\ln(1-\mu)$	$1-\exp(\eta)$	$\hat{\mu} \leq 1$
Negative log-log	$-\ln(-\ln(\mu))$	$\exp(-\exp(-\eta))$	$\hat{\mu} \in [0, 1]$

Note: In the power link function, if  $|\alpha| < 2.2\text{e-}16$ ,  $\alpha$  is treated as 0.

Table 19-4  
The first and second derivatives of link function

Link function	First derivative $g'(\mu) = \frac{\partial \eta}{\partial \mu} = \Delta$	Second derivative $g''(\mu) = \frac{\partial^2 \eta}{\partial \mu^2}$
Identity	1	0
Log	$\frac{1}{\mu}$	$-\Delta^2$
Logit	$\frac{1}{\mu(1-\mu)}$	$\Delta^2(2\mu - 1)$
Probit	$\frac{1}{\phi(\Phi^{-1}(\mu))}$ , where $\phi(z) = \frac{1}{\sqrt{2\pi}} e^{-z^2/2}$	$\Delta^2 \Phi^{-1}(\mu)$
Complementary log-log	$\frac{1}{(\mu-1) \ln(1-\mu)}$	$-\Delta^2(1 + \ln(1-\mu))$
Power( $\alpha$ ) $\begin{cases} \alpha \neq 0 \\ \alpha = 0 \end{cases}$	$\begin{cases} \alpha \mu^{\alpha-1} \\ \frac{1}{\mu} \end{cases}$	$\begin{cases} \Delta \frac{\alpha-1}{\mu} \\ -\Delta^2 \end{cases}$
Log-complement	$\frac{-1}{1-\mu}$	$-\Delta^2$
Negative log-log	$\frac{-1}{\mu \ln(\mu)}$	$\Delta^2(1 + \ln(\mu))$

When the canonical parameter is equal to the linear predictor,  $\theta = \eta$ , then the link function is called the **canonical link function**. Although the canonical links lead to desirable statistical properties of the model, particularly in small samples, there is in general no a priori reason why the systematic effects in a model should be additive on the scale given by that link. The canonical link functions for probability distributions are given in the following table.

Table 19-5  
Canonical and default link functions for probability distributions

Distribution	Canonical link function
Normal	Identity
Inverse Gaussian	Power(-2)
Gamma	Power(-1)
Negative binomial	Negative binomial
Poisson	Log
Binomial	Logit

The variance of  $\mathbf{y}$ , conditional on the random effects, is

$$\text{var}(\mathbf{y}|\boldsymbol{\gamma}) = \mathbf{A}^{1/2} \mathbf{R} \mathbf{A}^{1/2}$$

The matrix  $\mathbf{A}$  is a diagonal matrix and contains the variance function of the model, which is the function of the mean  $\boldsymbol{\mu}$ , divided by the corresponding scale weight variable; that is,  $\mathbf{A} = \text{diag}(V(\mu_i)/\omega_i), i = 1, \dots, n$ . The variance functions,  $V(\mu)$ , are different for different distributions. The matrix  $\mathbf{R}$  is the variance matrix for repeated measures.

Generalized linear mixed models allow correlation and/or heterogeneity from random effects ( $\mathbf{G}$ -side) and/or heterogeneity from residual effects ( $\mathbf{R}$ -side). resulting in 4 types of models:

1. If a GLMM has no  $\mathbf{G}$ -side or  $\mathbf{R}$ -side effects, then it reduces to a GZLM;  $\mathbf{G}=\mathbf{0}$  and  $\mathbf{R} = \phi\mathbf{I}$ , where  $\mathbf{I}$  is the identity matrix and  $\phi$  is the scale parameter. For continuous distributions (normal, inverse Gauss and gamma),  $\phi$  is an unknown parameter and is estimated jointly with the regression parameters by the maximum likelihood (ML) method. For discrete distributions (negative binomial, Poisson, binomial and multinomial),  $\phi$  is estimated by Pearson chi-square as follows:

$$\hat{\phi} = \frac{1}{N^*} \sum_{i=1}^n f_i \omega_i \frac{(y_i - \mu_i)^2}{V(\mu_i)},$$

where  $N^* = N - p_x$  for the restricted maximum pseudo-likelihood (REPL) method.

2. If a model only has  $\mathbf{G}$ -side random effects, then the  $\mathbf{G}$  matrix is user-specified and  $\mathbf{R} = \phi\mathbf{I}$ .  $\phi$  is estimated jointly with the covariance parameters in  $\mathbf{G}$  for continuous distributions and  $\phi = 1$  for discrete distributions..
3. If a model only has  $\mathbf{R}$ -side residual effects, then  $\mathbf{G} = \mathbf{0}$  and the  $\mathbf{R}$  matrix is user-specified. All covariance parameters in  $\mathbf{R}$  are estimated using the REPL method, defined in “Estimation ” on p. 192.
4. If a model has both  $\mathbf{G}$ -side and  $\mathbf{R}$ -side effects, all covariance parameters in  $\mathbf{G}$  and  $\mathbf{R}$  are jointly estimated using the REPL method.

For the negative binomial distribution, there is the ancillary parameter  $k$ , which is first estimated by the ML method, ignoring random and residual effects, then fixed to that estimate while other regression and covariance parameters are estimated.

### **Fixed effects transformation**

To improve numerical stability, the  $\mathbf{X}$  matrix is transformed according to the following rules.

The  $i$ th row of  $\mathbf{X}$  is  $\mathbf{x}_i = (x_{i1}, \dots, x_{ip})^T$ ,  $i=1, \dots, n$  with  $x_{i1} = 1$  if the model has an intercept. Suppose  $\mathbf{x}_i^*$  is the transformation of  $\mathbf{x}_i$  then the  $j$ th entry of  $\mathbf{x}_i^*$  is defined as

$$x_{ij}^* = \frac{x_{ij} - c_j}{s_j}$$

where  $c_j$  and  $s_j$  are centering and scaling values for  $x_{ij}$ , respectively, for  $j=1, \dots, p$  and choices of  $c_j$  and  $s_j$ , are listed as follows:

- For a non-constant continuous predictor or a derived predictor which includes a continuous predictor, if the model has an intercept,  $c_1 = 0$  and  $c_j = \bar{x}_j, j \neq 1$ , where  $\bar{x}_j$  is the sample mean of the  $j$ th predictor,  $\bar{x}_j = \frac{1}{N} \sum_{i=1}^n f_i x_{ij}$  and  $s_1 = 1$  and  $s_j = \sqrt{s_{x_j}^2}, j \neq 1$ , where  $\sqrt{s_{x_j}^2}$  is the sample standard deviation of the  $j$ th predictor and  $s_{x_j}^2 = \frac{1}{N-1} \sum_{i=1}^n f_i (x_{ij} - \bar{x}_j)^2$ . Note that the intercept column is not transformed. If the model has no intercept,  $c_j = 0$  and  $s_j = \sqrt{s_{x_j}^2 + \bar{x}_j^2}$ .
- For a constant predictor  $x_{ij} = a \neq 0, \forall i, c_j = 0$  and  $s_j = a$ , that is, scale it to 1.
- For a dummy predictor that is derived from a factor or a factor interaction,  $c_j = 0$  and  $s_j = 1$ ; that is, leave it unchanged.

## Estimation

We estimate GLMMs using linearization-based methods, also called the pseudo likelihood approach (PL; Wolfinger and O'Connell (1994)), penalized quasi-likelihood (PQL; Breslow and Clayton (1993)), marginal quasi-likelihood (MQL; Goldstein (1991)). They are based on the similar principle that the GLMMs are approximated by an LMM so that well-established estimation methods for LMMs can be applied. More specifically, the mean target function; that is, the inverse link function is approximated by a linear Taylor series expansion around the current estimates of the fixed-effect regression coefficients and different solutions of random effects (0 is used for MQL and the empirical Bayes estimates are used for PQL). Applying this linear approximation of the mean target leads to a linear mixed model for a transformation of the original target. The parameters of this LMM can be estimated by Newton-Raphson or Fisher scoring technique and the estimates then are used to update the linear approximation. The algorithm iterates between two steps until convergence. In general, the method is a doubly iterative process. The outer iterations are to update the transformed target for an LMM and the inner iterations are to estimate parameters of the LMM.

It is well known that parameter estimation for an LMM can be based on maximum likelihood (ML) or restricted (or residual) maximum likelihood (REML). Similarly, parameter estimation for a GLMM in the inner iterations can be based on maximum pseudo-likelihood (PL) or restricted maximum pseudo-likelihood (REPL).

## Linear mixed pseudo model

Following Wolfinger and O'Connell (1993), a first-order Taylor series of  $\boldsymbol{\mu}$  in (1) about  $\tilde{\boldsymbol{\beta}}$  and  $\tilde{\boldsymbol{\gamma}}$  yields

$$\boldsymbol{\mu} \approx \tilde{\boldsymbol{\mu}} + (g^{-1})' \left( \mathbf{X}\tilde{\boldsymbol{\beta}} + \mathbf{Z}\tilde{\boldsymbol{\gamma}} + \mathbf{0} \right) \left[ \mathbf{X}(\boldsymbol{\beta} - \tilde{\boldsymbol{\beta}}) + \mathbf{Z}(\boldsymbol{\gamma} - \tilde{\boldsymbol{\gamma}}) \right]$$

where  $(g^{-1})'(\mathbf{X}\tilde{\beta} + \mathbf{Z}\tilde{\gamma} + \mathbf{O})$  is a diagonal matrix with elements consisting of evaluations of the 1st derivative of  $g^{-1}$ . Since  $(g^{-1})'(\mathbf{X}\tilde{\beta} + \mathbf{Z}\tilde{\gamma} + \mathbf{O}) = (g'(\tilde{\mu}))^{-1}$ , this equation can be rearranged as

$$g'(\tilde{\mu})(\boldsymbol{\mu} - \tilde{\boldsymbol{\mu}}) + \mathbf{X}\tilde{\beta} + \mathbf{Z}\tilde{\gamma} \approx \mathbf{X}\beta + \mathbf{Z}\gamma$$

If we define a pseudo target variable as

$$\mathbf{v} \equiv g'(\tilde{\mu})(\mathbf{y} - \tilde{\boldsymbol{\mu}}) + \mathbf{X}\tilde{\beta} + \mathbf{Z}\tilde{\gamma} = g'(\tilde{\mu})(\mathbf{y} - \tilde{\boldsymbol{\mu}}) + g(\tilde{\boldsymbol{\mu}}) - \mathbf{O},$$

then the conditional expectation and variance of  $\mathbf{v}$ , based on  $E(\mathbf{y}|\boldsymbol{\gamma})$  and  $\text{var}(\mathbf{y}|\boldsymbol{\gamma}) = \mathbf{A}^{1/2}\mathbf{R}\mathbf{A}^{1/2}$ , are

$$E(\mathbf{v}|\boldsymbol{\gamma}) = g'(\tilde{\mu})(\boldsymbol{\mu} - \tilde{\boldsymbol{\mu}}) + \mathbf{X}\tilde{\beta} + \mathbf{Z}\tilde{\gamma}$$

$$\text{var}(\mathbf{v}|\boldsymbol{\gamma}) = g'(\tilde{\mu})\mathbf{A}_{\tilde{\mu}}^{1/2}\mathbf{R}\mathbf{A}_{\tilde{\mu}}^{1/2}g'(\tilde{\mu})$$

where  $\mathbf{A}_{\tilde{\mu}}^{1/2} = \text{diag}[(V(\tilde{\mu}_i)/\omega_i)^{1/2}]$ ,  $i = 1, \dots, n$ .

Furthermore, we also assume  $\mathbf{v}|\boldsymbol{\gamma}$  is normally distributed. Then we consider the model of  $\mathbf{v}$

$$\mathbf{v} = \mathbf{X}\beta + \mathbf{Z}\gamma + \boldsymbol{\varepsilon}$$

as a weighted linear mixed model with fixed effects  $\beta$ , random effects  $\boldsymbol{\gamma} \sim N(\mathbf{0}, \mathbf{G})$ , error terms  $\boldsymbol{\varepsilon} \sim N(\mathbf{0}, g'(\tilde{\mu})\mathbf{A}_{\tilde{\mu}}^{1/2}\mathbf{R}\mathbf{A}_{\tilde{\mu}}^{1/2}g'(\tilde{\mu}))$ , because  $\text{var}(\boldsymbol{\varepsilon}) = \text{var}(\mathbf{v}|\boldsymbol{\gamma})$ , and diagonal weight matrix

$\tilde{\mathbf{W}} = \mathbf{A}_{\tilde{\mu}} [g'(\tilde{\mu})]^{-2}$ . Note that the new target  $\mathbf{v}$  (with  $\mathbf{O}$  if an offset variable exists) is a Taylor series approximation of the linked target  $g(\mathbf{y})$ . The estimation method of unknown parameters of  $\beta$  and  $\boldsymbol{\theta}$ , which contains all unknowns in  $\mathbf{G}$  and  $\mathbf{R}$ , for traditional linear mixed models can be applied to this linear mixed pseudo model.

The Gaussian log pseudo-likelihood (PL) and restricted log pseudo-likelihood (REPL), which are expressed as the functions of covariance parameters in  $\boldsymbol{\theta}$ , corresponding to the linear mixed model for  $\mathbf{v}$  are the following:

$$\ell(\boldsymbol{\theta}; \mathbf{v}) = -\frac{1}{2} \ln |\mathbf{V}(\boldsymbol{\theta})| - \frac{1}{2} \mathbf{r}(\boldsymbol{\theta})^T \mathbf{V}(\boldsymbol{\theta})^{-1} \mathbf{r}(\boldsymbol{\theta}) - \frac{N}{2} \ln(2\pi)$$

$$\ell_R(\boldsymbol{\theta}; \mathbf{v}) = -\frac{1}{2} \ln |\mathbf{V}(\boldsymbol{\theta})| - \frac{1}{2} \mathbf{r}(\boldsymbol{\theta})^T \mathbf{V}(\boldsymbol{\theta})^{-1} \mathbf{r}(\boldsymbol{\theta}) - \frac{1}{2} \ln |\mathbf{X}^T \mathbf{V}(\boldsymbol{\theta})^{-1} \mathbf{X}| - \frac{N - p_x}{2} \ln(2\pi)$$

where

$\mathbf{V}(\boldsymbol{\theta}) = \mathbf{Z}\mathbf{G}(\boldsymbol{\theta})\mathbf{Z} + \tilde{\mathbf{W}}^{-1/2}\mathbf{R}(\boldsymbol{\theta})\tilde{\mathbf{W}}^{-1/2}$ ,  $\mathbf{r}(\boldsymbol{\theta}) = \mathbf{v} - \mathbf{X}(\mathbf{X}^T\mathbf{V}(\boldsymbol{\theta})^{-1}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{V}(\boldsymbol{\theta})^{-1}\mathbf{v} = \mathbf{v} - \mathbf{X}\hat{\beta}$ ,  $N$  denotes the effective sample size, and  $p_x$  denotes the rank of the design matrix of  $\mathbf{X}$  or the number of non-redundant parameters in  $\mathbf{X}$ . Note that the regression parameters in  $\beta$  are profiled from the above equations because the estimation of  $\beta$  can be obtained analytically. The covariance

parameters in  $\theta$  are estimated by Newton-Raphson or Fisher scoring algorithm. Following the tradition in linear mixed models, the objection functions of minimization for estimating  $\theta$  would be  $-2\ell(\theta; \mathbf{v})$  or  $-2\ell_R(\theta; \mathbf{v})$ . Upon obtaining  $\hat{\theta}$ , estimates for  $\beta$  and  $\gamma$  are computed as

$$\hat{\beta} = \left( \mathbf{X}^T \mathbf{V}(\hat{\theta})^{-1} \mathbf{X} \right)^{-1} \mathbf{X}^T \mathbf{V}(\hat{\theta})^{-1} \mathbf{v}$$

$$\hat{\gamma} = \hat{G} \mathbf{Z}^T \mathbf{V}(\hat{\theta})^{-1} \hat{r}$$

where  $\hat{\beta}$  is the best linear unbiased estimator (BLUE) of  $\beta$  and  $\hat{\gamma}$  is the estimated best linear unbiased predictor (BLUP) of  $\gamma$  in the linear mixed pseudo model. With these statistics,  $\mathbf{v}$  and  $\tilde{W}$  are recomputed based on  $\tilde{\mu}$  and the objective function is minimized again to obtain updated  $\hat{\theta}$ . Iteration between  $-2\ell(\theta; \mathbf{v})$  and the above equation yields the PL estimation procedure and between  $-2\ell_R(\theta; \mathbf{v})$  and the above equation the REPL procedure.

There are two choices for  $\tilde{\gamma}$  (the current estimates of  $\gamma$ ):

1.  $\hat{\gamma}$  for PQL; and
2. 0 for MQL.

On the other hand,  $\hat{\beta}$  is always used as the current estimate of the fixed effects. Based on the two objective functions (PL or REPL) and two choices of random effect estimates (PQL or MQL), 4 estimation methods can be implemented for GLMMs:

1. PL-PQL: pseudo-likelihood with  $\tilde{\gamma}=\hat{\gamma}$ ;
2. PL-MQL: pseudo-likelihood with  $\tilde{\gamma}=0$ ;
3. REPL-PQL: residual pseudo-likelihood with  $\tilde{\gamma}=\hat{\gamma}$ ;
4. REPL-MQL: residual pseudo-likelihood with  $\tilde{\gamma}=0$ .

We use method 3, REPL-PQL.

## Iterative process

The doubly iterative process for the estimation of  $\theta$  is as follows:

1. Obtain an initial estimate of  $\mu$ ,  $\mu^{(0)}$ . Specifically,  $\mu_i^0 = (y_i m_i + 0.5)/(m_i + 1)$  for a binomial distribution ( $y_i$  can be a proportion or 0/1 value) and  $\mu_i^0 = y_i$  for a non-binomial distribution. Also set the outer iteration index  $j = 0$ .
2. Based on  $\tilde{\mu}$ , compute

$$\mathbf{v} = g(\tilde{\mu}) - \mathbf{O} + g'(\tilde{\mu})(\mathbf{y} - \tilde{\mu}) \text{ and } \tilde{W} = \mathbf{A}_{\tilde{\mu}}^{-1} \left[ g'(\tilde{\mu}) \right]^{-2}.$$

Fit a weighted linear mixed model with pseudo target  $\mathbf{v}$ , fixed effects design matrix  $\mathbf{X}$ , random effects design matrix  $\mathbf{Z}$ , and diagonal weight matrix  $\tilde{W}$ . The fitting procedure, which is called the inner iteration, yields the estimates of  $\theta$ , and is denoted as  $\theta^{(j)}$ . The procedure uses the

specified settings for parameter, log-likelihood, and Hessian convergence criteria for determining convergence of the linear mixed model. If  $j = 0$ , go to step 4; otherwise go to the next step.

3. Check if the following criterion with tolerance level  $\xi$  is satisfied:

$$\max_i \left( 2 \times \frac{|\theta_i^{(j)} - \theta_i^{(j-1)}|}{|\theta_i^{(j-1)}| + |\theta_i^{(j-1)}|} \right) < \xi.$$

If it is met or maximum number of outer iterations is reached, stop. Otherwise, go to the next step.

4. Compute  $\hat{\beta}$  by setting  $\hat{\theta} = \theta^{(j)}$  then set  $\tilde{\beta} = \hat{\beta}$ . Depending on the choice of random effect estimates, set  $\tilde{\gamma} = \hat{\gamma}$ .
5. Compute the new estimate of  $\mu$  by

$$\tilde{\mu} = g^{-1}(\mathbf{X}\tilde{\beta} + Z\tilde{\gamma} + \mathbf{O}),$$

set  $j = j + 1$  and go to step 2.

### **Wald confidence intervals for covariance parameter estimates**

Here we assume that the estimated parameters of  $\mathbf{G}$  and  $\mathbf{R}$  are obtained through the above doubly iterative process. Then their asymptotic covariance matrix can be approximated by  $2\mathbf{H}^{-1}$ , where  $\mathbf{H}$  is the Hessian matrix of the objective function  $(-2\ell(\theta; \mathbf{v})$  or  $-2\ell_R(\theta; \mathbf{v})$ ) evaluated at  $\hat{\theta}$ . The standard error for the  $i$ th covariance parameter estimate in the  $\hat{\theta}$  vector, say  $\hat{\theta}_i$ , is the square root of the  $i$ th diagonal element of  $2\mathbf{H}^{-1}$ .

Thus, a simple Wald's type confidence interval or test statistic for any covariance parameter can be obtained by using the asymptotic normality. However, these can be unreliable in small samples, especially for variance and correlation parameters that have a range of  $[0, \infty)$  and  $[-1, 1]$  respectively. Therefore, following the same method used in linear mixed models, these parameters are transformed to parameters that have range  $(-\infty, \infty)$ . Using the delta method, these transformed estimates still have asymptotic normal distributions.

For variance type parameters in  $\mathbf{G}$  and  $\mathbf{R}$ , such as  $\sigma^2$  in the autoregressive, autoregressive moving average, compound symmetry, diagonal, Toeplitz, and variance components, and  $\theta_{ii}$  in the unstructured type, the  $100(1 - \alpha)\%$  Wald confidence interval is given, assuming the variance parameter estimate is  $\hat{\sigma}^2$  and its standard error is  $\text{se}(\hat{\sigma}^2)$  from the corresponding diagonal element of  $2\mathbf{H}^{-1}$ , by

$$\exp \left( \ln(\hat{\sigma}^2) \pm z_{1-\alpha/2} \cdot \hat{\sigma}^{-2} \cdot \text{se}(\hat{\sigma}^2) \right)$$

For correlation type parameters in  $\mathbf{G}$  and  $\mathbf{R}$ , such as  $\rho$  in the autoregressive, autoregressive moving average, and Toeplitz types and  $\varphi$  in the autoregressive moving average type, which usually come with the constraint of  $|\rho| \leq 1$ , the  $100(1 - \alpha)\%$  Wald confidence interval is given, assuming the correlation parameter estimate is  $\hat{\rho}$  and its standard error is  $\text{se}(\hat{\rho})$  from the corresponding diagonal element of  $2\mathbf{H}^{-1}$ , by

$$\tanh \left( \tanh^{-1}(\hat{\rho}) \pm z_{1-\alpha/2} \cdot (1 - \hat{\rho}^2)^{-1} \cdot \text{se}(\hat{\rho}) \right)$$

where  $\tanh x = \frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)}$  and  $\tanh^{-1} x = \frac{1}{2} \ln \left[ \frac{1+x}{1-x} \right]$  are hyperbolic tangent and inverse hyperbolic tangent, respectively.

For general type parameters, other than variance and correlation types, in  $\mathbf{G}$  and  $\mathbf{R}$ , such as  $\sigma_1$  in the compound symmetry type and  $\theta_{ij}, i \neq j$ , (off-diagonal elements) in the unstructured type, no transformation is done. Then the  $100(1 - \alpha)\%$  Wald confidence interval is simply, assuming the parameter estimate is  $\hat{\sigma}_1$  and its standard error is  $\text{se}(\hat{\sigma}_1)$  from the corresponding diagonal element of  $2\mathbf{H}^{-1}$ ,

$$(\hat{\sigma}_1 - z_{1-\alpha/2} \cdot \text{se}(\hat{\sigma}_1)), \hat{\sigma}_1 + z_{1-\alpha/2} \cdot \text{se}(\hat{\sigma}_1))$$

The  $100(1 - \alpha)\%$  Wald confidence interval for  $\phi$  is

$$(\exp(\hat{\tau} - z_{1-\alpha/2} \hat{\sigma}_\tau), \exp(\hat{\tau} + z_{1-\alpha/2} \hat{\sigma}_\tau))$$

where  $\tau = \ln(\phi)$ .

Note that the  $z$ -statistics for the hypothesis  $H_{0i} : \theta_i = 0$ , where  $\theta_i$  is a covariance parameter in  $\theta$  vector, are calculated; however, the Wald tests should be considered as an approximation and used with caution because the test statistics might not have a standardized normal distribution.

### **Statistics for estimates of fixed and random effects**

The approximate covariance matrix of  $(\hat{\beta} - \beta, \hat{\gamma} - \gamma)$  is

$$\hat{C} = \begin{bmatrix} \mathbf{X}^T \mathbf{R}^{*-1} \mathbf{X} & \mathbf{X}^T \mathbf{R}^{*-1} \mathbf{Z} \\ \mathbf{Z}^T \mathbf{R}^{*-1} \mathbf{X} & \mathbf{Z}^T \mathbf{R}^{*-1} \mathbf{Z} + \mathbf{G}(\hat{\theta})^{-1} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{C}_{11} & \mathbf{C}_{21}^T \\ \mathbf{C}_{21} & \mathbf{C}_{22} \end{bmatrix}$$

where  $\mathbf{R}^* \equiv \text{var}(\mathbf{v}|\gamma) = g'(\hat{\mu}) \mathbf{A}_{\hat{\mu}}^{1/2} \mathbf{R} \mathbf{A}_{\hat{\mu}}^{1/2} g'(\hat{\mu})$  is evaluated at the converged estimates and

$$\hat{C}_{11} = (\mathbf{X}^T \hat{\mathbf{V}}^{-1} \mathbf{X})^{-1}$$

$$\hat{C}_{21} = -\hat{\mathbf{G}} \mathbf{Z}^T \hat{\mathbf{V}}^{-1} \mathbf{X} \hat{C}_{11}$$

$$\hat{C}_{22} = (\mathbf{Z}^T \hat{\mathbf{R}}^{-1} \mathbf{Z} + \hat{\mathbf{G}}^{-1})^{-1} - \hat{C}_{21} \mathbf{X}^T \hat{\mathbf{V}}^{-1} \mathbf{Z} \hat{\mathbf{G}}$$

### **Statistics for estimates of fixed effects on original scale**

If the  $\mathbf{X}$  matrix is transformed, the restricted log pseudo-likelihood (REPL) would be different based on transformed and original scale, so the REPL on the transformed scale should be transformed back on the final iteration so that any post-estimation statistics based on REPL can be calculated correctly. Suppose the final objective function value based on the transformed and

original scales are  $-2\ell_R^*(\theta; \mathbf{v})$  and  $-2\ell_R(\theta; \mathbf{v})$ , respectively, then  $-2\ell_R(\theta; \mathbf{v})$  can be obtained from  $-2\ell_R^*(\theta; \mathbf{v})$  as follows:

$$-2\ell_R(\theta; \mathbf{v}) = -2\ell_R^*(\theta; \mathbf{v}) - 2 \ln |\mathbf{A}|$$

Because REPL has the following extra term involved the X matrix

$$\begin{aligned} -\frac{1}{2} \ln \left| \mathbf{X}^{*\mathbf{T}} \mathbf{V}(\theta)^{-1} \mathbf{X}^* \right| &= -\frac{1}{2} \ln \left| (\mathbf{X}\mathbf{A})^{\mathbf{T}} \mathbf{V}(\theta)^{-1} \mathbf{X}\mathbf{A} \right| \\ &= -\frac{1}{2} \ln \left( \left| \mathbf{A}^{\mathbf{T}} \right| \times \left| \mathbf{X}\mathbf{V}(\theta)^{-1} \mathbf{X} \right| \times |\mathbf{A}| \right) \\ &= -\frac{1}{2} \left( \ln \left| \mathbf{X}\mathbf{V}(\theta)^{-1} \mathbf{X} \right| + \ln |\mathbf{A}| + \ln \left| \mathbf{A}^{\mathbf{T}} \right| \right) \\ &= -\frac{1}{2} \ln \left| \mathbf{X}\mathbf{V}(\theta)^{-1} \mathbf{X} \right| - \ln |\mathbf{A}| \end{aligned}$$

then  $-\frac{1}{2} \ln \left| \mathbf{X}\mathbf{V}(\theta)^{-1} \mathbf{X} \right| = -\frac{1}{2} \ln \left| \mathbf{X}^{*\mathbf{T}} \mathbf{V}(\theta)^{-1} \mathbf{X}^* \right| + \ln |\mathbf{A}|$  and  $\ell_R(\theta; \mathbf{v}) = \ell_R^*(\theta; \mathbf{v}) + \ln |\mathbf{A}|$ . Please note that PL values are the same whether the X matrix is transformed or not.

In addition, the final estimates of  $\boldsymbol{\beta}$ ,  $\mathbf{C}_{11}$ ,  $\mathbf{C}_{21}$  and  $\mathbf{C}_{22}$  are based on the transformed scale, denoted as  $\hat{\boldsymbol{\beta}}^*$ ,  $\hat{\mathbf{C}}_{11}^*$ ,  $\hat{\mathbf{C}}_{21}^*$  and  $\hat{\mathbf{C}}_{22}^*$ , respectively. They are transformed back to the original scale, denoted as  $\hat{\boldsymbol{\beta}}$ ,  $\hat{\mathbf{C}}_{11}$ ,  $\hat{\mathbf{C}}_{21}$  and  $\hat{\mathbf{C}}_{22}$ , respectively, as follows:

$$\hat{\boldsymbol{\beta}} = \mathbf{A}\hat{\boldsymbol{\beta}}^*,$$

$$\hat{\mathbf{C}}_{11} = \mathbf{A}\hat{\mathbf{C}}_{11}^*\mathbf{A}^{\mathbf{T}},$$

$$\hat{\mathbf{C}}_{21} = \hat{\mathbf{C}}_{21}^*\mathbf{A}^{\mathbf{T}},$$

$$\hat{\mathbf{C}}_{22} = \hat{\mathbf{C}}_{22}^*.$$

Note that  $\mathbf{A}$  could reduce to  $\mathbf{S}^{-1}$ ; hereafter, the superscript \* denotes a quantity on the transformed scale.

### **Estimated covariance matrix of the fixed effects parameters**

Two estimated covariance matrices of the fixed effects parameters can be calculated: model-based and robust.

The model-based estimated covariance matrix of the fixed effects parameters is given by

$$\boldsymbol{\Sigma}_m = \hat{\mathbf{C}}_{11}$$

The robust estimated covariance matrix of the fixed effects parameters for a GLMM is defined as the classical sandwich estimator. It is similar to that for a generalized linear model or a generalized estimating equation (GEE). If the model is a generalized linear mixed model and it is processed by subjects, then the robust estimator is defined as follows

$$\Sigma_{\mathbf{r}} = \Sigma_{\mathbf{m}} \left( \sum_{j=1}^S \mathbf{X}_j^T \hat{V}_j^{-1} \hat{r}_j \hat{r}_j^T \hat{V}_j^{-1} \mathbf{X}_j \right) \Sigma_{\mathbf{m}}$$

where  $\hat{r}_j = \mathbf{v}_j - \mathbf{X}_j \hat{\beta}$ .

#### **Standard errors for estimates in fixed effects and predictions in random effects**

Let  $\hat{\beta}_i$  denote a non-redundant parameter estimate in fixed effects. Its standard error is the square root of the  $i$ th diagonal element of  $\Sigma_{\mathbf{m}}$  or  $\Sigma_{\mathbf{r}}$ ,

$$\hat{\sigma}_{\beta_i} = \sqrt{\sigma_{ii}}$$

The standard error for redundant parameter estimates is set to a system missing value.

Let  $\hat{\gamma}_i$  denote a prediction in random effects. Its standard error is the square root of the  $i$ th diagonal element of  $\hat{C}_{22}$ :

$$\hat{\sigma}_{\gamma_i} = \sqrt{\hat{C}_{22,ii}}$$

#### **Test statistics for estimates in fixed effects and predictions in random effects**

The hypothesis  $H_{0i} : \beta_i = 0$  is tested for each non-redundant parameter in fixed effects using the  $t$  statistic:

$$t_i = \frac{\hat{\beta}_i}{\hat{\sigma}_{\beta_i}}$$

which has an asymptotic  $t$  distribution with  $\nu$  degrees of freedom. See “Method for computing degrees of freedom” on p. 203 for details on computing the degrees of freedom.

#### **Wald confidence intervals for estimates in fixed effects and predictions in random effects**

The  $100(1 - \alpha)\%$  Wald confidence interval for  $\beta_i$  is given by

$$\left( \hat{\beta}_i - t_{\nu, \alpha/2} \hat{\sigma}_{\beta_i}, \hat{\beta}_i + t_{\nu, \alpha/2} \hat{\sigma}_{\beta_i} \right)$$

where  $t_{\nu, \alpha/2}$  is the  $(1 - \alpha/2)$  100th percentile of the  $t_{\nu}$  distribution.

For some models (see the list below), the exponentiated parameter estimates, their standard errors, and confidence intervals are computed. Using the delta method, the estimate of  $\exp(\beta_i)$  is  $\exp(\hat{\beta}_i)$ , the standard error estimate is  $\left( \exp(\hat{\beta}_i) \cdot \hat{\sigma}_{\beta_i} \right)$  and the corresponding  $100(1 - \alpha)\%$  Wald confidence interval for  $\exp(\beta_i)$  is

$$\left( \exp\left(\hat{\beta}_i - t_{\nu, \alpha/2} \hat{\sigma}_{\beta_i}\right), \exp\left(\hat{\beta}_i + t_{\nu, \alpha/2} \hat{\sigma}_{\beta_i}\right) \right).$$

The list of models is as follows:

1. Logistic regression (binomial distribution + logit link).
2. Nominal logistic regression (nominal multinomial distribution + generalized logit link).
3. Ordinal logistic regression (ordinal multinomial distribution + cumulative logit link).
4. Log-linear model (Poisson distribution + log link).
5. Negative binomial regression (negative binomial distribution + log link).

## Testing

After estimating parameters and calculating relevant statistics, several tests for the given model are performed.

## Goodness of fit

### Information criteria

Information criteria are used when comparing different models for the same data. The formulas for various criteria are as follows.

$$\begin{aligned} \text{Finite sample corrected (AICC)} & \quad -2\ell + \frac{2d \cdot N}{(N-d-1)} \\ \text{Bayesian information criteria (BIC)} & \quad -2\ell + d \ln(N) \end{aligned}$$

where  $\ell$  is the restricted log-pseudo-likelihood evaluated at the parameter estimates. For REPL,  $N$  is the effective sample size minus the number of non-redundant parameters in fixed effects ( $\sum_{i=1}^n f_i - p_x$ ) and  $d$  is the number of covariance parameters.

Note that the restricted log-pseudo-likelihood values are of the linearized model, not on the original scale. Thus the information criteria should not be compared across models with different distribution and link function and they should be interpreted with caution.

## Tests of fixed effects

For each effect specified in the model, a type III test matrix  $\mathbf{L}$  is constructed and  $H_0: \mathbf{L}_i \boldsymbol{\beta} = \mathbf{0}$  is tested. Construction of  $\mathbf{L}$  and the generating estimable function (GEF) is based on the generating matrix  $\mathbf{H}_\omega = (\mathbf{X}^T \boldsymbol{\Psi} \mathbf{X})^{-1} \mathbf{X}^T \boldsymbol{\Psi} \mathbf{X}$ , where  $\boldsymbol{\Psi} = \text{diag}(f_1 \omega_1, \dots, f_n \omega_n)$ , such that  $\mathbf{L}_i \boldsymbol{\beta}$  is estimable; that is,  $\mathbf{L}_i = \mathbf{L}_i \mathbf{H}_\omega$ . It involves parameters only for the given effect and the effects containing the given effect. For type III analysis,  $\mathbf{L}$  does not depend on the order of effects specified in the model. If such a matrix cannot be constructed, the effect is not testable.

Then the  $\mathbf{L}$  matrix is then used to construct the test statistic

$$\mathbf{F} = \frac{\hat{\beta}^T \mathbf{L}^T (\mathbf{L} \Sigma \mathbf{L}^T)^{-1} \mathbf{L} \hat{\beta}}{r_c}$$

where  $r_c = \text{rank}(\mathbf{L} \Sigma \mathbf{L}^T)$ . The statistic has an approximate  $F$  distribution. The numerator degrees of freedom is  $r_c$  and the denominator degrees of freedom is  $v$ . See “Method for computing degrees of freedom” on p. 203 for details on computing the denominator degrees of freedom.

In addition, we test a null hypothesis that all regression parameters (except intercept if there is one) equal zero. The test statistic would be the same as the above  $F$  statistic except the  $L$  matrix is from GEF. If there is no intercept, the  $L$  matrix is the whole GEF. If there is an intercept, the  $L$  matrix is GEF without the first row which corresponds to the intercept. This test is similar to the “corrected model” in linear models.

### **Estimated marginal means**

There are two types of estimated marginal means calculated here. One corresponds to the specified factors for the linear predictor of the model and the other corresponds to those for the original scale of the target.

Estimated marginal means are based on the estimated cell means. For a given fixed set of factors, or their interactions, we estimate marginal means as the mean value averaged over all cells generated by the rest of the factors in the model. Covariates may be fixed at any specified value. If not specified, the value for each covariate is set to its overall mean estimate.

Estimated marginal means are not available for the multinomial distribution.

### **Estimated marginal means for the linear predictor**

#### **Calculating estimated marginal means for the linear predictor**

Estimated marginal means for the linear predictor are based on the link function transformation, and constructed such that  $\mathbf{L}\mathbf{B}$  is estimable.

Suppose there are  $r$  combined levels of the specified categorical effect. This  $r \times 1$  vector can be expressed in the form  $\hat{\mathbf{u}} = \mathbf{L}\hat{\beta}$ . The variance matrix of  $\hat{\mathbf{u}}$  is then computed by

$$V(\hat{\mathbf{u}}) = \mathbf{L} \Sigma \mathbf{L}^T$$

The standard error for the  $j$ th element of  $\hat{\mathbf{u}}$  is the square root of the  $j$ th diagonal element of  $V(\hat{\mathbf{u}})$ . Let the  $j$ th element of  $\hat{\mathbf{u}}$  and its standard error be  $\hat{u}_j$  and  $\hat{\sigma}_{u_j}$ , respectively, then the corresponding  $100(1 - \alpha)\%$  confidence interval for  $u_j, j = 1, \dots, r$ , is given by

$$\hat{u}_j \pm t_{v, \alpha/2} \hat{\sigma}_{u_j}$$

where  $t_{v^j, \alpha/2}$  is the  $(1 - \alpha/2)$ 100th percentile of the  $t$  distribution with  $v^j$  degrees of freedom. See “Method for computing degrees of freedom” on p. 203 for details on computing the degrees of freedom.

### **Comparing estimated marginal means for the linear predictor**

We can compare estimated marginal means for the linear predictor based on a selected contrast type, for which a set of contrasts for the factor is created. Let this set of contrasts define matrix  $\mathbf{C}$  used for testing the hypothesis  $H_0 : \mathbf{C}\mathbf{u} = 0$ . An  $F$  statistic is used for testing given set of contrasts for the factor as follows:

$$F = \frac{(\mathbf{C}\hat{\mathbf{u}})^{\mathbf{T}} \left( \mathbf{C}\mathbf{V}(\hat{\mathbf{u}})\mathbf{C}^{\mathbf{T}} \right)^{-1} (\mathbf{C}\hat{\mathbf{u}})}{r_I}$$

which has an asymptotic  $F$  distribution with  $r_I$  degrees of freedom, where  $r_I = \text{rank}(\mathbf{C}\mathbf{V}(\hat{\mathbf{u}})\mathbf{C}^{\mathbf{T}})$ . See “Method for computing degrees of freedom” on p. 203 for details on computing the denominator degrees of freedom. The  $p$ -values can be calculated accordingly. Note that adjusted  $p$ -values based on multiple comparisons adjustments won’t be computed for the overall test.

Each row  $\mathbf{c}_i^{\mathbf{T}}$  of matrix  $\mathbf{C}$  is also tested separately. The estimate for the  $i$ th row is given by  $\mathbf{c}_i^{\mathbf{T}}\hat{\mathbf{u}}$  and its standard error by  $\sqrt{\mathbf{c}_i^{\mathbf{T}}\mathbf{V}(\hat{\mathbf{u}})\mathbf{c}_i}$ . The corresponding  $100(1 - \alpha)\%$  confidence interval is given by  $\mathbf{c}_i^{\mathbf{T}}\hat{\mathbf{u}} \pm t_{v^i, \alpha/2}\hat{\sigma}_{cu_i}$

The test statistic for  $H_0 : \mathbf{c}_i^{\mathbf{T}}\mathbf{u} = 0$  is

$$t_i = \frac{\mathbf{c}_i^{\mathbf{T}}\hat{\mathbf{u}}}{\hat{\sigma}_{cu_i}}$$

It has an asymptotic  $t$  distribution. See “Method for computing degrees of freedom” on p. 203 for details on computing the degrees of freedom. The  $p$ -values can be calculated accordingly. In addition, adjusted  $p$ -values for multiple comparisons can also be computed.

### **Estimated marginal means in the original scale**

Estimated marginal means for the target are based on the original scale. As a conditional predictor defined by Lane and Nelder (1982), estimated marginal means for the target are derived from those for the linear predictor.

#### **Calculating estimated marginal means for the target**

The estimated marginal means for the target are defined as

$$\hat{\mathbf{M}} = g^{-1}(\mathbf{L}\hat{\boldsymbol{\beta}}) = g^{-1}(\hat{\mathbf{u}})$$

The variance of estimated marginal means for the target is

$$V(\hat{\mathbf{M}}) = \text{diag}\left(\frac{\partial g^{-1}(\hat{v}_j)}{\partial \hat{u}_j}\right) L \Sigma L^T \text{diag}\left(\frac{\partial g^{-1}(\hat{u}_j)}{\partial \hat{v}_j}\right)$$

where  $\text{diag}(\partial g^{-1}(\hat{u}_j)/\partial \hat{u}_j)$  is a  $r \times r$  matrix and  $\partial g^{-1}(\hat{u}_j)/\partial \hat{u}_j$  is the derivative of the inverse of the link with respect to the  $j$ th value in  $\hat{\mathbf{u}}$  and  $\partial g^{-1}(\hat{u}_j)/\partial \hat{u}_j = 1/g'(\hat{M}_j)$  where  $g'(\hat{M}_j)$  is from Table 19-4 on p. 190.

The  $100(1 - \alpha)\%$  confidence interval for  $M_i, i = 1, \dots, r$ , is given by

$$g^{-1}(\hat{u}_i \pm t_{v, \alpha/2} \hat{\sigma}_{u_i}).$$

*Note:*  $\hat{\mathbf{M}}$  is estimated marginal means for the proportion, not for the number of events when events and trials variables are used for the binomial distribution.

### **Comparing estimated marginal means for the target**

This is similar to comparing estimated marginal means for the linear predictor; just replace  $\hat{\mathbf{u}}$  with  $\hat{\mathbf{M}}$  and  $V(\hat{\mathbf{u}})$  with  $V(\hat{\mathbf{M}})$ . For more information, see the topic “Estimated marginal means for the linear predictor” on p. 200.

### **Multiple comparisons**

The hypothesis  $H_0 : \mathbf{C}\mathbf{u} = \mathbf{0}$  can be tested using the multiple row hypotheses testing technique. Let  $\mathbf{c}_i^T$  be the  $i$ th row vector of matrix  $\mathbf{C}$ . The  $i$ th row hypothesis is  $H_{0i} : \mathbf{c}_i^T \mathbf{u} = 0$ . Testing  $H_0$  is the same as testing multiple non-redundant row hypotheses  $\{H_{0i}^*\}_{i=1}^R$  simultaneously, where  $R$  is the number of non-redundant row hypotheses, and  $H_{0i}^*$  represents the  $i$ th non-redundant hypothesis. A hypothesis  $H_{0i}$  is redundant if there exists another hypothesis  $H_{0j}, j \neq i$  such that  $\mathbf{c}_i = a\mathbf{c}_j, a \neq 0$ .

**Adjusted  $p$ -values.** For each individual hypothesis  $H_{0i}$ , test statistics can be calculated. Let  $p_i$  denote the  $p$ -value for testing  $H_{0i}$  and  $p_i^*$  denote the adjusted  $p$ -value. The conclusion from multiple testing is, at level  $\alpha$  (the family-wise type I error),

reject  $H_{0i} : \mathbf{c}_i^T \mathbf{u} = 0$  if  $p_i^* < \alpha$ ;

reject  $H_0 : \mathbf{C}\mathbf{u} = \mathbf{0}$  if  $\min_i (p_i^*) < \alpha$ .

Several different methods to adjust  $p$ -values are provided here. Please note that if the adjusted  $p$ -value is bigger than 1, it is set to 1 in all the methods.

**Adjusted confidence intervals.** Note that if confidence intervals are also calculated for the above hypothesis, then adjusting confidence intervals is required to correspond to adjusted  $p$ -values. The only item needed to be adjusted in the confidence intervals is the critical value from the standard normal distribution. Assume that the original critical value is  $z_{1-\alpha/2}$  and the adjusted critical value is  $z^*$ .

**LSD (Least Significant Difference)**

The adjusted  $p$ -values are the same as the original  $p$ -values:

$$p_i^* = p_i$$

The adjusted critical value is:

$$t^* = t_{v^i, \alpha/2}$$

**Sequential Bonferroni**

The adjusted  $p$ -values are:

$$p_{(i)}^* = \begin{cases} Rp_{(1)} & i = 1 \\ \max\left((R - i + 1)p_{(i)}, p_{(i-1)}^*\right) & i \geq 2 \end{cases}$$

The adjusted critical values will correspond to the ordered adjusted  $p$ -values as follows:

$$t_{v^{(i)}}^* = \begin{cases} t_{v^{(i)}, \frac{\alpha}{2R}} & \text{if } i = 1 \\ t_{v^{(i)}, \frac{\alpha}{2(R-i+1)}} & \text{if } p_{(i)}^* = (R - i + 1)p_{(i)} \text{ for } i \geq 2 \\ t_{v^{(i)}, \frac{\alpha}{2(p_{(i-1)}^*/p_{(i)})}} & \text{if } p_{(i)}^* = p_{(i-1)}^* \text{ for } i \geq 2 \end{cases}$$

**Sequential Sidak**

The adjusted  $p$ -values are:

$$p_{(i)}^* = \begin{cases} 1 - (1 - p_{(1)})^R & i = 1 \\ \max\left(1 - (1 - p_{(i)})^{R-i+1}, p_{(i-1)}^*\right) & i \geq 2 \end{cases}$$

The adjusted critical values will correspond to the ordered adjusted  $p$ -values as follows:

$$t_{v^{(i)}}^* = \begin{cases} t_{v^{(i)}, \frac{1-(1-\alpha)^{1/R}}{2}} & \text{if } i = 1, \\ t_{v^{(i)}, \frac{1-(1-\alpha)^{1/(R-i+1)}}{2}} & \text{if } p_{(i)}^* = (R - i + 1)p_{(i)} \text{ for } i \geq 2; \\ t_{v^{(i)}, \frac{1-(1-\alpha)^{1/x}}{2}} & \text{if } p_{(i)}^* = p_{(i-1)}^* \text{ for } i \geq 2 \end{cases}$$

$$\text{where } x = \frac{\ln(1-p_{(i-1)}^*)}{\ln(1-p_{(i)})}.$$

**Method for computing degrees of freedom****Residual method**

The value of degrees of freedom is given by  $N - \text{rank}(\mathbf{X})$ , where  $N$  is the effective sample size and  $\mathbf{X}$  is the design matrix of fixed effects.

**Satterthwaite's approximation**

First perform the spectral decomposition  $\mathbf{L}\hat{\mathbf{C}}\mathbf{L}^T = \mathbf{\Gamma}^T\mathbf{D}\mathbf{\Gamma}$  where  $\mathbf{\Gamma}$  is an orthogonal matrix of eigenvectors and  $\mathbf{D}$  is a diagonal matrix of eigenvalues. If  $l_m$  is the  $m$ th row of  $\mathbf{\Gamma}\mathbf{L}$ ,  $d_m$  is the  $m$ th eigenvalues and

$$\nu_m = \frac{2d_m}{\mathbf{g}_m \Sigma(\hat{\theta})^{-1} \mathbf{g}_m}$$

where  $\mathbf{g}_m = \frac{\partial l_m \mathbf{C} \mathbf{L}^T}{\partial \theta} \Big|_{\theta = \hat{\theta}}$  and  $\Sigma_{\hat{\theta}}$  is the asymptotic covariance matrix of  $\hat{\theta}$  obtained from the Hessian matrix of the objective function; that is,  $\Sigma_{\hat{\theta}} = 2\mathbf{H}^{-1}$ . If

$$E = \sum_{m=1}^q \frac{\nu_m}{\nu_m - 2} I(\nu_m > 2)$$

then the denominator degree of freedom is given by

$$\nu = \frac{2E}{E - q}$$

Note that the degrees of freedom can only be computed when  $E > q$ .

**Scoring**

For GLMMs, predicted values and relevant statistics can be computed based on solutions of random effects. PQL-type predictions use  $\hat{\gamma}$  as the solution for the random effects to compute predicted values and relevant statistics.

**PQL-type predicted values and relevant statistics**

Predicted value of the linear predictor

$$\mathbf{x}_i^T \hat{\beta} + \mathbf{z}_i^T \hat{\gamma} + o_i$$

Standard error of the linear predictor

$$\hat{\sigma}_\eta = \sqrt{\mathbf{x}_i^T \Sigma \mathbf{x}_i + \mathbf{z}_i^T \hat{\mathbf{C}}_{22} \mathbf{z}_i + 2\mathbf{z}_i^T \hat{\mathbf{C}}_{21} \mathbf{x}_i}$$

Predicted value of the mean

$$g^{-1}(\mathbf{x}_i^T \hat{\beta} + \mathbf{z}_i^T \hat{\gamma} + o_i)$$

For the binomial distribution with 0/1 binary target variable, the predicted category  $c(\mathbf{x}_i)$  is

$$c(\mathbf{x}_i) = \begin{cases} 1 \text{ (or success)} & \text{if } \hat{\mu}_i \geq 0.5 \\ 0 \text{ (or failure)} & \text{otherwise} \end{cases}$$

Approximate  $100(1-\alpha)\%$  confidence intervals for the mean

$$g^{-1}\left(\mathbf{x}_i^T \hat{\beta} + \mathbf{z}_i^T \hat{\gamma} + o_i \pm t_{v, \alpha/2} \hat{\sigma}_\eta\right)$$

Raw residual on the link function transformation

$$r_{\eta, i}^R = v_i - \hat{\eta}_i$$

Raw residual on the original scale of the target

$$r_i^R = y_i - \hat{\mu}_i$$

Pearson-type residual on the link function transformation

$$r_{\eta, i}^P = \frac{r_{\eta, i}^R}{\sqrt{\hat{v}ar(v_i|\gamma)}},$$

where  $\hat{v}ar(v_i|\gamma)$  is the  $i$ th diagonal element of  $\hat{v}ar(\mathbf{v}|\gamma)$  and  $\hat{v}ar(\mathbf{v}|\gamma) = g'(\hat{\mu})\mathbf{A}_{\hat{\mu}}^{1/2}\hat{R}\mathbf{A}_{\hat{\mu}}^{1/2}g'(\hat{\mu})$  where  $\hat{\mu}$  is an  $n \times 1$  vector of PQL-type predicted values of the mean.

Pearson-type residual on the original scale of the target

$$r_i^P = \frac{r_i^R}{\sqrt{\hat{v}ar(y_i|\gamma)}},$$

where  $\hat{v}ar(y_i|\gamma)$  is the  $i$ th diagonal element of  $\hat{v}ar(\mathbf{y}) = \mathbf{A}_{\hat{\mu}_m}^{1/2}\hat{R}\mathbf{A}_{\hat{\mu}_m}^{1/2}$  and  $\hat{\mu}_m = \hat{\mu}$ .

### **Classification Table**

Suppose that  $c(j, j')$  is the sum of the frequencies for the observations whose actual target category is  $j$  (as row) and predicted target category is  $j'$  (as column),  $j, j' = 1, \dots, J$  (note that  $J=2$  for binomial), then

$$c(j, j') = \sum_{i=1}^n f_i I(y_i = j, c(x_i) = j')$$

where  $I(\cdot)$  is indicator function.

Suppose that  $p(j, j')$  is the  $(j, j')$ <sup>th</sup> element of the classification table, which is the row percentage, then

$$p_{j,j'} = \left( \frac{c(j,j')}{\sum_{j'=1}^J c(j,j')} \right) \times 100\%$$

The percentage of total correct predictions of the model (or “overall percent correct”) is

$$p_{total} = \left( \frac{\sum_{j=1}^J c(j,j)}{\sum_{j=1}^J \sum_{j'=1}^J c(j,j')} \right) \times 100\%$$

## Nominal multinomial distribution

The nominal multinomial distribution requires some extra notation and explanation.

### Notation

The following notation is used throughout this section unless otherwise stated:

$S$	Number of super subjects.
$T_s$	Number of cases in the $s$ th super subject.
$y_{st}$	Nominal categorical target for the $t$ th case in the $s$ th super subject. Its category values are denoted as 1, 2, and so on.
$J$	The total number of categories for target.
$y_{st}$	Dummy vector of $y_{st}$ , $y_{st} = (y_{st,1}, \dots, y_{st,J-1})^T$ , where $y_{st,j} = 1$ if $y_{st} = j$ , otherwise $y_{st,j} = 0$ . The superscript $T$ means the transpose of a matrix or vector.
$y_s$	$y_s = (y_{s1}^T, \dots, y_{sT_s}^T)^T$ , $s = 1, \dots, S$ .
$y$	$y = (y_1^T, \dots, y_S^T)^T$
$\pi_{st,j}$	Probability of category $j$ for the $t$ th case in the $s$ th super subject; that is, $\pi_{st,j} = P(y_{st} = j)$ .
$\pi_{st}$	$\pi_{st} = (\pi_{st,1}, \dots, \pi_{st,J-1})^T$
$\pi_s$	$\pi_s = (\pi_{s1}^T, \dots, \pi_{sT_s}^T)^T$ , $s = 1, \dots, S$
$\pi$	$\pi = (\pi_1^T, \dots, \pi_S^T)^T$

$\eta_{st,j}$	Linear predictor value for category $j$ of the $t$ th case in the $s$ th super subject.
$\eta_{st}$	$\eta_{st} = (\eta_{st,1}, \dots, \eta_{st,J-1})^T$
$\eta_s$	$\eta_s = (\eta_{s1}^T, \dots, \eta_{sT_s}^T)^T, s = 1, \dots, S$
$\eta$	$(n(J-1)) \times 1$ vector of linear predictor. $\eta = (\eta_1^T, \dots, \eta_S^T)^T$
$x_{st}$	$p \times 1$ vector of predictor variables for the $t$ th case in the $s$ th super subject. The first element is 1 if there is an intercept.
$X_s$	$X_s = (I_{J-1} \otimes x_{s1}, \dots, I_{J-1} \otimes x_{sT_s})^T, s = 1, \dots, S$
$X$	$(n(J-1)) \times (J-1)p$ design matrix of fixed effects, $X = (X_1^T, \dots, X_S^T)^T$
$z_{st}$	$r \times 1$ vector of coefficients for the random effect corresponding to the $t$ th case in the $s$ th super subject.
$Z_s$	$Z_s = (I_{J-1} \otimes z_{s1}, \dots, I_{J-1} \otimes z_{sT_s})^T, s = 1, \dots, S$
$Z$	Design matrix of random effects, $Z = \bigoplus_{s=1}^S Z_s$ , where $\bigoplus$ is the direct sum of matrices.
$O$	$n \times 1$ vector of offsets, $O = (o_{11}, \dots, o_{1T_1}, \dots, o_{ST_S})^T$ , where $o_{st}$ is the offset value of the $t$ th case in the $s$ th super subject. This can't be the target ( $y$ ) or one of the predictors ( $X$ ). The offset must be continuous.
$O^*$	$O^* = O \otimes 1_{J-1}$ , where $1_q$ is a length $q$ vector of 1.
$\beta_j$	$p \times 1$ vector of unknown parameters for category $j$ , $\beta_j = (\beta_{j1}, \dots, \beta_{jp})^T, j = 1, \dots, J$ . The first element in $\beta_j$ is the intercept for the category $j$ , if there is one.
$\beta$	$\beta = (\beta_1^T, \dots, \beta_{J-1}^T)^T$
$\gamma_{sj}$	$r \times 1$ vector of random effects for category $j$ in the $s$ th super subject, $j = 1, \dots, J-1$ .
$\gamma_s$	Random effects for the $s$ th super subject, $\gamma_s = (\gamma_{s,1}^T, \dots, \gamma_{s,J-1}^T)^T$ .
$\gamma$	$\gamma = (\gamma_1^T, \dots, \gamma_S^T)^T$
$\omega_{st}$	Scale weight of the $t$ th case in the $s$ th super subject. It does not have to be integers. If it is less than or equal to 0 or missing, the corresponding case is not used.
$\omega$	$n \times 1$ vector of scale weight variable, $\omega = (\omega_{11}, \dots, \omega_{1T_1}, \dots, \omega_{S1}, \dots, \omega_{ST_S})^T$ .
$f_{st}$	Frequency weight of the $t$ th case in the $s$ th super subject. If it is a non-integer value, it is treated by rounding the value to the nearest integer. If it is less than 0.5 or missing, the corresponding cases are not used.
$f$	$n \times 1$ vector of frequency count variable, $f = (f_{11}, \dots, f_{1T_1}, \dots, f_{S1}, \dots, f_{ST_S})^T$ .
$N$	Effective sample size, $N = \sum_{i=1}^n f_i$ . If frequency count variable $f$ is not used, $N = n$ .

## Model

The form of a generalized linear mixed model for nominal target with the random effects is

$$\eta = g(E(y) | \gamma) = X\beta + Z\gamma + O^*$$

where  $\eta$  is the linear predictor;  $\mathbf{X}$  is the design matrix for fixed effects;  $\mathbf{Z}$  is the design matrix for random effects;  $\gamma$  is a vector of random effects which are assumed to be normally distributed with mean  $\mathbf{0}$  and variance matrix  $\mathbf{G}$ ;  $g(\cdot)$  is the logit link function such that

$$\eta_{st,j} = g(\pi_{st,j}) = \log \left( \frac{\pi_{st,j}}{\pi_{st,J}} \right)$$

And its inverse function is

$$\pi_{st,j} = g^{-1}(\eta_{st,j}) = \begin{cases} \frac{\exp(\eta_{st,j})}{J-1}, j = 1, \dots, J-1, \\ 1 + \sum_{k=1}^{J-1} \exp(\eta_{st,k}) \\ \frac{1}{J-1}, j = J. \\ 1 + \sum_{k=1}^{J-1} \exp(\eta_{st,k}) \end{cases}$$

The variance of  $\mathbf{y}$ , conditional on the random effects is

$$Var(y|\gamma) = A_{\mu}^{1/2} R A_{\mu}^{1/2}$$

where  $A_{\mu} = \bigoplus_{s=1}^S \bigoplus_{t=1}^{T_s} \left( \text{diag}(\pi_{st}) - \pi_{st} \pi_{st}^T \right) / \omega_{st}$  and  $R = \phi \mathbf{I}$  which means that R-side effects are not supported for the multinomial distribution.  $\phi$  is set to 1.

## Estimation

### Linear mixed pseudo model

Similarly to “Linear mixed pseudo model” on p. 192, we can obtain a weighted linear mixed model

$$v = X\beta + Z\gamma + \epsilon$$

where  $v \equiv \mathbf{D}^{-1}(\mathbf{y} - \tilde{\pi}) + g(\tilde{\pi}) - \mathbf{O}^*$  and error terms  $\epsilon \sim N\left(0, \mathbf{D}^{-1} A_{\tilde{\pi}}^{1/2} R A_{\tilde{\pi}}^{1/2} \mathbf{D}^{-1}\right)$  with

$$\mathbf{D} = \bigoplus_{s=1}^S \bigoplus_{t=1}^{T_s} \mathbf{D}_{st} = \bigoplus_{s=1}^S \bigoplus_{t=1}^{T_s} \frac{\mathbf{d}g^{-1}(\tilde{\eta}_{st})}{\mathbf{d}\tilde{\eta}_{st}} = \bigoplus_{s=1}^S \bigoplus_{t=1}^{T_s} \left( \text{diag}(\tilde{\pi}_{st}) - \tilde{\pi}_{st} \tilde{\pi}_{st}^T \right)$$

and

$$A_{\tilde{\mu}} = \bigoplus_{s=1}^S \bigoplus_{t=1}^{T_s} \left( \text{diag}(\tilde{\pi}_{st}) - \tilde{\pi}_{st} \tilde{\pi}_{st}^T \right) / \omega_{st}.$$

And block diagonal weight matrix is

$$\tilde{W} = \mathbf{D}A_{\tilde{\mu}}^{-1}\mathbf{D} = \bigoplus_{s=1}^S \bigoplus_{t=1}^{T_s} \omega_{st} \mathbf{D}_{st}.$$

The Gaussian log pseudo-likelihood (PL) and restricted log pseudo-likelihood (REPL), which are expressed as the functions of covariance parameters in  $\theta$ , corresponding to the linear mixed model for  $v$  are the following:

$$\ell(\theta; v) = -\frac{1}{2} \ln |\mathbf{V}(\theta)| - \frac{1}{2} \mathbf{r}(\theta)^T \mathbf{V}(\theta)^{-1} \mathbf{r}(\theta) - \frac{N}{2} \ln(2\pi)$$

$$\ell_R(\theta; v) = -\frac{1}{2} \ln |\mathbf{V}(\theta)| - \frac{1}{2} \mathbf{r}(\theta)^T \mathbf{V}(\theta)^{-1} \mathbf{r}(\theta) - \frac{1}{2} \ln |\mathbf{X}^T \mathbf{V}(\theta)^{-1} \mathbf{X}| - \frac{N - p_x}{2} \ln(2\pi)$$

where  $\mathbf{V}(\theta) = \mathbf{Z}\mathbf{G}(\theta)\mathbf{Z}^T + \tilde{W}^{-1/2}\mathbf{R}(\theta)\tilde{W}^{-1/2}$ ,  $\mathbf{r}(\theta) = v - \mathbf{X}\hat{\beta}$ ,  $N$  denotes the effective sample size, and  $p_x$  denotes the total number of non-redundant parameters for  $\beta$ .

The parameter  $\theta$  can be estimated by linear mixed model using the objection function  $-2\ell(\theta; v)$  or  $-2\ell_R(\theta; v)$ ,  $\beta$  and  $\gamma$  are computed as

$$\hat{\beta} = \left( \mathbf{X}^T \mathbf{V}(\hat{\theta})^{-1} \mathbf{X} \right)^{-1} \mathbf{X}^T \mathbf{V}(\hat{\theta})^{-1} v$$

$$\hat{\gamma} = \hat{G} \mathbf{Z}^T \mathbf{V}(\hat{\theta})^{-1} \hat{r}$$

### **Iterative process**

The doubly iterative process for the estimation of  $\theta$  is the same as that for other distributions, if we replace  $\tilde{\mu}$  and  $\mathbf{X}\hat{\beta} + \mathbf{Z}\hat{\gamma} + O$  with  $\tilde{\pi}$  and  $\mathbf{X}\hat{\beta} + \mathbf{Z}\hat{\gamma} + O^*$  respectively, and set initial estimation of  $\pi$  as

$$\pi^{(0)} = \frac{y + 1/J}{2}$$

For more information, see the topic “Iterative process ” on p. 194.

## **Post-estimation statistics**

### **Wald confidence intervals**

The Wald confidence intervals for covariance parameter estimates are described in “Wald confidence intervals for covariance parameter estimates ” on p. 195.

### **Statistics for estimates of fixed and random effects**

Similarly to “Statistics for estimates of fixed and random effects ” on p. 196, the approximate covariance matrix of  $(\hat{\beta} - \beta, \hat{\gamma} - \gamma)$  is

$$\hat{C} = \begin{bmatrix} X^T R^{*-1} X & X^T R^{*-1} Z \\ Z^T R^{*-1} X & Z^T R^{*-1} Z + G(\hat{\theta})^{-1} \end{bmatrix}^{-1} = \begin{bmatrix} C_{11} & C_{21}^T \\ C_{21} & C_{22} \end{bmatrix}$$

Where  $R^* = \text{var}(v|\gamma) = \hat{D}^{-1} A_{\hat{\pi}}^{1/2} R A_{\hat{\pi}}^{1/2} \hat{D}^{-1}$  with  $\hat{D} = \bigoplus_{s=1}^S \bigoplus_{t=1}^{T_s} \left( \text{diag}(\hat{\pi}_{st}) - \hat{\pi}_{st} \hat{\pi}_{st}^T \right)$ , and

$$\hat{C}_{11} = \left( X^T \hat{V}^{-1} X \right)^{-1}$$

$$\hat{C}_{21} = -\hat{G} Z^T \hat{V}^{-1} X \hat{C}_{11}$$

$$\hat{C}_{22} = \left( Z^T \hat{R}^{-1} Z + \hat{G}^{-1} \right)^{-1} - \hat{C}_{21} X^T \hat{V}^{-1} Z \hat{G}$$

### **Statistics for estimates of fixed and random effects on original scale**

If the fixed effects are transformed when constructing matrix  $\mathbf{X}$ , then the final estimates of  $\beta$ ,  $C_{11}$ ,  $C_{21}$ , and  $C_{22}$  above are based on transformed scale, denoted as  $\hat{\beta}^*$ ,  $\hat{C}_{11}^*$ ,  $\hat{C}_{21}^*$  and  $\hat{C}_{22}^*$ , respectively. They would be transformed back on the original scale, denoted as  $\hat{\beta}$ ,  $\hat{C}_{11}$ ,  $\hat{C}_{21}$ , and  $\hat{C}_{22}$ , respectively, as follows:

$$\hat{\beta} = T \hat{\beta}^*$$

$$\hat{C}_{11} = T \hat{C}_{11}^* T^T$$

$$\hat{C}_{21} = \hat{C}_{21}^* T^T$$

$$\hat{C}_{22} = \hat{C}_{22}^*$$

$$\text{where } T = \bigoplus_{j=1}^{J-1} A_j.$$

### **Estimated covariance matrix of the fixed effects parameters**

Model-based estimated covariance

$$\Sigma_m = \hat{C}_{11}$$

Robust estimated covariance of the fixed effects parameters

$$\Sigma_r = \Sigma_m \left( \sum_{s=1}^S X_s^T \hat{V}_s^{-1} \hat{r}_s \hat{r}_s^T \hat{V}_s^{-1} X_s \right) \Sigma_m$$

where  $\hat{r}_s = v_s - X_s \hat{\beta}$ , and  $v_s$  is a part of  $v$  corresponding to the  $s$ th super subject.

### **Standard error for estimates in fixed effects and predictions in random effects**

Let  $\hat{\beta}_{jc}$  denote a non-redundant fixed effects parameter estimate. Its standard error is the square root of the  $((j-1)p+c)$ th diagonal element of  $\Sigma$

$$\hat{\sigma}_{\beta_{jc}} = \sqrt{\sigma_{((j-1)p+c),((j-1)p+c)}}$$

The standard error for redundant parameter estimates is set to system missing value.

Similarly, let  $\hat{\gamma}_i$  denote the  $i$ th random effects prediction. Its standard error is the square root of the  $i$ th diagonal element of  $\hat{C}_{22}$ :

$$\hat{\sigma}_{\gamma_i} = \sqrt{\hat{C}_{22,ii}}$$

### **Test statistics for estimates in fixed effects and predictions in random effects**

Test statistics for estimates in fixed effects and predictions in random effects are as those described in “Statistics for estimates of fixed and random effects ” on p. 196.

### **Wald confidence intervals for estimates in fixed effects and random effects predictions**

Wald confidence intervals are as those described in “Statistics for estimates of fixed and random effects ” on p. 196.

## **Testing**

### **Information criteria**

These are as described in “Goodness of fit ” on p. 199.

### **Tests of fixed effects**

For each effect specified in the model, a type III test matrix  $\mathbf{L}$  is constructed from the generating matrix  $H_\omega = (x^T \Omega x)^{-1} x^T \Omega x$ , where  $x = (x_{11}^T, \dots, x_{st}^T, \dots, x_{ST_s}^T)^T$  and  $\Omega = \text{diag}(\omega_{11}, \dots, \omega_{1T_1}, \dots, \omega_{S1}, \dots, \omega_{ST_s})$ . Then the test statistic is

$$F = \frac{\hat{\beta}^T L^* T (L^* \Sigma L^{*T})^{-1} L^* \hat{\beta}}{r_c}$$

where  $r_c = \text{rank}(L^* \Sigma L^{*T})$  and  $L^* = I_{J-1} \otimes L$ . The statistic has an approximate  $F$  distribution. The numerator degrees of freedom is  $r_c$  and the denominator degree of freedom is  $v$ . For more information, see the topic “Method for computing degrees of freedom ” on p. 203.

## Scoring

### PQL-type predicted values and relevant statistics

$(J - 1) \times 1$  predicted vector of the linear predictor

$$\hat{\eta}_{st} = (I_{J-1} \otimes x_{st})^T \hat{\beta} + (I_{J-1} \otimes z_{st})^T \hat{\gamma}_s + 1_{J-1} \otimes o_{st}$$

Estimated covariance matrix of the linear predictor

$$\begin{aligned} \Sigma_{\hat{\eta}_{st}} = & (I_{J-1} \otimes x_{st})^T \Sigma (I_{J-1} \otimes x_{st}) + (I_{J-1} \otimes z_{st})^T \hat{C}_{22}^s (I_{J-1} \otimes z_{st}) \\ & + (I_{J-1} \otimes z_{st})^T \hat{C}_{21}^s (I_{J-1} \otimes x_{st}) + (I_{J-1} \otimes x_{st})^T \left( \hat{C}_{21}^s \right)^T (I_{J-1} \otimes z_{st}) \end{aligned}$$

where  $\hat{C}_{22}^s$  is a diagonal block corresponding to the  $s$ th super subject, the approximate covariance matrix of  $\hat{\gamma}_s - \gamma_s$ ;  $\hat{C}_{21}^s$  is a part of  $\hat{C}_{21}$  corresponding to the  $s$ th super subject.

The estimated standard error of the  $j$ th element in  $\hat{\eta}_{st}$ ,  $\hat{\eta}_{st,j}$ , is the square root of the  $j$ th diagonal element of  $\Sigma_{\hat{\eta}_{st}}$ ,

$$\sigma_{\hat{\eta}_{st,j}} = \sqrt{\sigma_{\hat{\eta}_{st,jj}}}$$

Predicted value of the probability for category  $j$

$$\hat{\pi}_{st,j} = g^{-1}(\hat{\eta}_{st,j}) = \begin{cases} \frac{\exp(\hat{\eta}_{st,j})}{J-1 + \sum_{k=1}^{J-1} \exp(\hat{\eta}_{st,k})}, j = 1, \dots, J-1, \\ \frac{1}{J-1 + \sum_{k=1}^{J-1} \exp(\hat{\eta}_{st,k})}, j = J. \end{cases}$$

Predicted category

$$c(x_{st}) = \arg \max_j \hat{\pi}_{st,j},$$

If there is a tie in determining the predicted category, the tie will be broken by choosing the category with the highest  $N_j = \sum_{s=1}^S \sum_{t=1}^{T_s} f_{st} y_{st,j}$ . If there is still a tie, the one with the lowest category number is chosen.

Approximate  $100(1-\alpha)\%$  confidence intervals for the predicted probabilities

The covariance matrix of  $\hat{\pi}_{st}$  can be computed as

$$Cov(\hat{\pi}_{st}) = \nabla g^{-1}(\hat{\eta}_{st})^T \Sigma_{\hat{\eta}_{st}} \nabla g^{-1}(\hat{\eta}_{st})$$

where

$$\nabla g^{-1}(\hat{\eta}_{st}) = \begin{bmatrix} \frac{\partial \hat{\pi}_{st,1}}{\partial \hat{\eta}_{st,1}} & \cdots & \frac{\partial \hat{\pi}_{st,J-1}}{\partial \hat{\eta}_{st,1}} & \frac{\partial \hat{\pi}_{st,J}}{\partial \hat{\eta}_{st,1}} \\ \vdots & & \vdots & \vdots \\ \frac{\partial \hat{\pi}_{st,1}}{\partial \hat{\eta}_{st,J-1}} & \cdots & \frac{\partial \hat{\pi}_{st,J-1}}{\partial \hat{\eta}_{st,J-1}} & \frac{\partial \hat{\pi}_{st,J}}{\partial \hat{\eta}_{st,J-1}} \end{bmatrix}$$

with

$$\frac{\partial \hat{\pi}_{st,j}}{\partial \hat{\eta}_{st,k}} = \begin{cases} \hat{\pi}_{st,j}(1 - \hat{\pi}_{st,j}), & j = k \\ -\hat{\pi}_{st,j}\hat{\pi}_{st,k}, & j \neq k \end{cases}$$

then the confidence interval is

$$\hat{\pi}_{st,j} \pm t_{v,\alpha/2} \hat{\sigma}_{\pi_{st,j}}, j = 1, \dots, J$$

where  $\hat{\sigma}_{\pi_{st,j}}^2$  is the  $j$ th diagonal element of  $Cov(\hat{\pi}_{st})$  and the estimated variance of  $\hat{\pi}_{st,j}$ ,  $j = 1, \dots, J$ .

## Ordinal multinomial distribution

The ordinal multinomial distribution requires some extra notation and explanation.

### Notation

The following notation is used throughout this section unless otherwise stated:

$S$	Number of super subjects.
$T_s$	Number of cases in the $s$ th super subject.
$y_{st}$	Ordinal categorical target for the $t$ th case in the $s$ th super subject. Its category values are denoted as consecutive integers from 1 to $J$ .
$J$	The total number of categories for target.
$y_{st}$	Indicator vector of $y_{st}$ , $y_{st} = (y_{st,1}, \dots, y_{st,J-1})^T$ , where $y_{st,j} = 1$ if $y_{st} = j$ , otherwise $y_{st,j} = 0$ . The superscript $T$ means the transpose of a matrix or vector.
$y_s$	$y_s = (y_{s1}^T, \dots, y_{sT_s}^T)^T$ , $s = 1, \dots, S$ .
$y$	$y = (y_1^T, \dots, y_S^T)^T$
$\lambda_{st,j}$	Cumulative target probability for category $j$ for the $t$ th case in the $s$ th super subject; $\lambda_{st,j} = P(y_{st} \leq j)$ .
$\lambda$	$\lambda = (\lambda_1^T, \dots, \lambda_S^T)^T$ , where $\lambda_s = (\lambda_{s1}^T, \dots, \lambda_{sT_s}^T)^T$ and $\lambda_{st}^T = (\lambda_{st,1}, \dots, \lambda_{st,J-1})$ , $s = 1, \dots, S$ and $t = 1, \dots, T_s$ .
$\pi_{st,j}$	Probability of category $j$ for the $t$ th case in the $s$ th super subject; that is, $\pi_{st,j} = P(y_{st} = j)$ and $\pi_{st,j} = \lambda_{st,j} - \lambda_{st,j-1}$ .

$\pi_{st}$	$\pi_{st} = (\pi_{st,1}, \dots, \pi_{st,J-1})^T$
$\pi_s$	$\pi_s = (\pi_{s1}^T, \dots, \pi_{sT_s}^T)^T, s = 1, \dots, S$
$\pi$	$\pi = (\pi_1^T, \dots, \pi_S^T)^T$
$\eta_{st,j}$	Linear predictor value for category $j$ of the $t$ th case in the $s$ th super subject.
$\eta_{st}$	$\eta_{st} = (\eta_{st,1}, \dots, \eta_{st,J-1})^T$
$\eta_s$	$\eta_s = (\eta_{s1}^T, \dots, \eta_{sT_s}^T)^T, s = 1, \dots, S$
$\eta$	$(n(J-1)) \times 1$ vector of linear predictor. $\eta = (\eta_1^T, \dots, \eta_S^T)^T$
$x_{st}$	$p \times 1$ vector of predictors for the $t$ th case in the $s$ th super subject.
$z_{st}$	$r \times 1$ vector of coefficients for the random effect corresponding to the $t$ th case in the $s$ th super subject.
$O$	$n \times 1$ vector of offsets, $O = (o_{11}, \dots, o_{1T_1}, \dots, o_{ST_S})^T$ , where $o_{si}$ is the offset value of the $t$ th case in the $s$ th super subject. This can't be the target ( $y$ ) or one of the predictors ( $X$ ). The offset must be continuous.
$O^*$	$O^* = O \otimes 1_{J-1}$ , where $1_q$ is a length $q$ vector of 1's.
$\Psi$	$J-1 \times 1$ vector of threshold parameters, $\Psi = (\psi_1, \psi_2, \dots, \psi_{J-1})^T$ and $\psi_1 < \psi_2 < \dots < \psi_{J-1}$
$\beta$	$p \times 1$ vector of unknown parameters.
$B$	$(J-1+p) \times 1$ vector of all parameters $B = (\Psi^T, \beta^T)^T$
$\omega_{st}$	Scale weight of the $t$ th case in the $s$ th super subject. It does not have to be integers. If it is less than or equal to 0 or missing, the corresponding case is not used.
$\omega$	$n \times 1$ vector of scale weight variable, $\omega = (\omega_{11}, \dots, \omega_{1T_1}, \dots, \omega_{S1}, \dots, \omega_{ST_S})^T$ .
$f_{st}$	Frequency weight of the $t$ th case in the $s$ th super subject. If it is a non-integer value, it is treated by rounding the value to the nearest integer. If it is less than 0.5 or missing, the corresponding cases are not used.
$f$	$n \times 1$ vector of frequency count variable, $f = (f_{11}, \dots, f_{1T_1}, \dots, f_{S1}, \dots, f_{ST_S})^T$ .
$N$	Effective sample size, $N = \sum_{i=1}^n f_i$ . If frequency count variable $f$ is not used, $N = n$ .
$A \otimes B$	direct (or Kronecker) product of $A$ and $B$ , which is equal to $\begin{bmatrix} a_{11}B & a_{12}B & a_{13}B \\ a_{21}B & a_{22}B & a_{23}B \\ a_{31}B & a_{32}B & a_{33}B \end{bmatrix}$
$1_m$	$m \times 1$ vector of 1's; $1_m = (1, \dots, 1)^T$

## Model

The form of a generalized linear mixed model for an ordinal target with random effects is

$$\eta = g(\lambda) = XB + Z\gamma + O^*$$

where  $\eta$  is the expanded linear predictor vector;  $\lambda$  is the expanded cumulative target probability vector;  $g(\cdot)$  is a cumulative link function;  $\mathbf{X}$  is the expanded design matrix for fixed effects arranged as follows

$$\begin{aligned} \mathbf{X} &= \begin{pmatrix} \mathbf{X}_1 \\ \vdots \\ \mathbf{X}_S \end{pmatrix}, \\ \mathbf{X}_s &= \begin{pmatrix} \mathbf{X}_{s1} \\ \vdots \\ \mathbf{X}_{sT_s} \end{pmatrix}_{T_s(J-1) \times (J-1+p)}, \\ \mathbf{X}_{st} &= \begin{pmatrix} \mathbf{I}_{J-1} & \mathbf{1}_{J-1} \otimes -\mathbf{x}_{st}^T \end{pmatrix}_{(J-1) \times (J-1+p)} \\ &= \begin{pmatrix} 1 & \cdots & 0 & -\mathbf{x}_{st}^T \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & 1 & -\mathbf{x}_{st}^T \end{pmatrix} \\ &= \begin{pmatrix} 1 & \cdots & 0 & -x_{st,1} & \cdots & -x_{st,p} \\ \vdots & \ddots & \vdots & \vdots & \cdots & \vdots \\ 0 & \cdots & 1 & -x_{st,1} & \cdots & -x_{st,p} \end{pmatrix} \end{aligned}$$

$\mathbf{B} = (\boldsymbol{\psi}^T, \boldsymbol{\beta}^T)^T = ((\psi_1, \dots, \psi_{J-1}), \boldsymbol{\beta}^T)^T$ ;  $\mathbf{Z}$  is the expanded design matrix for random effects arranged as follows

$$\begin{aligned} \mathbf{Z} &= \begin{pmatrix} \mathbf{Z}_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{Z}_S \end{pmatrix}, \\ \mathbf{Z}_s &= \begin{pmatrix} \mathbf{Z}_{s1} \\ \vdots \\ \mathbf{Z}_{sT_s} \end{pmatrix}_{T_s(J-1) \times r}, \\ \mathbf{Z}_{st} &= \left( \mathbf{1}_{J-1} \otimes -\mathbf{z}_{st}^T \right)_{(J-1) \times r}, \end{aligned}$$

$\boldsymbol{\gamma}$  is a vector of random effects which are assumed to be normally distributed with mean  $\mathbf{0}$  and variance matrix  $\mathbf{G}$ .

The variance of  $\mathbf{y}$ , conditional on the random effects is

$$\text{Var}(y|\boldsymbol{\gamma}) = A_\mu^{1/2} \mathbf{R} A_\mu^{1/2}$$

where  $A_\mu = \bigoplus_{s=1}^S \bigoplus_{t=1}^{T_s} \left( \text{diag}(\pi_{st}) - \pi_{st} \boldsymbol{\pi}_{st}^T \right) / \omega_{st}$  and  $\mathbf{R} = \phi \mathbf{I}$  which means that R-side effects are not supported for the multinomial distribution.  $\phi$  is set to 1.

## Estimation

### Linear mixed pseudo model

Similarly to “Linear mixed pseudo model” on p. 192, we can obtain a weighted linear mixed model

$$v = X\beta + Z\gamma + \epsilon$$

where  $v \equiv D^{-1}(y - \tilde{\pi}) + g(\tilde{\lambda}) - O^*$  and error terms  $\epsilon \sim N\left(0, D^{-1}A_{\tilde{\pi}}^{1/2}RA_{\tilde{\pi}}^{1/2}(D^{-1})^T\right)$  with

$$D = \begin{matrix} S & T_s \\ \oplus & \oplus \\ s=1 & t=1 \end{matrix} D_{st} = \begin{matrix} S & T_s \\ \oplus & \oplus \\ s=1 & t=1 \end{matrix} \frac{dg^{-1}(\tilde{\eta}_{st})}{d\tilde{\eta}_{st}} = \begin{matrix} S & T_s \\ \oplus & \oplus \\ s=1 & t=1 \end{matrix} \frac{d\tilde{\lambda}_{st}}{d\tilde{\eta}_{st}}$$

$$D_{st} = \begin{bmatrix} \frac{\partial \tilde{\lambda}_{st,1}}{\partial \tilde{\eta}_{st,1}} & 0 & \cdots & 0 & 0 \\ -\frac{\partial \tilde{\lambda}_{st,1}}{\partial \tilde{\eta}_{st,1}} & \frac{\partial \tilde{\lambda}_{st,2}}{\partial \tilde{\eta}_{st,2}} & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \ddots & \frac{\partial \tilde{\lambda}_{st,J-2}}{\partial \tilde{\eta}_{st,J-2}} & 0 \\ 0 & 0 & \cdots & -\frac{\partial \tilde{\lambda}_{st,J-2}}{\partial \tilde{\eta}_{st,J-2}} & \frac{\partial \tilde{\lambda}_{st,J-1}}{\partial \tilde{\eta}_{st,J-1}} \end{bmatrix}$$

and

$$A_{\tilde{\mu}} = \begin{matrix} S & T_s \\ \oplus & \oplus \\ s=1 & t=1 \end{matrix} \left( \text{diag}(\tilde{\pi}_{st}) - \tilde{\pi}_{st}\tilde{\pi}_{st}^T \right) / \omega_{st}.$$

And block diagonal weight matrix is

$$\tilde{W} = D^T A_{\tilde{\mu}}^{-1} D$$

The Gaussian log pseudo-likelihood (PL) and restricted log pseudo-likelihood (REPL), which are expressed as the functions of covariance parameters in  $\theta$ , corresponding to the linear mixed model for  $v$  are the following:

$$\ell(\theta; v) = -\frac{1}{2} \ln |\mathbf{V}(\theta)| - \frac{1}{2} \mathbf{r}(\theta)^T \mathbf{V}(\theta)^{-1} \mathbf{r}(\theta) - \frac{N}{2} \ln(2\pi)$$

$$\ell_R(\theta; v) = -\frac{1}{2} \ln |\mathbf{V}(\theta)| - \frac{1}{2} \mathbf{r}(\theta)^T \mathbf{V}(\theta)^{-1} \mathbf{r}(\theta) - \frac{1}{2} \ln |\mathbf{X}^T \mathbf{V}(\theta)^{-1} \mathbf{X}| - \frac{N - p_x}{2} \ln(2\pi)$$

where  $\mathbf{V}(\theta) = Z\mathbf{G}(\theta)Z^T + \tilde{W}^{-1/2}\mathbf{R}(\theta)\tilde{W}^{-1/2}$ ,  $\mathbf{r}(\theta) = v - X\hat{\mathbf{B}}$ ,  $N$  denotes the effective sample size, and  $p_x$  denotes the total number of non-redundant parameters for  $\mathbf{B}$ .

The parameter  $\theta$  can be estimated by linear mixed model using the objection function  $-2\ell(\theta; v)$  or  $-2\ell_R(\theta; v)$ ,  $\mathbf{B}$  and  $\gamma$  are computed as

$$\hat{\mathbf{B}} = \left( X^T V(\hat{\theta})^{-1} X \right)^{-1} X^T V(\hat{\theta})^{-1} v$$

$$\hat{\gamma} = \hat{G} Z^T V(\hat{\theta})^{-1} \hat{r}$$

### **Iterative process**

The doubly iterative process for the estimation of  $\theta$  is the same as that for other distributions, if we replace  $\tilde{\mu}$  and  $X\tilde{\mathbf{B}} + Z\tilde{\gamma} + O$  with  $\tilde{\pi}$  and  $X\tilde{\mathbf{B}} + Z\tilde{\gamma} + O^*$  respectively, and set initial estimation of  $\pi$  as

$$\pi^{(0)} = \frac{y + 1/J}{2}$$

For more information, see the topic “Iterative process ” on p. 194.

## **Post-estimation statistics**

### **Wald confidence intervals**

The Wald confidence intervals for covariance parameter estimates are described in “Wald confidence intervals for covariance parameter estimates ” on p. 195.

### **Statistics for estimates of fixed and random effects**

$\hat{C}$  is the approximate covariance matrix of  $(\hat{\mathbf{B}} - \mathbf{B}, \hat{\gamma} - \gamma)$  and  $R^*$  in  $\hat{C}$  should be

$$R^* = \text{var}(v|\gamma) = D^{-1} A_{\tilde{\pi}}^{1/2} R A_{\tilde{\pi}}^{1/2} (D^{-1})^T.$$

### **Statistics for estimates of fixed and random effects on original scale**

If the fixed effects are transformed when constructing matrix  $\mathbf{X}$ , then the final estimates of  $\mathbf{B}$ , denoted as  $\hat{B}^*$ . They would be transformed back on the original scale, denoted as  $\hat{B}$ , as follows:

$$\mathbf{B} = \begin{pmatrix} \psi \\ \beta \end{pmatrix} = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_{J-1} \\ \beta \end{pmatrix} = \mathbf{A} \begin{pmatrix} \Psi^* \\ \beta^* \end{pmatrix} = \mathbf{A} \mathbf{B}^*$$

where

$$\mathbf{A} = \begin{pmatrix} \mathbf{I}_{J-1} & \mathbf{1}_{J-1} \otimes (\mathbf{c}^T \mathbf{S}^{-1}) \\ 0 & \mathbf{S}^{-1} \end{pmatrix}$$

### **Estimated covariance matrix of the fixed effects parameters**

The estimated covariance matrix of the fixed effects parameters are described in “Statistics for estimates of fixed and random effects ” on p. 196.

### **Standard error for estimates in fixed effects and predictions in random effects**

Let  $\hat{\psi}_j, j = 1, \dots, J - 1$ , be threshold parameter estimates and  $\hat{\beta}_i, i = 1, \dots, p$ , denote non-redundant regression parameter estimates. Their standard errors are the square root of the diagonal elements of  $\Sigma_M$  or  $\Sigma_R$ :  $\hat{\sigma}_{\psi_j} = \sqrt{\sigma_{jj}}$  and  $\hat{\sigma}_{\beta_i} = \sqrt{\sigma_{(J-1+i),(J-1+i)}}$ , respectively, where  $\sigma_{ii}$  is the  $i$ th diagonal element of  $\Sigma_M$  or  $\Sigma_R$ .

Standard errors for predictions in random effects are as those described in “Statistics for estimates of fixed and random effects ” on p. 196.

### **Test statistics for estimates in fixed effects and predictions in random effects**

The hypotheses  $H_{0j} : \psi_j = 0, j = 1, \dots, J - 1$ , are tested for threshold parameters using the  $t$  statistic:

$$t_{\psi_j} = \frac{\hat{\psi}_j}{\hat{\sigma}_{\psi_j}}$$

Test statistics for estimates in fixed effects and predictions in random effects are otherwise as those described in “Statistics for estimates of fixed and random effects ” on p. 196.

### **Wald confidence intervals for estimates in fixed effects and random effects predictions**

The  $100(1 - \alpha)\%$  Wald confidence interval for threshold parameter is given by

$$\left( \hat{\psi}_j - t_{v, \alpha/2} \hat{\sigma}_{\psi_j}, \hat{\psi}_j + t_{v, \alpha/2} \hat{\sigma}_{\psi_j} \right)$$

Wald confidence intervals are otherwise as those described in “Statistics for estimates of fixed and random effects ” on p. 196.

The degrees of freedom can be computed by the residual method or Satterthwaite method. For the residual method,  $v = N - (J - 1 + p_x)$ . For the Satterthwaite method, it should be similar to that described in “Method for computing degrees of freedom ” on p. 203.

## **Testing**

### **Information criteria**

These are as described in “Goodness of fit ” on p. 199, with the following modifications.

For REPL, the value of  $N$  is chosen to be effective sample size minus number of non-redundant parameters in fixed effects,  $\sum_{i=1}^n f_i - (J - 1 + p_x)$ , where  $p_x$  is the number of non-redundant parameters in fixed effects, and  $d$  is the number of covariance parameters.

For PL, the value of  $N$  is effective sample size,  $\sum_{i=1}^n f_i$ , and  $d$  is the number of number of non-redundant parameters in fixed effects,  $J - 1 + p_x$ , plus the number of covariance parameters.

### **Tests of fixed effects**

For each effect specified in the model excluding threshold parameters, a type I or III test matrix  $\mathbf{L}_i$  is constructed and  $H_0: \mathbf{L}_i\mathbf{B} = \mathbf{0}$  is tested. Construction of matrix  $\mathbf{L}_i$  is based on matrix  $\mathbf{H}_\omega = (\mathbf{X}_1^T \boldsymbol{\Omega} \mathbf{X}_1)^{-1} \mathbf{X}_1^T \boldsymbol{\Omega} \mathbf{X}_1$ , where  $\mathbf{X}_1 = (1, -\mathbf{X})$  and such that  $\mathbf{L}_i\mathbf{B}$  is estimable. Note that  $\mathbf{L}_i\mathbf{B}$  is estimable if and only if  $\mathbf{L}_0 = \mathbf{L}_0\mathbf{H}_\omega$ , where  $\mathbf{L}_0 = (\mathbf{l}_0, \mathbf{L}(\beta))$ . Construction of  $\mathbf{L}_0$  considers a partition of the more general test matrix  $\mathbf{L}_i = (\mathbf{L}_i(\psi), \mathbf{L}_i(\beta))$  first, where  $\mathbf{L}_i(\psi) = (\mathbf{l}_1, \dots, \mathbf{l}_{J-1})$  consists of columns corresponding to the threshold parameters and  $\mathbf{L}_i(\beta)$  is the part of  $\mathbf{L}_i$  corresponding to regression parameters, then replace  $\mathbf{L}_i(\psi)$  with their sum  $\mathbf{l}_0 = \sum_{j=1}^{J-1} \mathbf{l}_j$  to get  $\mathbf{L}_0$ .

Note that the threshold-parameter effect is not tested for both type I and III analyses and construction of  $\mathbf{L}_i$  is the same as in GENLIN. For more information, see the topic “Default Tests of Model Effects” on p. 182. Similarly, if the fixed effects are transformed when constructing matrix  $\mathbf{X}$ , then  $\mathbf{H}_\omega$  should be constructed based on transformed values.

## **Scoring**

### **PQL-type predicted values and relevant statistics**

$(J - 1) \times 1$  predicted vector of the linear predictor

$$\hat{\eta}_{st} = X_{st}\hat{\mathbf{B}} + Z_{st}\hat{\gamma}_s + \mathbf{1}_{J-1} \otimes o_{st}$$

Estimated covariance matrix of the linear predictor

$$\Sigma_{\hat{\eta}_{st}} = X_{st}\Sigma X_{st}^T + Z_{st}\hat{C}_{22}^s Z_{st}^T + Z_{st}\hat{C}_{21}^s X_{st}^T + X_{st}(\hat{C}_{21}^s)^T Z_{st}^T$$

where  $\hat{C}_{22}^s$  is a diagonal block corresponding to the  $s$ th super subject, the approximate covariance matrix of  $\hat{\gamma}_s - \gamma_s$ ;  $\hat{C}_{21}^s$  is a part of  $\hat{C}_{21}$  corresponding to the  $s$ th super subject.

The estimated standard error of the  $j$ th element in  $\hat{\eta}_{st}$ ,  $\hat{\eta}_{st,j}$ , is the square root of the  $j$ th diagonal element of  $\Sigma_{\hat{\eta}_{st}}$ ,

$$\sigma_{\hat{\eta}_{st,j}} = \sqrt{\sigma_{\hat{\eta}_{st},jj}}$$

Predicted value of the cumulative probability for category  $j$

$$\hat{\gamma}_{st,j} = g^{-1}(\hat{\eta}_{st,j}), j = 1, \dots, J - 1$$

with  $\hat{\gamma}_{i,J} = 1$ .

Predicted category

$$c(x_{st}) = \arg \max_j \hat{\pi}_{st,j},$$

where  $\hat{\pi}_{st,j} = \hat{\gamma}_{st,j} - \hat{\gamma}_{st,j-1}$ .

If there is a tie in determining the predicted category, the tie will be broken by choosing the category with the highest  $N_j = \sum_{s=1}^S \sum_{t=1}^{T_s} f_{st} y_{st,j}$ . If there is still a tie, the one with the lowest category number is chosen.

Approximate  $100(1-\alpha)\%$  confidence intervals for the cumulative predicted probabilities

$$g^{-1}(\hat{\eta}_{st,j} \pm t_{v,\alpha/2} \hat{\sigma}_{\hat{\eta}_{st,j}}), j = 1, \dots, J - 1,$$

If either endpoint in the argument is outside the valid range for the inverse link function, the corresponding confidence interval endpoint is set to a system missing value.

The degrees of freedom can be computed by the residual method or Satterthwaite method.

For the residual method,  $v = N - (J - 1 + p_x)$ . For Satterthwaite's approximation, the  $\mathbf{L}$  matrix is constructed by  $(X_{st,j}, Z_{st,j})$ , where  $X_{st,j}$  and  $Z_{st,j}$  are the  $j$ th rows of  $X_{st}$  and  $Z_{st}$ , respectively, corresponding to the  $j$ th category. For example, the  $\mathbf{L}$  matrix is  $(1, 0, \dots, 0, -x_{st}^T, -z_{st}^T)_{1 \times (J-1+p+r)}$  for the 1st category. The computation should then be similar to that described in "Method for computing degrees of freedom" on p. 203.

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# Imputation of Missing Values

The following methods are available for imputing missing values:

**Fixed.** Substitutes a fixed value (either the field mean, midpoint of the range, or a constant that you specify).

**Random.** Substitutes a random value based on a normal or uniform distribution.

**Expression.** Allows you to specify a custom expression. For example, you could replace values with a global variable created by the Set Globals node.

**Algorithm.** Substitutes a value predicted by a model based on the C&RT algorithm. For each field imputed using this method, there will be a separate C&RT model, along with a Filler node that replaces blanks and nulls with the value predicted by the model. A Filter node is then used to remove the prediction fields generated by the model.

Details of each imputation method are provided below.

## Imputing Fixed Values

For fixed value imputation, three options are available:

**Mean.** Substitutes the mean of the valid training data values for the field being imputed,

$$\frac{\sum_{i=1}^{n_{valid}} x_i}{n_{valid}}$$

where  $x_i$  is the value of field  $x$  for record  $i$ , excluding missing values, and  $n_{valid}$  is the number of records with valid values for field  $x$ .

**Midrange.** Substitutes the value halfway between the minimum and maximum valid values for the field being imputed,

$$x_{\min} + \frac{x_{\max} - x_{\min}}{2} = \frac{x_{\max} + x_{\min}}{2}$$

where  $x_{\min}$  and  $x_{\max}$  are the minimum and maximum observed valid values for field  $x$ , respectively.

**Constant.** Substitutes the user-specified constant value.

For imputing fixed missing values in set or flag fields, only the Constant option is available.

*Note:* Using fixed imputed values for scale fields will artificially reduce the variance for that field, which can interfere with model building using the field. If you impute using fixed values and find that the field no longer has the expected effect in a model, consider imputing with a different method that has a smaller impact on the field's variance.

## Imputing Random Values

For random value imputation, the options depend on the type of the field being imputed.

### Range Fields

For range fields, you can select from a uniform distribution or a normal distribution.

**Uniform distribution.** Values are generated randomly on the interval  $[x_{\min}, x_{\max}]$ , where each value in the interval is equally likely to be generated.

**Normal distribution.** Values are generated from a normal distribution with mean  $\bar{x}_{valid}$  and variance  $s_{valid}^2$ , where  $\bar{x}_{valid}$  and  $s_{valid}^2$  are derived from the valid observed values of  $x$  in the training data,

$$\bar{x}_{valid} = \frac{\sum_{i=1}^{n_{valid}} x_i}{n_{valid}}$$

$$s_{valid}^2 = \frac{\sum_{i=1}^{n_{valid}} (x_i - \bar{x}_{valid})^2}{n_{valid} - 1}$$

### Set Fields

For set fields, random imputed values are selected from the list of observed values. By default, the probabilities of all values are equal,

$$p(k) = \frac{1}{j}$$

for the  $j$  possible values of  $k$ . The Equalize button will return any modified values to the default equal probabilities.

If you select Based on Audit, probabilities are assigned proportional to the relative frequencies of the values in the training data

$$p(k) = \frac{n_k}{n_{valid}}$$

where  $n_k$  is the number of records for which  $x_i = k$ .

If you select Normalize, values are adjusted to sum to 1.0, maintaining the same relative proportions,

$$p_{normalized}(k) = \frac{p(k)}{\sum_k p(k)}$$

This is useful if you want to enter your own weights for generated random values, but they aren't expressed as probabilities. For example, if you know you want twice as many *No* values as *Yes* values, you can enter 2 for *No* and 1 for *Yes* and click Normalize. Normalization will adjust the values to 0.667 and 0.333, preserving the relative weights but expressing them as probabilities.

## ***Imputing Values Derived from an Expression***

For expression-based imputation, imputed values are based on a user-specified CLEM expression. The expression is evaluated just as it would be for a filler node. Note that some expressions may return \$null or other missing values, with the result that missing values may exist even after imputation with this method.

## ***Imputing Values Derived from an Algorithm***

For the Algorithm method, a C&RT model is built for each field to be imputed, using all other input fields as predictors. For each record that is imputed, the model for the field to be imputed is applied to the record to produce a prediction, which is used as the imputed value. For more information, see the topic “Overview of C&RT” on p. 59.



# ***K-Means Algorithm***

## ***Overview***

The *k*-means method is a clustering method, used to group records based on similarity of values for a set of input fields. The basic idea is to try to discover *k* clusters, such that the records within each cluster are similar to each other and distinct from records in other clusters. *K*-means is an iterative algorithm; an initial set of clusters is defined, and the clusters are repeatedly updated until no more improvement is possible (or the number of iterations exceeds a specified limit).

## ***Primary Calculations***

In building the *k*-means model, input fields are encoded to account for differences in measurement scale and type, and the clusters are defined and updated to generate the final model. These calculations are described below.

## ***Field Encoding***

Input fields are recoded before the values are input to the algorithm as described below.

### ***Scaling of Range Fields***

In most datasets, there's a great deal of variability in the scale of range fields. For example, consider *age* and *number of cars per household*. Depending on the population of interest, *age* may take values up to 80 or even higher. Values for *number of cars per household*, however, are unlikely to exceed three or four in the vast majority of cases.

If you use both of these fields in their natural scale as inputs for a model, the *age* field is likely to be given much more weight in the model than *number of cars per household*, simply because the values (and therefore the differences between records) for the former are so much larger than for the latter.

To compensate for this effect of scale, range fields are transformed so that they all have the same scale. In IBM® SPSS® Modeler, range fields are rescaled to have values between 0 and 1. The transformation used is

$$x'_i = \frac{x_i - x_{\min}}{x_{\max} - x_{\min}},$$

where  $x'_i$  is the rescaled value of input field *x* for record *i*,  $x_i$  is the original value of *x* for record *i*,  $x_{\min}$  is the minimum value of *x* for all records, and  $x_{\max}$  is the maximum value of *x* for all records.

### ***Numeric Coding of Symbolic Fields***

For modeling algorithms that base their calculations on numerical differences between records, symbolic fields pose a special challenge. How do you calculate a numeric difference for two categories?

A common approach to the problem, and the approach used in IBM® SPSS® Modeler, is to recode a symbolic field as a group of numeric fields with one numeric field for each category or value of the original field. For each record, the value of the derived field corresponding to the category of the record is set to 1.0, and all the other derived field values are set to 0.0. Such derived fields are sometimes called **indicator fields**, and this recoding is called **indicator coding**.

For example, consider the following data, where  $x$  is a symbolic field with possible values A, B, and C:

Record #	$X$	$X_1'$	$X_2'$	$X_3'$
1	B	0	1	0
2	A	1	0	0
3	C	0	0	1

In this data, the original set field  $x$  is recoded into three derived fields  $x_1'$ ,  $x_2'$ , and  $x_3'$ .  $x_1'$  is an indicator for category A,  $x_2'$  is an indicator for category B, and  $x_3'$  is an indicator for category C.

### Applying the Set Encoding Value

After recoding set fields as described above, the algorithm can calculate a numerical difference for the set field by taking the differences on the  $k$  derived fields (where  $k$  is the number of categories in the original set). However, there is an additional problem. For algorithms that use the Euclidean distance to measure differences between records, the difference between two records with different values  $i$  and  $j$  for the set is

$$\sqrt{\sum_{k=1}^J (x_{k1} - x_{k2})^2}$$

where  $J$  is the number of categories, and  $x_{kn}$  is value of the derived indicator for category  $k$  for record  $n$ . But the values will be different on *two* of the derived indicators,  $x_i$  and  $x_j$ . Thus, the sum will be  $\sqrt{(1-0)^2 + (0-1)^2} = \sqrt{2} \approx 1.414$ , which is larger than 1.0. That means that based on this coding, set fields will have more weight in the model than range fields that are rescaled to 0-1 range.

To account for this bias,  $k$ -means applies a scaling factor to the derived set fields, such that a difference of values on a set field produces a Euclidean distance of 1.0. The default scaling factor is  $\sqrt{\frac{1}{2}} \approx 0.707$ . You can see that this value gives the desired result by inserting the value into the distance formula:

$$\sqrt{\left(\sqrt{\frac{1}{2}} - 0\right)^2 + \left(0 - \sqrt{\frac{1}{2}}\right)^2} = \sqrt{\frac{1}{2} + \frac{1}{2}} = 1$$

The user can specify a different scaling factor by changing the Encoding value for sets parameter in the K-Means node expert options.

### **Encoding of Flag Fields**

Flag fields are a special case of symbolic fields. However, because they have only two values in the set, they can be handled in a slightly more efficient way than other set fields. Flag fields are represented by a single numeric field, taking the value of 1.0 for the “true” value and 0.0 for the “false” value. Blanks for flag fields are assigned the value 0.5.

### **Model Parameters**

The primary calculation in  $k$ -means is an iterative process of calculating cluster centers and assigning records to clusters. The primary steps in the procedure are:

1. Select initial cluster centers
2. Assign each record to the nearest cluster
3. Update the cluster centers based on the records assigned to each cluster
4. Repeat steps 2 and 3 until either:
  - In step 3, there is no change in the cluster centers from the previous iteration, or
  - The number of iterations exceeds the maximum iterations parameter

Clusters are defined by their centers. A **cluster center** is a vector of values for the (encoded) input fields. The vector values are based on the mean values for records assigned to the cluster.

### **Selecting Initial Cluster Centers**

The user specifies  $k$ , the number of clusters in the model. Initial cluster centers are chosen using a maximin algorithm:

1. Initialize the first cluster center as the values of the input fields for the first data record.
2. For each data record, compute the minimum (Euclidean) distance between the record and each defined cluster center.
3. Select the record with the largest minimum distance from the defined cluster centers. Add a new cluster center with values of the input fields for the selected record.
4. Repeat steps 2 and 3 until  $k$  cluster centers have been added to the model.

Once initial cluster centers have been chosen, the algorithm begins the iterative assign/update process.

### **Assigning Records to Clusters**

In each iteration of the algorithm, each record is assigned to the cluster whose center is closest. Closeness is measured by the usual squared Euclidean distance

$$d_{ij} = \|X_i - C_j\|^2 = \sum_{q=1}^Q (x_{qi} - c_{qj})^2$$

where  $X_i$  is the vector of encoded input fields for record  $i$ ,  $C_j$  is the cluster center vector for cluster  $j$ ,  $Q$  is the number of encoded input fields,  $x_{qi}$  is the value of the  $q$ th encoded input field for the  $i$ th record, and  $c_{qj}$  is the value of the  $q$ th encoded input field for the  $j$ th record.

For each record, the distance between the record and each cluster center is calculated, and the cluster center whose distance from the record is smallest is assigned as the record's new cluster. When all records have been assigned, the cluster centers are updated.

### **Updating Cluster Centers**

After records have been (re)assigned to their closest clusters, the cluster centers are updated. The cluster center is calculated as the mean vector of the records assigned to the cluster:

$$C_j = \bar{X}_j$$

where the components of the mean vector  $\bar{X}_j$  are calculated in the usual manner,

$$\bar{x}_{qj} = \frac{\sum_{i=1}^{n_j} x_{qi}(j)}{n_j}$$

where  $n_j$  is the number of records in cluster  $j$ ,  $x_{qi}(j)$  is the  $q$ th encoded field value for record  $i$  which is assigned to cluster  $j$ .

### **Blank Handling**

In  $k$ -means, blanks are handled by substituting “neutral” values for the missing ones. For range and flag fields with missing values (blanks and nulls), the missing value is replaced with 0.5. For set fields, the derived indicator field values are all set to 0.0.

### **Effect of Options**

There are several options that affect the way the model calculations are carried out.

#### **Maximum Iterations**

The maximum iterations parameter controls how long the algorithm will continue searching for a stable cluster solution. The algorithm will repeat the classify/update cycle no more than the number of times specified. If and when this limit is reached, the algorithm terminates and produces the current set of clusters as the final model.

**Error Tolerance**

The error tolerance parameter provides another means of controlling how long the algorithm will continue searching for a stable cluster solution. The maximum change in cluster means for an iteration  $t$  is calculated as

$$\max_j \|C_j(t) - C_j(t - 1)\|$$

where  $C_j(t)$  is the cluster center vector for the  $j$ th cluster at iteration  $t$  and  $C_j(t - 1)$  is the cluster center vector at the previous iteration. If the maximum change is less than the specified tolerance for the current iteration, the algorithm terminates and produces the current set of clusters as the final model.

**Encoding Value for Sets**

The encoding value for sets parameter controls the relative weighting of set fields in the  $k$ -means algorithm. The default value of  $\sqrt{0.5} \approx 0.707$  provides an equal weighting between range fields and set fields. To emphasize set fields more heavily, you can set the encoding value closer to 1.0; to emphasize range fields more, set the encoding value closer to 0.0. For more information, see the topic “Numeric Coding of Symbolic Fields” on p. 227.

**Model Summary Statistics**

Cluster proximities are calculated as the Euclidean distance between cluster centers,

$$d_{ij} = \|C_i - C_j\| = \sqrt{\sum_{q=1}^Q (c_{qi} - c_{qj})^2}$$

**Generated Model/Scoring**

Generated  $k$ -means models provide predicted cluster memberships and distance from cluster center for each record.

**Predicted Cluster Membership**

When assigning a new record with a predicted cluster membership, the Euclidean distance between the record and each cluster center is calculated (in the same manner as for assigning records during the model building phase), and the cluster center closest to the record is assigned as the predicted cluster for the record.

**Distances**

The value of the **distance field** for each record, if requested, is calculated as the Euclidean distance between the record and its assigned cluster center,

$$d_{ij} = \|X_i - C_j\| = \sqrt{\sum_{q=1}^Q (x_{qi} - c_{qj})^2}$$

***Blank Handling***

In *k*-means, scoring records with a generated model handles blanks in the same way they are handled during model building. For more information, see the topic “Blank Handling” on p. 230.

# Kohonen Algorithms

## Overview

Kohonen models (Kohonen, 2001) are a special kind of neural network model that performs **unsupervised learning**. It takes the input vectors and performs a type of spatially organized clustering, or feature mapping, to group similar records together and collapse the input space to a two-dimensional space that approximates the multidimensional proximity relationships between the clusters.

The Kohonen network model consists of two layers of neurons or units: an input layer and an output layer. The input layer is fully connected to the output layer, and each connection has an associated weight. Another way to think of the network structure is to think of each output layer unit having an associated center, represented as a vector of inputs to which it most strongly responds (where each element of the center vector is a weight from the output unit to the corresponding input unit).

## Primary Calculations

### Field Encoding

#### Scaling of Range Fields

In most datasets, there's a great deal of variability in the scale of range fields. For example, consider *age* and *number of cars per household*. Depending on the population of interest, *age* may take values up to 80 or even higher. Values for *number of cars per household*, however, are unlikely to exceed three or four in the vast majority of cases.

If you use both of these fields in their natural scale as inputs for a model, the *age* field is likely to be given much more weight in the model than *number of cars per household*, simply because the values (and therefore the differences between records) for the former are so much larger than for the latter.

To compensate for this effect of scale, range fields are transformed so that they all have the same scale. In IBM® SPSS® Modeler, range fields are rescaled to have values between 0 and 1. The transformation used is

$$x_i' = \frac{x_i - x_{\min}}{x_{\max} - x_{\min}},$$

where  $x_i'$  is the rescaled value of input field  $x$  for record  $i$ ,  $x_i$  is the original value of  $x$  for record  $i$ ,  $x_{\min}$  is the minimum value of  $x$  for all records, and  $x_{\max}$  is the maximum value of  $x$  for all records.

#### Numeric Coding of Symbolic Fields

For modeling algorithms that base their calculations on numerical differences between records, symbolic fields pose a special challenge. How do you calculate a numeric difference for two categories?

A common approach to the problem, and the approach used in IBM® SPSS® Modeler, is to recode a symbolic field as a group of numeric fields with one numeric field for each category or value of the original field. For each record, the value of the derived field corresponding to the category of the record is set to 1.0, and all the other derived field values are set to 0.0. Such derived fields are sometimes called **indicator fields**, and this recoding is called **indicator coding**.

For example, consider the following data, where  $x$  is a symbolic field with possible values A, B, and C:

Record #	$X$	$X_1'$	$X_2'$	$X_3'$
1	B	0	1	0
2	A	1	0	0
3	C	0	0	1

In this data, the original set field  $x$  is recoded into three derived fields  $x_1'$ ,  $x_2'$ , and  $x_3'$ .  $x_1'$  is an indicator for category A,  $x_2'$  is an indicator for category B, and  $x_3'$  is an indicator for category C.

### Encoding of Flag Fields

Flag fields are a special case of symbolic fields. However, because they have only two values in the set, they can be handled in a slightly more efficient way than other set fields. Flag fields are represented by a single numeric field, taking the value of 1.0 for the “true” value and 0.0 for the “false” value. Blanks for flag fields are assigned the value 0.5.

### Model Parameters

In a Kohonen model, the parameters are represented as **weights** between input units and output units, or alternately, as a **cluster center** associated with each output unit. Input records are presented to the network, and the cluster centers are updated in a manner similar to that used in building a  $k$ -means model, with an important difference: the clusters are arranged spatially in a two-dimensional grid, and each record affects not only the unit (cluster) to which it is assigned but also units within a **neighborhood** about the winning unit. For more information, see the topic “Neighborhoods” on p. 235.

Training of the Kohonen network proceeds as follows:

- ▶ The network is initialized with small random weights.
- ▶ Input records are presented to the network in random order. As each record is presented, the output unit with the closest center to the input vector is identified as the winning unit. For more information, see the topic “Distances” on p. 235.
- ▶ The weights of the winning unit are adjusted to move the cluster center closer to the input vector. For more information, see the topic “Weight Updates” on p. 235.
- ▶ If the neighborhood size is greater than zero, then other output units that are within the neighborhood of the winning unit are also updated so their centers are closer to the input vector.
- ▶ At the end of each cycle, the learning rate parameter  $\eta$  (eta) is updated.

- ▶ This process repeats until one of the stopping criteria is met. Training proceeds in two phases, a gross structure phase and a fine tuning phase. Typically the first phase has a relatively large neighborhood size and large eta to learn the overall structure of the data, and the second phase uses a smaller neighborhood and smaller eta to fine tune the cluster centers.

### **Distances**

Distances in a Kohonen network are calculated as Euclidean distance between the encoded input vector and the cluster center for the output unit,

$$d_{ij} = \sqrt{\sum_k (x_{ik} - w_{jk})^2}$$

where  $x_{ik}$  is the value of the  $k$ th input field for the  $i$ th record, and  $w_{jk}$  is the weight for the  $k$ th input field on the  $j$ th output unit.

The activation of an output unit is simply the Euclidean distance between the output unit's weight vector (its center) and the input vector. Note that for Kohonen networks, the output unit with the *lowest* activation is the winning unit. This is in contrast to other types of neural networks, where higher activation represents stronger response.

### **Neighborhoods**

The neighborhood function is based on the Chebychev distance, which considers only the maximum distance on any single dimension:

$$d_c(x, y) = \max_i |x_i - y_i|$$

where  $x_i$  is the location of unit  $x$  on dimension  $i$  of the output grid, and  $y_i$  is the location of another unit  $y$  on the same dimension.

An output unit  $o_j$  is considered to be in the neighborhood of another output unit  $o_i$  if  $d_c(o_i, o_j) < n$ , where  $n$  is the neighborhood size.

Neighborhood size remains constant during each phase, but different phases usually use different neighborhood sizes. By default,  $n = 2$  for Phase 1 and  $n = 1$  for Phase 2.

### **Weight Updates**

For the winning output node, and its neighbors if the neighborhood is  $> 0$ , the weights are adjusted by adding a portion of the difference between the input vector and the current weight vector. The magnitude of the change is determined by the learning rate parameter  $\eta$  (eta). The weight change is calculated as

$$\Delta W = \eta \cdot (W - I)$$

where  $W$  is the weight vector for the output unit being updated,  $I$  is the input vector, and  $\eta$  is the learning rate parameter. In individual unit terms,

$$\Delta w_j = \eta \cdot (w_j - i_j)$$

where  $w_j$  is the weight corresponding to input unit  $j$  for the output unit being updated, and  $i_j$  is the  $j$ th input unit.

### **Eta Decay**

At the end of each cycle, the value of  $\eta$  is updated. The value of  $\eta$  generally decreases across training cycles. The user can control the rate of decrease by selecting either linear or exponential decay.

**Linear decay.** This is the default decay rate. When this option is selected, the value of  $\eta$  decays in a linear fashion, decreasing by a fixed amount each cycle, according to the formula

$$\eta(t + 1) = \eta(t) - \left( \frac{\eta(0) - \eta_{low}}{c} \right)$$

where  $\eta(0)$  is the initial eta value for the current phase, and  $\eta_{low}$  is the low eta for the current training phase, calculated as the lesser of the initial eta values for the current phase and the following phase, and  $c$  is the number of cycles set for the current phase.

**Exponential decay.** When this option is selected, the value of  $\eta$  decays in an exponential fashion, decreasing by a fixed proportion each cycle, according to the formula

$$\eta(t + 1) = \eta(t) \cdot \exp \left( \frac{\log \left( \frac{\eta_{low}}{\eta(0)} \right)}{c} \right)$$

The value of  $\eta_{low}$  has a minimum value of 0.0001 to prevent arithmetic errors in taking the logarithm.

### **Blank Handling**

In Kohonen networks, blanks are handled by substituting “neutral” values for the missing ones. For range and flag fields with missing values (blanks and nulls), the missing value is replaced with 0.5. For range fields, numeric values outside the range limits found in the field’s type information are coerced to the type-defined range. For set fields, the derived indicator field values are all set to 0.0.

### **Effect of Options**

**Stop on.** By default, training executes the specified number of cycles for each phase. If the Time option is selected, training stops when the elapsed time reaches the specified limit (or sooner if the specified number of cycles for both phases is completed before the time limit is reached).

**Random seed.** Sets the seed for the random number generator used to initialize the weights of the new network as well as the order of presentation for training records. Select a fixed seed value to create a reproducible network.

## ***Generated Model/Scoring***

### ***Cluster Membership***

Cluster membership for a new record is derived by presenting the input vector for the record to the network and identifying the output neuron with the closest weight vector, as described in Distances above. The predicted value is returned as the  $x$  and  $y$  coordinates of the winning neuron in the output grid.

### ***Blank Handling***

Blank handling for scoring is the same as during model building. For more information, see the topic “Blank Handling” on p. 236.



# Logistic Regression Algorithms

## Logistic Regression Models

Logistic regression is a well-established statistical method for predicting binomial or multinomial outcomes. IBM® SPSS® Modeler now offers two distinct algorithms for logistic regression modeling:

**Multinomial Logistic.** This is the original logistic regression algorithm used in SPSS Modeler, introduced in version 6.0. It can produce models when the target field is a set field with more than two possible values. See below for more information. It can also produce models for flag or binary outcomes, though it doesn't give the same level of statistical detail for such models as the newer binomial logistic algorithm.

**Binomial Logistic.** This algorithm, introduced in SPSS Modeler 11, is limited to models where the target field is a flag, or binary field. This algorithm provides some enhanced statistical output, relative to the output of the multinomial algorithm, and is less susceptible to problems when the number of cells (unique combinations of predictor values) is large relative to the number of records. For more information, see the topic "Binomial Logistic Regression" on p. 251.

For models with a flag output field, selection of a logistic algorithm is controlled in the modeling node by the Procedure option.

## Multinomial Logistic Regression

The purpose of the Multinomial Logistic Regression procedure is to model the dependence of a nominal (symbolic) output field on a set of symbolic and/or numeric predictor (input) fields.

### Primary Calculations

#### Field Encoding

In logistic regression, each symbolic (set) field is recoded as a group of numeric fields, with one numeric field for each category or value of the original field, except the last category, which is defined as a reference category. For each record, the value of the derived field corresponding to the category of the record is set to 1.0, and all of the other derived field values are set to 0.0. For records which have the value of the reference category, all derived fields are set to 0.0. Such derived fields are sometimes called **dummy fields**, and this recoding is called **dummy coding**.

For example, consider the following data, where  $x$  is a symbolic field with possible values A, B, and C:

Record #	$X$	$X_1'$	$X_2'$
1	B	0	1
2	A	1	0
3	C	0	0

In this data, the original set field  $x$  is recoded into two derived fields  $x_1'$  and  $x_2'$ .  $x_1'$  is an indicator for category A, and  $x_2'$  is an indicator for category B. The last category, category C, is the reference category; records belonging to this category have both  $x_1'$  and  $x_2'$  set to 0.0.

### Notation

The following notation is used throughout this chapter unless otherwise stated:

$Y$	The output field, which takes integer values from 1 to $J$ .
$J$	The number of categories of the output field.
$m$	The number of subpopulations.
$\mathbf{X}^A$	$m \times p^A$ matrix with vector-element $x_i^A$ , the observed values at the $i$ th subpopulation, determined by the input fields specified in the command.
$\mathbf{X}$	$m \times p$ matrix with vector-element $x_i^A$ , the observed values of the location model's input fields at the $i$ th subpopulation.
$n_{ij}$	The sum of frequency weights of the observations that belong to the cell corresponding to $Y = j$ at subpopulation $i$ .
$N$	The sum of all $n_{ij}$ 's.
$\pi_{ij}$	The cell probability corresponding to $Y = j$ at subpopulation $i$ .
$\log(\pi_{ij}/\pi_{ik})$	The logit of response category $j$ relative to response category $k$ .
$\beta_j = (\beta_{j1}, \dots, \beta_{jp})'$	$p \times 1$ vector of unknown parameters in the $j$ th logit (that is, logit of response category $j$ to response category $J$ ).
$p$	Number of parameters in each logit. $p \geq 1$ .
$p_j^{nr}$	Number of non-redundant parameters in logit $j$ after maximum likelihood estimation. $p \geq p_j^{nr} \geq 0$ .
$p^{nr}$	The total number of non-redundant parameters after maximum likelihood estimation. $p^{nr} = \sum_{j=1}^{k-1} p_j^{nr}$ .
$\mathbf{B} = (\beta'_1, \dots, \beta'_{J-1})'$	$(k-1)p \times 1$ vector of unknown parameters in the model.
$\hat{\mathbf{B}} = (\hat{\beta}'_1, \dots, \hat{\beta}'_{J-1})'$	The maximum likelihood estimate of $\mathbf{B}$ .
$\hat{\pi}_{ij}$	The maximum likelihood estimate of $\pi_{ij}$ .

### Data Aggregation

Observations are aggregated by the definition of subpopulations. Subpopulations are defined by the cross-classifications of the set of input fields.

Let  $n_i$  be the marginal count of subpopulation  $i$ ,

$$n_i = \sum_{j=1}^k n_{ij}$$

If there is no observation for the cell of  $Y = j$  at subpopulation  $i$ , it is assumed that  $n_{ij} = 0$ , provided that  $n_i \neq 0$ . A non-negative scalar  $\delta \in [0, 1)$  may be added to any zero cell (that is, cell with  $n_{ij} = 0$ ) if its marginal count  $n_i$  is nonzero. The value of  $\delta$  is zero by default.

### Generalized Logit Model

In a generalized logit model, the probability  $\pi_{ij}$  of response category  $j$  at subpopulation  $i$  is

$$\pi_{ij} = \frac{\exp(\mathbf{x}'_i \beta_j)}{1 + \sum_{k=1}^{J-1} \exp(\mathbf{x}'_i \beta_k)}$$

where the last category  $J$  is assumed to be the reference category.

In terms of logits, the model can be expressed as

$$\log\left(\frac{\pi_{ij}}{\pi_{iJ}}\right) = \mathbf{x}'_i \beta_j$$

for  $j = 1, \dots, J-1$ .

When  $J = 2$ , this model is equivalent to the binary logistic regression model. Thus, the above model can be thought of as an extension of the binary logistic regression model from binary response to polytomous nominal response.

### Log-Likelihood

The log-likelihood of the model is given by

$$\begin{aligned} l(\mathbf{B}) &= \sum_{i=1}^m \sum_{j=1}^J n_{ij} \log(\pi_{ij}) \\ &= \sum_{i=1}^m \sum_{j=1}^J n_{ij} \log\left(\frac{\exp(\mathbf{x}'_i \beta_j)}{1 + \sum_{k=1}^{J-1} \exp(\mathbf{x}'_i \beta_k)}\right) \end{aligned}$$

A constant that is independent of parameters has been excluded here. The value of the constant is  $c = \sum_{i=1}^m \log(n_i! / (n_{i1}! \dots n_{iJ}!))$ .

### Model Parameters

#### Derivatives of the Log-Likelihood

For any  $j = 1, \dots, J-1, s = 1, \dots, p$ , the first derivative of  $l$  with respect to  $\beta_{js}$  is

$$\frac{\partial l}{\partial \beta_{js}} = \sum_{i=1}^m x_{is} (n_{ij} - n_i \pi_{ij}).$$

For any  $j, j' = 1, \dots, J-1$  and  $s, t = 1, \dots, p$ , the second derivative of  $l$  with respect to  $\beta_{js}$  and  $\beta_{j't}$  is

$$\frac{\partial^2 l}{\partial \beta_{js} \partial \beta_{j't}} = - \sum_{i=1}^m n_i x_{is} x_{it} \pi_{ij} (\delta_{jj'} - \pi_{ij'})$$

where  $\delta_{jj'} = 1$  if  $j = j'$ , 0 otherwise.

### Maximum Likelihood Estimate

To obtain the maximum likelihood estimate of  $\mathbf{B}$ , a Newton-Raphson iterative estimation method is used. Notice that this method is the same as Fisher-Scoring iterative estimation method in this model, since the expectation of the second derivative of  $l$  with respect to  $\mathbf{B}$  is the same as the observed one.

Let  $\partial l / \partial \mathbf{B}$  be the  $(J-1)p \times 1$  vector of the first derivative of  $l$  with respect to  $\mathbf{B}$ . Moreover, let  $[\partial^2 l / \partial \mathbf{B} \partial \mathbf{B}]$  be the  $(J-1)p \times (J-1)p$  matrix of the second derivative of  $l$  with respect to  $\mathbf{B}$ . Notice that  $-[\partial^2 l / \partial \mathbf{B} \partial \mathbf{B}] = \sum_{i=1}^m \mathbf{X}_i^* \Delta_i \mathbf{X}_i^{*'}$  where  $\Delta_i$  is a  $(J-1) \times (J-1)$  matrix as

$$\Delta_i = n_i \left( \text{Diag} \left( \pi_i^{(-J)} \right) - \pi_i^{(-J)} \pi_i^{(-J)'} \right)$$

in which  $\pi_i^{(-J)} = (\pi_{i1}, \dots, \pi_{iJ-1})'$  and  $\text{Diag} \left( \pi_i^{(-J)} \right)$  is a  $\beta_{js}$  diagonal matrix of  $\pi_i^{(-J)}$ . Let  $B^{(\nu)}$  be the parameter estimate at iteration  $\nu$ , the parameter estimate  $B^{(\nu+1)}$  at iteration  $\nu + 1$  is updated as

$$\mathbf{B}^{(\nu+1)} = \mathbf{B}^{(\nu)} + \xi \left( \sum_{i=1}^m \mathbf{X}_i^* \Delta_i^{(\nu)} \mathbf{X}_i^{*'} \right) \frac{\partial l}{\partial \mathbf{B}^{(\nu)}}$$

and  $\xi > 0$  is a stepping scalar such that  $l(\mathbf{B}^{(\nu+1)}) - l(\mathbf{B}^{(\nu)}) \geq 0$ ,  $\mathbf{X}^*$  is a  $(J-1)p \times (J-1)$  matrix of independent vectors,

$$\mathbf{X}_i^* = \begin{pmatrix} \mathbf{x}_i & 0 & \dots & 0 \\ 0 & \mathbf{x}_i & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \dots & 0 & \mathbf{x}_i \end{pmatrix}$$

and  $\Delta_i^{(\nu)}$  is  $\Delta_i$  and  $\partial l / \partial \mathbf{B}^{(\nu)}$  is  $\partial l / \partial \mathbf{B}$ , both evaluated at  $\mathbf{B} = \mathbf{B}^{(\nu)}$ .

### Stepping

Use step-halving method if  $l(\mathbf{B}^{(\nu+1)}) - l(\mathbf{B}^{(\nu)}) < 0$ . Let  $V$  be the maximum number of steps in step-halving, the set of values of  $\xi$  is  $\{1/2^\nu : \nu = 0, \dots, V-1\}$ .

### Starting Values of the Parameters

If intercepts are included in the model, set  $\beta_j^{(0)} = (\beta_{j1}^{(0)}, 0, \dots, 0)'$  where

$$\beta_{j1}^{(0)} = \log \left( \frac{\tilde{\pi}_{ij}}{\tilde{\pi}_{iJ}} \right) = \log \left( \frac{\sum_{i=1}^m n_{ij}}{\sum_{i=1}^m n_{iJ}} \right)$$

for  $j = 1, \dots, J-1$ .

If intercepts are not included in the model, set

$$\beta_j^{(0)} = (0, \dots, 0)'$$

for  $j = 1, \dots, J-1$ .

### **Convergence Criteria**

Given two convergence criteria  $\epsilon_k > 0$  and  $\epsilon_p > 0$ , the iteration is considered to be converged if one of the following criteria are satisfied:

1.  $|l(\mathbf{B}^{(\nu+1)}) - l(\mathbf{B}^{(\nu)})| < \epsilon_k$ .
2.  $\max_i |\mathbf{B}_i^{(\nu+1)} - \mathbf{B}_i^\nu| < \epsilon_p$ .
3. The maximum above element in  $\partial l / \partial \mathbf{B}^{(\nu+1)}$  is less than  $\min(\epsilon_k, \epsilon_p)$ .

### **Checking for Separation**

The algorithm checks for separation in the data starting with iteration  $\nu^{chksep}$  (20 by default). To check for separation:

1. For each subpopulation  $i$ , find  $j^* : \hat{\pi}_{ij^*} = \max_j (\hat{\pi}_{ij})$ .
2. If  $n_{ij^*} = n_i$ , then there is a perfect prediction for subpopulation  $i$ .
3. If all subpopulations have perfect prediction, then there is complete separation. If some patterns have perfect prediction and the Hessian of  $\hat{\mathbf{B}}$  is singular, then there is quasi-complete separation.

### **Blank Handling**

All records with missing values for any input or output field are excluded from the estimation of the model.

## Secondary Calculations

### Model Summary Statistics

#### Log-Likelihood

**Initial model with intercepts.** If intercepts are included in the model, the predicted probability for the initial model (that is, the model with intercepts only) is

$$\tilde{\pi}_{ij} = \frac{\sum_{i=1}^m n_{ij}}{N}$$

and the value of  $-2$  log-likelihood of the initial model is

$$-2l(\tilde{\pi}) = -2 \sum_{i=1}^m \sum_{j=1}^J n_{ij} \log(\tilde{\pi}_{ij}).$$

**Initial model with no intercepts.** If intercepts are not included in the model, the predicted probability for the initial model is

$$\tilde{\pi}_{ij} = \frac{1}{J}$$

and the value of  $-2$  log-likelihood of the initial model is

$$-2l(\tilde{\pi}) = -2N \log\left(\frac{1}{J}\right).$$

**Final model.** The value of  $-2$  log-likelihood of the final model is

$$-2l(\tilde{\pi}) = -2 \sum_{i=1}^m \sum_{j=1}^J n_{ij} \log(\hat{\pi}_{ij}).$$

#### Model Chi-Square

The model chi-square is given by

$$-2l(\tilde{\pi}) - \{-2l(\hat{\pi})\}$$

If the final model includes intercepts, then the initial model is an intercept-only model. Under the null hypothesis that  $H_0 : \beta^{intercepts} = \mathbf{0}$ , the model chi-square is asymptotically chi-squared distributed with  $p^{nr} - (J - 1)$  degrees of freedoms.

If the model does not include intercepts, then the initial model is an empty model. Under the null hypothesis that  $H_0 : \beta = \mathbf{0}$ , the Model Chi-square is asymptotically chi-squared distributed with  $p^{nr}$  degrees of freedoms.

### **Pseudo R-Square Measures**

**Cox and Snell.** Cox and Snell's  $R^2$  is calculated as

$$R_{CS}^2 = 1 - \left( \frac{L(\tilde{\pi})}{L(\hat{\pi})} \right)^{\frac{2}{n}}.$$

**Nagelkerke.** Nagelkerke's  $R^2$  is calculated as

$$R_N^2 = \frac{R_{CS}^2}{1 - L(\tilde{\pi})^{2/n}}.$$

**McFadden.** McFadden's  $R^2$  is calculated as

$$R_M^2 = 1 - \left( \frac{l(\hat{\pi})}{l(\tilde{\pi})} \right).$$

### **Goodness-of-Fit Measures**

**Pearson.** The Pearson goodness-of-fit measure is

$$\chi^2 = \sum_{i=1}^m \sum_{j=1}^J \frac{(n_{ij} - n_i \hat{\pi}_{ij})^2}{n_i \hat{\pi}_{ij}}.$$

Under the null hypothesis, the Pearson goodness-of-fit statistic is asymptotically chi-squared distributed with  $m(J - 1) - p^{nr}$  degrees of freedom.

**Deviance.** The deviance goodness-of-fit measure is

$$D = 2 \sum_{i=1}^m \sum_{j=1}^J n_{ij} \log \left( \frac{n_{ij}}{n_i \hat{\pi}_{ij}} \right).$$

Under the null hypothesis, the deviance goodness-of-fit statistic is asymptotically chi-squared distributed with  $m(J - 1) - p^{nr}$  degrees of freedom.

### **Field Statistics and Other Calculations**

The statistics shown in the advanced output for the logistic equation node are calculated in the same manner as in the NOMREG procedure in IBM® SPSS® Statistics. For more details, see the SPSS Statistics Nomreg algorithm document, available at <http://www.ibm.com/support>.

## **Stepwise Variable Selection**

Several methods are available for selecting independent variables. With the forced entry method, any variable in the variable list is entered into the model. The forward stepwise, backward stepwise, and backward entry methods use either the Wald statistic or the likelihood ratio statistic for variable removal. The forward stepwise, forward entry, and backward stepwise use the score statistic or the likelihood ratio statistic to select variables for entry into the model.

### **Forward Stepwise (FSTEP)**

1. Estimate the parameter and likelihood function for the initial model and let it be our current model.
2. Based on the MLEs of the current model, calculate the score statistic or likelihood ratio statistic for every variable eligible for inclusion and find its significance.
3. Choose the variable with the smallest significance (p-value). If that significance is less than the probability for a variable to enter, then go to step 4; otherwise, stop FSTEP.
4. Update the current model by adding a new variable. If this results in a model which has already been evaluated, stop FSTEP.
5. Calculate the significance for each variable in the current model using LR or Wald's test.
6. Choose the variable with the largest significance. If its significance is less than the probability for variable removal, then go back to step 2. If the current model with the variable deleted is the same as a previous model, stop FSTEP; otherwise go to the next step.
7. Modify the current model by removing the variable with the largest significance from the previous model. Estimate the parameters for the modified model and go back to step 5.

### **Forward Only (FORWARD)**

1. Estimate the parameter and likelihood function for the initial model and let it be our current model.
2. Based on the MLEs of the current model, calculate the score or LR statistic for every variable eligible for inclusion and find its significance.
3. Choose the variable with the smallest significance. If that significance is less than the probability for a variable to enter, then go to step 4; otherwise, stop FORWARD.
4. Update the current model by adding a new variable. If there are no more eligible variable left, stop FORWARD; otherwise, go to step 2.

### **Backward Stepwise (BSTEP)**

1. Estimate the parameters for the full model that includes the final model from previous method and all eligible variables. Only variables listed on the BSTEP variable list are eligible for entry and removal. Let current model be the full model.
2. Based on the MLEs of the current model, calculate the LR or Wald's statistic for every variable in the BSTEP list and find its significance.

3. Choose the variable with the largest significance. If that significance is less than the probability for a variable removal, then go to step 5. If the current model without the variable with the largest significance is the same as the previous model, stop BSTEP; otherwise go to the next step.
4. Modify the current model by removing the variable with the largest significance from the model. Estimate the parameters for the modified model and go back to step 2.
5. Check to see any eligible variable is not in the model. If there is none, stop BSTEP; otherwise, go to the next step.
6. Based on the MLEs of the current model, calculate LR statistic or score statistic for every variable not in the model and find its significance.
7. Choose the variable with the smallest significance. If that significance is less than the probability for the variable entry, then go to the next step; otherwise, stop BSTEP.
8. Add the variable with the smallest significance to the current model. If the model is not the same as any previous models, estimate the parameters for the new model and go back to step 2; otherwise, stop BSTEP.

### **Backward Only (BACKWARD)**

1. Estimate the parameters for the full model that includes all eligible variables. Let the current model be the full model.
2. Based on the MLEs of the current model, calculate the LR or Wald's statistic for all variables eligible for removal and find its significance.
3. Choose the variable with the largest significance. If that significance is less than the probability for a variable removal, then stop BACKWARD; otherwise, go to the next step.
4. Modify the current model by removing the variable with the largest significance from the model. Estimate the parameters for the modified model. If all the variables in the BACKWARD list are removed then stop BACKWARD; otherwise, go back to step 2.

### **Stepwise Statistics**

The statistics used in the stepwise variable selection methods are defined as follows.

### **Score Function and Information Matrix**

The score function for a model with parameter  $B$  is:

$$U(B) = \frac{\partial l(B)}{\partial B}$$

The  $(j,s)$ th element of the score function can be written as

$$\begin{aligned} [U(B)]_{js} &= \frac{\partial l(B)}{\partial \beta_{js}} \\ &= \sum_{i=1}^m x_{is} (n_{ij} - n_i \pi_{ij}) \end{aligned}$$

Similarly, elements of the information matrix are given by

$$\begin{aligned} [I(B)]_{js,j't} &= \frac{\partial^2 l(B)}{\partial \beta_{js} \partial \beta_{jt}} \\ &= - \sum_{i=1}^m n_i x_{is} x_{it} \pi_{ij} (\delta_{jj'} - \pi_{ij'}) \end{aligned}$$

where  $\delta_{jj'} = 1$  if  $j = j'$ , 0 otherwise.

(Note that  $\pi_{ij}$  in the formula are functions of  $B$ )

### Block Notations

By partitioning the parameter  $B$  into two parts,  $B_1$  and  $B_2$ , the score function, information matrix, and inverse information matrix can be written as partitioned matrices:

$$\begin{aligned} U(B_1, B_2) &= \begin{pmatrix} U_1(B_1, B_2) \\ U_2(B_1, B_2) \end{pmatrix} \\ &= \begin{pmatrix} \frac{\partial l(B_1, B_2)}{\partial B_1} \\ \frac{\partial l(B_1, B_2)}{\partial B_2} \end{pmatrix} \end{aligned}$$

where  $l(B_1, B_2) = l(B)$

$$\begin{aligned} I(B) &= I(B_1, B_2) \\ &= \begin{pmatrix} I_{11}(B_1, B_2) & I_{12}(B_1, B_2) \\ I_{21}(B_1, B_2) & I_{22}(B_1, B_2) \end{pmatrix} \\ &= \begin{pmatrix} \frac{\partial^2 l(B_1, B_2)}{\partial B_1 \partial B_1} & \frac{\partial^2 l(B_1, B_2)}{\partial B_1 \partial B_2} \\ \frac{\partial^2 l(B_1, B_2)}{\partial B_2 \partial B_1} & \frac{\partial^2 l(B_1, B_2)}{\partial B_2 \partial B_2} \end{pmatrix} \end{aligned}$$

$$J(B) = I(B_1, B_2)^{-1} = \begin{pmatrix} J_{11}(B_1, B_2) & J_{12}(B_1, B_2) \\ J_{21}(B_1, B_2) & J_{22}(B_1, B_2) \end{pmatrix}$$

where

$$\begin{aligned} J_{11} &= I_{11}^{-1} + I_{11}^{-1} I_{12} J_{22} I_{21} I_{11}^{-1} \\ J_{12} &= -I_{11}^{-1} I_{12} J_{22} \\ J_{21} &= J_{12}^T \\ J_{22} &= [I_{22} - I_{21} I_{11}^{-1} I_{12}]^{-1} \end{aligned}$$

Typically,  $B_1$  and  $B_2$  are parameters corresponding to two different sets of effects. The dimensions of the 1st and 2nd partition in  $U$ ,  $I$  and  $J$  are equal to the numbers of parameters in  $B_1$  and  $B_2$  respectively.

### Score Test

Suppose a base model with parameter vector  $B_{base}$  with the corresponding maximum likelihood estimate  $\hat{B}_{base}$ . We are interested in testing the significance of an extra effect E if it is added to the base model. For convenience, we will call the model with effect E the augmented model. Let  $B_E$  be the vector of extra parameters associated with the effect E, then the hypothesis can be written as

$$H_0 : B_E = 0 \text{ v.s. } H_1 : B_E \neq 0$$

Using the block notations, the score function, information matrix and inverse information of the augmented model can be written as

$$U(B_{base}, B_E) = \begin{pmatrix} U_{base}(B_{base}, B_E) \\ U_E(B_{base}, B_E) \end{pmatrix}$$

$$I(B_{base}, B_E) = \begin{pmatrix} I_{base,base}(B_{base}, B_E) & I_{base,E}(B_{base}, B_E) \\ I_{E,base}(B_{base}, B_E) & I_{E,E}(B_{base}, B_E) \end{pmatrix}$$

$$J(B_{base}, B_E) = \begin{pmatrix} J_{base,base}(B_{base}, B_E) & J_{base,E}(B_{base}, B_E) \\ J_{E,base}(B_{base}, B_E) & J_{E,E}(B_{base}, B_E) \end{pmatrix}$$

Then the score statistic for testing our hypothesis will be

$$s = U_E(\hat{B}_{base}, 0)^T J_{E,E}(\hat{B}_{base}, 0) U_E(\hat{B}_{base}, 0)$$

where  $U_E(\hat{B}_{base}, 0)$  and  $J_{E,E}(\hat{B}_{base}, 0)$  are the 2nd partition of score function and inverse information matrix evaluated at  $B_{base} = \hat{B}_{base}$  and  $B_E = 0$ .

Under the null hypothesis, the score statistic  $s$  has a chi-square distribution with degrees of freedom equal to the rank of  $J_{E,E}(B_1, B_2)$ . If the rank of  $J_{E,E}(B_1, B_2)$  is zero, then the score statistic will be set to 0 and the  $p$ -value will be 1. Otherwise, if the rank of  $J_{E,E}(B_1, B_2)$  is  $r_E : r_E > 0$ , then the  $p$ -value of the test is equal to  $1 - F(s; r_E)$ , where  $F(\cdot, r_E)$  is the cumulative distribution function of a chi-square distribution with  $r_E$  degrees of freedom.

### Computational Formula for Score Statistic

When we compute the score statistic  $s$ , it is not necessary to re-compute  $U(\hat{B}_{base}, 0)$  and  $I(\hat{B}_{base}, 0)$  from scratch. The score function and information matrix of the base model can be reused in the calculation. Using the block notations introduced earlier, we have

$$U(\hat{B}_{base}, 0) = \begin{pmatrix} U_{base}(\hat{B}_{base}, 0) \\ U_E(\hat{B}_{base}, 0) \end{pmatrix} = \begin{pmatrix} U(\hat{B}_{base}) \\ U_E(\hat{B}_{base}, 0) \end{pmatrix}$$

and

$$I(\hat{B}_{base}, 0) = \begin{pmatrix} I(\hat{B}_{base}) & I_{base,E}(\hat{B}_{base}, 0) \\ I_{E,base}(\hat{B}_{base}, 0) & I_{E,E}(\hat{B}_{base}, 0) \end{pmatrix}$$

In stepwise logistic regression, it is necessary to compute one score test for each effect that are not in the base model. Since the 1st partition of  $U(\hat{B}_{base}, 0)$  and  $I(\hat{B}_{base}, 0)$  depend only on the base model, we only need to compute  $U_E(\hat{B}_{base}, 0)$ ,  $I_{base,E}(\hat{B}_{base}, 0)$  and  $I_{E,E}(\hat{B}_{base}, 0)$  for each new effect.

If  $\beta_{js}$  is the  $s$ -th parameter of the  $j$ -th logit in  $B_{base}$  and  $\beta_{kt}$  is the  $t$ -th parameter of  $k$ -th logit in  $B_E$ , then the elements of  $U_E(\hat{B}_{base}, 0)$ ,  $I_{base,E}(\hat{B}_{base}, 0)$  and  $I_{E,E}(\hat{B}_{base}, 0)$  can be expressed as follows:

$$\left[ U_E(\hat{B}_{base}, 0) \right]_{kt} = \sum_{i=1}^m x_{it} (n_{ik} - n_i \hat{\pi}_{ik})$$

$$\left[ I_{E,E}(\hat{B}_{base}, 0) \right]_{kt,k't'} = - \sum_{i=1}^m n_i x_{it} x_{it'} \hat{\pi}_{ik} (\delta_{kk'} - \hat{\pi}_{ik'})$$

$$\left[ I_{base,E}(\hat{B}_{base}, 0) \right]_{js,kt} = - \sum_{i=1}^m n_i x_{is} x_{it} \hat{\pi}_{ij} (\delta_{jk} - \hat{\pi}_{ik})$$

where  $\hat{\pi}_{ik}$ ,  $\hat{\pi}_{ik'}$  are computed under the base model.

### Wald's Test

In backward stepwise selection, we are interested in removing an effect  $F$  from an already fitted model. For a given base model with parameter vector  $B_{base}$ , we want to use Wald's statistic to test if effect  $F$  should be removed from the base model. If the parameter vector for the effect  $F$  is  $B_F$ , then the hypothesis can be formulated as

$$H_0 : B_F = 0 \text{ vs. } H_1 : B_F \neq 0$$

In order to write down the expression of the Wald's statistic, we will partition our parameter vector (and its estimate) into two parts as follows:

$$B_{base} = \begin{pmatrix} B_{base \setminus F} \\ B_F \end{pmatrix} \text{ and } \hat{B}_{base} = \begin{pmatrix} \hat{B}_{base \setminus F} \\ \hat{B}_F \end{pmatrix}$$

The first partition contains parameters that we intended to keep in the model and the 2nd partition contains the parameters of the effect  $F$ , which may be removed from the model. The information matrix and inverse information will be partitioned accordingly,

$$I(B_{base}) = \begin{pmatrix} I_{base \setminus F, base \setminus F}(B_{base \setminus F}, B_{base \setminus F}) & I_{base \setminus F, F}(B_{base \setminus F}, B_F) \\ I_{F, base \setminus F}(B_{base \setminus F}, B_F) & I_{F, F}(B_{base \setminus F}, B_F) \end{pmatrix}$$

and

$$J(B_{base}) = \begin{pmatrix} J_{base \setminus F, base \setminus F}(B_{base \setminus F}, B_{base \setminus F}) & J_{base \setminus F, F}(B_{base \setminus F}, B_F) \\ J_{F, base \setminus F}(B_{base \setminus F}, B_F) & J_{F, F}(B_{base \setminus F}, B_F) \end{pmatrix}$$

Using the above notations, the Wald's statistic for effect  $F$  can be expressed as

$$w = \hat{B}_F [J_{F, F}(B_{base \setminus F}, B_F)]^{-1} \hat{B}_F$$

Under the null hypothesis,  $w$  has a chi-square distribution with degrees of freedom equal to the rank of  $J_{F, F}(B_{base \setminus F}, B_F)$ . If the rank of  $J_{F, F}(B_{base \setminus F}, B_F)$  is zero, then Wald's statistic will be set to 0 and the  $p$ -value will be 1. Otherwise, if the rank of  $J_{F, F}(B_{base \setminus F}, B_F)$  is  $r_F : r_F > 0$ , then

the  $p$ -value of the test is equal to  $1 - F(w; r_F)$ , where  $F(w; r_F)$  is the cumulative distribution function of a chi-square distribution with  $r_F$  degrees of freedom.

## Generated Model/Scoring

### Predicted Values

The predicted value for a record  $i$  is the output field category  $j$  with the largest logit value  $r_{ij}$ ,

$$r_{ij} = \log \left( \frac{\pi_{ij}}{\pi_{iJ}} \right) = \mathbf{x}'_i \beta_j$$

for  $j = 1, \dots, J-1$ . The logit for reference category  $J, r_{iJ}$ , is 1.0.

### Predicted Probability

The probability for the predicted category  $j^*$  for scored record  $i$  is derived from the logit for category  $j^*$ ,

$$\hat{\pi}_{ij} = \frac{\exp(r_{ij'})}{1 + \sum_{k=1}^{J-1} \exp(r_{ij'})} = \frac{\exp(\mathbf{x}'_i \beta_j)}{1 + \sum_{k=1}^{J-1} \exp(\mathbf{x}'_i \beta_k)}$$

If the Append all probabilities option is selected, the probability is calculated for all  $J$  categories in a similar manner.

### Blank Handling

Records with missing values for any input field cannot be scored and are assigned a predicted value and probability value(s) of \$null\$.

## Binomial Logistic Regression

For binomial models (models with a flag field as the target), IBM® SPSS® Modeler uses an algorithm optimized for such models, as described here.

### Notation

The following notation is used throughout this chapter unless otherwise stated:

$n$	The number of observed cases
$p$	The number of parameters
$y$	$n \times 1$ vector with element $y_i$ , the observed value of the $i$ th case of the dichotomous dependent variable
$X$	$n \times p$ matrix with element $x_{ij}$ , the observed value of the $i$ th case of the $j$ th parameter

$\beta$	$p \times 1$ vector with element $\beta_j$ , the coefficient for the $j$ th parameter
$\mathbf{w}$	$n \times 1$ vector with element $w_i$ , the weight for the $i$ th case
$l$	Likelihood function
$L$	Log-likelihood function
$\mathbf{I}$	Information matrix

## Model

The linear logistic model assumes a dichotomous dependent variable  $Y$  with probability  $\pi$ , where for the  $i$ th case,

$$\pi_i = \frac{\exp(\eta_i)}{1 + \exp(\eta_i)}$$

or

$$\ln\left(\frac{\pi_i}{1 - \pi_i}\right) = \eta_i = \mathbf{X}'_i \beta$$

Hence, the likelihood function  $l$  for  $n$  observations  $y_1, \dots, y_n$ , with probabilities  $\pi_1, \dots, \pi_n$  and case weights  $w_1, \dots, w_n$ , can be written as

$$l = \prod_{i=1}^n \pi_i^{w_i y_i} (1 - \pi_i)^{w_i(1 - y_i)}$$

It follows that the logarithm of  $l$  is

$$L = \ln(l) = \sum_{i=1}^n (w_i y_i \ln(\pi_i) + w_i(1 - y_i) \ln(1 - \pi_i))$$

and the derivative of  $L$  with respect to  $\beta_j$  is

$$L^*_{X_j} = \frac{\partial L}{\partial \beta_j} = \sum_{i=1}^n w_i (y_i - \pi_i) x_{ij}$$

## Maximum Likelihood Estimates (MLE)

The maximum likelihood estimates for  $\beta$  satisfy the following equations

$$\sum_{i=1}^n w_i (y_i - \hat{\pi}_i) x_{ij} = 0, \text{ for the } j\text{th parameter}$$

where  $x_{i0} = 1$  for  $i = 1, \dots, n$ .

Note the following:

1. A Newton-Raphson type algorithm is used to obtain the MLEs. Convergence can be based on
  - Absolute difference for the parameter estimates between the iterations

- Percent difference in the log-likelihood function between successive iterations
  - Maximum number of iterations specified
2. During the iterations, if  $\hat{\pi}_i(1 - \hat{\pi}_i)$  is smaller than  $10^{-8}$  for all cases, the log-likelihood function is very close to zero. In this situation, iteration stops and the message “All predicted values are either 1 or 0” is issued.

After the maximum likelihood estimates  $\hat{\beta}$  are obtained, the asymptotic covariance matrix is estimated by  $I^{-1}$ , the inverse of the information matrix  $I$ , where

$$I = - \left[ E \left( \frac{\partial^2 L}{\partial \beta_i \partial \beta_j} \right) \right] = \mathbf{X}' \mathbf{W} \hat{\mathbf{V}} \mathbf{X},$$

$$\hat{\mathbf{V}} = \text{Diag}\{\hat{\pi}_1(1 - \hat{\pi}_1), \dots, \hat{\pi}_n(1 - \hat{\pi}_n)\},$$

$$\mathbf{W} = \text{Diag}\{w_1, \dots, w_n\},$$

$$\hat{\pi}_i = \frac{\exp(\hat{\eta}_i)}{1 + \exp(\hat{\eta}_i)},$$

and

$$\hat{\eta}_i = \mathbf{X}_i' \hat{\beta}$$

### **Stepwise Variable Selection**

Several methods are available for selecting independent variables. With the forced entry method, any variable in the variable list is entered into the model. There are two stepwise methods: forward and backward. The stepwise methods can use either the Wald statistic, the likelihood ratio, or a conditional algorithm for variable removal. For both stepwise methods, the score statistic is used to select variables for entry into the model.

#### **Forward Stepwise (FSTEP)**

1. If FSTEP is the first method requested, estimate the parameter and likelihood function for the initial model. Otherwise, the final model from the previous method is the initial model for FSTEP. Obtain the necessary information: MLEs of the parameters for the current model, predicted probability, likelihood function for the current model, and so on.
2. Based on the MLEs of the current model, calculate the score statistic for every variable eligible for inclusion and find its significance.
3. Choose the variable with the smallest significance. If that significance is less than the probability for a variable to enter, then go to step 4; otherwise, stop FSTEP.
4. Update the current model by adding a new variable. If this results in a model which has already been evaluated, stop FSTEP.
5. Calculate LR or Wald statistic or conditional statistic for each variable in the current model. Then calculate its corresponding significance.

6. Choose the variable with the largest significance. If that significance is less than the probability for variable removal, then go back to step 2; otherwise, if the current model with the variable deleted is the same as a previous model, stop FSTEP; otherwise, go to the next step.
7. Modify the current model by removing the variable with the largest significance from the previous model. Estimate the parameters for the modified model and go back to step 5.

### **Backward Stepwise (BSTEP)**

1. Estimate the parameters for the full model which includes the final model from previous method and all eligible variables. Only variables listed on the BSTEP variable list are eligible for entry and removal. Let the current model be the full model.
2. Based on the MLEs of the current model, calculate the LR or Wald statistic or conditional statistic for every variable in the model and find its significance.
3. Choose the variable with the largest significance. If that significance is less than the probability for a variable removal, then go to step 5; otherwise, if the current model without the variable with the largest significance is the same as the previous model, stop BSTEP; otherwise, go to the next step.
4. Modify the current model by removing the variable with the largest significance from the model. Estimate the parameters for the modified model and go back to step 2.
5. Check to see any eligible variable is not in the model. If there is none, stop BSTEP; otherwise, go to the next step.
6. Based on the MLEs of the current model, calculate the score statistic for every variable not in the model and find its significance.
7. Choose the variable with the smallest significance. If that significance is less than the probability for variable entry, then go to the next step; otherwise, stop BSTEP.
8. Add the variable with the smallest significance to the current model. If the model is not the same as any previous models, estimate the parameters for the new model and go back to step 2; otherwise, stop BSTEP.

### **Stepwise Statistics**

The statistics used in the stepwise variable selection methods are defined as follows.

#### **Score Statistic**

The score statistic is calculated for each variable not in the model to determine whether the variable should enter the model. Assume that there are  $r_1$  variables, namely,  $\alpha_1, \dots, \alpha_{r_1}$  in the model and  $r_2$  variables,  $\gamma_1, \dots, \gamma_{r_2}$ , not in the model. The score statistic for  $\gamma_i$  is defined as

$$S_i = (\mathbf{L}_{\gamma_i}^*)^2 \mathbf{B}_{22,i}$$

if  $\gamma_i$  is not a categorical variable. If  $\gamma_i$  is a categorical variable with  $m$  categories, it is converted to a  $(m - 1)$ -dimension dummy vector. Denote these new  $m - 1$  variables as  $\tilde{\gamma}_i, \dots, \tilde{\gamma}_{i+m-2}$ . The score statistic for  $\gamma_i$  is then

$$\mathbf{S}_i = (\mathbf{L}_{\tilde{\gamma}}^*)' \mathbf{B}_{22,i} \mathbf{L}_{\tilde{\gamma}}^*$$

where  $(\mathbf{L}_{\tilde{\gamma}}^*)' = (L_{\tilde{\gamma}_i}^*, \dots, L_{\tilde{\gamma}_{i+m-2}}^*)$  and the  $(m - 1) \times (m - 1)$  matrix  $\mathbf{B}_{22,i}$  is

$$\mathbf{B}_{22,i} = (\mathbf{A}_{22,i} - \mathbf{A}_{21,i} \mathbf{A}_{11}^{-1} \mathbf{A}_{12,i})^{-1}$$

with

$$\begin{aligned} \mathbf{A}_{11} &= \alpha' \tilde{\mathbf{V}} \alpha, \\ \mathbf{A}_{12,i} &= \alpha' \tilde{\mathbf{V}} \tilde{\gamma}_i, \\ \mathbf{A}_{22,i} &= \tilde{\gamma}_i' \tilde{\mathbf{V}} \tilde{\gamma}_i \end{aligned}$$

in which  $\alpha$  is the design matrix for variables  $\alpha_1, \dots, \alpha_{r_1}$  and  $\tilde{\gamma}_i$  is the design matrix for dummy variables  $\tilde{\gamma}_i, \dots, \tilde{\gamma}_{i+m-2}$ . Note that  $\tilde{\mathbf{V}}$  contains a column of ones unless the constant term is excluded from  $\eta$ . Based on the MLEs for the parameters in the model,  $\mathbf{V}$  is estimated by  $\tilde{\mathbf{V}} = \text{Diag}\{\hat{\pi}_1(1 - \hat{\pi}_1), \dots, \hat{\pi}_n(1 - \hat{\pi}_n)\}$ . The asymptotic distribution of the score statistic is a chi-square with degrees of freedom equal to the number of variables involved.

Note the following:

1. If the model is through the origin and there are no variables in the model,  $\mathbf{B}_{22,i}$  is defined by  $\mathbf{A}_{22,i}^{-1}$  and  $\tilde{\mathbf{V}}$  is equal to  $\frac{1}{4} \mathbf{I}_n$ .
2. If  $\mathbf{B}_{22,i}$  is not positive definite, the score statistic and residual chi-square statistic are set to be zero.

### **Wald Statistic**

The Wald statistic is calculated for the variables in the model to determine whether a variable should be removed. If the  $i$ th variable is not categorical, the Wald statistic is defined by

$$Wald_i = \frac{\hat{\beta}_i^2}{\hat{\sigma}_{\hat{\beta}_i}^2}$$

If it is a categorical variable, the Wald statistic is computed as follows:

Let  $\hat{\beta}_i$  be the vector of maximum likelihood estimates associated with the  $m - 1$  dummy variables, and  $\mathbf{C}$  the asymptotic covariance matrix for  $\hat{\beta}_i$ . The Wald statistic is

$$Wald_i = \hat{\beta}_i' \mathbf{C}^{-1} \hat{\beta}_i$$

The asymptotic distribution of the Wald statistic is chi-square with degrees of freedom equal to the number of parameters estimated.

### Likelihood Ratio (LR) Statistic

The LR statistic is defined as two times the log of the ratio of the likelihood functions of two models evaluated at their MLEs. The LR statistic is used to determine if a variable should be removed from the model. Assume that there are  $r_1$  variables in the current model which is referred to as a full model. Based on the MLEs of the full model,  $l(full)$  is calculated. For each of the variables removed from the full model one at a time, MLEs are computed and the likelihood function  $l(reduced)$  is calculated. The LR statistic is then defined as

$$LR = -2 \ln \left( \frac{l(reduced)}{l(full)} \right) = -2(L(reduced) - L(full))$$

LR is asymptotically chi-square distributed with degrees of freedom equal to the difference between the numbers of parameters estimated in the two models.

### Conditional Statistic

The conditional statistic is also computed for every variable in the model. The formula for the conditional statistic is the same as the LR statistic except that the parameter estimates for each reduced model are conditional estimates, not MLEs. The conditional estimates are defined as follows. Let  $\hat{\beta} = (\hat{\beta}_1, \dots, \hat{\beta}_{r_1})$  be the MLE for the  $r_1$  variables in the model and  $\mathbf{C}$  be the asymptotic covariance matrix for  $\hat{\beta}$ . If variable  $x_i$  is removed from the model, the conditional estimate for the parameters left in the model given  $\hat{\beta}$  is

$$\tilde{\beta}_{(i)} = \hat{\beta}_{(i)} - \mathbf{c}_{12}^{(i)} \left( \mathbf{c}_{22}^{(i)} \right)^{-1} \hat{\beta}_i$$

where  $\hat{\beta}_i$  is the MLE for the parameter(s) associated with  $x_i$  and  $\hat{\beta}_{(i)}$  is  $\hat{\beta}$  with  $\hat{\beta}_i$  removed,  $\mathbf{c}_{12}^{(i)}$  is the covariance between  $\hat{\beta}_{(i)}$  and  $\hat{\beta}_i$ , and  $\mathbf{c}_{22}^{(i)}$  is the covariance of  $\hat{\beta}_i$ . Then the conditional statistic is computed by

$$-2 \left( L(\tilde{\beta}_{(i)}) - L(full) \right)$$

where  $L(\tilde{\beta}_{(i)})$  is the log-likelihood function evaluated at  $\tilde{\beta}_{(i)}$ .

## Statistics

The following output statistics are available.

### Initial Model Information

If  $\beta_0$  is not included in the model, the predicted probability is estimated to be 0.5 for all cases and the log-likelihood function  $L(0)$  is

$$L(0) = W \ln(0.5) = -0.6931472W$$

with  $W = \sum_{i=1}^n w_i$ . If  $\beta_0$  is included in the model, the predicted probability is estimated as

$$\hat{\pi}_0 = \frac{\sum_{i=1}^n w_i y_i}{W}$$

and  $\beta_0$  is estimated by

$$\hat{\beta}_0 = \ln \left( \frac{\hat{\pi}_0}{1 - \hat{\pi}_0} \right)$$

with asymptotic standard error estimated by

$$\hat{\sigma}_{\hat{\beta}_0} = \frac{1}{\sqrt{W \hat{\pi}_0 (1 - \hat{\pi}_0)}}$$

The log-likelihood function is

$$L(0) = W \left[ \hat{\pi}_0 \ln \left( \frac{\hat{\pi}_0}{1 - \hat{\pi}_0} \right) + \ln (1 - \hat{\pi}_0) \right]$$

### **Model Information**

The following statistics are computed if a stepwise method is specified.

#### **-2 Log-Likelihood**

$$-2 \sum_{i=1}^n (w_i y_i \ln(\hat{\pi}_i) + w_i (1 - y_i) \ln(1 - \hat{\pi}_i))$$

#### **Model Chi-Square**

2(log-likelihood function for current model – log-likelihood function for initial model)

The initial model contains a constant if it is in the model; otherwise, the model has no terms. The degrees of freedom for the model chi-square statistic is equal to the difference between the numbers of parameters estimated in each of the two models. If the degrees of freedom is zero, the model chi-square is not computed.

#### **Block Chi-Square**

2(log-likelihood function for current model – log-likelihood function for the final model from the previous method)

The degrees of freedom for the block chi-square statistic is equal to the difference between the numbers of parameters estimated in each of the two models.

#### **Improvement Chi-Square**

2(log-likelihood function for current model – log-likelihood function for the model from the last step)

The degrees of freedom for the improvement chi-square statistic is equal to the difference between the numbers of parameters estimated in each of the two models.

**Goodness of Fit**

$$\sum_{i=1}^n \frac{w_i (y_i - \hat{\pi}_i)^2}{\hat{\pi}_i (1 - \hat{\pi}_i)}$$

**Cox and Snell's R-Square (Cox and Snell, 1989; Nagelkerke, 1991)**

$$R_{CS}^2 = 1 - \left( \frac{l(0)}{l(\hat{\beta})} \right)^{\frac{2}{W}}$$

where  $l(\hat{\beta})$  is the likelihood of the current model and  $l(0)$  is the likelihood of the initial model; that is,  $l(0) = W \log(0.5)$  if the constant is not included in the model;  $l(0) = W[\hat{\pi}_o \log\{\hat{\pi}_o/(1 - \hat{\pi}_o)\} + \log(1 - \hat{\pi}_o)]$  if the constant is included in the model, where  $\hat{\pi}_o = \sum_i^n w_i y_i / W$ .

**Nagelkerke's R-Square (Nagelkerke, 1981)**

$$R_N^2 = R_{CS}^2 / \max(R_{CS}^2)$$

where  $\max(R_{CS}^2) = 1 - \{l(0)\}^{2/W}$ .

**Hosmer-Lemeshow Goodness-of-Fit Statistic**

The test statistic is obtained by applying a chi-square test on a  $2 \times g$  contingency table. The contingency table is constructed by cross-classifying the dichotomous dependent variable with a grouping variable (with  $g$  groups) in which groups are formed by partitioning the predicted probabilities using the percentiles of the predicted event probability. In the calculation, approximately 10 groups are used ( $g=10$ ). The corresponding groups are often referred to as the “deciles of risk” (Hosmer and Lemeshow, 2000).

If the values of independent variables for observation  $i$  and  $i'$  are the same, observations  $i$  and  $i'$  are said to be in the same block. When one or more blocks occur within the same decile, the blocks are assigned to this same group. Moreover, observations in the same block are not divided when they are placed into groups. This strategy may result in fewer than 10 groups (that is,  $g \leq 10$ ) and consequently, fewer degrees of freedom.

Suppose that there are  $Q$  blocks, and the  $q$ th block has  $m_q$  number of observations,  $q = 1, \dots, Q$ . Moreover, suppose that the  $k$ th group ( $k = 1, \dots, g$ ) is composed of the  $q_1$ th,  $\dots$ ,  $q_k$ th blocks of observations. Then the total number of observations in the  $k$ th group is  $s_k = \sum_{q_1}^{q_k} m_j$ . The total observed frequency of events (that is,  $Y=1$ ) in the  $k$ th group, call it  $O_{1k}$ , is the total number of observations in the  $k$ th group with  $Y=1$ . Let  $E_{1k}$  be the total expected frequency of the event in the  $k$ th group; then  $E_{1k}$  is given by  $E_{1k} = s_k \xi_k$ , where  $\xi_k$  is the average predicted event probability for the  $k$ th group.

$$\xi_k = \sum_{q_1}^{q_k} m_j \hat{\pi}_j / s_k$$

The Hosmer-Lemeshow goodness-of-fit statistic is computed as

$$\chi_{HL}^2 = \sum_{k=1}^g \frac{(O_{1k} - E_{1k})^2}{E_{1k}(1 - \xi_k)}$$

The  $p$  value is given by  $\Pr(\chi^2 \geq \chi_{HL}^2)$  where  $\chi^2$  is the chi-square statistic distributed with degrees of freedom  $(g-2)$ .

### Information for the Variables Not in the Equation

For each of the variables not in the equation, the score statistic is calculated along with the associated degrees of freedom, significance and partial  $R$ . Let  $X_i$  be a variable not currently in the model and  $S_i$  the score statistic. The partial  $R$  is defined by

$$Partial\_R = \begin{cases} \sqrt{\frac{S_i - 2 \times df}{-2L(initial)}} & \text{if } S_i > 2 \times df \\ 0 & \text{otherwise} \end{cases}$$

where  $df$  is the degrees of freedom associated with  $S_i$ , and  $L(initial)$  is the log-likelihood function for the initial model.

The residual Chi-Square printed for the variables not in the equation is defined as

$$R_{CS} = (L_{\mathbf{g}}^*)' B_{22} L_{\mathbf{g}}^*$$

$$\text{where } L_{\mathbf{g}}^* = (L_{\gamma_1}^*, \dots, L_{\gamma_{r_2}}^*)'$$

### Information for the Variables in the Equation

For each of the variables in the equation, the MLE of the Beta coefficients is calculated along with the standard errors, Wald statistics, degrees of freedom, significances, and partial  $R$ . If  $X_i$  is not a categorical variable currently in the equation, the partial  $R$  is computed as

$$Partial\_R = \begin{cases} sign(\hat{\beta}_i) \sqrt{\frac{Wald_i - 2}{-2L(initial)}} & \text{if } Wald_i > 2 \\ 0 & \text{otherwise} \end{cases}$$

If  $X_i$  is a categorical variable with  $m$  categories, the partial  $R$  is then

$$Partial\_R = \begin{cases} \sqrt{\frac{Wald_i - 2(m-1)}{-2L(initial)}} & \text{if } Wald_i > 2(m-1) \\ 0 & \text{otherwise} \end{cases}$$

### Casewise Statistics

The following statistics are computed for each case.

### Individual Deviance

The deviance of the  $i$ th case,  $G_i$ , is defined as

$$G_i = \begin{cases} \sqrt{2(y_i \ln(\hat{\pi}_i) + (1 - y_i) \ln(1 - \hat{\pi}_i))} & \text{if } y_i > \hat{\pi}_i \\ -\sqrt{2(y_i \ln(\hat{\pi}_i) + (1 - y_i) \ln(1 - \hat{\pi}_i))} & \text{otherwise} \end{cases}$$

**Leverage**

The leverage of the  $i$ th case,  $h_i$ , is the  $i$ th diagonal element of the matrix

$$\hat{\mathbf{V}}^{\frac{1}{2}} \mathbf{X} (\mathbf{X}' \mathbf{C} \hat{\mathbf{V}} \mathbf{X})^{-1} \mathbf{X}' \hat{\mathbf{V}}^{\frac{1}{2}}$$

where

$$\hat{\mathbf{V}} = \text{Diag}\{\hat{\pi}_1(1 - \hat{\pi}_1), \dots, \hat{\pi}_n(1 - \hat{\pi}_n)\}$$

**Studentized Residual**

$$\tilde{G}_i^* = \frac{G_i}{\sqrt{1-h_i}}$$

**Logit Residual**

$$\tilde{e}_i = \frac{e_i}{\hat{\pi}_i(1-\hat{\pi}_i)}$$

where  $e_i = y_i - \hat{\pi}_i$

**Standardized Residual**

$$z_i = \frac{e_i}{\sqrt{\hat{\pi}_i(1-\hat{\pi}_i)}}$$

**Cook's Distance**

$$D_i = \frac{z_i^2 h_i}{1-h_i}$$

**DFBETA**

Let  $\Delta\beta_i$  be the change of the coefficient estimates from the deletion of case  $i$ . It is computed as

$$\Delta\beta_i = \frac{(\mathbf{X}' \mathbf{C} \hat{\mathbf{V}} \mathbf{X})^{-1} \mathbf{X}'_i e_i}{1-h_i}$$

**Predicted Group**

If  $\hat{\pi}_i \geq 0.5$ , the predicted group is the group in which  $y=1$ .

Note the following:

For the unselected cases with nonmissing values for the independent variables in the analysis, the leverage ( $\tilde{h}_i$ ) is computed as

$$\tilde{h}_i = h_i - \frac{\hat{V}_i h_i^2}{1 + \hat{V}_i h_i}$$

where

$$h_i = \hat{V}_i \mathbf{X}'_i (\mathbf{X}' \mathbf{C} \hat{\mathbf{V}} \mathbf{X})^{-1} \mathbf{X}_i$$

For the unselected cases, the Cook's distance and DFBETA are calculated based on  $\tilde{h}_i$ .

### **Generated Model/Scoring**

For each record passed through a generated binomial logistic regression model, a predicted value and confidence score are calculated as follows:

#### **Predicted Value**

The probability of the value  $y = 1$  for record  $i$  is calculated as

$$\hat{\pi}_i = \frac{\exp(\hat{\eta}_i)}{1 + \exp(\hat{\eta}_i)}$$

where

$$\hat{\eta}_i = \mathbf{X}_i' \hat{\beta}$$

If  $\hat{\pi} > 0.5$ , the predicted value is 1; otherwise, the predicted value is 0.

#### **Confidence**

For records with a predicted value of  $y = 1$ , the confidence value is  $\hat{\pi}$ . For records with a predicted value of  $y = 0$ , the confidence value is  $(1 - \hat{\pi})$ .

#### **Blank Handling (generated model)**

Records with missing values for any input field in the final model cannot be scored, and are assigned a predicted value of \$null\$.



# KNN Algorithms

Nearest Neighbor Analysis is a method for classifying cases based on their similarity to other cases. In machine learning, it was developed as a way to recognize patterns of data without requiring an exact match to any stored patterns, or cases. Similar cases are near each other and dissimilar cases are distant from each other. Thus, the distance between two cases is a measure of their dissimilarity.

Cases that are near each other are said to be “neighbors.” When a new case (holdout) is presented, its distance from each of the cases in the model is computed. The classifications of the most similar cases – the nearest neighbors – are tallied and the new case is placed into the category that contains the greatest number of nearest neighbors.

You can specify the number of nearest neighbors to examine; this value is called  $k$ . The pictures show how a new case would be classified using two different values of  $k$ . When  $k = 5$ , the new case is placed in category  $I$  because a majority of the nearest neighbors belong to category  $I$ . However, when  $k = 9$ , the new case is placed in category  $\theta$  because a majority of the nearest neighbors belong to category  $\theta$ .

Nearest neighbor analysis can also be used to compute values for a continuous target. In this situation, the average or median target value of the nearest neighbors is used to obtain the predicted value for the new case.

## Notation

The following notation is used throughout this chapter unless otherwise stated:

$Y$	Optional $1 \times N$ vector of responses with element $y_n$ , where $n=1, \dots, N$ indexes the cases.
$X^0$	$P^0 \times N$ matrix of features with element $x_{pn}^0$ , where $p=1, \dots, P^0$ indexes the features and $n=1, \dots, N$ indexes the cases.
$X$	$P \times N$ matrix of encoded features with element $x_{pn}$ , where $p=1, \dots, P$ indexes the features and $n=1, \dots, N$ indexes the cases.
$P$	Dimensionality of the feature space; the number of continuous features plus the number of categories across all categorical features.
$N$	Total number of cases.
$N_j, j = 1, 2, \dots, J$	The number of cases with $Y = j$ , where $Y$ is a response variable with $J$ categories
$\hat{N}_j$	The number of cases which belong to class $j$ and are correctly classified as $j$ .
$\hat{N}_j^*$	The total number of cases which are classified as $j$ .

## Preprocessing

Features are coded to account for differences in measurement scale.

**Continuous**

Continuous features are optionally coded using adjusted normalization:

$$x_{pn} = \frac{2(x_{pn}^0 - \min(x_p^0))}{\max(x_p^0) - \min(x_p^0)} - 1$$

where  $x_{pn}$  is the normalized value of input feature  $p$  for case  $n$ ,  $x_p^0$  is the original value of the feature for case  $n$ ,  $\min(x_p^0)$  is the minimum value of the feature for all training cases, and  $\max(x_p^0)$  is the maximum value for all training cases.

**Categorical**

Categorical features are always temporarily recoded using one-of- $c$  coding. If a feature has  $c$  categories, then it is stored as  $c$  vectors, with the first category denoted  $(1,0,\dots,0)$ , the next category  $(0,1,0,\dots,0)$ , ..., and the final category  $(0,0,\dots,0,1)$ .

**Training**

Training a nearest neighbor model involves computing the distances between cases based upon their values in the feature set. The nearest neighbors to a given case have the smallest distances from that case. The distance metric, choice of number of nearest neighbors, and choice of the feature set have the following options.

**Distance Metric**

We use one of the following metrics to measure the similarity of query cases and their nearest neighbors.

**Euclidean Distance.** The distance between two cases is the square root of the sum, over all dimensions, of the weighted squared differences between the values for the cases.

$$Euclidean_{ih} = \sqrt{\sum_{p=1}^P w_{(p)} (x_{(p)i} - x_{(p)h})^2}$$

**City Block Distance.** The distance between two cases is the sum, over all dimensions, of the weighted absolute differences between the values for the cases.

$$CityBlock_{ih} = \sum_{p=1}^P w_{(p)} |x_{(p)i} - x_{(p)h}|$$

The feature weight  $w_{(p)}$  is equal to 1 when feature importance is not used to weight distances; otherwise, it is equal to the normalized feature importance:

$$w_{(p)} = FI_{(p)} / \sum_{p=1}^P FI_{(p)}$$

See “Output Statistics ” for the computation of feature importance  $FI_{(p)}$ .

### **Crossvalidation for Selection of $k$**

Cross validation is used for automatic selection of the number of nearest neighbors, between a minimum  $k_{\min}$  and maximum  $k_{\max}$ . Suppose that the training set has a cross validation variable with the integer values  $1, 2, \dots, V$ . Then the cross validation algorithm is as follows:

- ▶ For each  $k \in [k_{\min}, k_{\max}]$ , compute the average error rate or sum-of square error of  $k$ :  $CV_k = \sum_{v=1}^V e_v / V$ , where  $e_v$  is the error rate or sum-of square error when we apply the Nearest Neighbor model to make predictions on the cases with  $X = v$ ; that is, when we use the other cases as the training dataset.
- ▶ Select the optimal  $k$  as:  $\hat{k} = \arg\{\min CV_k : k_{\min} \leq k \leq k_{\max}\}$ .

*Note:* If multiple values of  $k$  are tied on the lowest average error, we select the smallest  $k$  among those that are tied.

### **Feature Selection**

Feature selection is based on the wrapper approach of Cunningham and Delany (2007) and uses forward selection which starts from  $J_{\text{Forced}}$  features which are entered into the model. Further features are chosen sequentially; the chosen feature at each step is the one that causes the largest decrease in the error rate or sum-of squares error.

Let  $S_J$  represent the set of  $J$  features that are currently chosen to be included,  $S_J^c$  represents the set of remaining features and  $e_J$  represents the error rate or sum-of-squares error associated with the model based on  $S_J$ .

The algorithm is as follows:

- ▶ Start with  $J = J_{\text{Forced}}$  features.
- ▶ For each feature in  $S_J^c$ , fit the  $k$  nearest neighbor model with this feature plus the existing features in  $S_J$  and calculate the error rate or sum-of square error for each model. The feature in  $S_J^c$  whose model has the smallest error rate or sum-of square error is the one to be added to create  $S_{J+1}$ .
- ▶ Check the selected stopping criterion. If satisfied, stop and report the chosen feature subset. Otherwise,  $J=J+1$  and go back to the previous step.

*Note:* the set of encoded features associated with a categorical predictor are considered and added together as a set for the purpose of feature selection.

### Stopping Criteria

One of two stopping criteria can be applied to the feature selection algorithm.

**Fixed number of features.** The algorithm adds a fixed number of features,  $J_{add}$ , in addition to those forced into the model. The final feature subset will have  $J_{add} + J_{Forced}$  features.  $J_{add}$  may be user-specified or computed automatically; if computed automatically the value is

$$J_{add} = \max \{ \min (20, P^0) - J_{Forced}, 0 \}$$

When this is the stopping criterion, the feature selection algorithm stops when  $J_{add}$  features have been added to the model; that is, when  $J_{add} = J + 1$ , stop and report  $S_{J+1}$  as the chosen feature subset.

*Note:* if  $J_{add} = 0$ , no features are added and  $S_J$  with  $J = J_{Forced}$  is reported as the chosen feature subset.

**Change in error rate or sum of squares error.** The algorithm stops when the change in the absolute error ratio indicates that the model cannot be further improved by adding more features. Specifically, if  $e_{J+1} = 0$  or  $e_J \geq e_{J+1}$  and

$$\frac{|e_J - e_{J+1}|}{e_J} \leq \Delta_{\min}$$

where  $\Delta_{\min}$  is the specified minimum change, stop and report  $S_{J+1}$  as the chosen feature subset.

If  $e_J < e_{J+1}$  and

$$\frac{|e_J - e_{J+1}|}{e_J} > 2\Delta_{\min}$$

stop and report  $S_J$  as the chosen feature subset.

*Note:* if  $e_J = 0$  for  $J = J_{Forced}$ , no features are added and  $S_J$  with  $J = J_{Forced}$  is reported as the chosen feature subset.

### Combined $k$ and Feature Selection

The following method is used for combined neighbors and features selection.

1. For each  $k$ , use the forward selection method for feature selection.
2. Select the  $k$ , and accompanying feature set, with the lowest error rate or the lowest sum-of-squares error.

### Blank Handling

All records with missing values for any input or output field are excluded from the estimation of the model.

## Output Statistics

The following statistics are available.

### Percent correct for class $j$

$$\frac{\hat{N}_j}{N_j} \times 100\%$$

### Overall percent for class $j$

$$\frac{\hat{N}_j^*}{N} \times 100\%$$

### Intersection of Overall percent and percent correct

$$\left( \sum_{j=1}^J \hat{N}_j / N \right) \times 100\%$$

### Error rate of classification

$$\left( 1 - \sum_{j=1}^J \hat{N}_j / N \right) \times 100\%$$

### Sum-of-Square Error for continuous response

$$\sum_{n=1}^N (y_n - \hat{y}_n)^2$$

where  $\hat{y}_n$  is the estimated value of  $y_n$ .

### Feature Importance

Suppose there are  $X_{(1)}, X_{(2)} \cdots X_{(m)}$  ( $1 \leq m \leq P^0$ ) in the model from the forward selection process with the error rate or sum-of-squares error  $e$ . The importance of feature  $X_{(p)}$  in the model is computed by the following method.

- ▶ Delete the feature  $X_{(p)}$  from the model, make predictions and evaluate the error rate or sum-of-squares error  $e_{(p)}$  based on features  $X_{(1)}, X_{(2)} \cdots X_{(p-1)}, X_{(p+1)}, \cdots, X_{(m)}$ .
- ▶ Compute the error ratio  $e_{(p)} + \frac{1}{m}$ .

The feature importance of  $X_{(p)}$  is  $FI_{(p)} = e_{(p)} + \frac{1}{m}$

## Scoring

After we find the  $k$  nearest neighbors of a case, we can classify it or predict its response value.

### **Categorical response**

Classify each case by majority vote of its  $k$  nearest neighbors among the training cases.

- ▶ If multiple categories are tied on the highest predicted probability, then the tie should be broken by choosing the category with largest number of cases in training set.
- ▶ If multiple categories are tied on the largest number of cases in the training set, then choose the category with the smallest data value among the tied categories. In this case, categories are assumed to be in the ascending sort or lexical order of the data values.

We can also compute the predicted probability of each category. Suppose  $k_j$  is the number of cases of the  $j$ th category among the  $k$  nearest neighbors. Instead of simply estimating the predicted probability for the  $j$ th category by  $\frac{k_j}{k}$ , we apply a Laplace correction as follows:

$$\frac{k_j + 1}{k + J}$$

where  $J$  is the number of categories in the training data set.

The effect of the Laplace correction is to shrink the probability estimates towards to  $1/J$  when the number of nearest neighbors is small. In addition, if a query case has  $k$  nearest neighbors with the same response value, the probability estimates are less than 1 and larger than 0, instead of 1 or 0.

### **Continuous response**

Predict each case using the mean or median function.

**Mean function.**  $\hat{y}_n = \sum_{m \in \text{Nearest}(n)} y_m / k$ , where  $\text{Nearest}(n)$  is the index set of those cases that are the nearest neighbors of case  $n$  and  $y_m$  is the value of the continuous response variable for case  $m$ .

**Median function.** Suppose that  $y_m, m \in \text{Nearest}(n)$  are the values of the continuous response variable, and we arrange  $y_m, m \in \text{Nearest}(n)$  from the lowest value to the highest value and denote them as  $y_{(j_1)} \leq y_{(j_2)} \leq \dots \leq y_{(j_k)}$ , then the median is

$$\hat{y}_n = \begin{cases} y_{(\frac{k+1}{2})} & k \text{ is odd} \\ \frac{y_{(\frac{k}{2})} + y_{(\frac{k}{2}+1)}}{2} & k \text{ is even} \end{cases}$$

## Blank Handling

Records with missing values for any input field cannot be scored and are assigned a predicted value and probability value(s) of \$null\$.

## References

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# Linear modeling algorithms

Linear models predict a continuous target based on linear relationships between the target and one or more predictors.

For algorithms on enhancing model accuracy, enhancing model stability, or working with very large datasets, see “Ensembles Algorithms” on p. 125.

## Notation

The following notation is used throughout this chapter unless otherwise stated:

$n$	Number of distinct records in the dataset. It is an integer and $n \geq 1$ .
$p$	Number of parameters (including parameters for dummy variables but excluding the intercept) in the model. It is an integer and $p \geq 0$ .
$p^*$	Number of non-redundant parameters (excluding the intercept) currently in the model. It is an integer and $0 \leq p^* \leq p$ .
$p^c$	Number of non-redundant parameters currently in the model. $p^c = p^* + 1$
$p^e$	Number of effects excluding the intercept. It is an integer and $0 \leq p^e \leq p$
$\mathbf{y}$	$n \times 1$ target vector with elements $y_i$ .
$f$	$n \times 1$ frequency weight vector.
$g$	$n \times 1$ regression weight vector.
$N$	Effective sample size. It is an integer and $N = \sum_{i=1}^n f_i$ . If there is no frequency weight vector, $N=n$ .
$\mathbf{X}$	$n \times (p + 1)$ design matrix with element $x_{ij}$ . The rows represent the records and the columns represent the parameters.
$\epsilon$	$n \times 1$ vector of unobserved errors.
$\beta$	$(p + 1) \times 1$ vector of unknown parameters; $\beta = (\beta_0, \beta_1, \dots, \beta_p)$ . $\beta_0$ is the intercept.
$\hat{\beta}$	$(p + 1) \times 1$ vector of parameter estimates.
$b$	$(p + 1) \times 1$ vector of standardized parameter estimates. It is the result of a sweep operation on matrix $\mathbf{R}$ . $b_0$ is the standardized estimate of the intercept and is equal to 0.
$\hat{\mathbf{y}}$	$n \times 1$ vector of predicted target values.
$\bar{X}_j$	Weighted sample mean for $X_j$ , $j = 1, 2, \dots, p$
$\bar{y}$	Weighted sample mean for $\mathbf{y}$ .
$S_{ij}$	Weighted sample covariance between $X_i$ and $X_j$ , $i, j = 1, 2, \dots, p$ .
$S_{iy}$	Weighted sample covariance between $X_i$ and $\mathbf{y}$ .
$S_{yy}$	Weighted sample variance for $\mathbf{y}$ .
$\mathbf{R}$	$(p + 1) \times (p + 1)$ weighted sample correlation matrix for $\mathbf{X}$ (excluding the intercept, if it exists) and $\mathbf{y}$ .
$\tilde{\mathbf{R}}$	The resulting matrix after a sweep operation whose elements are $\tilde{r}_{ij}$ .

## Model

Linear regression has the form

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

where  $\boldsymbol{\varepsilon}$  follows a normal distribution with mean 0 and variance  $\sigma^2\mathbf{D}^{-1}$ , where  $\mathbf{D}^{-1} = \text{diag}(1/g_1, \dots, 1/g_n)$ . The elements of  $\boldsymbol{\varepsilon}$  are independent with respect to each other.

Notes:

- $\mathbf{X}$  can be any combination of continuous and categorical effects.
- Constant columns in the design matrix are not used in model building.
- If  $n=1$  or the target is constant, no model is built.

### Missing values

Records with missing values are deleted listwise.

## Least squares estimation

The coefficients are estimated by the least squares (LS) method. First, we transform the model by pre-multiplying  $\mathbf{D}^{1/2}$  as follows:

$$\mathbf{D}^{1/2}\mathbf{y} = \mathbf{D}^{1/2}\mathbf{X}\boldsymbol{\beta} + \mathbf{D}^{1/2}\boldsymbol{\varepsilon}$$

so that the new unobserved error  $\mathbf{D}^{1/2}\boldsymbol{\varepsilon}$  follows a normal distribution  $N_n(0, \sigma^2\mathbf{I})$ , where  $\mathbf{I}$  is an identity matrix and  $\mathbf{D}^{1/2} = \text{diag}(\sqrt{g_1}, \dots, \sqrt{g_n})$ . Then the least squares estimates of  $\boldsymbol{\beta}$  can be obtained from the following formula

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\text{arg min}} \left( \mathbf{D}^{1/2}\mathbf{y} - \mathbf{D}^{1/2}\mathbf{X}\boldsymbol{\beta} \right)^T F \left( \mathbf{D}^{1/2}\mathbf{y} - \mathbf{D}^{1/2}\mathbf{X}\boldsymbol{\beta} \right)$$

where  $F = \text{diag}(f_1, \dots, f_n)$ . Note that

$$\begin{aligned} & \left( \mathbf{D}^{1/2}\mathbf{y} - \mathbf{D}^{1/2}\mathbf{X}\boldsymbol{\beta} \right)^T F \left( \mathbf{D}^{1/2}\mathbf{y} - \mathbf{D}^{1/2}\mathbf{X}\boldsymbol{\beta} \right) \\ &= (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T \mathbf{D}^{1/2} F \mathbf{D}^{1/2} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \\ &= (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T \mathbf{W} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \end{aligned}$$

where  $\mathbf{W} = \text{diag}(w_1, \dots, w_n) = \text{diag}(g_1 f_1, \dots, g_n f_n)$ , so the closed form solution of  $\hat{\boldsymbol{\beta}}$  is

$$\hat{\boldsymbol{\beta}} = \left( \mathbf{X}^T \mathbf{W} \mathbf{X} \right)^{-1} \mathbf{X}^T \mathbf{W} \mathbf{y}$$

$\hat{\beta}$  is computed by applying sweep operations instead of the equation above. In addition, sweep operations are applied to the transformed scale of  $\mathbf{X}$  and  $\mathbf{y}$  to achieve numerical stability. Specifically, we construct the weighted sample correlation matrix  $\mathbf{R}$  then apply sweep operations to it. The  $\mathbf{R}$  matrix is constructed as follows.

First, compute weighted sample means, variances and covariances among  $\mathbf{X}_i$ ,  $\mathbf{X}_j$ ,  $i, j = 1, \dots, p$ , and  $\mathbf{y}$  :

Weighted sample means of  $\mathbf{X}_i$  and  $\mathbf{y}$  are  $\bar{X}_i = \frac{1}{\sum_{k=1}^n w_k} \sum_{k=1}^n w_k x_{ki}$  and  $\bar{y} = \frac{1}{\sum_{k=1}^n w_k} \sum_{k=1}^n w_k y_k$ ;

Weighted sample covariance for  $\mathbf{X}_i$  and  $\mathbf{X}_j$  is  $S_{ij} = \frac{1}{N-1} \sum_{k=1}^n w_k (x_{ki} - \bar{X}_i) (x_{kj} - \bar{X}_j)$ ;

Weighted sample covariance for  $\mathbf{X}_i$  and  $\mathbf{y}$  is  $S_{iy} = \frac{1}{N-1} \sum_{k=1}^n w_k (x_{ki} - \bar{X}_i) (y_k - \bar{y})$ ;

Weighted sample variance for  $\mathbf{y}$  is  $S_{yy} = \frac{1}{N-1} \sum_{k=1}^n w_k (y_k - \bar{y})^2$ .

Second, compute weighted sample correlations  $r_{ij} = \frac{S_{ij}}{\sqrt{S_{ii}S_{jj}}}$ ,  $i, j = 1, \dots, p$  and  $y$ .

Then the matrix  $\mathbf{R}$  is

$$\mathbf{R} = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1p} & r_{1y} \\ r_{21} & r_{22} & \cdots & r_{2p} & r_{2y} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ r_{p1} & r_{p2} & \cdots & r_{pp} & r_{py} \\ r_{y1} & r_{y2} & \cdots & r_{yp} & r_{yy} \end{bmatrix} = \begin{bmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} \\ \mathbf{R}_{12}^T & R_{22} \end{bmatrix}$$

If the sweep operations are repeatedly applied to each row of  $\mathbf{R}_{11}$ , where  $\mathbf{R}_{11}$  contains the predictors in the model at the current step, the result is

$$\tilde{\mathbf{R}} = \begin{bmatrix} \mathbf{R}_{11}^{-1} & \mathbf{R}_{11}^{-1}\mathbf{R}_{12} \\ -\mathbf{R}_{12}^T\mathbf{R}_{11}^{-1} & R_{22} - \mathbf{R}_{12}^T\mathbf{R}_{11}^{-1}\mathbf{R}_{12} \end{bmatrix}$$

The last column  $\mathbf{R}_{11}^{-1}\mathbf{R}_{12}$  contains the standardized coefficient estimates; that is,  $\mathbf{b} = \mathbf{R}_{11}^{-1}\mathbf{R}_{12}$ . Then the coefficient estimates, except the intercept estimate if there is an intercept in the model, are:

$$\hat{\beta}_j = b_j \sqrt{\frac{S_{yy}}{S_{jj}}}$$

## Model selection

The following model selection methods are supported:

- None, in which no selection method is used and effects are force entered into the model. For this method, the singularity tolerance is set to 1e-12 during the sweep operation.

- Forward stepwise, which starts with no effects in the model and adds and removes effects one step at a time until no more can be added or removed according to the stepwise criteria.
- Best subsets, which checks “all possible” models, or at least a larger subset of the possible models than forward stepwise, to choose the best according to the best subsets criterion.

### Forward stepwise

The basic idea of the forward stepwise method is to add effects one at a time as long as these additions are worthy. After an effect has been added, all effects in the current model are checked to see if any of them should be removed. Then the process continues until a stopping criterion is met. The traditional criterion for effect entry and removal is based on their  $F$ -statistics and corresponding  $p$ -values, which are compared with some specified entry and removal significance levels; however, these statistics may not actually follow an  $F$  distribution so the results might be questionable. Hence the following additional criteria for effect entry and removal are offered:

- Maximum adjusted  $R^2$ ;
- Minimum corrected Akaike information criterion (AICC); and
- Minimum average squared error (ASE) over the overfit prevention data

### Candidate statistics

Some additional notations are needed describe the addition or removal of a continuous effect  $X_j$  or categorical effect  $\{X_{j_s}\}_{s=1}^{\ell}$ , where  $\ell$  is the number of categories.

$\ell^*$	The number of non-redundant parameters of the eligible effect $\mathbf{X}_j$ or $\{X_{j_s}\}_{s=1}^{\ell}$ .
$p^c$	The number of non-redundant parameters in the current model (including the intercept).
$p^r$	The number of non-redundant parameters in the resulting model (including the intercept). Note that $p^r = \begin{cases} p^c + \ell^* & \text{for entering an effect} \\ p^c - \ell^* & \text{for removing an effect} \end{cases}$
$SSE_p$	The weighted residual sum of squares for the current model.
$SSE_{p+\ell}$	The weighted residual sum of squares for the resulting model after entering the effect.
$SSE_{p-\ell}$	The weighted residual sum of squares for the resulting model after removing the effect.
$r_{yy}$	The last diagonal element in the current $\mathbf{R}$ matrix.
$\tilde{r}_{yy}$	The last diagonal element in the resulting $\tilde{\mathbf{R}}$ matrix.

**F statistics.** The  $F$  statistics for entering or removing an effect from the current model are:

$$F_{enter_j} = \frac{(SSE_p - SSE_{p+\ell})/\ell^*}{SSE_{p+\ell}/(N - p^r)} = \frac{(r_{yy} - \tilde{r}_{yy})(N - p^r)}{\tilde{r}_{yy} \times \ell^*}$$

$$F_{remove_j} = \frac{(SSE_{p-\ell} - SSE_p)/\ell^*}{SSE_p/(N - p^c)} = \frac{(\tilde{r}_{yy} - r_{yy})(N - p^c)}{r_{yy} \times \ell^*}$$

and their corresponding  $p$ -values are:

$$p_{enter_j} = P(F_{\ell^*, N-p^r} \geq F_{enter_j}) = 1 - P(F_{\ell^*, N-p^r} \leq F_{enter_j})$$

$$p_{remove_j} = P(F_{\ell^*, N-p^c} \geq F_{remove_j}) = 1 - P(F_{\ell^*, N-p^c} \leq F_{remove_j})$$

**Adjusted R-squared.** The adjusted  $R^2$  value for entering or removing an effect from the current model is:

$$\text{adj.}R^2 = 1 - \frac{(N-1)\tilde{r}_{yy}}{N-p^r}$$

**Corrected Akaike Information Criterion (AICC).** The AICC value for entering or removing an effect from the current model is:

$$AICC = N \ln \left( \frac{(N-1)S_{yy} \times \tilde{r}_{yy}}{N} \right) + \frac{2p^r N}{N-p^r-1}$$

**Average Squared Error (ASE).** The ASE value for entering or removing an effect from the current model is:

$$ASE = \frac{1}{\sum_{t=1}^T f_t} \sum_{t=1}^T w_t (y_t - \hat{y}_t)^2$$

where  $\hat{y}_t = x_t \hat{\beta}$  are the predicted values of  $y_t$  and  $T$  is the number of distinct testing cases in the overfit prevention set.

### The Selection Process

There are slight variations in the selection process, depending upon the model selection criterion:

- The  $F$  statistic criterion is to select an effect for entry (removal) with the minimum (maximum)  $p$ -value and continue doing it until the  $p$ -values of all candidates for entry (removal) are equal to or greater than (less than) a specified significance level.
- The other three criteria are to compare the statistic (adjusted  $R^2$ , AICC or ASE) of the resulting model after entering (removing) an effect with that of the current model. Selection stops at a local optimal value (a maximum for the adjusted  $R^2$  criterion and a minimum for the AICC and ASE).

The following additional definitions are needed for the selection process:

<b>FLAG</b>	A $p^e \times 1$ index vector which records the status of each effect. $FLAG_i = 1$ means the effect $i$ is in the current model, $FLAG_i = 0$ means it is not. $ \{i   FLAG_i = 1\} $ denotes the number of effects with $FLAG_i = 1$ .
<b>MAXSTEP</b>	The maximum number of iteration steps. The default value is $3 \times p^e$ .
<b>MAXEFFECT</b>	The maximum number of effects (excluding intercept if exists). The default value is $p^e$ .

$P_{in}$	The significance level for effect entry when the $F$ -statistic criterion is used. The default is 0.05.
$P_{out}$	The significance level for effect removal when the $F$ statistic criterion is used. The default is 0.1.
$\Delta F$	The $F$ statistic change. It is $F_{enter_j}$ or $F_{remove_j}$ for entering or removing an effect $X_j$ (here $X_j$ could represent continuous or categorical for simpler notation).
$p_{\Delta F}$	The corresponding $p$ -value for $\Delta F$ .
$MSC_{current}$	The adjusted $R^2$ , AICC, or ASE value for the current model.

1. Set  $\{FLAG_i\}_{i=1}^{p^e} = 0$  and  $iter = 0$ . The initial model is  $\hat{y} = \bar{y}$ . If the adjusted  $R^2$ , AICC, or ASE criterion is used, compute the statistic for the initial model and denote it as  $MSC_{current}$ .
2. If  $\{i|FLAG_i = 0\} \neq \emptyset$ ,  $iter \leq MAXSTEP$  and  $|\{i|FLAG_i = 1\}| < MAXEFFECT$ , go to the next step; otherwise stop and output the current model .
3. Based on the current model, for every effect  $j$  eligible for entry (see Condition below),
 

If FC (the  $F$  statistic criterion) is used, compute  $F_{enter_j}$  and  $p_{enter_j}$ ;

If MSC (the adjusted  $R^2$ , AICC, or ASE criterion) is used, compute  $MSC_j$ .
4. If FC is used, choose the effect  $X_{j^*}$ ,  $j^* = \arg \min_j \{p_{enter_j}\}$  and if  $p_{enter_{j^*}} < P_{in}$ , enter  $X_{j^*}$  to the current model.
 

If MSC is used, choose the effect  $X_{j^*}$ ,  $j^* = \arg \min_j \{MSC_j\}$  and if  $MSC_{j^*} < MSC_{current}$ , enter  $X_{j^*}$  to the current model. (For the adjusted  $R^2$  criterion, replace min with max and reverse the inequality)

If the inequality is not satisfied, stop and output the current model.
5. If the model with the new effect is the same as any previously obtained model, stop and output the current model; otherwise update the current model by doing the sweep operation on corresponding row(s) and column(s) associated with  $X_{j^*}$  in the current  $\mathbf{R}$  matrix. Set  $FLAG_{j^*} = 1$  and  $iter = iter + 1$ .
 

If FC is used, let  $\Delta F = F_{enter_{j^*}}$  and  $p_{\Delta F} = p_{enter_{j^*}}$ ;

If MSC is used, let  $MSC_{current} = MSC_{j^*}$ .
6. For every effect  $k$  in the current model; that is,  $FLAG_k = 1, \forall k$ ,
 

If FC is used, compute  $F_{remove_k}$  and  $p_{remove_k}$ ;

If MSC is used, compute  $MSC_k$ .
7. If FC is used, choose the effect  $X_{k^*}$ ,  $k^* = \arg \max_k \{p_{remove_k}\}$  and if  $p_{remove_{k^*}} > P_{out}$ , remove  $X_{k^*}$  from the current model.
 

If MSC is used, choose the effect  $X_{k^*}$ ,  $k^* = \arg \min_k \{MSC_k\}$  and if  $MSC_{k^*} < MSC_{current}$ , remove  $X_{k^*}$  from the current model. (For the adjusted  $R^2$  criterion, replace min with max and reverse the inequality)

If the inequality is met, go to the next step; otherwise go back to step 2.

8. If the model with the effect removed is the same as any previously obtained model, stop and output the current model; otherwise update the current model by doing the sweep operation on corresponding row(s) and column(s) associated with  $X_{j^*}$  in the current  $\mathbf{R}$  matrix. Set  $FLAG_{j^*} = 0$  and  $iter = iter + 1$ .

If FC is used, let  $\Delta F = F_{remove_{k^*}}$  and  $p_{\Delta F} = p_{remove_{k^*}}$ ;

If AC is used, let  $AICC_{current} = AICC_{k^*}$ . Then go back to step 6.

**Condition.** In order for effect  $j$  to be eligible for entry into the model, the following conditions must be met:

For continuous a effect  $X_j$ ,  $r_{jj} \geq t$ ; ( $t$  is the singularity tolerance with a value of  $1e-4$ )

For categorical effect  $\{X_{j_s}\}_{s=1}^{\ell}$ ,  $\max\{r_{j_1j_1}, r_{j_2j_2}, \dots, r_{j_{\ell}j_{\ell}}\} \geq t$ ;

where  $t$  is the singularity tolerance, and  $r_{jj}$  and  $r_{j_sj_s}$ ,  $s = 1, \dots, \ell$ , are diagonal elements in the current  $\mathbf{R}$  matrix (before entering).

For each continuous effect  $X_k$  that is currently in the model,  $\tilde{r}_{kk}t \leq 1$ .

For each categorical effect  $\{X_{k_s}\}_{s=1}^{\ell'}$  with  $\ell'$  levels that is currently in the model,  $\max\{\tilde{r}_{k_1k_1}, \tilde{r}_{k_2k_2}, \dots, \tilde{r}_{k_{\ell'}k_{\ell'}}\}t \leq 1$ .

where  $\tilde{r}_{kk}$  and  $\tilde{r}_{k_s k_s}$ ,  $s = 1, \dots, \ell'$ , are diagonal elements in the resulting  $\mathbf{R}$  matrix; that is, the results after doing the sweep operation on corresponding row(s) and column(s) associated with  $X_k$  or  $\{X_{k_s}\}_{s=1}^{\ell'}$  in the current  $\mathbf{R}$  matrix. The above condition is imposed so that entry of the effect does not reduce the tolerance of other effects already in the model to unacceptable levels.

## Best subsets

Stepwise methods search fewer combinations of sub-models and rarely select the best one, so another option is to check all possible models and select the “best” based upon some criterion. The available criteria are the maximum adjusted  $R^2$ , minimum AICC, and minimum ASE over the overfit prevention set.

Since there are  $p^e$  free effects, we do an exhaustive search over  $2^{p^e}$  models, which include intercept-only model ( $\hat{y} = \bar{y}$ ). Because the number of calculations increases exponentially with  $p^e$ , it is important to have an efficient algorithm for carrying out the necessary computations. However, if  $p^e$  is too large, it may not be practical to check all of the possible models.

We divide the problem into 2 tiers in terms of the number of effects:

- when  $p^e \leq 20$ , we search all possible subsets
- when  $p^e > 20$ , we apply a hybrid method which combines the forward stepwise method and the all possible subsets method.

### Searching All Possible Subsets

An efficient method that minimizes the number of sweep operations on the  $\mathbf{R}$  matrix (Schatzoff 1968), is applied to traverse all the models and outlined as follows:

Each sweep step(s) on an effect results in a model. So  $2^{p^e}$  models can be obtained through a sequence of exactly  $2^{p^e}$  sweeps on effects. Assuming that the all possible models on  $p^e - 1$  effects can be obtained in a sequence  $S_{p^e-1}$  of exactly  $2^{p^e-1}$  sweeps on the first  $2^{p^e-1}$  pivotal effects, and sweeping on the last effect will produce a new model which adds the last effect to the model produced by the sequence  $S_{p^e-1}$ , then repeating the sequence  $S_{p^e-1}$  will produce another  $2^{p^e-1}$  distinct models (including the last effect). It is a recursive algorithm for constructing the sequence; that is,  $S_{p^e} = (S_{p^e-1}, k, S_{p^e-1}) = (S_{p^e-2}, k-1, S_{p^e-2}, k, S_{p^e-2}, k-1, S_{p^e-2}) = \dots$ , and so on.

The sequence of models produced is demonstrated in the following table:

$k$	$S_k$	Sequence of models produced
0	0	Only intercept
1	1	(1)
2	121	(1),(12),(2)
3	1213121	(1),(12),(2),(23),(123),(13),(3)
4	121312141213121	(1),(12),(2),(23),(123),(13),(3),(34),(134),(1234),(234),(24),(124),(14),(4)
...	...	...
$p^e$	$S_{p^e-1}, p^e, S_{p^e-1}$	All $2^{p^e}$ models including the intercept model.

The second column indicates the indexes of effects which are pivoted on. Each parenthesis in the third column represents a regression model. The numbers in the parentheses indicate the effects which are included in that model.

### Hybrid Method

If  $p^e > 20$ , we apply a hybrid method by combining the forward stepwise method with the all possible subsets method as follows:

Select the effects using the forward stepwise method with the same criterion chosen for best subsets. Say that  $p^s$  is the number of effects chosen by the forward stepwise method.

Apply one of the following approaches, depending on the value of  $p^s$ , as follows:

- If  $p^s \leq 20$ , do an exhaustive search of all possible subsets on these selected effects, as described above.
- If  $20 < p^s \leq 40$ , select  $p^s - 20$  effects based on the  $p$ -values of type III sum of squares tests from all  $p^s$  effects (see ANOVA in “Model evaluation ” on p. 279) and enter them into the model, then do an exhaustive search of the remaining 20 effects via the method described above.
- If  $40 < p^s$ , do nothing and assume the best model is the one with these  $p^s$  effects (with a warning message that the selected model is based on the forward stepwise method).

## Model evaluation

The following output statistics are available.

### ANOVA

#### Weighted total sum of squares

$$SS_t = \sum_{i=1}^n w_i (y_i - \bar{y})^2 = (N - 1) S_{yy} \text{ with d.f.} = df_t = N - 1$$

where d.f. means degrees of freedom. It is called “SS (sum of squares) for Corrected Total”.

#### Weighted residual sum of squares

$$SS_e = \sum_{i=1}^n w_i (y_i - \hat{y}_i)^2 = \tilde{r}_{yy} (N - 1) S_{yy}$$

with d.f. =  $df_e = N - p^c$ . It is also called “SS for Error”.

#### Weighted regression sum of squares

$$SS_r = \sum_{i=1}^n w_i (\hat{y}_i - \bar{y})^2 = (1 - \tilde{r}_{yy}) (N - 1) S_{yy} = SS_t - SS_e$$

with d.f. =  $df_r = p^*$ . It is called “SS for Corrected Model” if there is an intercept.

#### Regression mean square error

$$SS_r / df_r$$

#### Residual mean square error

$$SS_e / df_e$$

#### F statistic for corrected model

$$F = \frac{SS_r / df_r}{SS_e / df_e} = \frac{SS_r \cdot df_e}{SS_e \cdot df_r}$$

which follows an  $F$  distribution with degrees of freedom  $df_r$  and  $df_e$ , and the corresponding  $p$ -value can be calculated accordingly.

#### Type III sum of squares for each effect

To compute type III SS for the effect  $j$ ,  $j = 1, \dots, p^e$ , the type III test matrix  $\mathbf{L}_j$  needs to be constructed first. Construction of  $\mathbf{L}_j$  is based on the generating matrix  $\mathbf{H}_\omega = (\mathbf{X}^T \mathbf{D} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{D} \mathbf{X}$ , where  $\mathbf{D} = \text{diag}(g_1, \dots, g_n)$ , such that  $\mathbf{L}_j \boldsymbol{\beta}$  is estimable. It involves parameters only for the given effect and the effects containing the given effect. For type III analysis,  $\mathbf{L}_j$  doesn't depend on the order of effects specified in the model. If such a matrix cannot be constructed, the effect is not testable. For each effect  $j$ , the type III SS is calculated as follows

$$\mathbf{S}_j = \hat{\boldsymbol{\beta}}^T \mathbf{L}_j^T \left( \mathbf{L}_j \mathbf{G} \mathbf{L}_j^T \right)^{-1} \mathbf{L}_j \hat{\boldsymbol{\beta}}$$

where  $\mathbf{G} = (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1}$ .

### F statistic for each effect

The SS for the effect  $j$  is also used to compute the  $F$  statistic for the hypothesis test  $H_0: \mathbf{L}_j \boldsymbol{\beta} = \mathbf{0}$  as follows:

$$F_j = \frac{\mathbf{S}_j / r_j}{SS_e / df_e}$$

where  $r_j$  is the full row rank of  $\mathbf{L}_j$ . It follows an  $F$  distribution with degrees of freedom  $r_j$  and  $df_e$ , then the  $p$ -values can be calculated accordingly.

### Model summary

#### Adjusted R square

$$\text{adj.}R^2 = 1 - \frac{SS_e / df_e}{SS_t / df_t} = R^2 - \frac{(1 - R^2) p^*}{df_e} = 1 - \frac{df_t \times \tilde{r}_{yy}}{df_e}$$

where

$$R^2 = \frac{SS_r}{SS_t} = 1 - \frac{SS_e}{SS_t} = 1 - \tilde{r}_{yy}.$$

### Model information criteria

#### Corrected Akaike information criterion (AICC)

$$AICC = N \ln \left( \frac{SS_e}{N} \right) + \frac{2p^c N}{N - p^c - 1}$$

## Coefficients and statistical inference

After the model selection process, we can get the coefficients and related statistics from the swept correlation matrix. The following statistics are computed based on the  $\mathbf{R}$  matrix.

**Unstandardized coefficient estimates**

$$\hat{\beta}_j = b_j \sqrt{\frac{S_{yy}}{S_{jj}}} = \tilde{r}_{jy} \sqrt{\frac{S_{yy}}{S_{jj}}}$$

for  $j = 1, \dots, p^*$ .

**Standard errors of regression coefficients**

The standard error of  $\hat{\beta}_j$  is

$$\hat{\sigma}_{\hat{\beta}_j} = \sqrt{\text{var}(\hat{\beta}_j)} = \sqrt{\frac{\tilde{r}_{jj} \tilde{r}_{yy} S_{yy}}{S_{jj} df_e}}$$

**Intercept estimation**

The intercept is estimated by all other parameters in the model as

$$\hat{\beta}_0 = \bar{y} - \sum_{j=1}^p \hat{\beta}_j \bar{X}_j$$

The standard error of  $\hat{\beta}_0$  is estimated by

$$\hat{\sigma}_{\hat{\beta}_0} = \sqrt{\hat{\sigma}_{\hat{\beta}_0}^2}$$

where

$$\begin{aligned} \hat{\sigma}_{\hat{\beta}_0}^2 &= \frac{(N-1)\tilde{r}_{yy}S_{yy}}{N(N-p^*-1)} + \sum_{j=1}^p \bar{X}_j^2 \hat{\sigma}_{\hat{\beta}_j}^2 + 2 \sum_{j=1}^{p-1} \sum_{k=j+1}^p \bar{X}_k \bar{X}_j \text{cov}(\hat{\beta}_k, \hat{\beta}_j) \\ &= \frac{SS_e}{N \times df_e} + \sum_{j=1}^p \bar{X}_j^2 \hat{\sigma}_{\hat{\beta}_j}^2 + 2 \sum_{j=1}^{p-1} \sum_{k=j+1}^p \bar{X}_k \bar{X}_j \frac{\tilde{r}_{kj} \times SS_e}{\sqrt{S_{kk} S_{jj}} \times (N-1) df_e}. \end{aligned}$$

$\hat{\sigma}_{\hat{\beta}_0}^2 = \frac{(N-1)\tilde{r}_{yy}S_{yy}}{N(N-p^*-1)} + \sum_{j=1}^p \bar{X}_j^2 \hat{\sigma}_{\hat{\beta}_j}^2 + 2 \sum_{j=1}^{p-1} \sum_{k=j+1}^p \bar{X}_k \bar{X}_j \text{cov}(\hat{\beta}_k, \hat{\beta}_j)$  and  $\text{cov}(\hat{\beta}_k, \hat{\beta}_j)$  is the  $k$ th row and  $j$ th column element in the parameter estimates covariance matrix.

**t statistics for regression coefficients**

$$t = \frac{\hat{\beta}_j}{\hat{\sigma}_{\hat{\beta}_j}} = \tilde{r}_{jy} \sqrt{\frac{df_e}{\tilde{r}_{yy} \tilde{r}_{jj}}}$$

for  $j = 1, \dots, p^*$ , with degrees of freedom  $df_e$  and the  $p$ -value can be calculated accordingly.

**100(1- $\alpha$ )% confidence intervals**

$$\hat{\beta}_j \pm \hat{\sigma}_{\hat{\beta}_j} \times t_{\alpha/2, df_e}$$

*Note:* For redundant parameters, the coefficient estimates are set to zero and standard errors, t statistics, and confidence intervals are set to missing values.

## Scoring

### Predicted values

$$\hat{y}_k = \sum_{i=0}^p x_{ki} \hat{\beta}_i, k = 1, \dots, n.$$

## Diagnostics

The following values are computed to produce various diagnostic charts and tables.

### Residuals

$$e_k = y_k - \hat{y}_k$$

### Studentized residuals

This is the ratio of the residual to its standard error.

$$SRES_k = \frac{e_k}{s \sqrt{\frac{(1-h_k)}{g_k}}}$$

where  $s$  is the square root of the mean square error; that is,  $s = \sqrt{SS_e/df_e}$ , and  $h_k$  is the leverage value for the  $k$ th case (see below).

### Cook's distance

$$COOK_k = \frac{e_k^2 h_k g_k}{s^2 (1 - h_k)^2 p^c}$$

where the “leverage”

$$h_k = g_k \mathbf{x}_k \mathbf{G} \mathbf{x}_k^T$$

is the  $k$ th diagonal element of the hat matrix

$$\mathbf{H} = \mathbf{W}^{1/2} \mathbf{X} (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{W}^{1/2} = \mathbf{W}^{1/2} \mathbf{X} \mathbf{G} \mathbf{X}^T \mathbf{W}^{1/2}$$

A record with Cook's distance larger than  $\frac{4}{N-p^c}$  is considered influential (Fox, 1997).

## Predictor importance

We use the leave-one-out method to compute the predictor importance, based on the residual sum of squares (SSE) by removing one predictor at a time from the final full model.

If the final full model contains  $p$  predictors,  $X_1, X_2, \dots, X_p$ , then the predictor importance can be calculated as follows:

1.  $i=1$
2. If  $i > p$ , go to step 5.
3. Do a sweep operation on the corresponding row(s) and column(s) associated with  $X_i$  in the  $\tilde{\mathbf{R}}$  matrix of the full final model.
4. Get the last diagonal element in the current  $\tilde{\mathbf{R}}$  and denote it  $\tilde{r}_{yy}^{(i)}$ . Then the predictor importance of  $X_i$  is  $VI_i = \left( \tilde{r}_{yy}^{(i)} - \tilde{r}_{yy} \right) (N - 1) SS_{yy}$ . Let  $i = i + 1$ , and go to step 2.
5. Compute the normalized predictor importance of  $X_i$ :

$$NormVI_i = \frac{VI_i}{\sum_{i=1}^p VI_i}$$

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# Neural Networks Algorithms

Neural networks predict a continuous or categorical target based on one or more predictors by finding unknown and possibly complex patterns in the data.

For algorithms on enhancing model accuracy, enhancing model stability, or working with very large datasets, see “Ensembles Algorithms” on p. 125.

## Multilayer Perceptron

The multilayer perceptron (MLP) is a feed-forward, supervised learning network with up to two hidden layers. The MLP network is a function of one or more predictors that minimizes the prediction error of one or more targets. Predictors and targets can be a mix of categorical and continuous fields.

### Notation

The following notation is used for multilayer perceptrons unless otherwise stated:

$X^{(m)} = (x_1^{(m)}, \dots, x_P^{(m)})$	Input vector, pattern $m$ , $m=1, \dots, M$ .
$Y^{(m)} = (y_1^{(m)}, \dots, y_R^{(m)})$	Target vector, pattern $m$ .
$I$	Number of layers, discounting the input layer.
$J_i$	Number of units in layer $i$ . $J_0 = P$ , $J_1 = R$ , discounting the bias unit.
$\Gamma^c$	Set of categorical outputs.
$\Gamma$	Set of continuous outputs.
$\Gamma_h$	Set of subvectors of $Y^{(m)}$ containing 1-of- $c$ coded $h$ th categorical field.
$a_{i:j}^m$	Unit $j$ of layer $i$ , pattern $m$ , $j = 0, \dots, J_i$ ; $i = 0, \dots, I$ .
$w_{i:j,k}$	Weight leading from layer $i-1$ , unit $j$ to layer $i$ , unit $k$ . No weights connect $a_{i-1:j}^m$ and the bias $a_{i:0}^m$ ; that is, there is no $w_{i:j,0}$ for any $j$ .
$c_{i:k}^m$	$\sum_{j=0}^{J_{i-1}} w_{i:j,k} a_{i-1:j}^m$ , $i=1, \dots, I$ .
$\gamma_i(c)$	Activation function for layer $i$ .
$\mathbf{w}$	Weight vector containing all weights $(w_{1:0,1}, w_{1:0,2}, \dots, w_{I:J_{I-1},J_I})$ .

### Architecture

The general architecture for MLP networks is:

**Input layer:**  $J_0=P$  units,  $a_{0:1}, \dots, a_{0:J_0}$ ; with  $a_{0:j} = x_j$ .

**$i$ th hidden layer:**  $J_i$  units,  $a_{i:1}, \dots, a_{i:J_i}$ ; with  $a_{i:k} = \gamma_i(c_{i:k})$  and  $c_{i:k} = \sum_{j=0}^{J_{i-1}} w_{i:j,k} a_{i-1:j}$  where  $a_{i-1:0} = 1$ .

**Output layer:**  $J_I=R$  units,  $a_{I:1}, \dots, a_{I:J_I}$ ; with  $a_{I:k} = \gamma_I(c_{I:k})$  and  $c_{I:k} = \sum_{j=0}^{J_1} w_{I:j,k} a_{i-1:j}$  where  $a_{i-1:0} = 1$ .

Note that the pattern index and the bias term of each layer are not counted in the total number of units for that layer.

### Activation Functions

#### Hyperbolic Tangent

$$\gamma(c) = \tanh(c) = \frac{e^c - e^{-c}}{e^c + e^{-c}}$$

This function is used for hidden layers.

#### Identity

$$\gamma(c) = c$$

This function is used for the output layer when there are continuous targets.

#### Softmax

$$\gamma(c_k) = \frac{\exp(c_k)}{\sum_{j \in \Gamma_h} \exp(c_j)}$$

This function is used for the output layer when all targets are categorical.

### Error Functions

#### Sum-of-Squares

$$E_T(w) = \sum_{m=1}^M E_m(w)$$

where

$$E_m(w) = \frac{1}{2} \sum_{r=1}^R \left( y_r^{(m)} - a_{I:r}^m \right)^2$$

This function is used when there are continuous targets.

**Cross-Entropy**

$$E_T(w) = \sum_{m=1}^M E_m(w)$$

where

$$E_m(w) = - \sum_{r \in \Gamma^c} y_r^{(m)} \log \left( \frac{a_{I:r}^m}{y_r^{(m)}} \right)$$

This function is used when all targets are categorical.

**Expert Architecture Selection**

Expert architecture selection determines the “best” number of hidden units in a single hidden layer.

A random sample is taken from the entire data set and split into training (70%) and testing samples (30%). The size of random sample is  $N = 1000$ . If entire dataset has less than  $N$  records, use all of them. If training and testing data sets are supplied separately, the random samples for training and testing should be taken from the respective datasets.

Given  $K_{\min}$  and  $K_{\max}$ , the algorithm is as follows.

1. Start with an initial network of  $k$  hidden units. The default is  $k = \min(g(R, P), 20, h(R, P))$ , where

$$g(R, P) = \begin{cases} \lfloor 4.5 + \sqrt{P + R} \rfloor & R < 5, P \geq 8 \\ \lfloor 0.5 + 0.5(P + R) \rfloor & \text{otherwise} \end{cases}$$

where  $\lfloor x \rfloor$  denotes the largest integer less than or equal to  $x$ .  $h(R, P) = \left\lfloor \frac{M - R}{P + R + 1} \right\rfloor$  is the maximum number of hidden units that will not result in more weights than there are records in the entire training set.

If  $k < K_{\min}$ , set  $k = K_{\min}$ . Else if  $k > K_{\max}$ , set  $k = K_{\max}$ . Train this network once via the alternated simulated annealing and training procedure (steps 1 to 5).

2. If  $k > K_{\min}$ , set  $DOWN = TRUE$ . Else if training error ratio  $> 0.01$ ,  $DOWN = FALSE$ . Else stop and report the initial network.
3. If  $DOWN = TRUE$ , remove the weakest hidden unit (see below);  $k = k - 1$ . Else add a hidden unit;  $k = k + 1$ .
4. Using the previously fit weights as initial weights for the old weights and random weights for the new weights, train the old and new weights for the network once through the alternated simulated annealing and training procedure (steps 3 to 5) until the stopping conditions are met.
5. If the error on test data has dropped:

If  $DOWN = FALSE$ , If  $k < K_{\max}$  and the training error has dropped but the error ratio is still above 0.01, return to step 3. Else if  $k > K_{\min}$ , return to step 3. Else, stop and report the network with the minimum test error.

Else if  $DOWN=TRUE$ , If  $|k-k_0|>1$ , stop and report the network with the minimum test error. Else if training error ratio for  $k=k_0$  is bigger than 0.01, set  $DOWN=FALSE$ ,  $k=k_0$  return to step 3. Else stop and report the initial network.

Else stop and report the network with the minimum test error.

If more than one network attains the minimum test error, choose the one with fewest hidden units.

If the resulting network from this procedure has training error ratio (training error divided by error from the model using average of an output field to predict that field) bigger than 0.1, repeat the architecture selection with different initial weights until either the error ratio is  $\leq 0.1$  or the procedure is repeated 5 times, then pick the one with smallest test error.

Using this network with its weights as initial values, retrain the network on the entire training set.

### **The weakest hidden unit**

For each hidden unit  $j$ , calculate the error on the test data when  $j$  is removed from the network. The weakest hidden unit is the one having the smallest total test error upon its removal.

## **Training**

The problem of estimating the weights consists of the following parts:

- ▶ Initializing the weights. Take a random sample and apply the alternated simulated annealing and training procedure on the random sample to derive the initial weights. Training in step 3 is performed using all default training parameters.
- ▶ Computing the derivative of the error function with respect to the weights. This is solved via the error backpropagation algorithm.
- ▶ Updating the estimated weights. This is solved by the gradient descent or scaled conjugate gradient method.

### **Alternated Simulated Annealing and Training**

The following procedure uses simulated annealing and training alternately up to  $K_1$  times. Simulated annealing is used to break out of the local minimum that training finds by perturbing the local minimum  $K_2$  times. If break out is successful, simulated annealing sets a better initial weight for the next training. We hope to find the global minimum by repeating this procedure  $K_3$  times. This procedure is rather expensive for large data sets, so it is only used on a random sample to search for initial weights and in architecture selection. Let  $K_1=K_2=4$ ,  $K_3=3$ .

1. Randomly generate  $K_2$  weight vectors between  $[a_0-a, a_0+a]$ , where  $a_0=0$  and  $a=0.5$ . Calculate the training error for each weight vector. Pick the weights that give the minimum training error as the initial weights.
2. Set  $k_1=0$ .
3. Train the network with the specified initial weights. Call the trained weights  $\mathbf{w}$ .

4. If the training error ratio  $\leq 0.05$ , stop the  $k_1$  loop and use  $\mathbf{w}$  as the result of the loop. Else set  $k_1 = k_1 + 1$ .
5. If  $k_1 < K_1$ , perturb the old weight to form  $K_2$  new weights  $\mathbf{w}' = \mathbf{w} + \mathbf{w}_n$  by adding  $K_2$  different random noise  $\mathbf{w}_n$  between  $[a(k_1), a(k_1)]$  where  $a(k_1) = (0.5)^{k_1} a$ . Let  $\mathbf{w}_{\min}$  be the weights that give the minimum training error among all the perturbed weights. If  $E_T(\mathbf{w}_{\min}) < E_T(\mathbf{w})$ , set the initial weights to be  $\mathbf{w}_{\min}$ , return to step 3. Else stop and report  $\mathbf{w}$  as the final result.

Else stop the  $k_1$  loop and use  $\mathbf{w}$  as the result of the loop.

If the resulting weights have training error ratio bigger than 0.1, repeat this algorithm until either the training error ratio is  $\leq 0.1$  or the procedure is repeated  $K_3$  times, then pick the one with smallest test error among the result of the  $k_1$  loops.

### Error Backpropagation

Error-backpropagation is used to compute the first partial derivatives of the error function with respect to the weights.

$$\text{First note that } \gamma'(c) = \begin{cases} 1 - [\gamma(c)]^2 & \text{tanh} \\ 1 & \text{identity} \end{cases}$$

The backpropagation algorithm follows:

For each  $i, j, k$ , set  $\frac{\partial E_T}{\partial w_{i:k,j}} = 0$ .

For each  $m$  in group  $T$ ; For each  $p=1, \dots, J_1$ , let

$$\delta_{I:p}^m = \frac{\partial E_m}{\partial c_{I:p}^m} = \begin{cases} a_{I:p}^m - y_p^{(m)} & \text{if cross-entropy error is used} \\ \gamma'(c_{I:p}^m) (a_{I:p}^m - y_p^{(m)}) & \text{otherwise} \end{cases}$$

For each  $i=I, \dots, 1$  (start from the output layer); For each  $j=1, \dots, J_i$ ; For each  $k=0, \dots, J_{i-1}$

- ▶ Let  $\frac{\partial E_m}{\partial w_{i:k,j}} = \delta_{i:j}^m a_{i-1:k}^m$ , where  $\delta_{i:j}^m = \frac{\partial E_m}{\partial c_{i:j}^m}$
- ▶ Set  $\frac{\partial E_T}{\partial w_{i:k,j}} = \frac{\partial E_T}{\partial w_{i:k,j}} + \frac{\partial E_m}{\partial w_{i:k,j}}$
- ▶ If  $k > 0$  and  $i > 1$ , set  $\delta_{i-1:k}^m = \gamma'_{i-1}(c_{i-1:k}^m) \sum_{j=1}^{J_i} \delta_{i:j}^m w_{i:k,j}$

This gives us a vector of  $\sum_{i=0}^{I-1} (J_i + 1) J_{i+1}$  elements that form the gradient of  $E_T(w_k)$ .

### Gradient Descent

Given the learning rate parameter  $\eta_0$  (set to 0.4) and momentum rate  $\alpha$  (set to 0.9), the gradient descent method is as follows.

1. Let  $k=0$ . Initialize the weight vector to  $w_0$ , learning rate to  $\eta_0$ . Let  $\Delta w_0 = 0$ .

2. Read all data and find  $E_T(w_k)$  and its gradient  $g_k = \nabla E_T(w_k)$ . If  $|g_k| < 10^{-6}$ , stop and report the current network.
3. If  $\eta_k |g_k| \leq \alpha |\Delta w_k|$ ,  $\alpha = 0.9 \eta_k \frac{|g_k|}{|\Delta w_k|}$ . This step is to make sure that the steepest gradient descent direction dominates weight change in next step. Without this step, the weight change in next step could be along the opposite direction of the steepest descent and hence no matter how small  $\eta_k$  is, the error will not decrease.
4. Let  $v = w_k - \eta_k g_k + \alpha \Delta w_k$
5. If  $E_T(v) < E_T(w_k)$ , then set  $w_{k+1} = v$ ,  $\Delta w_{k+1} = w_{k+1} - w_k$ , and  $\eta_{k+1} = \eta_k$ , Else  $\eta_k = .5\eta_k$  and return to step 3.
6. If a stopping rule is met, exit and report the network as stated in the stopping criteria. Else let  $k=k+1$  and return to step 2.

### **Model Update**

Given the learning rate parameters  $\eta_0$  (set to 0.4) and  $\eta_{low}$  (set to 0.001), momentum rate  $\alpha$  (set to 0.9), and learning rate decay factor  $\beta = (1/pK) * \ln(\eta_0/\eta_{low})$ , the gradient descent method for online and mini-batch training is as follows.

1. Let  $k=0$ . Initialize the weight vector to  $w_0$ , learning rate to  $\eta_0$ . Let  $\Delta w_0 = 0$ .
2. Read records in  $T_k$  ( $T_k$  is randomly chosen) and find  $E_{T_k}(w_k)$  and its gradient  $g_k = \nabla E_{T_k}(w_k)$ .
3. If  $\eta_k |g_k| \leq \alpha |\Delta w_k|$ ,  $\alpha = 0.9 \eta_k \frac{|g_k|}{|\Delta w_k|}$ . This step is to make sure that the steepest gradient descent direction dominates weight change in next step. Without this step, the weight change in next step could be along the opposite direction of the steepest descent and hence no matter how small  $\eta_k$  is, the error will not decrease.
4. Let  $v = w_k - \eta_k g_k + \alpha \Delta w_k$ .
5. If  $E_{T_k}(v) < E_{T_k}(w_k)$ , then set  $w_{k+1} = v$  and  $\Delta w_{k+1} = w_{k+1} - w_k$ , Else  $w_{k+1} = w_k$ ,  $\Delta w_{k+1} = \Delta w_k$ .
6.  $\eta_{k+1} = e^{-\beta} \eta_k$ . If  $\eta_{k+1} < \eta_{low}$ , then set  $\eta_{k+1} = \eta_{low}$ .
7. If a stopping rule is met, exit and report the network as stated in the stopping criteria. Else let  $k=k+1$  and return to step 2.

### **Scaled Conjugate Gradient**

To begin, initialize the weight vector to  $w_0$ , and let  $N$  be the total number of weights.

1.  $k=0$ . Set scalars  $\lambda_0 = 5.0E-7$ ,  $\sigma = 5.0E-5$ ,  $\bar{\lambda}_0 = 0$ . Set  $r_0 = p_0 = -\nabla E_T(w_0)$ , and  $success=true$ .
2. If  $success=true$ , find the second-order information:  $\sigma_k = \frac{\sigma}{|p_k|}$ ,  $s_k = \frac{\nabla E_T(w_k + \sigma_k p_k) - \nabla E_T(w_k)}{\sigma_k}$ ,  $\delta_k = p_k^t s_k$ , where the superscript  $t$  denotes the transpose.

3. Set  $\delta_k = \delta_k + (\lambda_k - \bar{\lambda}_k) |\mathbf{p}_k|^2$ .
4. If  $\delta_k \leq 0$ , make the Hessian positive definite:  $\bar{\lambda}_k = 2 \left( \lambda_k - \frac{\delta_k}{|\mathbf{p}_k|^2} \right)$ ,  $\delta_k = -\delta_k + \lambda_k |\mathbf{p}_k|^2$ ,  $\lambda_k = \bar{\lambda}_k$ .
5. Calculate the step size:  $\mu_k = \mathbf{p}_k^t \mathbf{r}_k$ ,  $\alpha_k = \frac{\mu_k}{\delta_k}$ .
6. Calculate the comparison parameter:  $\Delta_k = 2\delta_k \frac{[E_T(\mathbf{w}_k) - E_T(\mathbf{w}_k + \alpha_k \mathbf{p}_k)]}{\mu_k}$ .
7. If  $\Delta_k \geq 0$ , error can be reduced. Set  $\mathbf{w}_{k+1} = \mathbf{w}_k + \alpha_k \mathbf{p}_k$ ,  $\mathbf{r}_{k+1} = -\nabla E_T(\mathbf{w}_{k+1})$ , If  $|\mathbf{r}_{k+1}| < 10^{-6}$ , return  $\mathbf{w}_{k+1}$  as the final weight vector and exit. Set  $\bar{\lambda}_k = 0$ , *success=true*. If  $k \bmod N = 0$ , restart the algorithm:  $\mathbf{p}_{k+1} = \mathbf{r}_{k+1}$ , else set  $\beta_k = \frac{|\mathbf{r}_{k+1}|^2 - \mathbf{r}_{k+1}^t \mathbf{r}_k}{\mu_k}$ ,  $\mathbf{p}_{k+1} = \mathbf{r}_{k+1} + \beta_k \mathbf{p}_k$ . If  $\Delta_k \geq .75$ , reduce the scale parameter:  $\lambda_k = \frac{1}{4} \lambda_k$ . else (if  $\Delta_k < 0$ ): Set  $\bar{\lambda}_k = \lambda_k$ , *success=false*.
8. If  $\Delta_k < .25$ , increase the scale parameter:  $\lambda_k = \lambda_k + \frac{\delta_k(1 - \Delta_k)}{|\mathbf{p}_k|^2}$ .
9. If *success=false*, return to step 2. Otherwise if a stopping rule is met, exit and report the network as stated in the stopping criteria. Else set  $k=k+1$ ,  $\bar{\lambda}_{k+1} = \bar{\lambda}_k$ ,  $\lambda_{k+1} = \lambda_k$  and return to step 2.

*Note:* each iteration requires at least two data passes.

### Stopping Rules

Training proceeds through at least one complete pass of the data. Then the search should be stopped according to following criteria. These stopping criteria should be checked in the listed order. When creating a new model, check after completing an iteration. During a model update, check criteria 1, 3, 4, 5 and 6 is after completing a data pass, and only check criterion 2 after an iteration. In the descriptions below, a “step” means an iteration when building a new model and a data pass when performing a model update. Let  $E_1$  denote the current minimum error and  $K_1$  denote the iteration where it occurs for the training set,  $E_2$  and  $K_2$  are that for the overfit prevention set, and  $K_3 = \min(K_1, K_2)$ .

1. At the end of each step compute the total error for the overfit prevention set. From step  $K_2$ , if the testing error does not decrease below  $E_2$  over the next  $n=1$  steps, stop. Report the weights at step  $K_2$ . If there is no overfit prevention set, this criterion is not used for building a new model; for a model update when there is no overfit prevention set, compute the total error for training data at the end of each step. From step  $K_1$ , if the training error does not decrease below  $E_1$  over the next  $n=1$  steps, stop. Report the weights at step  $K_1$ .
2. The search has lasted beyond some maximum allotted time. For building a new model, simply report the weights at step  $K_3$ . For a model update, even though training stops before the completion of current step, treat this as a complete step. Calculate current errors for training and testing datasets and update  $E_1$ ,  $K_1$ ,  $E_2$ ,  $K_2$  correspondingly. Report the weights at step  $K_3$ .
3. The search has lasted more than some maximum number of data passes. Report the weights at step  $K_3$ .
4. Stop if the relative change in training error is small:  $\frac{|E_T(w_k) - E_T(w_{k-1})|}{\frac{1}{2}(E_T(w_k) + E_T(w_{k-1})) + \delta} < \epsilon_1$  for  $\delta = 10^{-10}$  and  $\epsilon_1 = 10^{-4}$ , where  $w_{k-1}$ ,  $w_k$  are the weight vectors of two consecutive steps. Report weights at step  $K_3$ .

5. The current training error ratio is small compared with the initial error:  $\left| \frac{E_T(w_k)}{\bar{E}_T + \delta} \right| < \epsilon_2$  for  $\delta = 10^{-10}$  and  $\epsilon_2 = 10^{-3}$ , where  $\bar{E}_T$  is the total error from the model using the average of an output field to predict that field;  $\bar{E}_T$  is calculated by using  $a_{I:r}^m = \frac{1}{M} \sum_{m=1}^M y_r^{(m)}$  in the error function, where  $w_k$  is the weight vector of one step. Report weights at step  $K_3$ .
6. The current accuracy meets a specified threshold. Accuracy is computed based on the overfit prevention set if there is one, otherwise the training set.

*Note:* In criteria 4 and 5, the total error for whole training data is needed. For model updates, these criteria will not be checked if there is an overfit prevention set.

### Model Updates

When new records become available, the synaptic weights can be updated. The new records are split into groups of the size  $R = \min(M, 2N, 1000)$ , where  $M$  is the number of training records and  $N$  is the number of weights in the network. A single data pass is made through the new groups to update the weights. If the last of the new groups has more than one-quarter of the records of a normal group, then it is processed normally; otherwise, it remains in the internal buffer so that these records can be used during the next update. Thus, after the last update there may be some unused records remaining in the buffer that will be lost.

## Radial Basis Function

A radial basis function (RBF) network is a feed-forward, supervised learning network with only one hidden layer, called the radial basis function layer. The RBF network is a function of one or more predictors that minimizes the prediction error of one or more targets. Predictors and targets can be a mix of categorical and continuous fields.

### Notation

The following notation is used throughout this chapter unless otherwise stated:

$X^{(m)} = (x_1^{(m)}, \dots, x_P^{(m)})$	Input vector, pattern $m$ , $m=1, \dots, M$ .
$Y^{(m)} = (y_1^{(m)}, \dots, y_R^{(m)})$	Target vector, pattern $m$ .
$I$	Number of layers, discounting the input layer. For an RBF network, $I=2$ .
$J_i$	Number of units in layer $i$ . $J_0 = P$ , $J_1 = R$ , discounting the bias unit. $J_1$ is the number of RBF units.
$\phi_j(X^{(m)})$	$j$ th RBF unit for input $X^{(m)}$ , $j=1, \dots, J_1$ .
$\mu_j$	center of $\phi_j$ , it is $P$ -dimensional.
$\sigma_j$	width of $\phi_j$ , it is $P$ -dimensional.
$h$	the RBF overlapping factor.

$a_{i:j}^m$	Unit $j$ of layer $i$ , pattern $m$ , $j = 0, \dots, J_i$ ; $i = 0, \dots, I$ .
$w_{rj}$	weight connecting $r$ th output unit and $j$ th hidden unit of RBF layer.

## Architecture

There are three layers in the RBF network:

**Input layer:**  $J_0=P$  units,  $a_{0:1}, \dots, a_{0:J_0}$ ; with  $a_{0:j} = x_j$ .

**RBF layer:**  $J_1$  units,  $a_{1:1}, \dots, a_{1:J_1}$ ; with  $a_{1:j} = \phi_j(X)$  and

$$\phi_j(X) = \exp\left(-\sum_{p=1}^P \frac{1}{2\sigma_{jp}^2} (x_p - \mu_{jp})^2\right) / \sum_{j=1}^{J_1} \exp\left(-\sum_{p=1}^P \frac{1}{2\sigma_{jp}^2} (x_p - \mu_{jp})^2\right).$$

**Output layer:**  $J_2=R$  units,  $a_{I:1}, \dots, a_{I:J_2}$ ; with  $a_{I:r} = w_{r0} + \sum_{j=1}^{J_1} w_{rj} \phi_j(X)$ .

## Error Function

Sum-of-squares error is used:

$$E_T(w) = \sum_{m=1}^M E_m(w)$$

where

$$E_m(w) = \frac{1}{2} \sum_{r=1}^R \left( y_r^{(m)} - a_{I:r}^m \right)^2$$

The sum-of-squares error function with identity activation function for output layer can be used for both continuous and categorical targets. For continuous targets,  $a_{I:r}^m$  approximates the conditional expectation of the target value  $E(y_r | X^{(m)})$ . For categorical targets,  $a_{I:r}^m$  approximates the posterior probability of class  $k$ :  $P(y_r = 1 | X^{(m)})$ .

*Note:* though  $\sum a_{I:r}^m = 1$  (the sum is over all classes of the same categorical target field),  $a_{I:r}^m$  may not lie in the range  $[0, 1]$ .

## Training

The network is trained in two stages:

1. **Determine the basis functions by clustering methods.** The center and width for each basis function is computed.
2. **Determine the weights given the basis functions.** For the given basis functions, compute the ordinary least-squares regression estimates of the weights.

The simplicity of these computations allows the RBF network to be trained very quickly.

### Determining Basis Functions

The two-step clustering algorithm is used to find the RBF centers and widths. For each cluster, the mean and standard deviation for each continuous field and proportion of each category for each categorical field are derived. Using the results from clustering, the center of the  $j$ th RBF is set as:

$$\mu_{jp} = \begin{cases} \bar{x}_{jp} & \text{if } p\text{th field is continuous} \\ \pi_{jp} & \text{if } p\text{th field is a dummy field of a categorical field} \end{cases}$$

where  $\bar{x}_{jp}$  is the  $j$ th cluster mean of the  $p$ th input field if it is continuous, and  $\pi_{jp}$  is the proportion of the category of a categorical field that the  $p$ th input field corresponds to. The width of the  $j$ th RBF is set as

$$\sigma_{jp} = h^{1/2} \begin{cases} s_{jp} & \text{if } p\text{th field is continuous} \\ \sqrt{p_{jp}(1-p_{jp})} & \text{if } p\text{th field is a dummy field of a categorical field} \end{cases}$$

where  $s_{jp}$  is the  $j$ th cluster standard deviation of the  $p$ th field and  $h > 0$  is the RBF overlapping factor that controls the amount of overlap among the RBFs. Since some  $\sigma_{jp}$  may be zeros, we use spherical shaped Gaussian bumps; that is, a common width

$$\sigma_j = \sqrt{\frac{1}{P} \sum_{p=1}^P \sigma_{jp}^2}$$

in for all predictors. In the case that  $\sigma_j$  is zero for some  $j$ , set it to be  $\min\{\sigma_j : \sigma_j \neq 0, \}_{j=1}^{J_1}$ . If all  $\sigma_j$  are zero, set all of them to be  $\sqrt{h}$ .

When there are a large number of predictors,  $\sum_{p=1}^P (x_p - \mu_{jp})^2$  could be easily very large and hence

$\exp\left(-\sum_{p=1}^P \frac{1}{2\sigma_j^2} (x_p - \mu_{jp})^2\right)$  is practically zero for every record and every RBF unit if  $\sigma_j$  is relatively small. This is especially bad for ORBF because there would be only a constant term in the model when this happens. To avoid this,  $\sigma_j$  is increased by setting the default overlapping factor  $h$  proportional to the number of inputs:  $h = 1 + 0.1 P$ .

### Automatic Selection of Number of Basis Functions

The algorithm tries a reasonable range of numbers of hidden units and picks the “best”. By default, the reasonable range  $[K_1, K_2]$  is determined by first using the two-step clustering method to automatically find the number of clusters,  $K$ . Then set  $K_1 = \min(K, R)$  for ORBF and  $K_1 = \max\{2, \min(K, R)\}$  for NRBF and  $K_2 = \max(10, 2K, R)$ .

If a test data set is specified, then the “best” model is the one with the smaller error in the test data. If there is no test data, the BIC (Bayesian information criterion) is used to select the “best” model. The BIC is defined as

$$BIC = MR \ln(MSE) + k \ln(M)$$

where  $MSE = \frac{1}{MR} \sum_{m=1}^M \sum_{r=1}^R (y_r^{(m)} - a_{I,r}^m)^2$  is the mean squared error and  $k = (P+1+R)J_1$  for NRBF and  $(P+1+R)J_1+R$  for ORBF is the number of parameters in the model.

### Model Updates

When new records become available, you can update the weights connecting the RBF layer and output layer. Again, given the basis functions, updating the weights is a least-squares regression problem. Thus, it is very fast.

For best results, the new records should have approximately the same distribution as the original records.

### Missing Values

The following options for handling missing values are available:

- Records with missing values are excluded listwise.
- Missing values are imputed. Continuous fields impute the average of the minimum and maximum observed values; categorical fields impute the most frequently occurring category.

### Output Statistics

The following output statistics are available. Note that, for continuous fields, output statistics are reported in terms of the rescaled values of the fields.

#### Accuracy

For continuous targets, it is

$$R^2 = 1 - \frac{\sum_{k=1}^K f_k (y_k - \hat{y}_k)^2}{\sum_{k=1}^K f_k (y_k - \bar{y})^2}$$

where  $\bar{y} = \frac{1}{N} \sum_{k=1}^K f_k y_k$

Note that  $R^2$  can never be greater than one, but can be less than zero.

For the naïve model,  $\hat{y}_k$  is the modal category for categorical targets and the mean for continuous targets.

For each categorical target, this is the percentage of records for which the predicted value matches the observed value.

### **Predictor Importance**

For more information, see the topic “Predictor Importance Algorithms” on p. 305.

## **Confidence**

Confidence values for neural network predictions are calculated based on the type of output field being predicted. Note that no confidence values are generated for numeric output fields.

### **Difference**

The difference method calculates the confidence of a prediction by comparing the best match with the second-best match as follows, depending on output field type and encoding used.

- **Flag fields.** Confidence is calculated as  $c = 2 \cdot |0.5 - o|$ , where  $o$  is the output activation for the output unit.
- **Set fields.** With the standard encoding, confidence is calculated as  $c = o_1 - o_2$ , where  $o_1$  is the output unit in the fields group of units with the highest activation, and  $o_2$  is the unit with the second-highest activation.

With binary set encoding, the sum of the errors comparing the output activation and the encoded set value is calculated for the closest and second-closest matches, and the confidence is calculated as  $c = e_2 - e_1$ , where  $e_2$  is the error for the second-best match and  $e_1$  is the error for the best match.

### **Simplemax**

Simplemax returns the highest predicted probability as the confidence.

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# OPTIMAL BINNING Algorithms

The Optimal Binning procedure performs MDLP (minimal description length principle) discretization of scale variables. This method divides a scale variable into a small number of intervals, or bins, where each bin is mapped to a separate category of the discretized variable.

MDLP is a univariate, supervised discretization method. Without loss of generality, the algorithm described in this document only considers one continuous attribute in relation to a categorical guide variable — the discretization is “optimal” with respect to the categorical guide. Therefore, the input data matrix  $S$  contains two columns, the scale variable  $A$  and categorical guide  $C$ .

Optimal binning is applied in the Binning node when the binning method is set to Optimal.

## Notation

The following notation is used throughout this chapter unless otherwise stated:

$S$	The input data matrix, containing a column of the scale variable $A$ and a column of the categorical guide $C$ . Each row is a separate observation, or instance.
$A$	A scale variable, also called a continuous attribute.
$S(i)$	The value of $A$ for the $i$ th instance in $S$ .
$N$	The number of instances in $S$ .
$D$	A set of all distinct values in $S$ .
$S_i$	A subset of $S$ .
$C$	The categorical guide, or class attribute; it is assumed to have $k$ categories, or classes.
$T$	A cut point that defines the boundary between two bins.
$T_A$	A set of cut points.
$\text{Ent}(S)$	The class entropy of $S$ .
$E(A, T, S)$	The class entropy of partition induced by $T$ on $A$ .
$\text{Gain}(A, T, S)$	The information gain of the cut point $T$ on $A$ .
$n$	A parameter denoting the number of cut points for the equal frequency method.
$W$	A weight attribute denoting the frequency of each instance. If the weight values are not integer, they are rounded to the nearest whole numbers before use. For example, 0.5 is rounded to 1, and 2.4 is rounded to 2. Instances with missing weights or weights less than 0.5 are not used.

## Simple MDLP

This section describes the supervised binning method (MDLP) discussed in Fayyad and Irani (1993).

### Class Entropy

Let there be  $k$  classes  $C_1, \dots, C_k$  and let  $P(C_i, S)$  be the proportion of instances in  $S$  that have class  $C_i$ . The class entropy  $\text{Ent}(S)$  is defined as

$$Ent(S) = - \sum_{i=1}^k P(C_i, S) \log_2(P(C_i, S))$$

### **Class Information Entropy**

For an instance set  $S$ , a continuous attribute  $A$ , and a cut point  $T$ , let  $S_1 \subset S$  be the subset of instances in  $S$  with the values of  $A \leq T$ , and  $S_2 = S - S_1$ . The class information entropy of the partition induced by  $T$ ,  $E(A, T; S)$ , is defined as

$$E(A, T; S) = \frac{|S_1|}{|S|} Ent(S_1) + \frac{|S_2|}{|S|} Ent(S_2)$$

### **Information Gain**

Given a set of instances  $S$ , a continuous attribute  $A$ , and a cut point  $T$  on  $A$ , the information gain of a cut point  $T$  is

$$Gain(A, T; S) = Ent(S) - E(A, T; S)$$

### **MDLP Acceptance Criterion**

The partition induced by a cut point  $T$  for a set  $S$  of  $N$  instances is accepted if and only if

$$Gain(A, T; S) > \frac{\log_2(N-1)}{N} + \frac{\Delta(A, T; S)}{N}$$

and it is rejected otherwise.

Here  $\Delta(A, T; S) = \log_2(3^k - 2) - [k \cdot Ent(S) - k_1 Ent(S_1) - k_2 Ent(S_2)]$  in which  $k_i$  is the number of classes in the subset  $S_i$  of  $S$ .

*Note:* While the MDLP acceptance criterion uses the association between  $A$  and  $C$  to determine cut points, it also tries to keep the creation of bins to a small number. Thus there are situations in which a high association between  $A$  and  $C$  will result in no cut points. For example, consider the following data:

$D$	Class	
	2	3
1	1	0
2	0	6

Then the potential cut point is  $T = 1$ . In this case:

$$Gain(A, T; S) = 0.5916728$$

$$\frac{\log_2(N-1)}{N} + \frac{\Delta(A, T; S)}{N} = 0.6530774$$

Since  $0.5916728 < 0.6530774$ ,  $T$  is not accepted as a cut point, even though there is a clear relationship between  $A$  and  $C$ .

### Algorithm: BinaryDiscretization

1. Calculate  $E(A, d_i; S)$  for each distinct value  $d_i \in D$  for which  $d_i$  and  $d_{i+1}$  do not belong to the same class. A distinct value belongs to a class if all instances of this value have the same class.
2. Select a cut point  $T$  for which  $E(A, T; S)$  is minimum among all the candidate cut points, that is,
 
$$T = \arg \min_{d_i} E(A, d_i; S)$$

### Algorithm: MDLPCut

1. BinaryDiscretization( $A, T; D, S$ ).
2. Calculate Gain( $A, T; S$ ).
3. If  $Gain(A, T; S) > \frac{\log_2(N-1)}{N} + \frac{\Delta(A, T; S)}{N}$  then
  - a)  $T_A = T_A \cup T$ .
  - b) Split  $D$  into  $D_1$  and  $D_2$ , and  $S$  into  $S_1$  and  $S_2$ .
  - c) MDLPCut( $A, T_A; D_1, S_1$ ).
  - d) MDLPCut( $A, T_A; D_2, S_2$ ). where  $S_1 \subset S$  be the subset of instances in  $S$  with  $A$ -values  $\leq T$ , and  $S_2 = S - S_1$ .  $D_1$  and  $D_2$  are the sets of all distinct values in  $S_1$  and  $S_2$ , respectively.

Also presented is the iterative version of MDLPCut( $A, T_A; D, S$ ). The iterative implementation requires a stack to store the  $D$  and  $S$  remaining to be cut.

First push  $D$  and  $S$  into *stack*. Then, while ( $stack \neq \emptyset$ ) do

1. Obtain  $D$  and  $S$  by popping *stack*.
2. BinaryDiscretization( $A, T; D, S$ ).
3. Calculate Gain( $A, T; S$ ).
4. If  $Gain(A, T; S) > \frac{\log_2(N-1)}{N} + \frac{\Delta(A, T; S)}{N}$  then
  - i)  $T_A = T_A \cup T$ .
  - ii) Split  $D$  into  $D_1$  and  $D_2$ , and  $S$  into  $S_1$  and  $S_2$ .
  - iii) Push  $D_1$  and  $S_1$  into *stack*.
  - iv) Push  $D_2$  and  $S_2$  into *stack*.

*Note:* In practice, all operations within the algorithm are based on a global matrix  $M$ . Its element,  $m_{ij}$ , denotes the total number of instances that have value  $d_i \in D$  and belong to the  $j$ th class in  $S$ . In addition,  $D$  is sorted in ascending order. Therefore, we do not need to push  $D$  and  $S$  into *stack*, but only two integer numbers, which denote the bounds of  $D$ , into *stack*.

### **Algorithm: SimpleMDLP**

1. Sort the set  $S$  with  $N$  instances by the value  $A$  in ascending order.
2. Find a set of all distinct values,  $D$ , in  $S$ .
3.  $T_A = \emptyset$ .
4. MDLPCut( $A, T_A; D, S$ )
5. Sort the set  $T_A$  in ascending order, and output  $T_A$ .

### **Hybrid MDLP**

When the set  $D$  of distinct values in  $S$  is large, the computational cost to calculate  $E(A, d_i; S)$  for each  $d_i \in D$  is large. In order to reduce the computational cost, the unsupervised equal frequency binning method is used to reduce the size of  $D$  and obtain a subset  $D_{ef} \in D$ . Then the MDLPCut( $A, T_A; D_s, S$ ) algorithm is applied to obtain the final cut point set  $T_A$ .

### **Algorithm: EqualFrequency**

It divides a continuous attribute  $A$  into  $n$  bins where each bin contains  $N/n$  instances.  $n$  is a user-specified parameter, where  $1 < n < N$ .

1. Sort the set  $S$  with  $N$  instances by the value  $A$  in ascending order.
2.  $D_{ef} = \emptyset$ .
3.  $j=1$ .
4. Use the empirical percentile method to generate the  $d_{p,i}$  which denote the  $(\frac{i \cdot N}{n} \times 100)$ th percentiles.
5.  $D_{ef} = D_{ef} \cup d_{p,i}; i=i+1$
6. If  $i \leq n$ , then go to step 4.
7. Delete the duplicate values in the set  $D_{ef}$ .

*Note:* If, for example, there are many occurrences of a single value of  $A$ , the equal frequency criterion may not be met. In this case, no cut points are produced.

### **Algorithm: HybridMDLP**

1.  $D = \emptyset$ ;

2. EqualFrequency( $A, n, D; S$ ).
3.  $T_A = \emptyset$ .
4. MDLPCut( $A, T_A; D, S$ ).
5. Output  $T_A$ .

## Model Entropy

The model entropy is a measure of the predictive accuracy of an attribute  $A$  binned on the class variable  $C$ . Given a set of instances  $S$ , suppose that  $A$  is discretized into  $I$  bins given  $C$ , where the  $i$ th bin has the value  $A_i$ . Letting  $S_i \subset S$  be the subset of instances in  $S$  with the value  $A_i$ , the model entropy is defined as:

$$E_m = \sum_{i=1}^I P(A_i) \left( - \sum_{j=1}^J P(C_j|A_i) \log_2 P(C_j|A_i) \right)$$

where  $P(A_i) = \frac{|S_i|}{|S|}$  and  $P(C_j|A_i) = \frac{P(C_j, A_i)}{P(A_i)} = P(C_j, S_i)$ .

## Merging Sparsely Populated Bins

Occasionally, the procedure may produce bins with very few cases. The following strategy deletes these pseudo cut points:

- For a given variable, suppose that the algorithm found  $n_{\text{final}}$  cut points, and thus  $n_{\text{final}}+1$  bins. For bins  $i = 2, \dots, n_{\text{final}}$  (the second lowest-valued bin through the second highest-valued bin), compute

$$\frac{\text{sizeof}(b_i)}{\min(\text{sizeof}(b_{i-1}), \text{sizeof}(b_{i+1}))}$$

where sizeof(bin) is the number of cases in the bin.

- When this value is less than a user-specified merging threshold,  $b_i$  is considered sparsely populated and is merged with  $b_{i-1}$  or  $b_{i+1}$ , whichever has the lower class information entropy. For more information, see the topic “Class Information Entropy” on p. 300.

The procedure makes a single pass through the bins.

## Blank Handling

In optimal binning, blanks are handled in pairwise fashion. That is, for every pair of fields {binning field, target field}, all records with valid values for both fields are used to bin that specific binning field, regardless of any blanks that may exist in other fields to be binned.

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# Predictor Importance Algorithms

Predictor importance can be determined by computing the reduction in variance of the target attributable to each predictor, via a sensitivity analysis. This method of computing predictor importance is used in the following models:

- Neural Networks
- C5.0
- C&RT
- QUEST
- CHAID
- Regression
- Logistic
- Discriminant
- GenLin
- SVM
- Bayesian Networks

## Notation

The following notation is used throughout this chapter unless otherwise stated:

$Y$	Target
$X_j$	Predictor, where $j=1,\dots,k$
$k$	The number of predictors
$Y = f(X_1, X_2, \dots, X_k)$	Model for $Y$ based on predictors $X_1$ through $X_k$

## Variance Based Method

Predictors are ranked according to the sensitivity measure defined as follows.

$$S_i = \frac{V_i}{V(Y)} = \frac{V(E(Y|X_i))}{V(Y)}$$

where  $V(Y)$  is the unconditional output variance. In the numerator, the expectation operator  $E$  calls for an integral over  $X_{-i}$ ; that is, over all factors but  $X_i$ , then the variance operator  $V$  implies a further integral over  $X_i$ .

Predictor importance is then computed as the normalized sensitivity.

$$VI_i = \frac{S_i}{\sum_{j=1}^k S_j}$$

Saltelli et al (2004) show that  $S_i$  is the proper measure of sensitivity to rank the predictors in order of importance for any combination of interaction and non-orthogonality among predictors.

The importance measure  $S_i$  is the first-order sensitivity measure, which is accurate if the set of the input factors ( $X_1, X_2, \dots, X_k$ ) is orthogonal/independent (a property of the factors), and the model is additive; that is, the model does not include interactions (a property of the model) between the input factors. For any combination of interaction and non-orthogonality among factors, Saltelli (2004) pointed out that  $S_i$  is still the proper measure of sensitivity to rank the input factors in order of importance, but there is a risk of inaccuracy due to the presence of interactions or/and non-orthogonality. For better estimation of  $S_i$ , the size of the dataset should be a few hundred at least. Otherwise,  $S_i$  may be biased heavily. In this case, the importance measure can be improved by bootstrapping.

### Computation

In the orthogonal case, it is straightforward to estimate the conditional variances  $V_i$  by computing the multidimensional integrals in the space of the input factors, via Monte Carlo methods as follows.

Let us start with two input sample matrices  $\mathbf{M}_1$  and  $\mathbf{M}_2$ , each of dimension  $N \times k$ :

$$\mathbf{M}_1 = \begin{matrix} x_1^{(1)} & x_2^{(1)} & \dots & x_k^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \dots & x_k^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{(\hat{N})} & x_2^{(\hat{N})} & \dots & x_k^{(\hat{N})} \end{matrix}$$

and

$$\mathbf{M}_2 = \begin{matrix} x_1^{(1')} & x_2^{(1')} & \dots & x_k^{(1')} \\ x_1^{(2')} & x_2^{(2')} & \dots & x_k^{(2')} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{(\hat{N}')} & x_2^{(\hat{N}')} & \dots & x_k^{(\hat{N}')} \end{matrix}$$

where  $N$  is the sample size of the Monte Carlo estimate which can vary from a few hundred to one thousand. Each row is an input sample. From  $\mathbf{M}_1$  and  $\mathbf{M}_2$ , we can build a third matrix  $\mathbf{N}_j$ .

$$\mathbf{N}_j = \begin{matrix} x_1^{(1)} & x_2^{(1)} & \dots & x_j^{(1)} & \dots & x_k^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \dots & x_j^{(2)} & \dots & x_k^{(2)} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_1^{(\hat{N})} & x_2^{(\hat{N})} & \dots & x_j^{(\hat{N})} & \dots & x_k^{(\hat{N})} \end{matrix}$$

We may think of  $\mathbf{M}_1$  as the “sample” matrix,  $\mathbf{M}_2$  as the “resample” matrix, and  $\mathbf{N}_j$  as the matrix where all factors except  $X_j$  are resampled. The following equations describe how to obtain the variances (Saltelli 2002). The ‘hat’ denotes the numeric estimates.

$$\hat{V}(Y) = \frac{1}{N-1} \sum_{r=1}^N f^2(x_1^{(r)}, x_2^{(r)}, \dots, x_k^{(r)}) - \hat{E}^2(Y)$$

where

$$\hat{E}^2(Y) = \left[ \frac{1}{N} \sum_{r=1}^N f(x_1^{(r)}, x_2^{(r)}, \dots, x_k^{(r)}) \right]^2$$

$$\hat{V}(E(Y|X_j)) = \hat{U}_j - \hat{E}^2(Y)$$

where

$$\hat{U}_j = \frac{1}{N-1} \sum_{r=1}^N f(x_1^{(r)}, x_2^{(r)}, \dots, x_k^{(r)}) f(x_1^{(r')}, x_2^{(r')}, \dots, x_{(j-1)}^{(r')}, x_j^{(r)}, x_{(j+1)}^{(r')}, \dots, x_k^{(r')})$$

and

$$\hat{E}^2(Y) = \frac{1}{N} \sum_{r=1}^N f(x_1^{(r)}, x_2^{(r)}, \dots, x_k^{(r)}) f(x_1^{(r')}, x_2^{(r')}, \dots, x_k^{(r')})$$

When the target is continuous, we simply follow the accumulation steps of variance and expectations. For a categorical target, the accumulation steps are for each category of  $Y$ . For each input factor,  $S_i$  is a vector with an element for each category of  $Y$ . The average of elements of  $S_i$  is used as the estimation of importance of the  $i$ th input factor on  $Y$ .

**Convergence.** In order to improve scalability, we use a subset of the records and predictors when checking for convergence. Specifically, the convergence is judged by the following criteria:

$$i \in I \frac{1}{D} \sum_{j=t-D+1}^t \frac{|S_i(j) - \bar{S}_i|}{\bar{S}_i} < \epsilon$$

where  $I = \{i | S_i(t) > 1/num\}$ ,  $D=100$  and denotes the width of interest,  $\bar{S}_i = \frac{1}{D} \sum_{j=t-D+1}^t S_i(j)$ , and  $\epsilon = 0.005$  defines the desired average relative error.

This specification focuses on “good” predictors; those whose importance values are larger than average.

**Record order.** This method of computing predictor importance is desirable because it scales well to large datasets, but the results are dependent upon the order of records in the dataset. However, with large, randomly ordered datasets, you can expect the predictor importance results to be consistent.

## **References**

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# QUEST Algorithms

## Overview of QUEST

QUEST stands for Quick, Unbiased, Efficient Statistical Tree. It is a relatively new binary tree-growing algorithm (Loh and Shih, 1997). It deals with split field selection and split-point selection separately. The univariate split in QUEST performs approximately unbiased field selection. That is, if all predictor fields are equally informative with respect to the target field, QUEST selects any of the predictor fields with equal probability.

QUEST affords many of the advantages of C&RT, but, like C&RT, your trees can become unwieldy. You can apply automatic cost-complexity pruning (see “Pruning” on p. 317) to a QUEST tree to cut down its size. QUEST uses surrogate splitting to handle missing values. For more information, see the topic “Blank Handling” on p. 313.

## Primary Calculations

The calculations directly involved in building the model are described below.

## Frequency Weight Fields

A **frequency field** represents the total number of observations represented by each record. It is useful for analyzing aggregate data, in which a record represents more than one individual. The sum of the values for a frequency field should always be equal to the total number of observations in the sample. Note that output and statistics are the same whether you use a frequency field or case-by-case data. The table below shows a hypothetical example, with the predictor fields *sex* and *employment* and the target field *response*. The frequency field tells us, for example, that 10 employed men responded *yes* to the target question, and 19 unemployed women responded *no*.

Table 29-1  
Dataset with frequency field

Sex	Employment	Response	Frequency
M	Y	Y	10
M	Y	N	17
M	N	Y	12
M	N	N	21
F	Y	Y	11
F	Y	N	15
F	N	Y	15
F	N	N	19

The use of a frequency field in this case allows us to process a table of 8 records instead of case-by-case data, which would require 120 records.

QUEST does not support the use of case weights.

## Model Parameters

QUEST deals with field selection and split-point selection separately. Note that you can specify the alpha level to be used in the Expert Options for QUEST—the default value is  $\alpha_{\text{nominal}} = 0.05$ .

### Field Selection

1. For each predictor field  $X$ , if  $X$  is a symbolic (categorical), or nominal, field, compute the  $p$  value of a Pearson chi-square test of independence between  $X$  and the dependent field. If  $X$  is scale-level (continuous), or ordinal field, use the  $F$  test to compute the  $p$  value.
2. Compare the smallest  $p$  value to a prespecified, Bonferroni-adjusted alpha level  $\alpha_B$ .
  - If the smallest  $p$  value is less than  $\alpha_B$ , then select the corresponding predictor field to split the node. Go on to step 3.
  - If the smallest  $p$  value is *not* less than  $\alpha_B$ , then for each  $X$  that is scale-level (continuous), use Levene's test for unequal variances to compute a  $p$  value. (In other words, test whether  $X$  has unequal variances at different levels of the target field.)
  - Compare the smallest  $p$  value from Levene's test to a new Bonferroni-adjusted alpha level  $\alpha_L$ .
  - If the  $p$  value is less than  $\alpha_L$ , select the corresponding predictor field with the smallest  $p$  value from Levene's test to split the node.
  - If the  $p$  value is greater than  $\alpha_L$ , the node is not split.

### Split Point Selection—Scale-Level Predictor

1. If  $Y$  has only two categories, skip to the next step. Otherwise, group the categories of  $Y$  into two superclasses as follows:
  - Compute the mean of  $X$  for each category of  $Y$ .
  - If all means are the same, the category with the largest weighted frequency is selected as one superclass and all other categories are combined to form the other superclass. (If all means are the same and there are multiple categories tied for largest weighted frequency, select the category with the smallest index as one superclass and combine the other categories to form the other.)
  - If the means are not all the same, apply a two-mean clustering algorithm to those means to obtain two superclasses of  $Y$ , with the initial cluster centers set at the two most extreme class means. (This is a special case of  $k$ -means clustering, where  $k = 2$ . For more information, see the topic "Overview" on p. 227.)
2. Apply quadratic discriminant analysis (QDA) to determine the split point. Notice that QDA usually produces two cut-off points—choose the one that is closer to the sample mean of the first superclass.

### Split Point Selection—Symbolic (Categorical) Predictor

QUEST first transforms the symbolic field into a continuous field  $\xi$  by assigning discriminant coordinates to categories of the predictor. The derived field  $\xi$  is then split as if it were any other continuous predictor as described above.

### Chi-Square Test

The Pearson chi-square statistic is calculated as

$$X^2 = \sum_{j=1}^J \sum_{i=1}^I \frac{(n_{ij} - \hat{m}_{ij})^2}{\hat{m}_{ij}}$$

where  $n_{ij} = \sum_n f_n I(x_n = i \wedge y_n = j)$  is the observed cell frequency and  $\hat{m}_{ij}$  is the expected cell frequency for cell  $(x_n = i, y_n = j)$  from the independence model as described below. The corresponding  $p$  value is calculated as  $p = \Pr(\chi_d^2 > X^2)$ , where  $\chi_d^2$  follows a chi-square distribution with  $d = (J - 1)(I - 1)$  degrees of freedom.

#### Expected Frequencies for Chi-Square Test

For models with no case weights, expected frequencies are calculated as

$$\hat{m}_{ij} = \frac{n_{i.} n_{.j}}{n_{..}}$$

where

$$n_{i.} = \sum_{j=1}^J n_{ij}, \quad n_{.j} = \sum_{i=1}^I n_{ij}, \quad n_{..} = \sum_{j=1}^J \sum_{i=1}^I n_{ij}.$$

### F Test

Suppose for node  $t$  there are  $J_t$  classes of target field  $Y$ . The  $F$  statistic for continuous predictor  $X$  is calculated as

$$F_X = \frac{\sum_{j=1}^{J_t} N_{f,j}(t) \left( \bar{x}^{(j)}(t) - \bar{x}(t) \right)^2 / (J_t - 1)}{\sum_{i \in t} f_i \left( x_i - \bar{x}^{(y_n)}(t) \right)^2 / (N_f(t) - J_t)}$$

where

$$\bar{x}^{(j)}(t) = \frac{\sum_{i \in t} f_n x_n I(y_n = j)}{N_{f,j}(t)}, \quad \bar{x}(t) = \frac{\sum_{i \in t} f_n x_n}{N_f(t)}$$

The corresponding  $p$  value is given by

$$p_X = \Pr \left( F(J_t - 1, N_f(t) - J_t) > F_X \right)$$

where  $F(J_t - 1, N_f(t) - J_t)$  follows an  $F$  distribution with degrees of freedom  $J_t - 1$  and  $N_f(t) - J_t$ .

**Levene's Test**

For continuous predictor  $X$ , calculate  $z_n = |x_n - \bar{x}^{(y_n)}(t)|$ , where  $\bar{x}$  is the mean of  $X$  for records in node  $t$  with target value  $y_n$ . Levene's  $F$  statistic for predictor  $X$  is the ANOVA  $F$  statistic for  $z_n$ .

**Bonferroni Adjustment**

The adjusted alpha level  $\alpha_B$  is calculated as the nominal value divided by the number of possible comparisons.

For QUEST, the Bonferroni adjusted alpha level  $\alpha_B$  for the initial predictor selection is

$$\alpha_B = \frac{\alpha_{nominal}}{m}$$

where  $m$  is the number of predictor fields in the model.

For the Levene test, the Bonferroni adjusted alpha level  $\alpha_L$  is

$$\alpha_L = \frac{\alpha_{nominal}}{m + m_c}$$

where  $m_c$  is the number of continuous predictor fields.

**Discriminant Coordinates**

For categorical predictor  $X$  with values  $\{b_1, \dots, b_I\}$ , QUEST assigns a score value from a continuous variable  $\xi$  to each category of  $X$ . The scores assigned are chosen to maximize the ratio of between-class to within-class sum of squares of  $\xi$  for the target field classes:

For each record, transform  $X$  into a vector of dummy fields  $\mathbf{g} = (g_1, \dots, g_I)'$ , where

$$g_i = \begin{cases} 1 & x = b_i \\ 0 & \text{otherwise} \end{cases}$$

Calculate the overall and class  $j$  mean of  $\mathbf{v}$ :

$$\bar{\mathbf{g}} = \frac{\sum_n f_n \mathbf{g}_n}{N_f}, \bar{\mathbf{g}}^{(j)} = \frac{\sum_n f_n \mathbf{g}_n I(y_n = j)}{N_{f,j}}$$

where  $f_n$  is the frequency weight for record  $n$ ,  $\mathbf{g}_n$  is the dummy vector for record  $n$ ,  $N_f$  is the total sum of frequency weights for the training data, and  $N_{f,j}$  is the sum of frequency weights for records with category  $j$ .

Calculate the following  $I \times I$  matrices:

$$\mathbf{B} = \sum_{j=1}^J N_{f,j} (\bar{\mathbf{g}}^{(j)} - \bar{\mathbf{g}}) (\bar{\mathbf{g}}^{(j)} - \bar{\mathbf{g}})'$$

$$\mathbf{T} = \sum_n f_n (\mathbf{g}_n - \bar{\mathbf{g}})(\mathbf{g}_n - \bar{\mathbf{g}})'$$

Perform singular value decomposition on  $\mathbf{T}$  to obtain  $\mathbf{T} = \mathbf{Q}\mathbf{D}\mathbf{Q}'$ , where  $\mathbf{Q}$  is an  $I \times I$  orthogonal matrix,  $\mathbf{D} = \text{diag}(d_1, \dots, d_I)$  such that  $d_1 \geq \dots \geq d_I \geq 0$ . Let  $\mathbf{D}^{-\frac{1}{2}} = \text{diag}(d_1^*, \dots, d_I^*)$  where  $d_i^* = d_i^{-\frac{1}{2}}$  if  $d_i > 0$ , 0 otherwise. Perform singular value decomposition on  $\mathbf{D}^{-\frac{1}{2}}\mathbf{Q}'\mathbf{B}\mathbf{Q}\mathbf{D}^{-\frac{1}{2}}$  to obtain its eigenvector  $\mathbf{a}$  which is associated with its largest eigenvalue.

The largest discriminant coordinate of  $\mathbf{g}$  is the projection

$$\xi = \mathbf{a}' \mathbf{D}^{-\frac{1}{2}} \mathbf{Q}' \mathbf{g}$$

### **Quadratic Discriminant Analysis (QDA)**

To determine the cutpoint for a continuous predictor, first group the categories of the target field  $Y$  to form two superclasses,  $A$  and  $B$ , as described above.

If  $\min(s_A^2, s_B^2) = 0$ , order the two superclasses by their variance in increasing order and denote the variances by  $s_1^2 \leq s_2^2$ , and the corresponding means by  $\bar{x}_1, \bar{x}_2$ . Let  $\epsilon$  be a very small positive number, say  $\epsilon = 10^{-12}$ . Set the cutpoint  $d$  based on  $\bar{x}_1$  and  $\epsilon$ :

$$d = \begin{cases} \bar{x}_1(1 + \epsilon) & \text{if } \bar{x}_1 < \bar{x}_2 \\ \bar{x}_1(1 - \epsilon) & \text{otherwise} \end{cases}$$

### **Blank Handling**

Records with missing values for the target field are ignored in building the tree model.

**Surrogate splitting** is used to handle blanks for predictor fields. If the best predictor field to be used for a split has a blank or missing value at a particular node, another field that yields a split similar to the predictor field in the context of that node is used as a surrogate for the predictor field, and its value is used to assign the record to one of the child nodes.

For example, suppose that  $X^*$  is the predictor field that defines the best split  $s^*$  at node  $t$ . The surrogate-splitting process finds another split  $s$ , the surrogate, based on another predictor field  $X$  such that this split is most similar to  $s^*$  at node  $t$  (for records with valid values for both predictors). If a new record is to be predicted and it has a missing value on  $X^*$  at node  $t$ , the surrogate split  $s$  is applied instead. (Unless, of course, this record also has a missing value on  $X$ . In such a situation, the next best surrogate is used, and so on, up to the limit of number of surrogates specified.)

In the interest of speed and memory conservation, only a limited number of surrogates is identified for each split in the tree. If a record has missing values for the split field and all surrogate fields, it is assigned to the child node with the higher weighted probability, calculated as

$$\frac{N_{f,j}(t)}{N_f(t)}$$

where  $N_{f,j}(t)$  is the sum of frequency weights for records in category  $j$  for node  $t$ , and  $N_f(t)$  is the sum of frequency weights for all records in node  $t$ .

If the model was built using equal or user-specified priors, the priors are incorporated into the calculation:

$$\frac{\pi(j)}{p_f(t)} \times \frac{N_{f,j}(t)}{N_f(t)}$$

where  $\pi(j)$  is the prior probability for category  $j$ , and  $p_f(t)$  is the weighted probability of a record being assigned to the node,

$$p_f(t) = \sum_j \frac{\pi(j)N_{f,j}(t)}{N_{f,j}}$$

where  $N_{f,j}(t)$  is the sum of the frequency weights (or the number of records if no frequency weights are defined) in node  $t$  belonging to category  $j$ , and  $N_{f,j}$  is the sum of frequency weights for records belonging to category  $j$  in the entire training sample.

#### **Predictive measure of association**

Let  $\tilde{h}_{X^* \cap X}$  (resp.  $\tilde{h}_{X^* \cap X}(t)$ ) be the set of learning cases (resp. learning cases in node  $t$ ) that has non-missing values of both  $X^*$  and  $X$ . Let  $p(s^* \approx s_X | t)$  be the probability of sending a case in  $\tilde{h}_{X^* \cap X}(t)$  to the same child by both  $s^*$  and  $s_X$ , and  $\tilde{s}_X$  be the split with maximized probability  $p(s^* \approx \tilde{s}_X | t) = \max_{s_X} (p(s^* \approx s_X | t))$ .

The predictive measure of association  $\lambda(s^* \approx \tilde{s}_X | t)$  between  $s^*$  and  $\tilde{s}_X$  at node  $t$  is

$$\lambda(s^* \approx \tilde{s}_X | t) = \frac{\min(p_L, p_R) - (1 - p(s^* \approx \tilde{s}_X | t))}{\min(p_L, p_R)}$$

where  $p_L$  (resp.  $p_R$ ) is the relative probability that the best split  $s^*$  at node  $t$  sends a case with non-missing value of  $X^*$  to the left (resp. right) child node. And where

$$p(s^* \approx s_X | t) = \begin{cases} \sum_j \frac{\pi(j) N_{w,j}(s^* \approx s_X, t)}{N_{w,j}(X^* \cap X)} & \text{if } Y \text{ is categorical} \\ \frac{N_w(s^* \approx s_X, t)}{N_w(X^* \cap X)} & \text{if } Y \text{ is continuous} \end{cases}$$

with

$$N_w(X^* \cap X) = \sum_{n \in \tilde{h}_{X^* \cap X}} w_n f_n, \quad N_w(X^* \cap X, t) = \sum_{n \in \tilde{h}_{X^* \cap X}(t)} w_n f_n$$

$$N_w(s^* \approx s_X, t) = \sum_{n \in \tilde{h}_{X^* \cap X}(t)} w_n f_n I(n : s^* \approx s_X)$$

$$N_{w,j}(X^* \cap X) = \sum_{n \in \tilde{h}_{X^* \cap X}} w_n f_n I(y_n = j), \quad N_{w,j}(X^* \cap X) = \sum_{n \in \tilde{h}_{X^* \cap X}(t)} w_n f_n I(y_n = j)$$

$$N_{w,j}(s^* \approx s_X, t) = \sum_{n \in \tilde{h}_{X^* \cap X}(t)} w_n f_n I(y_n = j) I(n : s^* \approx s_X)$$

and  $I(n : s^* \approx s_X)$  being the indicator function taking value 1 when both splits  $s^*$  and  $s_X$  send the case  $n$  to the same child, 0 otherwise.

## Effect of Options

### Stopping Rules

Stopping rules control how the algorithm decides when to stop splitting nodes in the tree. Tree growth proceeds until every leaf node in the tree triggers at least one stopping rule. Any of the following conditions will prevent a node from being split:

- The node is pure (all records have the same value for the target field)
- All records in the node have the same value for all predictor fields used by the model
- The tree depth for the current node (the number of recursive node splits defining the current node) is the *maximum tree depth* (default or user-specified).
- The number of records in the node is less than the *minimum parent node size* (default or user-specified)
- The number of records in any of the child nodes resulting from the node's best split is less than the *minimum child node size* (default or user-specified)

### Profits

**Profits** are numeric values associated with categories of a (symbolic) target field that can be used to estimate the gain or loss associated with a segment. They define the relative value of each value of the target field. Values are used in computing gains but not in tree growing.

Profit for each node in the tree is calculated as

$$\sum_j f_j(t) P_j$$

where  $j$  is the target field category,  $f_j(t)$  is the sum of frequency field values for all records in node  $t$  with category  $j$  for the target field, and  $P_j$  is the user-defined profit value for category  $j$ .

### Priors

**Prior probabilities** are numeric values that influence the misclassification rates for categories of the target field. They specify the proportion of records expected to belong to each category of the target field prior to the analysis. The values are involved both in tree growing and risk estimation.

There are three ways to derive prior probabilities.

**Empirical Priors**

By default, priors are calculated based on the training data. The prior probability assigned to each target category is the weighted proportion of records in the training data belonging to that category,

$$\pi(j) = \frac{N_{w,j}}{N_w}$$

In tree-growing and class assignment, the  $N$ s take both case weights and frequency weights into account (if defined); in risk estimation, only frequency weights are included in calculating empirical priors.

**Equal Priors**

Selecting equal priors sets the prior probability for each of the  $J$  categories to the same value,

$$\pi(j) = \frac{1}{J}$$

**User-Specified Priors**

When user-specified priors are given, the specified values are used in the calculations involving priors. The values specified for the priors must conform to the probability constraint: the sum of priors for all categories must equal 1.0. If user-specified priors do not conform to this constraint, adjusted priors are derived which preserve the proportions of the original priors but conform to the constraint, using the formula

$$\pi'(j) = \frac{\pi(j)}{\sum_J \pi(j)}$$

where  $\pi'(j)$  is the adjusted prior for category  $j$ , and  $\pi(j)$  is the original user-specified prior for category  $j$ .

**Costs**

If misclassification costs are specified, they are incorporated into split calculations by using altered priors. The altered prior is defined as

$$\pi'(t) = \frac{C(j)\pi(j)}{\sum_J C(j)\pi(j)}$$

where  $C(j) = \sum_i C(i|j)$ .

Misclassification costs also affect risk estimates and predicted values, as described below ( on p. 318 and on p. 319, respectively).

## Pruning

**Pruning** refers to the process of examining a fully grown tree and removing bottom-level splits that do not contribute significantly to the accuracy of the tree. In pruning the tree, the software tries to create the smallest tree whose misclassification risk is not too much greater than that of the largest tree possible. It removes a tree branch if the cost associated with having a more complex tree exceeds the gain associated with having another level of nodes (branch).

It uses an index that measures both the misclassification risk and the complexity of the tree, since we want to minimize both of these things. This cost-complexity measure is defined as follows:

$$R_\alpha(T) = R(T) + \alpha |\tilde{T}|$$

$R(T)$  is the misclassification risk of tree  $T$ , and  $|\tilde{T}|$  is the number of terminal nodes for tree  $T$ . The term  $\alpha$  represents the complexity cost *per terminal node* for the tree. (Note that the value of  $\alpha$  is calculated by the algorithm during pruning.)

Any tree you might generate has a maximum size ( $T_{\max}$ ), in which each terminal node contains only one record. With no complexity cost ( $\alpha = 0$ ), the maximum tree has the lowest risk, since every record is perfectly predicted. Thus, the larger the value of  $\alpha$ , the fewer the number of terminal nodes in  $T(\alpha)$ , where  $T(\alpha)$  is the tree with the lowest complexity cost for the given  $\alpha$ . As  $\alpha$  increases from 0, it produces a finite sequence of subtrees ( $T_1, T_2, T_3$ ), each with progressively fewer terminal nodes. Cost-complexity pruning works by removing the weakest split.

The following equations represent the cost complexity for  $\{t\}$ , which is any single node, and for  $T_t$ , the subbranch of  $\{t\}$ .

$$R_\alpha(\{t\}) = R(t) + \alpha$$

$$R_\alpha(T_t) = R(T_t) + \alpha |\tilde{T}_t|$$

If  $R_\alpha(T_t)$  is less than  $R_\alpha(\{t\})$ , then the branch  $T_t$  has a smaller cost complexity than the single node  $\{t\}$ .

The tree-growing process ensures that  $R_\alpha(\{t\}) \geq R_\alpha(T_t)$  for ( $\alpha = 0$ ). As  $\alpha$  increases from 0, both  $R_\alpha(\{t\})$  and  $R_\alpha(T_t)$  grow linearly, with the latter growing at a faster rate. Eventually, you will reach a threshold  $\alpha'$ , such that  $R_\alpha(\{t\}) < R_\alpha(T_t)$  for all  $\alpha > \alpha'$ . This means that when  $\alpha$  grows larger than  $\alpha'$ , the cost complexity of the tree can be reduced if we cut the subbranch  $T_t$  under  $\{t\}$ . Determining the threshold is a simple computation. You can solve this first inequality,  $R_\alpha(\{t\}) \geq R_\alpha(T_t)$ , to find the largest value of  $\alpha$  for which the inequality holds, which is also represented by  $g(t)$ . You end up with

$$\alpha \leq g(t) = \frac{R(t) - R(T_t)}{|\tilde{T}_t| - 1}$$

You can define the weakest link ( $t$ ) in tree  $T$  as the node that has the smallest value of  $g(t)$ :

$$g(\bar{t}) = \min_{t \in T} g(t)$$

Therefore, as  $\alpha$  increases,  $\bar{t}$  is the first node for which  $R_\alpha(\{\bar{t}\}) = R_\alpha(T)$ . At that point,  $\{\bar{t}\}$  becomes preferable to  $T_{\bar{t}}$ , and the subbranch is pruned.

With that background established, the pruning algorithm follows these steps:

- ▶ Set  $\alpha_1 = 0$  and start with the tree  $T_1 = T(0)$ , the fully grown tree.
- ▶ Increase  $\alpha$  until a branch is pruned. Prune the branch from the tree, and calculate the risk estimate of the pruned tree.
- ▶ Repeat the previous step until only the root node is left, yielding a series of trees,  $T_1, T_2, \dots, T_k$ .
- ▶ If the standard error rule option is selected, choose the smallest tree  $T_{opt}$  for which

$$R(T_{opt}) \leq \min_k R(T_k) + m \times SE(R(T))$$

- ▶ If the standard error rule option is not selected, then the tree with the smallest risk estimate  $R(T)$  is selected.

## Secondary Calculations

Secondary calculations are not directly related to building the model but give you information about the model and its performance.

### Risk Estimates

**Risk estimates** describe the risk of error in predicted values for specific nodes of the tree and for the tree as a whole.

#### Risk Estimates for Symbolic Target Field

For classification trees (with a symbolic target field), the risk estimate  $r(t)$  of a node  $t$  is computed as

$$r(t) = \frac{1}{N_f} \sum_j N_{f,j}(t) C(j^*(t)|j)$$

where  $C(j^*(t)|j)$  is the misclassification cost of classifying a record with target value  $j$  as  $j^*(t)$ ,  $N_{f,j}(t)$  is the sum of the frequency weights for records in node  $t$  in category  $j$  (or the number of records if no frequency weights are defined), and  $N_f$  is the sum of frequency weights for all records in the training data.

If the model uses user-specified priors, the risk estimate is calculated as

$$\sum_j \frac{\pi(j)N_{f,j}(t)}{N_{f,j}} C(j^*(t)|j)$$

### Gain Summary

The **gain summary** provides descriptive statistics for the terminal nodes of a tree.

If your target field is continuous (scale), the gain summary shows the weighted mean of the target value for each terminal node,

$$g(t) = \sum_{i \in t} w_i f_i x_i$$

If your target field is symbolic (categorical), the gain summary shows the weighted percentage of records in a selected target category,

$$g(t, j) = \frac{\sum_{i \in t} f_i x_i(j)}{\sum_{i \in t} f_i}$$

where  $x_i(j) = 1$  if record  $x_i$  is in target category  $j$ , and 0 otherwise. If profits are defined for the tree, the gain is the average profit value for each terminal node,

$$g(t) = \sum_{i \in t} f_i P(x_i)$$

where  $P(x_i)$  is the profit value assigned to the target value observed in record  $x_i$ .

### Generated Model/Scoring

Calculations done by the QUEST generated model are described below.

### Predicted Values

New records are scored by following the tree splits to a terminal node of the tree. Each terminal node has a particular predicted value associated with it, determined as follows:

For trees with a symbolic target field, each terminal node's predicted category is the category with the lowest weighted cost for the node. This weighted cost is calculated as

$$\min_i \sum_j C(i|j)p(j|t)$$

where  $C(i|j)$  is the user-specified misclassification cost for classifying a record as category  $i$  when it is actually category  $j$ , and  $p(j|t)$  is the conditional weighted probability of a record being in category  $j$  given that it is in node  $t$ , defined as

$$p(j|t) = \frac{p(j, t)}{\sum_j p(j, t)}, p(j, t) = \pi(j) \frac{N_{w,j}(t)}{N_{w,j}}$$

where  $\pi(j)$  is the prior probability for category  $j$ ,  $N_{w,j}(t)$  is the weighted number of records in node  $t$  with category  $j$  (or the number of records if no frequency or case weights are defined),

$$N_{w,j}(t) = \sum_{i \in t} w_i f_{ij}(i)$$

and  $N_{w,j}$  is the weighted number records in category  $j$  (any node),

$$N_{w,j} = \sum_{i \in T} w_i f_{ij}(i)$$

### **Confidence**

Confidence for a scored record is the proportion of weighted records in the training data in the scored record's assigned terminal node that belong to the predicted category, modified by the Laplace correction:

$$\frac{N_{f,j}(t) + 1}{N_f(t) + k}$$

### **Blank Handling**

In classification of new records, blanks are handled as they are during tree growth, using surrogates where possible, and splitting based on weighted probabilities where necessary. For more information, see the topic "Blank Handling" on p. 313.

# Linear Regression Algorithms

## Overview

This procedure performs ordinary least squares multiple linear regression with four methods for entry and removal of variables (Neter, Wasserman, and Kutner, 1990).

## Primary Calculations

### Notation

The following notation is used throughout this chapter unless otherwise stated:

$y_i$	Output field for record $i$ with variance $\frac{\sigma^2}{g_i}$
$c_i$	Case weight for record $i$ ; in IBM® SPSS® Modeler, $c_i \equiv 1$
$g_i$	Regression weight for record $i$ ; $g_i = 1$ if regression weight is not specified
$l$	Number of distinct records
$w_i$	$c_i \cdot g_i$
$W$	The sum of weights across records, $\sum_{i=1}^l w_i$
$p$	Number of input fields
$C$	Sum of case weights, $\sum_{i=1}^l c_i$
$x_{ki}$	The value of the $k$ th input field for record $i$
$\bar{X}_k$	Sample mean for the $k$ th input field, $\frac{\sum_{i=1}^l w_i x_{ki}}{W}$
$\bar{Y}$	Sample mean for the output field, $\frac{\sum_{i=1}^l w_i y_i}{W}$
$S_{kj}$	Sample covariance for input fields $X_k$ and $X_j$
$S_{yy}$	Sample variance for output field $Y$
$S_{ky}$	Sample covariance for $X_k$ and $Y$
$p^*$	Number of coefficients in the model. $p^* = p$ if the intercept is not included; otherwise $p^* = p + 1$
$\mathbf{R}$	Sample correlation matrix for $X_1 \dots X_p$ and $Y$

### Model Parameters

The summary statistics  $\bar{X}_i$  and covariance  $S_{ij}$  are computed using provisional means algorithms to update the values as each record is read:

$$\bar{X}_{i(k)} = \bar{X}_{i(k-1)} + (x_{ik} - \bar{X}_{i(k-1)}) \frac{w_k}{W_k}$$

and

$$S_{ij} = \frac{C_{ij}}{C - 1}$$

where, if the intercept is included,

$$C_{ij(k)} = C_{ij(k-1)} + (x_{ik} - \bar{X}_{i(k-1)}) (x_{jk} - \bar{X}_{j(k-1)}) \left( w_k - \frac{w_k^2}{W_k} \right)$$

or if the intercept is not included,

$$C_{ij(k)} = C_{ij(k-1)} + w_k x_{ik} x_{jk}$$

where  $W_k$  is the cumulative weight up to record  $k$ , and  $\bar{X}_{i(k)}$  is the estimate of  $\bar{X}_i$  up to record  $k$ .

For a regression model of the form

$$Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \dots + \beta_p X_{pi} + e_i$$

sweep operations are used to compute the least squares estimates  $\mathbf{b}$  of  $\beta$  and the associated regression statistics (Dempster, 1969). The sweeping starts with the correlation matrix  $\mathbf{R}$ ,

$$\mathbf{R} = \begin{bmatrix} r_{11} & \dots & r_{1p} & r_{1y} \\ r_{21} & \dots & r_{2p} & r_{2y} \\ \cdot & \dots & \cdot & \cdot \\ r_{y1} & \dots & r_{yp} & r_{yy} \end{bmatrix}$$

where

$$r_{kj} = \frac{S_{kj}}{\sqrt{S_{kk}S_{jj}}}$$

and

$$r_{yk} = r_{ky} = \frac{S_{ky}}{\sqrt{S_{kk}S_{yy}}}$$

Let  $\tilde{\mathbf{R}}$  be the new matrix produced by sweeping on the  $k$ th row and column of  $\mathbf{R}$ . The elements of  $\tilde{\mathbf{R}}$  are

$$\tilde{r}_{kk} = \frac{1}{r_{kk}}$$

$$\tilde{r}_{ik} = \frac{r_{ik}}{r_{kk}}, i \neq k$$

$$\tilde{r}_{kj} = \frac{r_{kj}}{r_{kk}}, j \neq k$$

and

$$\tilde{r}_{ij} = \frac{r_{ij}r_{kk} - r_{ik}r_{kj}}{r_{kk}}, i \neq k, j \neq k$$

If the above sweep operations are repeatedly applied to each row of  $\mathbf{R}_{11}$  in

$$\mathbf{R} = \begin{pmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} \\ \mathbf{R}_{21} & \mathbf{R}_{22} \end{pmatrix}$$

where  $\mathbf{R}_{11}$  contains the input fields in the equation at the current step, the result is

$$\tilde{\mathbf{R}} = \begin{pmatrix} \mathbf{R}_{11}^{-1} & -\mathbf{R}_{11}^{-1}\mathbf{R}_{12} \\ \mathbf{R}_{21}\mathbf{R}_{11}^{-1} & \mathbf{R}_{22} - \mathbf{R}_{21}\mathbf{R}_{11}^{-1}\mathbf{R}_{12} \end{pmatrix}$$

The last row of

$$\mathbf{R}_{21}\mathbf{R}_{11}^{-1}$$

contains the standardized coefficients (also called beta), and

$$\mathbf{R}_{22} - \mathbf{R}_{21}\mathbf{R}_{11}^{-1}\mathbf{R}_{12}$$

can be used to obtain the partial correlations for the variables not in the equation, controlling for the variables already in the equation. Note that this routine is its own inverse; that is, exactly the same operations are performed to remove an input field as to enter it.

The unstandardized coefficient estimates  $b_1 \dots b_p$  are calculated as

$$b_k = \frac{r_{yk}\sqrt{S_{yy}}}{\sqrt{S_{kk}}}$$

and the intercept  $b_0$ , if included in the model, is calculated as

$$b_0 = \bar{y} - \sum_{k=1}^p b_k \bar{X}_k$$

### **Automatic Field Selection**

Let  $r_{ij}$  be the element in the current swept matrix associated with  $X_i$  and  $X_j$ . Variables are entered or removed one at a time.  $X_k$  is eligible for entry if it is an input field not currently in the model such that

$$r_{kk} \geq t$$

and

$$\left( r_{jj} - \frac{r_{jk}r_{kj}}{r_{kk}} \right) t \leq 1$$

where  $t$  is the tolerance, with a default value of 0.0001.

The second condition above is imposed so that entry of the variable does not reduce the tolerance of variables already in the model to unacceptable levels.

The  $F$ -to-enter value for  $X_k$  is computed as

$$F - to - enter_k = \frac{(C - p^* - 1)V_k}{r_{yy} - V_k}$$

with 1 and  $C - p^* - 1$  degrees of freedom, where  $p^*$  is the number of coefficients currently in the model and

$$V_k = \frac{r_{yk}r_{ky}}{r_{kk}}$$

The  $F$ -to-remove value for  $X_k$  is computed as

$$F - to - remove_k = \frac{(C - p^*) |V_k|}{r_{yy}}$$

with 1 and  $C - p^*$  degrees of freedom.

### **Methods for Variable Entry and Removal**

Four methods for entry and removal of variables are available. The selection process is repeated until no more independent variables qualify for entry or removal. The algorithms for these four methods are described below.

#### **Enter**

The selected input fields are all entered in the model, with no field selection applied.

#### **Stepwise**

If there are independent variables currently entered in the model, choose  $X_k$  such that  $F - to - remove_k$  is minimum.  $X_k$  is removed if  $F - to - remove_k < F_{out}$  (default = 2.71) or, if probability criteria are used,  $P(F - to - remove_k) > P_{out}$  (default = 0.1). If the inequality does not hold, no variable is removed from the model.

If there are no independent variables currently entered in the model or if no entered variable is to be removed, choose  $X_k$  such that  $F - to - enter_k$  is maximum.  $X_k$  is entered if  $F - to - enter_k > F_{in}$  (default = 3.84) or,  $P(F - to - enter_k) < P_{in}$  (default = 0.05). If the inequality does not hold, no variable is entered.

At each step, all eligible variables are considered for removal and entry.

#### **Forward**

This procedure is the entry phase of the stepwise procedure.

### **Backward**

This procedure starts with all input fields in the model and applies the removal phase of the stepwise procedure.

### **Blank Handling**

By default, a case that has a missing value for any input or output field is deleted from the computation of the correlation matrix on which all consequent computations are based. If the Only use complete records option is deselected, each correlation in the correlation matrix  $\mathbf{R}$  is computed based on records with complete data for the two fields associated with the correlation, regardless of missing values on other fields. For some datasets, this approach can lead to a non-positive definite  $\mathbf{R}$  matrix, so that the model cannot be estimated.

## **Secondary Calculations**

### **Model Summary Statistics**

The multiple correlation coefficient  $R$  is calculated as

$$R = \sqrt{1 - r_{yy}}$$

R-square, the proportion of variance in the output field accounted for by the input fields, is calculated as

$$R^2 = 1 - r_{yy}$$

The adjusted R-square, which takes the complexity of the model relative to the size of the training data into account, is calculated as

$$R_{adj}^2 = R^2 - \frac{(1 - R^2)p}{C - p^*}$$

### **Field Statistics and Other Calculations**

The statistics shown in the advanced output for the regression equation node are calculated in the same manner as in the REGRESSION procedure in IBM® SPSS® Statistics. For more details, see the SPSS Statistics Regression algorithm document, available at <http://www.ibm.com/support>.

## **Generated Model/Scoring**

### **Predicted Values**

The predicted value for a new record is calculated as

$$\hat{y} = b_0 + \sum_{i=1}^p b_i X_i$$

**Blank Handling**

Records with missing values for any input field in the final model cannot be scored, and are assigned a predicted value of `$null$`.

# Sequence Algorithm

## Overview of Sequence Algorithm

The sequence node in IBM® SPSS® Modeler detects patterns in sequential data, such as purchases over time. The sequence node algorithm uses the following two-stage process for sequential pattern mining (Agrawal and Srikant, 1995):

- ▶ **Mine for the frequent sequences.** This part of the process extracts the information needed for quick responses to the pattern queries, yielding an adjacency lattice of the frequent sequences. This structure provides an optimal configuration for the second stage.
- ▶ **Generate sequential patterns online.** This stage uses a pre-computed adjacency lattice. You can extract the patterns according to specified criteria, such as support and confidence bounds, or place restrictions on the antecedent sequence.

## Primary Calculations

### Itemsets, Transactions, and Sequences

A group of items associated at a single point in time constitutes an **itemset**, which will be identified here using braces “{ }”. Consider the hypothetical data below representing sales at a gourmet store.

Table 31-1  
Example data - product purchases

Customer	Time 1	Time 2	Time 3	Time 4
1	cheese & crackers	wine	beer	-
2	wine	beer	cheese	-
3	bread	wine	cheese & beer	-
4	crackers	wine	beer	cheese
5	beer	cheese & crackers	bread	-
6	crackers	bread	-	-

Customer 1 yields three itemsets:  $\{cheese \& \textit{crackers}\}$ ,  $\{wine\}$ , and  $\{beer\}$ . The ampersand denotes items appearing in a single itemset. In this case, items separated by an ampersand appear in the same purchase. Notice that some itemsets may contain a single item only.

The complete group of itemsets for a single object, in this case a customer, constitutes a **transaction**. *Time* refers to a purchase occasion for a particular customer and does not represent a specific time across all customers. For example, the first purchase occasion for customer 1 may have been on January 23 while the first occasion for customer 4 was February 12. Although the dates are not identical, each itemset was the first for that customer. The analysis focuses on time relative to a specific customer instead of on absolute time.

Ordering the itemsets by time yields **sequences**. The symbol “>” denotes an ordering of itemsets, with the itemset on the right occurring after the itemset on the left. For example, customer 6 yields a sequence of  $[\{crackers\} > \{bread\}]$ .

Two common characteristics used to describe sequences are **size** and **length**. The number of items contained in a sequence corresponds to the sequence size. The number of itemsets in the sequence equals its length. For example, the three timepoints for customer 5 correspond to a sequence having a length of three and a size of four.

A sequence is a **subsequence** of another sequence if the first can be derived by deleting itemsets from the second. Consider the sequence:

$[\{wine\} > \{beer\} > \{cheese\}]$

Deleting the itemset *cheese* results in the sequence of length two  $[\{wine\} > \{beer\}]$ . This two itemset sequence is a subsequence of the original sequence. Similar deletions reveal that the three itemset sequence can be decomposed into three singleton subsequences ( $\{wine\}$ ,  $\{beer\}$ ,  $\{cheese\}$ ) and three subsequences involving two itemsets ( $[\{wine\} > \{beer\}]$ ,  $[\{beer\} > \{cheese\}]$ ,  $[\{wine\} > \{cheese\}]$ ). A sequence that is not a subsequence of another sequence is referred to as a **maximal sequence**.

### Support

The **support** for a sequence equals the proportion of transactions that contain the sequence. The table below shows support values for sequences that appear in at least one transaction for a set of gourmet store sales data (note that this is a different data set from the one shown previously).

For example, the support for sequence  $[\{wine\} > \{beer\}]$  is 0.67 because it occurs in four of the six transactions. Similarly, support for a sequential rule equals the proportion of transactions that contain both the antecedent and the consequent of the rule, in that order. The support for the sequential rule:

If  $\{cheese\} > \{wine\}$  then  $\{beer\}$

is 0.17 because only one of the six transactions contains these three itemsets in this order.

Sequences that do not appear in any transaction have support values of 0 and are excluded from the mining analysis.

Table 31-2  
Nonzero support values

Sequence	Support	Sequence	Support
$\{cheese\}$	0.83	$\{crackers\} > \{cheese\}$	0.17
$\{crackers\}$	0.67	$\{beer\} > \{cheese \& crackers\}$	0.17
$\{wine\}$	0.67	$\{cheese \& crackers\} > \{wine\}$	0.17
$\{beer\}$	0.83	$\{cheese \& crackers\} > \{beer\}$	0.17
$\{bread\}$	0.50	$\{bread\} > \{cheese \& beer\}$	0.17
$\{cheese \& crackers\}$	0.33	$\{wine\} > \{cheese \& beer\}$	0.17
$\{cheese \& beer\}$	0.17	$\{cheese \& crackers\} > \{bread\}$	0.17
$\{cheese\} > \{wine\}$	0.17	$\{cheese\} > \{wine\} > \{beer\}$	0.17
$\{cheese\} > \{beer\}$	0.17	$\{crackers\} > \{wine\} > \{beer\}$	0.33
$\{wine\} > \{beer\}$	0.67	$\{wine\} > \{beer\} > \{cheese\}$	0.33
$\{crackers\} > \{wine\}$	0.33	$\{bread\} > \{wine\} > \{beer\}$	0.17

Sequence	Support	Sequence	Support
{crackers} > {beer}	0.33	{bread} > {wine} > {cheese}	0.17
{wine} > {cheese}	0.50	{beer} > {cheese} > {bread}	0.17
{beer} > {cheese}	0.50	{beer} > {crackers} > {bread}	0.17
{bread} > {wine}	0.17	{crackers} > {wine} > {cheese}	0.17
{bread} > {beer}	0.17	{crackers} > {beer} > {cheese}	0.17
{bread} > {cheese}	0.17	{cheese & crackers} > {wine} > {beer}	0.17
{beer} > {bread}	0.17	{bread} > {wine} > {cheese & beer}	0.17
{beer} > {crackers}	0.17	{beer} > {cheese & crackers} > {bread}	0.17
{cheese} > {bread}	0.17	{crackers} > {wine} > {beer} > {cheese}	0.17
{crackers} > {bread}	0.33		

Typically, the analysis focuses on sequences having support values greater than a minimum threshold, the **support level**. This value, defined by the user, determines the minimum level for which sequences will be kept. Sequences with support values exceeding the threshold, referred to as **frequent sequences**, form the basis of the adjacency lattice. For example, for a threshold of 0.40, sequence [ {*wine*} > {*beer*} ] is a frequent sequence because its support level is 0.67. By relaxing the threshold, more sequences are classified as frequent.

### Time Constraints

Defining the time at which events occur has a dramatic impact on sequences. For instance, each purchase occasion in the gourmet data yields a new timed itemset. However, suppose a customer bought wine and realized while walking to his car that beer was needed too. He immediately returns to the store and buys the forgotten item. Should these two purchases be considered separately?

One method for controlling for itemsets that occur very close in time is through a **timestamp tolerance** parameter. This tolerance defines the length of time covering a single itemset. Specifying a tolerance larger than the difference between two consecutive times results in a single itemset at one time, such as {*wine & beer*} in the scenario described above.

Another time issue commonly arising in the analysis of sequences is **gap**. This statistic measures the difference in time between two items and can be used to make time-based predictions of future behavior. Gap statistics can be based on the gap between the last and penultimate sets in sequences, or on the gaps between the last and first sets in sequences.

### Sequential Patterns

**Sequential patterns**, or sequential association rules, identify items that frequently follow other items in transaction-based data. A sequential pattern is simply an ordered list of itemsets. All itemsets leading to the final itemset form the **antecedent** sequence, and the last itemset is the **consequent** sequence. These statements have the following form:

If [antecedent] then [consequent]

For example, a sequential pattern for *wine*, *beer*, and *cheese* is: “if a customer buys wine, then buys beer, he will buy cheese in the future”. *Wine* and *beer* form the antecedent, and *cheese* is the consequent.

Notationally, the symbol “=>” separates the antecedent from the consequent in a sequential rule. The sequence to the left of this symbol corresponds to the antecedent; the sequence on the right is the consequent. For instance, the rule above is denoted:

[{*wine*} > {*beer*} => {*cheese*}]

The only notational difference between a sequence and a sequential rule is the identification of a subsequence as a consequent.

## Adjacency Lattice

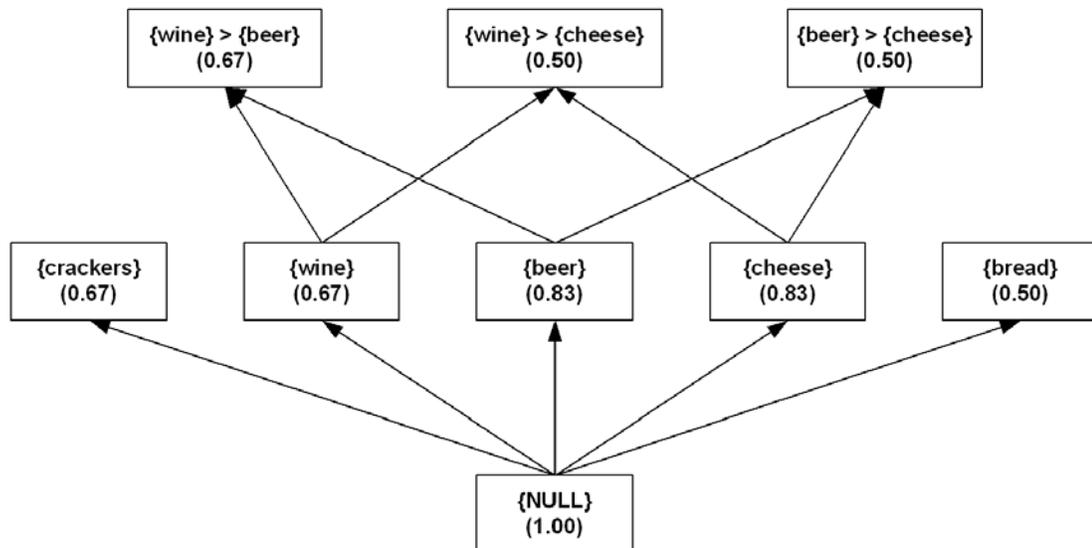
The number of itemsets and sequences for a collection of transactions grows very quickly as the number of items appearing in transactions gets larger. In practice, analyses typically involve many transactions and these transactions include a variety of itemsets. Larger datasets require complex methods to process the sequential patterns, particularly if rapid feedback is needed.

An adjacency lattice provides a structure for organizing sequences, permitting rapid generation of sequential patterns. Two sequences are **adjacent** if adding a single item to one yields the other, resulting in a hierarchical structure denoting which sequences are subsequences of other sequences. The lattice also includes sequence frequencies, as well as other information.

The adjacency lattice of all observed sequences is usually too large to be practical. It may be more useful to prune the lattice to frequent sequences in an effort to simplify the structure. All sequences contained in the resulting structure reach a specified support level. The adjacency lattice for the sample transactions using a support level of 0.40 is shown below.

Figure 31-1

Adjacency lattice for a threshold of 0.40 (support values in parentheses)



## Mining for Frequent Sequences

IBM® SPSS® Modeler uses a non-sequential association rule mining approach that performs very well with respect to minimizing I/O costs, time, and space requirements. The **continuous association rule mining algorithm** (Carma), uses only two data passes and allows changes in the support level during execution (Hidber, 1999). The final guaranteed support level depends on the provided series of support values.

For the first stage of the mining process, the component uses a variation of Carma to apply the approach to the sequential case. The general order of operations is:

- ▶ Read the transaction data.
- ▶ Identify frequent sequences, discarding infrequent sequences.
- ▶ Build an adjacency lattice of frequent sequences.

Carma is based upon transactions and requires only two passes through the data. In the first data pass, referred to as Phase I, the algorithm generates the frequent sequence candidates. The second data pass, Phase II, computes the exact frequency counts for the candidate sequences from Phase I.

### Phase I

Phase I corresponds to an estimation phase. In this phase, Carma generates candidate sequences successively for every transaction. Candidate sequences satisfy a version of the “apriori” principle where a sequence becomes a candidate only if all of its subsequences are candidates from the previous transactions. Therefore, the size of candidate sequences can grow with each transaction. To prevent the number of candidates from growing too large, Carma periodically prunes candidate sequences that have not reached a threshold frequency. Pruning may occur after processing any number of transactions. While pruning usually lowers the memory requirements, it increases the computational costs. At the end of the Phase I, the algorithm generates all sequences whose frequency exceeds the computed support level (which depends on the support series). Carma can use many support levels, up to one support level per transaction.

The table below represents support values during transaction processing with no pruning for the gourmet data. As the algorithm processes a transaction, support values adjust to account for items appearing in that transaction, as well as for the total number of processed transactions. For example, after the first transaction, the lattice contains *cheese*, *crackers*, *wine*, and *beer*, each having a support exceeding the threshold level. After processing the second transaction, the support for *crackers* drops from 1.0 to 0.50 because that item appears in only one of the two transactions. The support for the other items remains unchanged because both transactions contain the items. Furthermore, the sequences [*wine* > *beer*] and [*beer* > *cheese*] enter the lattice because their constituent subsequences already appear in the lattice.

Table 31-3  
Carma transaction processing

Sequence	Transaction					
	1	2	3	4	5	6
{cheese}	1	1	1	1	1	0.83
{crackers}	1	0.50	0.33	0.50	0.60	0.67
{wine}	1	1	1	1	0.80	0.67
{beer}	1	1	1	1	1	0.83

Sequence	Transaction					
	1	2	3	4	5	6
{wine} > {beer}		1	1	1	0.80	0.67
{beer} > {cheese}		0.50	0.33	0.50	0.60	0.50
{bread}			0.33	0.25	0.40	0.50
{wine} > {cheese}			0.67	0.75	0.60	0.50
{cheese & beer}			0.33	0.25	0.20	0.17
{crackers} > {wine}				0.50	0.40	0.33
{crackers} > {beer}				0.50	0.40	0.33
{crackers} > {cheese}				0.25	0.20	0.17
{wine} > {beer} > {cheese}				0.50	0.40	0.33
{cheese & crackers}					0.40	0.33
{beer} > {crackers}					0.20	0.17
{beer} > {bread}					0.20	0.17
{cheese} > {bread}					0.20	0.17
{crackers} > {bread}					0.20	0.33

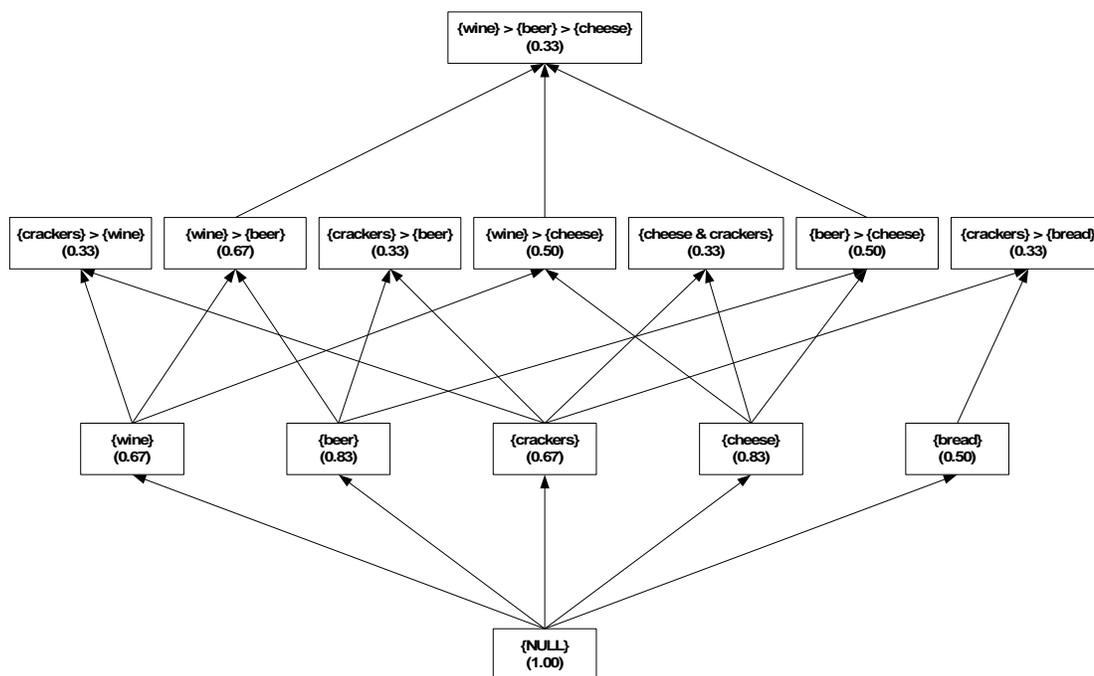
After completing the first data pass, the lattice contains five sequences containing one item, twelve sequences involving two items, and one sequence composed of three items.

### **Phase II**

Phase II is a validation phase requiring a second data pass, during which the algorithm determines accurate frequencies for candidate sequences. In this phase, Carma does not generate any candidate sequences and prunes infrequent sequences only once, making Phase II faster than Phase I. Moreover, depending on the entry points of candidate sequences during Phase I, a complete data pass may not even be necessary. In an online application, Carma skips Phase II altogether.

Suppose the threshold level is 0.30 for the lattice. Several sequences fail to reach this level and subsequently get pruned during Phase II. The resulting lattice appears below.

Figure 31-2  
Adjacency lattice for a threshold of 0.30 (support values in parentheses)



Notice that the lattice does not contain  $[\{crackers\} > \{wine\} > \{beer\}]$  although the support for this sequence exceeds the threshold. Although  $[\{crackers\} > \{wine\} > \{beer\}]$  occurs in one-third of the transactions, Carma cannot add this sequence to the lattice until all of its subsequences are included. The final two subsequences occur in the fourth transaction, after which the full three-itemset sequence is not observed. In general, however, the database of transactions will be much larger than the small example shown here, and exclusions of this type will be extremely rare.

## Generating Sequential Patterns

The second stage in the sequential pattern mining process queries the adjacency lattice of the frequent sequences produced in the first stage for the actual patterns. Aggarwal and Yu (1998a) IBM® SPSS® Modeler uses a set of efficient algorithms for generating association rules online from the adjacency lattice (Aggarwal and Yu, 1998). Applying these algorithms to the sequential case takes advantage of the monotonic properties for rule support and confidence preserved by the adjacency lattice data structures. The lattice efficiently saves all the information necessary for generating the sequential patterns and is orders of magnitude smaller than all the patterns it could possibly generate.

The queries contain the constraints that the resulting set of sequential patterns needs to satisfy. These constraints fall into two categories:

- constraints on statistical indices
- constraints on the items contained in the antecedent of the patterns

Statistical index constraints involve support, confidence, or cause. These queries require returned patterns to have values for these statistics within a specified range. Usually, lower confidence bound is the primary criterion. The lower bound for the pattern support level is given by the support level for the sequences in the corresponding adjacency lattice. Often, however, the support specified for pattern generation exceeds the value specified for lattice creation.

For the lattice shown above, specifying a support range between 0.30 and 1.00, a confidence range from 0.30 to 1.0, and a cause range from 0 to 1.0 results in the following seven rules:

- If [*crackers*] then [*beer*].
- If [*crackers*] then [*wine*].
- If [*crackers*] then [*bread*].
- If [*wine*] > [*beer*] then [*cheese*].
- If [*wine*] then [*beer*].
- If [*wine*] then [*cheese*].
- If [*beer*] then [*cheese*].

Limiting the set to only maximal sequences omits the final three rules because they are subsequences of the fourth.

The second type of query requires the specification of the sequential rule antecedent. This type of query returns a new singleton itemset after the final itemset in the antecedent. For example, consider an online shopper who has placed items in a shopping cart. A future item query looks at only the past purchases to derive a recommended item for the next time the shopper visits the site.

## Blank Handling

Blanks are ignored by the sequence rules algorithm. The algorithm will handle records containing blanks for input fields, but such a record will not be considered to match any rule containing one or more of the fields for which it has blank values.

## Secondary Calculations

### Confidence

Confidence is a measure of sequential rule accuracy and equals the proportion obtained by dividing the number of transactions that contain both the antecedent and consequent of the rule by the number of transactions containing the antecedent. In other words, confidence is the support for the rule divided by the support for the antecedent. For example, the confidence for the sequential rule:

```
If [wine] then
  [cheese]
```

is 3/4, or 0.75. Three-quarters of the transactions that include *wine* also include *cheese* at a later time. In contrast, the sequential rule:

```
If [cheese] then
  [wine]
```

includes the same itemsets but has a confidence of 0.20. Only one-fifth of the transactions that include *cheese* contain *wine* at a later time. In other words, *wine* is more likely to lead to *cheese* than *cheese* is to lead to *wine*.

displays the confidence for every sequential rule observed in the gourmet data. Rules with empty antecedents correspond to having no previous transaction history.

Table 31-4  
Nonzero confidence values

Sequence	Confidence	Sequence	Confidence
{cheese}	1.00	{crackers} => {cheese}	0.25
{crackers}	1.00	{beer} => {cheese & crackers}	0.20
{wine}	1.00	{cheese & crackers} => {wine}	0.50
{beer}	1.00	{cheese & crackers} => {beer}	0.50
{bread}	1.00	{bread} => {cheese & beer}	0.33
{cheese & crackers}	1.00	{wine} => {cheese & beer}	0.25
{cheese & beer}	1.00	{cheese & crackers} => {bread}	0.50
{cheese} => {wine}	0.20	{cheese} > {wine} => {beer}	1.00
{cheese} => {beer}	0.20	{crackers} > {wine} => {beer}	1.00
{wine} => {beer}	1.00	{wine} > {beer} => {cheese}	0.50
{crackers} => {wine}	0.50	{bread} > {wine} => {beer}	1.00
{crackers} => {beer}	0.50	{bread} > {wine} => {cheese}	1.00
{wine} => {cheese}	0.75	{beer} > {cheese} => {bread}	0.33
{beer} => {cheese}	0.60	{beer} > {crackers} => {bread}	1.00
{bread} => {wine}	0.33	{crackers} > {wine} => {cheese}	0.50
{bread} => {beer}	0.33	{crackers} > {beer} => {cheese}	0.50
{bread} => {cheese}	0.33	{cheese & crackers} > {wine} => {beer}	1.00
{beer} => {bread}	0.20	{bread} > {wine} => {cheese & beer}	1.00
{beer} => {crackers}	0.20	{beer} > {cheese & crackers} => {bread}	1.00
{cheese} => {bread}	0.20	{crackers} > {wine} > {beer} => {cheese}	0.50
{crackers} => {bread}	0.50		

## Generated Model/Scoring

### Predicted Values

When you pass data records into a Sequence Rules model, the model handles the records in a time-dependent manner (or order-dependent, if no timestamp field was used to build the model). Records should be sorted by the ID field and timestamp field (if present).

For each record, the rules in the model are compared to the set of transactions processed for the current ID so far, including the current record and any previous records with the same ID and earlier timestamp. The  $k$  rules with the highest confidence values that apply to this set of transactions are used to generate the  $k$  predictions for the record, where  $k$  is the number of predictions specified when the model was built. (If multiple rules predict the same outcome for the transaction set, only the rule with the highest confidence is used.)

Note that the predictions for each record do not necessarily depend on that record's transactions. If the current record's transactions do not trigger a specific rule, rules will be selected based on the previous transactions for the current ID. In other words, if the current record doesn't add any useful predictive information to the sequence, the prediction from the last useful transaction for this ID is carried forward to the current record.

For example, suppose you have a Sequence Rule model with the single rule

Jam -> Bread (0.66)

and you pass it the following records:

ID	Purchase	Prediction
001	jam	bread
001	milk	bread

Notice that the first record generates a prediction of *bread*, as you would expect. The second record also contains a prediction of *bread*, because there's no rule for *jam* followed by *milk*; therefore the *milk* transaction doesn't add any useful information, and the rule Jam -> Bread still applies.

## **Confidence**

The confidence associated with a prediction is the confidence of the rule that produced the prediction. For more information, see the topic "Confidence" on p. 334.

## **Blank Handling**

Blanks are ignored by the sequence rules algorithm. The algorithm will handle records containing blanks for input fields, but such a record will not be considered to match any rule containing one or more of the fields for which it has blank values.

# Self-Learning Response Model Algorithms

Self-Learning Response Models (SLRMs) use Naive Bayes classifiers to build models that can be easily updated to incorporate new data, without having to regenerate the entire model. The methods used for building, updating and scoring with SLRMs are described here.

## Primary Calculations

The model-building algorithm used in SLRMs is Naive Bayes. A Bayesian Network consisting of a Naive Bayes model for each target field is generated.

## Naive Bayes Algorithms

The Naive Bayes model is an old method for classification and predictor selection that is enjoying a renaissance because of its simplicity and stability.

## Notation

The following notation is used throughout this chapter unless otherwise stated:

Table 32-1

Notation

Notation	Description
$J_0$	Total number of predictors.
$\mathbf{X}$	Categorical predictor vector $\mathbf{X}' = (X_1, \dots, X_J)$ , where $J$ is the number of predictors considered.
$M_j$	Number of categories for predictor $X_j$ .
$Y$	Categorical target variable.
$K$	Number of categories of $Y$ .
$N$	Total number of cases or patterns in the training data.
$N_k$	The number of cases with $Y = k$ in the training data.
$N_{mk}^j$	The number of cases with $Y = k$ and $X_j = m$ in the training data.
$\pi_k$	The probability for $Y = k$ .
$p_{mk}^j$	The probability of $X_j = m$ given $Y = k$ .

## Naive Bayes Model

The Naive Bayes model is based on the conditional independence model of each predictor given the target class. The Bayesian principle is to assign a case to the class that has the largest posterior probability. By Bayes' theorem, the posterior probability of  $Y$  given  $\mathbf{X}$  is:

$$P(Y = k | \mathbf{X} = \mathbf{x}) = \frac{P(\mathbf{X} = \mathbf{x} | Y = k) P(Y = k)}{\sum_{i=1}^K P(\mathbf{X} = \mathbf{x} | Y = i) P(Y = i)}$$

Let  $X_1, \dots, X_J$  be the  $J$  predictors considered in the model. The Naive Bayes model assumes that  $X_1, \dots, X_J$  are conditionally independent given the target; that is:

$$P(\mathbf{X} = \mathbf{x} | Y = k) = \prod_{j=1}^J P(X_j = x_j | Y = k)$$

These probabilities are estimated from training data by the following equations:

$$\pi_k = P(Y = k) = \frac{N_k + \lambda}{N + K\lambda}$$

$$p_{mk}^j = P(X_j = m | Y = k) = \frac{N_{mk}^j + f}{\sum_{l=1}^{M_j} N_{lk}^j + M_j f}$$

Where  $N_k$  is calculated based on all non-missing  $Y$ ,  $N_{mk}^j$  is based on all non-missing pairs of  $X_j$  and  $Y$ , and the factors  $\lambda$  and  $f$  are introduced to overcome problems caused by zero or very small cell counts. These estimates correspond to Bayesian estimation of the multinomial probabilities with Dirichlet priors. Empirical studies suggest  $\lambda = f = \frac{1}{N}$  (Kohavi, Becker, and Sommerfield, 1997).

A single data pass is needed to collect all the involved counts.

For the special situation in which  $J = 0$ ; that is, there is no predictor at all,  $P(Y = k | \mathbf{X} = \mathbf{x}) = P(Y = k)$ . When there are empty categories in the target variable or categorical predictors, these empty categories should be removed from the calculations.

## Secondary Calculations

In addition to the model parameters, a model assessment is calculated.

### Model Assessment

For a trained model, we need to assess how reliable it is. Given this problem, we face two conditions which will result with different solutions:

- A sample of test data (not used in training or updating the model) is available. In this case we can directly feed these data into the model, and observe the outcome.
- No extra testing data are available. This is more common since users normally apply all available data to train the model. In this case, we have to simulate data first based on the calibrated model parameters, such as  $\pi_k$  and  $p_{mk}^j$ , then assess the trained model by scoring these pseudo random data.

#### Testing with Simulated Data

In our simulation,  $n_{round} \times n_{sample\_per\_round}$  data are generated. For each round, we can determine the corresponding accuracy; across all rounds, average accuracy and variance can be calculated, and they are explained as reliability statistics.

- ▶ For each round, we generate  $n_{sample}$  random cases as follows:
  - $y$  is assigned a random value based on the prior probabilities  $\pi_k$ .
  - Each  $X_i$  is randomly assigned based on conditional probabilities  $\hat{P}(X_j|Y = y)$
- ▶ The accuracy of each round is calculated by comparing the model's predicted value for each case to the case's generated outcome  $y$ ,  $P_{accuracy} = \frac{n_{correct}}{n_{sample}}$
- ▶ The mean, variance, minimum and maximum of the accuracy estimates are calculated across rounds.

## Blank Handling

If the target is missing, or all  $J_0$  predictors for a case are missing, the case is ignored. If every value for a predictor is missing, or all non-missing values for a predictor are the same, that predictor is ignored.

## Updating the Model

The model can be updated by updating the cell counts  $N_k$ ,  $N_{mk}^j$  to account for the new records and recalculating the probabilities  $\pi_k$  and  $p_{mk}^j$  as described in “Naive Bayes Model” on p. 337. Updating the model only requires a data pass of new records.

## Generated Model/Scoring

Scoring with a generated SLRM model is described below.

## Predicted Values and Confidences

By default, the first  $M$  offers with highest predicted value will be returned. However, sometimes low-probability offers are of interest for marketing strategy. Model settings allow you to bias the results toward particular offers, or include random components to the offers.

Some notation for scoring offers:

$N$	Number of offers modeled already
$P = \{P_1, P_2, \dots, P_N\}$	Scores for each offer
$P_r = \{P_{r1}, P_{r2}, \dots, P_{rN}\}$	Randomly generated scores for offers
$\alpha$	Randomization factor, ranging from 0.0 (offer based only on model prediction) to 1.0 (offer is completely random)
$W = \{W_1, W_2, \dots, W_N\}$	Number of cases used for training each offer
$W_{emp}$	Empirical value of the amount of training cases that will result in a reliable model. When “Take account of model reliability” is selected in the Settings tab, this is set to 500; otherwise 0.

$S = \{S_1, S_2, \dots, S_N\}$	User's preferences for offers, or the ratings of the offers. Can be any non-negative value, where larger values means stronger recommendations for the corresponding offers. The default setting is $S = \{1, 1, \dots, 1\}$
$F = \{F_1, F_2, \dots, F_N\}$	Mandatory inclusion/exclusion filters. $F_i \in \{0, 1\}$ , where 0 indicates an excluded offer.

The final score for each offer is calculated as

$$P_i = \left[ \alpha P_{ri} + (1 - \alpha) \left( \frac{W_i}{W_i + W_{emp}} P + \frac{W_{emp}}{W_i + W_{emp}} 0.5 \right) \right] \cdot \frac{S_i}{\max(S)} \cdot F_i$$

The outcomes  $P_i$  are ordered in specified order, ascending or descending, and the first  $M$  offers in the list are recommended. The calculated score is reported as the confidence for the score.

## Variable Assessment

Among all the features modeled, some are definitely more important to the accuracy of the model than others. Two different approaches to measuring importance are proposed here: Predictor Importance and Information Measure.

### Predictor Importance

The variance of predictive error can be used as the measure of importance. With this method, we leave out one predictor variable at a time, and observe the performance of remaining model. A variable is regarded as more important than another if it adds more variance compared to that of the complete model (with all variables).

When test data are available, they can be used for predictor importance calculations in a direct way. When test data are not available, they are simulated based on the model parameters  $\pi_k$  and  $p_{mk}^j$ .

In our simulation,  $n_{round} \times n_{sample\_per\_round}$  data are generated. For each round, we determine the corresponding accuracy for each submodel, excluding  $X_j$  for each of the  $j$  predictors; across all rounds, average accuracy and variance can be calculated.

- ▶ For each round, we generate  $n_{sample}$  random cases as follows:
  - $y$  is assigned a random value based on the prior probabilities  $\pi_k$ .
  - Each  $X_i$  is randomly assigned based on conditional probabilities  $\hat{P}(X_j|Y = y)$

Within a round, each of the  $X_j$  predictors is excluded from the model, and the accuracy is calculated based on the generated test data for each submodel in turn.

- ▶ The accuracies for each round are calculated by comparing the submodel's predicted value for each case to the case's generated outcome  $y$ ,  $P_{accuracy\_without\_xj} = \frac{n_{correct\_without\_xj}}{n_{sample}}$ , for each of the  $j$  submodels.

- The mean and variance of the accuracy estimates are calculated across rounds for each submodel. For each variable, the importance is measured as the difference between the accuracy of the full model and the mean accuracy for the submodels that excluded the variable.

### Information Measure

The importance of an explanatory variable  $X$  for a response variable  $Y$  is the extent to which the use of  $X$  reduces uncertainty in predicting outcomes of  $Y$ . The uncertainty about predicting an outcome  $Y$  is measured by the entropy of its distribution (Shannon 1948):

$$H_Y \equiv - \sum_i P(Y = i) \log P(Y = i)$$

Based on a value  $x$  of the explanatory variable, the probability distribution of the outcomes  $Y$  is the conditional distribution  $f_{y|x}$ . The information value of using the value  $x$  for the prediction is assessed by comparing the concentrations of the marginal distribution  $f_y$  and the conditional distribution  $f_{y|x}$ . The difference between the conditional and marginal distribution entropy is:

$$\Delta H(x_j) = H_Y - H_{Y|x_j}$$

where  $H_{Y|x_j}$  denotes the entropy of the conditional distribution  $f_{y|x_j}$ . The value  $x_j$  is informative about  $Y$  if the conditional distribution  $f_{y|x_j}$  is more concentrated than  $f_y$ .

The importance of a random variable  $X$  for predicting  $Y$  is measured by the expected uncertainty reduction, referred to as the *mutual information* between two variables:

$$\begin{aligned} M(Y, X) &\equiv \sum_i f_x(x_j) \Delta H(x_j) \\ &= H_Y - H_{Y|X} \\ &= H_Y + H_X - H_{Y,X} \end{aligned}$$

The expected fraction of uncertainty reduction due to  $X$  is a mutual information index given by

$$I_{y,x} = 1 - \frac{H_{Y|X}}{H_Y} = \frac{M_{Y,X}}{H_Y}$$

This index ranges from zero to one:  $I_{y,x} = 0$  if and only if the two variables are independent, and  $I_{y,x} = 100\%$  if and only if the two variables are functionally related in some form, linearly or nonlinearly.



# Simulation algorithms

Simulation in IBM® SPSS® Modeler refers to simulating input data to predictive models using the Monte Carlo method and evaluating the model based on the simulated data. You do this by using the Simulation Generation (also known as SimGen) source node. The distribution of predicted target values can then be used to evaluate the likelihood of various outcomes.

## Simulation algorithms

Creating a simulation includes specifying distributions for all inputs to a predictive model that are to be simulated. When historical data are present, the distribution that most closely fits the data for each input can be determined using the algorithms described in this section.

### Notation

The following notation is used throughout this section unless otherwise stated:

Table 33-1

Notation

Notation	Description
$x_i$	Value of the input variable in the $i$ th case of the historical data
$w_i$	Frequency weight associated with the $i$ th case of the historical data
$W$	Total effective sample size accounting for frequency weights
$\bar{x}_{obs}$	Sample mean
$s_{obs}^2$	Sample variance
$s_{obs}$	Sample standard deviation

### Distribution fitting

The historical data for a given input is denoted by:

$$\vec{x} = x_1, x_2, \dots, x_n$$

The total effective sample size is:

$$W = \sum_{i=1}^n w_i$$

The observed sample mean, sample variance and sample standard deviation are:

$$\bar{x}_{obs} = \frac{1}{W} \sum_{i=1}^n w_i x_i$$

$$s_{obs}^2 = \frac{1}{W-1} \sum_{i=1}^n w_i (x_i - \bar{x}_{obs})^2$$

$$s_{obs} = \sqrt{s_{obs}^2}$$

Parameter estimation for most distributions is based on the maximum likelihood (ML) method, and closed-form solutions for the parameters exist for many of the distributions. There is no closed-form ML solution for the distribution parameters for the following distributions: negative binomial, beta, gamma and Weibull. For these distributions, the Newton-Raphson method is used. This approach requires the following information: the log-likelihood function, the gradient vector, the Hessian matrix, and the initial values for the iterative Newton-Raphson process.

### **Discrete distributions**

Distribution fitting is supported for the following discrete distributions: binomial, categorical, Poisson and negative binomial.

#### **Binomial distribution: parameter estimation**

The probability mass function for a random variable  $x$  with a binomial distribution is:

$$Bin(x; N, P) = \binom{N}{x} P^x (1-P)^{N-x}, \text{ for } x = 0, 1, \dots, N$$

where  $0 \leq P \leq 1$  is the probability of success. The binomial distribution is used to describe the total number of successes in a sequence of  $N$  independent Bernoulli trials. The parameter estimates for the binomial distribution using the method of moments (see Johnson & Kotz (2005) for details) are:

$$\hat{P} = \begin{cases} 1 - \frac{s_{obs}^2}{\bar{x}_{obs}}, & \bar{x}_{obs} > s_{obs}^2 \\ NaN, & \bar{x}_{obs} < s_{obs}^2 \end{cases}$$

where  $NaN$  implies that the binomial distribution would not be an appropriate distribution to fit the data under this criterion, and where

$$\hat{N} = \frac{\bar{x}_{obs}}{\hat{P}}$$

If  $\hat{N}$  is not an integer, then the parameter estimates are:

$$\hat{N}^* = \lceil \hat{N} + 0.5 \rceil$$

$$\hat{P}^* = \frac{\bar{x}_{obs}}{\hat{N}^*}$$

where  $[x]$  denotes the integer part of  $x$ .

### **Categorical distribution: parameter estimation**

The categorical distribution can be considered a special case of the multinomial distribution in which  $N=1$ . Suppose  $x_i, i = 1, 2, \dots, n$ , has the categorical distribution and its categorical values are denoted as  $1, 2, \dots, J$ . Then an indicator variable of  $x_i$  for category  $j$  can be denoted as

$$x_{i,j} = \begin{cases} 1 & \text{if } x_i = j \\ 0 & \text{otherwise} \end{cases}$$

and the corresponding probability is  $P_j$ . Then the probability mass function for a random variable  $x_i$  with the categorical distribution can be described based on  $x_{i,j}$  and  $P_j$  as follows:

$$\text{Categorical}(x_i; P_1, \dots, P_J) = \prod_{j=1}^J P_j^{x_{i,j}}, \text{ with } \sum_{j=1}^J P_j = 1$$

The parameter estimates for  $P_j, j = 1, \dots, J$ , are:

$$\hat{P}_j = \frac{\sum_{i=1}^n w_i x_{i,j}}{W}, j = 1, \dots, J$$

### **Poisson distribution: parameter estimation**

The probability mass function for a random variable  $x$  with a Poisson distribution is:

$$\text{Pois}(x; \lambda) = \frac{e^{-\lambda} \lambda^x}{x!}, \text{ for } x = 0, 1, \dots$$

where  $\lambda > 0$  is the rate parameter of the Poisson distribution. The parameter of the Poisson distribution can be estimated as:

$$\hat{\lambda} = \bar{x}_{obs}$$

### **Negative binomial distribution: parameter estimation**

The distribution fitting component for simulation supports the parameterization of the negative binomial distribution that describes the distribution of the number of failures before the  $r^{\text{th}}$  success. For this parameterization, the probability mass function for a random variable  $x$  is:

$$\text{NB}(x; r, \theta) = \binom{x+r-1}{x} \theta^r (1-\theta)^x, \text{ for } x = 0, 1, \dots$$

where  $r \geq 0$ ,  $0 \leq \theta \leq 1$  are the two distribution parameters. There is no closed-form solution for the parameters  $r$  and  $\theta$ , so the Newton-Raphson method with step-halving will be used. The method requires the following information:

(1) The log likelihood function

$$L = \sum_{i=1}^n w_i \ln \Gamma(x_i + r) - \sum_{i=1}^n w_i \ln x_i! - W \ln \Gamma(r) + Wr \ln(\theta) + \ln(1 - \theta) \sum_{i=1}^n w_i x_i$$

(2) The gradient (1st derivative) vector with respect to  $r$  and  $\theta$

$$s = \begin{bmatrix} \frac{\partial L}{\partial \theta} \\ \frac{\partial L}{\partial r} \end{bmatrix} = \begin{bmatrix} \frac{Wr}{\theta} - \frac{1}{(1-\theta)} \sum_{i=1}^n w_i x_i \\ \sum_{i=1}^n w_i \psi(x_i + r) - W \psi(r) + W \ln(\theta) \end{bmatrix}$$

where  $\psi(\alpha) = \frac{\Gamma'(\alpha)}{\Gamma(\alpha)}$  is a digamma function, which is the derivative of the logarithm of the gamma function, evaluated at  $\alpha$ .

(3) The Hessian (2nd derivative) matrix with respect to  $r$  and  $\theta$  (since the Hessian matrix is symmetric, only the lower triangular portion is displayed)

$$H = \begin{bmatrix} \frac{\partial^2 L}{\partial \theta^2} & \\ \frac{\partial^2 L}{\partial r \partial \theta} & \frac{\partial^2 L}{\partial r^2} \end{bmatrix} = \begin{bmatrix} -\frac{Wr}{\theta^2} - \frac{1}{(1-\theta)^2} \sum_{i=1}^n w_i x_i & \\ \frac{W}{\theta} & \sum_{i=1}^n w_i \psi'(x_i + r) - W \psi'(r) \end{bmatrix}$$

where  $\psi'(\alpha)$  is the trigamma function, or the derivative of the digamma function.

(4) The initial values of  $\theta$  and  $r$  can be obtained from the closed-form estimates using the method of moments:

$$r^{(0)} = \begin{cases} \frac{\bar{x}_{obs}^2}{s_{obs}^2 - \bar{x}_{obs}} & \text{if } s_{obs}^2 > \bar{x}_{obs} \\ 1 & \text{otherwise} \end{cases}$$

$$\theta^{(0)} = \frac{r^{(0)}}{r^{(0)} + \bar{x}_{obs}}$$

Note

An alternative parameterization of the negative binomial distribution describes the distribution of the number of trials before the  $r^{\text{th}}$  success. Although it is not supported in distribution fitting, it is supported in simulation when explicitly specified by the user. The probability mass function for this parameterization, for a random variable  $x$  is:

$$NB(x; r, \theta) = \binom{x-1}{r-1} \theta^r (1-\theta)^{x-r}, \text{ for } x \geq r$$

where  $r \geq 0$ ,  $0 \leq \theta \leq 1$  are the two distribution parameters.

### Continuous distributions

Distribution fitting is supported for the following continuous distributions: triangular, uniform, normal, lognormal, exponential, beta, gamma and Weibull.

#### Triangular distribution: parameter estimation

The probability density function for a random variable  $x$  with a triangular distribution is:

$$Triag(x; a, m, b) = \begin{cases} \frac{2}{(b-a)} \frac{(x-a)}{(m-a)}, & x \in [a, m) \\ \frac{2}{(b-a)}, & x = m \\ \frac{2}{(b-a)} \frac{(b-x)}{(b-m)}, & x \in (m, b] \\ 0, & x \notin [a, b] \end{cases}$$

such that  $a \leq m \leq b$ . Parameter estimates of the triangular distribution are:

$$\hat{a} = \min \{x_1, x_2, \dots, x_n\}$$

$$\hat{b} = \max \{x_1, x_2, \dots, x_n\}$$

$$\hat{m} = mode \{x_1, x_2, \dots, x_n\}$$

Since the calculation of the mode for continuous data may be ambiguous, we transform the parameter estimates and use the method of moments as follows (see Kotz and Rene van Dorp (2004) for details):

$$z_i = \frac{x_i - \hat{a}}{\hat{b} - \hat{a}}$$

$$\theta = \frac{m - \hat{a}}{\hat{b} - \hat{a}}$$

$$\bar{z} = \frac{1}{W} \sum_{i=1}^n w_i z_i$$

From the method of moments we obtain

$$\hat{\theta} = 3\bar{z} - 1$$

from which it follows that

$$\hat{m} = \hat{a} + (\hat{b} - \hat{a}) \times (3\bar{z} - 1)$$

*Note:* For very skewed data or if the actual mode equals  $a$  or  $b$ , the estimated mode,  $\hat{m}$ , may be less than  $\hat{a}$  or greater than  $\hat{b}$ . In this case, the adjusted mode, defined as below, is used:

$$Adj. \hat{m} = \begin{cases} \hat{a} & \text{if } \hat{m} < \hat{a} \\ \hat{b} & \text{if } \hat{m} > \hat{b} \end{cases}$$

### **Uniform distribution: parameter estimation**

The probability density function for a random variable  $x$  with a uniform distribution is:

$$U(x; a, b) = \begin{cases} \frac{1}{b-a}, & x \in [a, b] \\ 0, & x \notin [a, b] \end{cases}$$

where  $a$  is the minimum and  $b$  is the maximum among the values of  $\vec{x}$ . Hence, the parameter estimates of the uniform distribution are:

$$\hat{a} = \min \{x_1, x_2, \dots, x_n\}$$

$$\hat{b} = \max \{x_1, x_2, \dots, x_n\}$$

### **Normal distribution: parameter estimation**

The probability density function for a random variable  $x$  with a normal distribution is:

$$Nor(x, \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}, \quad -\infty < x < \infty$$

Here,  $\mu$  is the measure of centrality and  $\sigma$  is the measure of dispersion of the normal distribution. The parameter estimates of the normal distribution are:

$$\hat{\mu} = \bar{x}_{obs}$$

$$\hat{\sigma} = \sqrt{\frac{1}{W} \sum_{i=1}^n w_i (x_i - \bar{x}_{obs})^2} = \sqrt{\frac{(W-1) s_{obs}^2}{W}}$$

### **Lognormal distribution: parameter estimation**

The lognormal distribution is a probability distribution where the natural logarithm of a random variable follows a normal distribution. In other words, if  $x$  has a lognormal( $\mu, \sigma$ ) distribution, then  $\ln(x)$  has a normal( $\ln(\mu), \sigma$ ) distribution. The probability density function for a random variable  $x$  with a lognormal distribution is:

$$LN(x, \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma x} e^{-\frac{1}{2}\left(\frac{\ln x - \ln \mu}{\sigma}\right)^2}, \quad 0 < x < \infty$$

Define  $\bar{\ln x}_{obs} = \frac{1}{W} \sum_{i=1}^n w_i \ln x_i$

Parameter estimates for the lognormal distribution are:

$$\hat{\mu} = e^{\bar{\ln x}_{obs}}$$

$$\hat{\sigma} = \sqrt{\frac{1}{W} \sum_{i=1}^n w_i (\ln x_i - \ln \hat{\mu})^2}$$

### **Exponential distribution: parameter estimation**

The probability density function for a random variable  $x$  with an exponential distribution is:

$$Exp(x; \lambda) = \lambda e^{-\lambda x}, \text{ for } x \geq 0 \text{ and } \lambda > 0$$

The estimate of the parameter for the exponential distribution is:

$$\hat{\lambda} = \frac{1}{\bar{x}_{obs}}$$

### **Beta distribution: parameter estimation**

The probability density function for a random variable  $x$  with a beta distribution is:

$$Beta(x; \alpha, \beta) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1}, \quad \alpha, \beta > 0$$

where,

$$B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)}$$

There is no closed-form solution for the parameters  $\alpha$  and  $\beta$ , so the Newton-Raphson method with step-halving will be used. The method requires the following information:

(1) The log likelihood function

$$L = W \ln(\Gamma(\alpha + \beta)) - W \ln(\Gamma(\alpha)) - W \ln(\Gamma(\beta))$$

$$+ (\alpha - 1) \sum_{i=1}^n w_i \ln x_i + (\beta - 1) \sum_{i=1}^n w_i \ln (1 - x_i)$$

(2) The gradient (1st derivative) vector with respect to  $\alpha$  and  $\beta$

$$s = \begin{bmatrix} \frac{\partial L}{\partial \alpha} \\ \frac{\partial L}{\partial \beta} \end{bmatrix} = \begin{bmatrix} W\psi(\alpha + \beta) - W\psi(\alpha) + \sum_{i=1}^n w_i \ln(x_i) \\ W\psi(\alpha + \beta) - W\psi(\beta) + \sum_{i=1}^n w_i \ln(1 - x_i) \end{bmatrix}$$

where  $\psi(\alpha) = \frac{\Gamma'(\alpha)}{\Gamma(\alpha)}$  is a digamma function, which is the derivative of the logarithm of the gamma function, evaluated at  $\alpha$ .

(3) The Hessian (2nd derivative) matrix with respect to  $\alpha$  and  $\beta$  (since the Hessian matrix is symmetric, only the lower triangular portion is displayed)

$$H = \begin{bmatrix} \frac{\partial^2 L}{\partial \alpha^2} & \\ \frac{\partial^2 L}{\partial \alpha \partial \beta} & \frac{\partial^2 L}{\partial \beta^2} \end{bmatrix} = \begin{bmatrix} W(\psi'(\alpha + \beta) - \psi'(\alpha)) & \\ W\psi'(\alpha + \beta) & W(\psi'(\alpha + \beta) - \psi'(\beta)) \end{bmatrix}$$

where  $\psi'(\alpha)$  is the trigamma function, or the derivative of the digamma function.

(4) The initial values of  $\alpha$  and  $\beta$  can be obtained from the closed-form estimates using the method of moments:

$$\alpha^{(0)} = \bar{x}_{obs} \left( \frac{\bar{x}_{obs} (1 - \bar{x}_{obs})}{s_{obs}^2} - 1 \right)$$

$$\beta^{(0)} = (1 - \bar{x}_{obs}) \left( \frac{\bar{x}_{obs} (1 - \bar{x}_{obs})}{s_{obs}^2} - 1 \right)$$

### **Gamma distribution: parameter estimation**

The probability density function for a random variable  $x$  with a gamma distribution is:

$$\text{Gamma}(x; \alpha, \beta) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x}, \text{ for } x \geq 0 \text{ and } \alpha, \beta > 0$$

If  $\alpha$  is a positive integer, then the gamma function is given by:  $\Gamma(\alpha) = (\alpha - 1)!$

There is no closed-form solution for the parameters  $\alpha$  and  $\beta$ , so the Newton-Raphson method with step-halving will be used. The method requires the following information:

(1) The log likelihood function

$$L = W\alpha \ln \beta - W \ln \Gamma(\alpha) + (\alpha - 1) \sum_{i=1}^n w_i \ln x_i - \beta \sum_{i=1}^n w_i x_i$$

(2) The gradient (1st derivative) vector with respect to  $\alpha$  and  $\beta$

$$s = \begin{bmatrix} \frac{\partial L}{\partial \alpha} \\ \frac{\partial L}{\partial \beta} \end{bmatrix} = \begin{bmatrix} W \ln \beta - W\psi(\alpha) + \sum_{i=1}^n w_i \ln x_i \\ \frac{W\alpha}{\beta} - \sum_{i=1}^n w_i x_i \end{bmatrix}$$

where  $\psi(\alpha) = \frac{\Gamma'(\alpha)}{\Gamma(\alpha)}$  is a digamma function, which is the derivative of the logarithm of the gamma function, evaluated at  $\alpha$ .

(3) The Hessian (2nd derivative) matrix with respect to  $\alpha$  and  $\beta$  (since the Hessian matrix is symmetric, only the lower triangular portion is displayed)

$$H = \begin{bmatrix} \frac{\partial^2 L}{\partial \alpha^2} & \frac{\partial^2 L}{\partial \alpha \partial \beta} \\ \frac{\partial^2 L}{\partial \alpha \partial \beta} & \frac{\partial^2 L}{\partial \beta^2} \end{bmatrix} = \begin{bmatrix} -W\psi'(\alpha) & \\ \frac{W}{\beta} & -\frac{W\alpha}{\beta^2} \end{bmatrix}$$

where  $\psi'(\alpha)$  is the trigamma function, or the derivative of the digamma function.

(4) The initial values of  $\alpha$  and  $\beta$  can be obtained from the closed-form estimates using the method of moments:

$$\alpha^{(0)} = \left( \frac{\bar{x}_{obs}}{s_{obs}} \right)^2$$

$$\beta^{(0)} = \frac{\bar{x}_{obs}}{s_{obs}^2}$$

### **Weibull distribution: parameter estimation**

Distribution fitting for the Weibull distribution is restricted to the two-parameter Weibull distribution, whose probability density function is given by:

$$Weib(x; \beta, \gamma) = \frac{\gamma}{\beta} \left( \frac{x}{\beta} \right)^{\gamma-1} e^{-\left(\frac{x}{\beta}\right)^\gamma}, \text{ for } x \geq 0 \text{ and } \beta, \gamma > 0$$

There is no closed-form solution for the parameters  $\beta$  and  $\gamma$ , so the Newton-Raphson method with step-halving will be used. The method requires the following information:

(1) The log likelihood function

$$L = W(\ln \gamma - \gamma \ln \beta) + (\gamma - 1) \sum_{i=1}^n w_i \ln(x_i) - \sum_{i=1}^n w_i \left( \frac{x_i}{\beta} \right)^\gamma$$

(2) The gradient (1st derivative) vector with respect to  $\beta$  and  $\gamma$

$$s = \begin{bmatrix} \frac{\partial L}{\partial \beta} \\ \frac{\partial L}{\partial \gamma} \end{bmatrix} = \begin{bmatrix} -\frac{W\gamma}{\beta} + \frac{\gamma}{\beta} \sum_{i=1}^n w_i \left( \frac{x_i}{\beta} \right)^\gamma \\ \frac{W}{\gamma} - W \ln \beta + \sum_{i=1}^n w_i \ln(x_i) - \sum_{i=1}^n w_i \left( \frac{x_i}{\beta} \right)^\gamma \ln \left( \frac{x_i}{\beta} \right) \end{bmatrix}$$

(3) The Hessian (2nd derivative) matrix with respect to  $\beta$  and  $\gamma$  (since the Hessian matrix is symmetric, only the lower triangular portion is displayed)

$$H = \begin{bmatrix} \frac{\partial^2 L}{\partial \beta^2} & \\ \frac{\partial^2 L}{\partial \beta \partial \gamma} & \frac{\partial^2 L}{\partial \gamma^2} \end{bmatrix}$$

where

$$\begin{aligned} \frac{\partial^2 L}{\partial \beta^2} &= \frac{\gamma}{\beta^2} \left[ W - (\gamma + 1) \sum_{i=1}^n w_i \left( \frac{x_i}{\beta} \right)^\gamma \right] \\ \frac{\partial^2 L}{\partial \beta \partial \gamma} &= -\frac{1}{\beta} \left[ W - \sum_{i=1}^n w_i \left( \frac{x_i}{\beta} \right)^\gamma - \gamma \sum_{i=1}^n w_i \left( \frac{x_i}{\beta} \right)^\gamma \ln \left( \frac{x_i}{\beta} \right) \right] \\ \frac{\partial^2 L}{\partial \gamma^2} &= -\frac{W}{\gamma^2} - \sum_{i=1}^n w_i \left( \frac{x_i}{\beta} \right)^\gamma \left[ \ln \left( \frac{x_i}{\beta} \right) \right]^2 \end{aligned}$$

(4) The initial values of  $\beta$  and  $\gamma$  are given by:

$$\gamma^{(0)} = 1$$

$$\beta^{(0)} = 1$$

### Goodness of fit measures

Goodness of fit measures are used to determine the distribution that most closely fits the data. For discrete distributions, the Chi-Square test is used. For continuous distributions, the Anderson-Darling test or the Kolmogorov-Smirnov test is used.

#### Discrete distributions

The Chi-Square goodness of fit test is used for discrete distributions (Dirk P. Kroese, 2011). The Chi-Square test statistic has the following form:

$$T = \sum_{i=1}^k \frac{(O_i - E_i)^2}{E_i}$$

where,

Table 33-2

Notation

Notation	Description
$k$	The number of classes, as defined in the table below for each discrete distribution
$O_i$	The total observed frequency for class $i$

<b>Notation</b>	<b>Description</b>
$PDF(i)$	Probability density function of the fitted distribution. For the Poisson and negative binomial distributions, the density function for the last class is computed as $PDF(k) = 1 - \sum_{i=1}^{k-1} PDF(i)$
$E_i$	Expected frequency for class $i$ : $E_i = W * PDF(i)$
$W$	The total effective sample size

For large  $W$ , the above statistic follows the Chi-Square distribution:

$$T \sim \chi_{k-1-r}^2$$

where  $r = \text{number of parameters estimated from the data}$ . The following table provides the values of  $k$  and  $r$  for the various distributions. The value  $Max$  in the table is the observed maximum value.

<b>Distribution</b>	<b>Notation</b>	<b><math>k</math> (classes)</b>	<b><math>r</math> (parameters)</b>
Binomial	$Bin(x; N, P)$	$N+1$	2
Categorical	$Categorical(x; p_1, \dots, p_J)$	$J$	$J-1$
Poisson	$Pois(x; \lambda)$	$Max + 1$	1
Negative binomial	$NB(x; r, \theta)$	$Max + 1$	2

This Chi-Square test is valid only if all values of  $E_i \geq 5$ .

The p-value for the Chi-Square test is then calculated as:

$$p = 1 - F(T, \chi_{k-1-r}^2)$$

where  $F(T, \chi_{k-1-r}^2) = CDF$  of the Chi-Square distribution.

*Note:* The p-value cannot be calculated for the Categorical distribution since the number of degrees of freedom is zero.

### **Continuous distributions**

For continuous distributions, the Anderson-Darling test or the Kolmogorov-Smirnov test is used to determine goodness of fit. The calculation consists of the following steps:

1. Transform the data to a Uniform(0,1) distribution
2. Sort the transformed data to generate the Order Statistics
3. Calculate the Anderson-Darling or Kolmogorov-Smirnov test statistic
4. Compute the approximate p-value associated with the test statistic

The first two steps are common to both the Anderson-Darling and Kolmogorov-Smirnov tests. The original data are transformed to a Uniform(0,1) distribution using the transformation:

$$y = F(x)$$

where the transformation function  $F(x)$  is given in the table below for each of the supported distributions.

Distribution	Transformation F(x)
$Triag(x; a, m, b)$	$\begin{cases} \frac{1}{(b-a)} \frac{(x-a)^2}{(m-a)}, & x \in [a, m) \\ \frac{(m-a)}{(b-a)}, & x = m \\ 1 - \frac{1}{(b-a)} \frac{(b-x)^2}{(b-m)}, & x \in (m, b] \\ 0, & x \notin [a, b] \end{cases}$
$U(x; a, b)$	$\frac{x-a}{b-a}$
$Nor(x, \mu, \sigma)$	$\Phi\left(\frac{x-\mu}{\sigma}\right)$
$LN(x, \mu, \sigma)$	$\Phi\left(\frac{\ln x - \ln \mu}{\sigma}\right)$
$Exp(x; \lambda)$	$1 - e^{-\lambda x}$
$Beta(x; \alpha, \beta)$	$\int_0^x \frac{1}{B(\alpha, \beta)} t^{\alpha-1} (1-t)^{\beta-1} dt$
$Gamma(x; \alpha, \beta)$	$\int_0^x \frac{\beta^\alpha}{\Gamma(\alpha)} t^{\alpha-1} e^{-\beta t} dt$
$Weib(x; \beta, \gamma)$	$1 - e^{-\left(\frac{x}{\beta}\right)^\gamma}$

The transformed data points  $y_i$  are sorted in ascending order to generate the Order Statistics:

$$y_{(1)} \leq y_{(2)} \leq \dots \leq y_{(n-1)} \leq y_{(n)}$$

Define  $w_i^*$  to be the corresponding frequency weight for  $y_{(i)}$ . The cumulative frequency up to and including  $y_{(i)}$  is defined as:

$$W_i^* = \sum_{k=1}^i w_k^*$$

and where we define  $W_0^* = 0$ .

**Anderson-Darling test**

The Anderson-Darling test statistic is given by:

$$z = -W_n^* - \frac{1}{W_n^*} \sum_{i=1}^n w_i^* (2W_{i-1}^* + w_i^*) \ln(y_{(i)}) + \frac{1}{W_n^*} \sum_{i=1}^n w_i^* (2W_{i-1}^* + w_i^*) \ln(1 - y_{(i)}) - 2 \sum_{i=1}^n w_i^* \ln(1 - y_{(i)})$$

For more information, see the topic “Anderson-Darling statistic with frequency weights” on p. 360.

The approximate p-value for the Anderson-Darling statistic can be computed for the following distributions: uniform, normal, lognormal, exponential, Weibull and gamma. The p-value is not available for the triangular and beta distributions.

**Uniform distribution: p-value**

The p-value for the Anderson-Darling statistic is computed based on the following result, provided by Marsaglia (2004):

$$p = \begin{cases} 1 - z^{-1/2} e^{-1.2337141/z} g(z) & \text{for } z \in (0, 2) \\ 1 - e^{(1.0776 - (2.30695 - (0.43424 - (0.082433 - (0.008056 - 0.0003146z)z)z)z)z)} & \text{for } z \in [2, \infty) \end{cases}$$

where

$$g(z) = (2.00012 + (0.247105 - (0.0649821 - (0.0347962 - (0.0116720 - 0.00168691z)z)z)z)z)$$

**Normal and lognormal distributions: p-value**

The p-value for the Anderson-Darling statistic is computed based on the following result, provided by D’Agostino and Stephens (1986):

$$p = \begin{cases} 1 - \exp(-13.436 + 101.14z^* - 223.73z^{*2}), & z^* \leq 0.2 \\ 1 - \exp(-8.318 + 42.796z^* - 59.938z^{*2}), & 0.2 < z^* \leq 0.34 \\ \exp(0.9177 - 4.279z^* - 1.38z^{*2}), & 0.34 < z^* \leq 0.6 \\ \exp(1.2937 - 5.709z^* + 0.0186z^{*2}), & 0.6 < z^* \leq 153.467 \\ 0 & z^* > 153.467 \end{cases}$$

where

$$z^* = z(1.0 + 0.75/W_n^* + 2.25/W_n^{*2})$$

**Exponential distribution: p-value**

The p-value for the Anderson-Darling statistic is computed based on the following result, provided by D'Agostino and Stephens (1986):

$$p = \begin{cases} 1 - \exp(-12.2204 + 67.459z^* - 110.3z^{*2}), & z^* \leq 0.260 \\ 1 - \exp(-6.1327 + 20.218z^* - 18.663z^{*2}), & 0.260 < z^* \leq 0.510 \\ \exp(0.9209 - 3.353z^* + 0.3z^{*2}), & 0.510 < z^* \leq 0.950 \\ \exp(0.731 - 3.009z^* + 0.15z^{*2}), & 0.950 < z^* \leq 10.03 \\ 0, & z^* > 10.03 \end{cases}$$

where

$$z^* = z(1.0 + 0.6/W_n^*)$$

**Weibull distribution: p-value**

The p-value for the Anderson-Darling statistic is computed based on Table 33-3 below, provided by D'Agostino and Stephens (1986). First, the adjusted Anderson-Darling statistic is computed from:

$$z^* = z \left( 1 + 0.2/\sqrt{W_n^*} \right)$$

If the value of  $z^*$  is between two probability levels (in the table), then linear interpolation is used to estimate the p-value. For example, if  $z^* = 0.543$  which is between  $z_1^* = 0.474$  and  $z_2^* = 0.637$ , then the corresponding probabilities of  $z_1^*$  and  $z_2^*$  are  $p_1 = 0.25$  and  $p_2 = 0.1$  respectively. Then the p-value of  $z^*$  is computed as

$$p = \frac{p_2 - p_1}{z_2^* - z_1^*} (z^* - z_1^*) + p_1 = \frac{0.1 - 0.25}{0.637 - 0.474} (0.543 - 0.474) + 0.25 = 0.1865$$

If the value of  $z^*$  is less than the smallest critical value in the table, then the p-value is  $\geq 0.25$ ; and if  $z^*$  is greater than the largest critical value in the table, then the p-value is  $\leq 0.01$ .

**Table 33-3**

*Upper tail probability and corresponding critical values for the Anderson-Darling test, for the Weibull distribution*

<b>p-value</b>	<b>0.25</b>	<b>0.10</b>	<b>0.05</b>	<b>0.025</b>	<b>0.01</b>
$z(1 + 0.2/\sqrt{W_n^*})$	0.474	0.637	0.757	0.877	1.038

**Gamma distribution: p-value**

Table 33-4, which is provided by D'Agostino and Stephens (1986), is used to compute the p-value of the Anderson-Darling test for the gamma distribution. First, the appropriate row in the table is determined from the range of the parameter  $\alpha$ . Then linear interpolation is used to compute the p-value, as done for the Weibull distribution. For more information, see the topic "Weibull distribution: p-value" on p. 356.

If the test statistic is less than the smallest critical value in the row, then the p-value is  $\geq 0.25$ ; and if the test statistic is greater than the largest critical value in the row, then the p-value is  $\leq 0.005$ .

Table 33-4

Upper tail probability and corresponding critical values for the Anderson-Darling test, for the gamma distribution with estimated parameter  $\alpha$

p-value	0.25	0.10	0.05	0.025	0.01	0.005
$\alpha \in (0, 1]$	0.486	0.657	0.786	0.917	1.092	1.227
$\alpha \in (1, 8]$	0.473	0.637	0.759	0.883	1.048	1.173
$\alpha \in (8, \infty)$	0.470	0.631	0.752	0.873	1.035	1.159

### Kolmogorov-Smirnov test

The Kolmogorov-Smirnov test statistic,  $D_n$ , is given by:

$$D^+ = \max_i \left| y_{(i)} - \frac{W_i^*}{W_n^*} \right| \quad D^- = \max_i \left| y_{(i)} - \frac{W_i^* - 1}{W_n^*} \right|$$

$$D_n = \max(D^+, D^-)$$

Computation of the p-value is based on the modified Kolmogorov-Smirnov statistic, which is distribution specific.

### Uniform distribution: p-value

The procedure proposed by Kroese (2011) is used to compute the p-value of the Kolmogorov-Smirnov statistic for the uniform distribution. First, the modified Kolmogorov-Smirnov statistic is computed as

$$D = \sqrt{W_n^*} D_n$$

The corresponding p-value is computed as follows:

1. Set  $k=100$
2. Define  $\alpha_k = \sum_{i=-k}^k (-1)^i e^{-2(iD)^2}$
3. Calculate  $\alpha_k$  and  $\alpha_{k+1}$
4. If  $|\alpha_k - \alpha_{k+1}| \geq 10^{-5}$  set  $k=k+1$  and repeat step 2; otherwise, go to step 5.
5. p-value =  $1 - \alpha_k$

### Normal and lognormal distributions: p-value

The modified Kolmogorov-Smirnov statistic is

$$D = D_n \left( \sqrt{W_n^*} - 0.01 + \frac{0.85}{\sqrt{W_n^*}} \right)$$

The p-value for the Kolmogorov-Smirnov statistic is computed based on Table 33-5 below, provided by D'Agostino and Stephens (1986). If the value of D is between two probability levels, then linear interpolation is used to estimate the p-value. For more information, see the topic "Weibull distribution: p-value" on p. 356.

If D is less than the smallest critical value in the table, then the p-value is  $\geq 0.15$ ; and if D is greater than the largest critical value in the table, then the p-value is  $\leq 0.01$ .

**Table 33-5**

*Upper tail probability and corresponding critical values for the Kolmogorov-Smirnov test, for the Normal and Lognormal distributions*

p-value	0.15	0.10	0.05	0.025	0.01
D	0.775	0.819	0.895	0.995	1.035

### **Exponential distribution: p-value**

The modified Kolmogorov-Smirnov statistic is

$$D = (D_n - 0.2/W_n^*) \left( \sqrt{W_n^*} + 0.26 + 0.5/\sqrt{W_n^*} \right)$$

The p-value for the Kolmogorov-Smirnov statistic is computed based on Table 33-6 below, provided by D'Agostino and Stephens (1986). If the value of D is between two probability levels, then linear interpolation is used to estimate the p-value. For more information, see the topic "Weibull distribution: p-value" on p. 356.

If D is less than the smallest critical value in the table, then the p-value is  $\geq 0.15$ ; and if D is greater than the largest critical value in the table, then the p-value is  $\leq 0.01$ .

**Table 33-6**

*Upper tail probability and corresponding critical values for the Kolmogorov-Smirnov test, for the Exponential distribution*

p-value	0.15	0.10	0.05	0.025	0.01
D	0.926	0.995	1.094	1.184	1.298

### **Weibull distribution: p-value**

The modified Kolmogorov-Smirnov statistic is

$$D = \sqrt{W_n^*} D_n$$

The p-value for the Kolmogorov-Smirnov statistic is computed based on Table 33-7 below, provided by D'Agostino and Stephens (1986). If the value of D is between two probability levels, then linear interpolation is used to estimate the p-value. For more information, see the topic "Weibull distribution: p-value" on p. 356.

If  $D$  is less than the smallest critical value in the table, then the  $p$ -value is  $\geq 0.10$ ; and if  $D$  is greater than the largest critical value in the table, then the  $p$ -value is  $\leq 0.01$ .

**Table 33-7**

*Upper tail probability and corresponding critical values for the Kolmogorov-Smirnov test, for the Weibull distribution*

<b><math>p</math>-value</b>	<b>0.10</b>	<b>0.05</b>	<b>0.025</b>	<b>0.01</b>
$D$	1.372	1.477	1.557	1.671

### **Gamma distribution: $p$ -value**

The modified Kolmogorov-Smirnov statistic is

$$D = D_n \left( \sqrt{W_n^*} + 0.3/\sqrt{W_n^*} \right)$$

The  $p$ -value for the Kolmogorov-Smirnov statistic is computed based on Table 33-8 below, provided by D'Agostino and Stephens (1986). If the value of  $D$  is between two probability levels, then linear interpolation is used to estimate the  $p$ -value. For more information, see the topic "Weibull distribution:  $p$ -value" on p. 356.

If  $D$  is less than the smallest critical value in the table, then the  $p$ -value is  $\geq 0.25$ ; and if  $D$  is greater than the largest critical value in the table, then the  $p$ -value is  $\leq 0.005$ .

**Table 33-8**

*Upper tail probability and corresponding critical values for the Kolmogorov-Smirnov test, for the Gamma distribution*

<b><math>p</math>-value</b>	<b>0.25</b>	<b>0.20</b>	<b>0.15</b>	<b>0.10</b>	<b>0.05</b>	<b>0.025</b>	<b>0.01</b>	<b>0.005</b>
$D$	0.74	0.780	0.800	0.858	0.928	0.990	1.069	1.13

### **Determining the recommended distribution**

The distribution fitting module is invoked by the user, who may specify an explicit set of distributions to test or rely on the default set, which is determined from the measurement level of the input to be fit. For continuous inputs, the user specifies either the Anderson-Darling test (the default) or the Kolmogorov-Smirnov test for the goodness of fit measure (for ordinal and nominal inputs, the Chi-Square test is always used). The distribution fitting module then returns the values of the specified test statistic along with the calculated  $p$ -values (if available) for each of the tested distributions, which are then presented to the user in ascending order of the test statistic. The recommended distribution is the one with the minimum value of the test statistic.

The above approach yields the distribution that most closely fits the data. However, if the  $p$ -value of the recommended distribution is less than 0.05, then the recommended distribution may not provide a close fit to the data.

### Anderson-Darling statistic with frequency weights

To obtain the expression for the Anderson-Darling statistic with frequency weights, we first give the expression where the frequency weight of each value is 1:

$$\begin{aligned}
 z &= -n - \frac{1}{n} \sum_{i=1}^n (2i - 1) [\ln (y_{(i)} (1 - y_{(n+1-i)}))] \\
 &= -n - \frac{1}{n} \sum_{i=1}^n (2i - 1) [\ln (y_{(i)}) + \ln (1 - y_{(n+1-i)})] \\
 &= -n - \frac{1}{n} \sum_{i=1}^n (2i - 1) [\ln (y_{(i)})] - \frac{1}{n} \sum_{i=1}^n (2(n + 1 - i) - 1) [\ln (1 - y_{(i)})] \\
 &= -n - \frac{1}{n} \sum_{i=1}^n (2i - 1) [\ln (y_{(i)})] - \frac{1}{n} \sum_{i=1}^n (1 - 2i) [\ln (1 - y_{(i)})] - \sum_{i=1}^n 2 [\ln (1 - y_{(i)})] \\
 &= A + B + C + D
 \end{aligned}$$

If there is a frequency weight variable, then the corresponding four terms of the above expression are given by:

$$A = -W_n^*$$

$$\begin{aligned}
 B &= -\frac{1}{W_n^*} \sum_{i=1}^n \sum_{j=1}^{w_i^*} (2(W_{i-1}^* + j) - 1) [\ln (y_{(i)})] \\
 &= -\frac{1}{W_n^*} \sum_{i=1}^n w_i^* (2W_{i-1}^* - 1) \ln (y_{(i)}) - \frac{1}{W_n^*} \sum_{i=1}^n w_i^* (w_i^* + 1) \ln (y_{(i)}) \\
 &= -\frac{1}{W_n^*} \sum_{i=1}^n w_i^* (2W_{i-1}^* + w_i^*) \ln (y_{(i)})
 \end{aligned}$$

$$\begin{aligned}
 C &= -\frac{1}{W_n^*} \sum_{i=1}^n \sum_{j=1}^{w_i^*} (1 - 2(W_{i-1}^* + j)) [\ln (1 - y_{(i)})] \\
 &= -\frac{1}{W_n^*} \sum_{i=1}^n w_i^* (1 - 2W_{i-1}^*) \ln (1 - y_{(i)}) + \frac{1}{W_n^*} \sum_{i=1}^n w_i^* (w_i^* + 1) \ln (1 - y_{(i)}) \\
 &= \frac{1}{W_n^*} \sum_{i=1}^n w_i^* (2W_{i-1}^* + w_i^*) \ln (1 - y_{(i)})
 \end{aligned}$$

$$D = -2 \sum_{i=1}^n w_i^* \ln (1 - y_{(i)})$$

where  $w_i^*$  and  $W_i^*$  are defined in the section on goodness of fit measures for continuous distributions. For more information, see the topic ‘‘Continuous distributions’’ on p. 353.

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## Simulation algorithms: run simulation

Running a simulation involves generating data for each of the simulated inputs, evaluating the predictive model based on the simulated data (along with values for any fixed inputs), and calculating metrics based on the model results.

### Generating correlated data

Simulated values of input variables are generated so as to account for any correlations between pairs of variables. This is accomplished using the NORTA (Normal-To-Anything) method described by Biller and Ghosh (2006). The central idea is to transform standard multivariate normal variables to variables with the desired marginal distributions and Pearson correlation matrix.

Suppose that the desired variables are  $X_j$ ,  $j = 1, \dots, k$ , with the desired Pearson correlation matrix  $\Sigma_X$ , where the elements of  $\Sigma_X$  are given by  $\rho_{ij}$ . Then the NORTA algorithm is as follows:

1. For each pair  $X_i$  and  $X_j$ , where  $i < j$ , use a stochastic root finding algorithm (described in the following section) and the correlation  $\rho_{ij}$  to search for an approximate correlation  $\rho_{ij}^*$  of standard bivariate normal variables.
2. Construct the symmetric matrix  $\Sigma_z$  whose elements are given by  $\rho_{ij}^*$ , where  $\rho_{ii}^* = 1$  and  $\rho_{ij}^* = \rho_{ji}^*$ .
3. Generate the standard multivariate normal variables  $Z_1, \dots, Z_k$  with Pearson correlation matrix  $\Sigma_z$ .
4. Transform the variables  $Z_1, \dots, Z_k$  to  $X_1, \dots, X_k$  using

$$X_i = F_i^{-1}(\Phi(Z_i)), i = 1, \dots, k$$

where  $F_i$  is the desired marginal cumulative distribution, and  $\Phi()$  is the cumulative standard normal distribution function. Then the correlation matrix of  $X_1, \dots, X_k$  will be close to the desired Pearson correlation matrix  $\Sigma_X$ .

### Stochastic root finding algorithm

Given a correlation  $\rho_{ij}$ , a stochastic root finding algorithm is used to find an approximate correlation  $\rho_{ij}^*$  such that if standard bivariate normal variables  $Z_i$  and  $Z_j$  have the Pearson correlation  $\rho_{ij}^*$ , then after transforming  $Z_i$  and  $Z_j$  to  $X_i$  and  $X_j$  (using the transformation described in Step 4 of the previous section) the Pearson correlation between  $X_i$  and  $X_j$  is close to  $\rho_{ij}$ . The stochastic root finding algorithm is as follows:

1. Let  $LowCorr = -1$  and  $HighCorr = 1$
2. Simulate N samples of standard normal variables  $Z_i^{(L)}$  and  $Z_j^{(L)}$ ,  $Z_i^{(H)}$  and  $Z_j^{(H)}$ , such that the Pearson correlation between  $Z_i^{(L)}$  and  $Z_j^{(L)}$  is  $LowCorr$  and the Pearson correlation between  $Z_i^{(H)}$  and  $Z_j^{(H)}$  is  $HighCorr$ . The sample size N is set to 1000.
3. Transform the variables  $Z_i^{(L)}$ ,  $Z_j^{(L)}$ ,  $Z_i^{(H)}$  and  $Z_j^{(H)}$  to the variables  $X_i^{(L)}$ ,  $X_j^{(L)}$ ,  $X_i^{(H)}$  and  $X_j^{(H)}$  using the transformation described in Step 4 of the previous section.

4. Compute the Pearson correlation between  $X_i^{(L)}$  and  $X_j^{(L)}$  and denote it as  $\rho_{ij}^L$ . Similarly, compute the Pearson correlation between  $X_i^{(H)}$  and  $X_j^{(H)}$  and denote it as  $\rho_{ij}^H$ .
5. If the desired correlation  $\rho_{ij} \leq \rho_{ij}^L$  or  $\rho_{ij} \geq \rho_{ij}^H$  then stop and set  $\rho_{ij}^* = LowCorr$  if  $\rho_{ij} \leq \rho_{ij}^L$  or set  $\rho_{ij}^* = HighCorr$  if  $\rho_{ij} \geq \rho_{ij}^H$ . Otherwise go to Step 6.
6. Simulate N samples of standard bivariate normal variables  $Z_i^{(M)}$  and  $Z_j^{(M)}$  with a Pearson correlation of  $MidCorr = \frac{1}{2}(LowCorr + HighCorr)$ . As in Steps 3 and 4, transform  $Z_i^{(M)}$  and  $Z_j^{(M)}$  to  $X_i^{(M)}$  and  $X_j^{(M)}$  and compute the Pearson correlation between  $X_i^{(M)}$  and  $X_j^{(M)}$ , which will be denoted  $\rho_{ij}^M$ .
7. If  $|\rho_{ij} - \rho_{ij}^M| \leq \epsilon$  or  $|HighCorr - LowCorr| \leq \epsilon$  where  $\epsilon$  is the tolerance level (set to 0.01), then stop and set  $\rho_{ij}^* = MidCorr$ . Otherwise go to Step 8.
8. If  $\rho_{ij} > \rho_{ij}^M$ , set  $LowCorr = MidCorr$ , else set  $HighCorr = MidCorr$  and return to Step 6.

### **Inverse CDF for binomial, Poisson and negative binomial distributions**

Use of the NORTA method for generating correlated data requires the inverse cumulative distribution function for each desired marginal distribution. This section describes the method for computing the inverse CDF for the binomial, Poisson and negative binomial distributions. Two parameterizations of the negative binomial distribution are supported. The first parameterization describes the distribution of the number of trials before the  $r^{\text{th}}$  success, whereas the second parameterization describes the distribution of the number of failures before the  $r^{\text{th}}$  success.

The choice of method for determining the CDF depends on the mean  $\mu$  of the distribution. If  $\mu \geq Threshold$ , where *Threshold* is set to 20, the following approximate normal method will be used to compute the inverse CDF for the binomial distribution, the Poisson distribution and the second parameterization of the negative binomial distribution.

$$X = [F^{-1}(\Phi(Z))] = [\sigma(\Phi^{-1}(\Phi(Z))) + \mu] = [\sigma Z + \mu]$$

For the first parameterization of the negative binomial distribution, the formula is as follows:

$$X = [\sigma Z + \mu] + r$$

The parameters  $\mu$  and  $\sigma$  are given by:

- **Binomial distribution.**  $\mu = NP$  and  $\sigma = \sqrt{NP(1-P)}$ , where N is the number of trials and P is the probability of success.
- **Poisson distribution.**  $\mu = \lambda$  and  $\sigma = \sqrt{\lambda}$ , where  $\lambda$  is the rate parameter.
- **Negative binomial distribution (both parameterizations).**  $\mu = r \frac{1-\theta}{\theta}$  and  $\sigma = \sqrt{r \frac{1-\theta}{\theta^2}}$ , where r is the specified number of successes and  $\theta$  is the probability of success.

The notation  $[x]$  used above denotes the integer part of  $x$ .

If  $\mu \leq Threshold$  then the bisection method will be used.

Suppose that  $x$  and  $z$  are the values of  $X$  and  $Z$  respectively, where  $X$  is a random variable with a binomial, Poisson or negative binomial distribution, and  $Z$  is a random variable with the standard normal distribution. The objective function  $f(x)$  to be used in the bisection search method is as follows:

- **Binomial distribution.**  $f(x) = 1 - \Pr(B(x+1, N-x) \leq P) - \Phi(z)$
- **Poisson distribution.**  $f(x) = 1 - \Pr(G(x+1, 1) \leq \lambda) - \Phi(z)$
- **Negative binomial distribution (second parameterization).**  $f(x) = \Pr(B(r, x+1) \leq \theta) - \Phi(z)$

where  $B(\alpha, \beta)$  and  $G(\alpha, \beta)$  are random variables with the beta distribution and gamma distribution, respectively, with parameters  $\alpha$  and  $\beta$ .

The bisection method is as follows:

1. If  $f(\mu) = 0$  then stop and set  $x = [\mu + 0.5]$ . Otherwise go to step 2 to determine two values  $x_1$  and  $x_2$  such that  $f(x_1) \times f(x_2) \leq 0$ .
2. If  $f(\mu) > 0$  then let  $x_1 = 0$  and  $x_2 = \mu$ . If  $f(\mu) < 0$  then let  $x_1 = 2^{J-1} \times \mu$  and  $x_2 = 2^J \times \mu$ , where  $J$  is the minimum integer such that  $f(x_1) \times f(x_2) \leq 0$ .
3. Let  $m = \frac{1}{2}(x_1 + x_2)$ . If  $|f(m)| < \epsilon$  or  $|x_1 - x_2| < 1$  where  $\epsilon$  is a tolerance level, which is set to  $10^{-6}$ , then stop and set  $x = [m + 0.5]$ . Otherwise go to Step 4.
4. If  $f(m) > 0$ , let  $x_2 = m$ , else let  $x_1 = m$  and return to Step 3.

*Note:* The inverse CDF for the first parameterization of the negative binomial distribution is determined by taking the inverse CDF for the second parameterization and adding the distribution parameter  $r$ , where  $r$  is the specified number of successes.

## Sensitivity measures

Sensitivity measures provide information on the relationship between the values of a target and the values of the simulated inputs that give rise to the target. The following sensitivity measures are supported (and rendered as Tornado charts in the output of the simulation):

- **Correlation.** Measures the Pearson correlation between a target and a simulated input.
- **One-at-a-time measure.** Measures the effect on the target of modulating a simulated input by plus or minus a specified number of standard deviations of the input.
- **Contribution to variance.** Measures the contribution to the variance of the target from a simulated input.

## Notation

The following notation is used throughout this section unless otherwise stated:

Table 33-9

### Notation

Notation	Description
$n$	Number of records of simulated data

$X$	An $n \times p$ matrix of values of the inputs to the predictive model. The rows $x_i = (x_{i1}, \dots, x_{ip})$ ; $i = 1, \dots, n$ contain the values of the inputs for each simulated record, excluding the target value. The columns $x_j^T = (x_{1j}, \dots, x_{nj})$ ; $j = 1, \dots, p$ represent the set of inputs.
$y$	An $n \times 1$ vector of values of the target variable, consisting of $y_i$ , $i = 1, \dots, n$
$F(X)$	A known model which can generate $y$ from $X$
$sa_j$	The value of a sensitivity measure for the input $x_j$

### Correlation measure

The correlation measure is the Pearson correlation coefficient between the values of a target and one of its simulated predictors. The correlation measure is not supported for targets with a nominal measurement level or for simulated inputs with a categorical distribution.

### One-at-a-time measure

The one-at-a-time measure is the change in the target due to modulating a simulated input by plus or minus a specified number of standard deviations of the distribution associated with the input. The one-at-a-time measure is not supported for targets with an ordinal or nominal measurement level, or for simulated inputs with any of the following distributions: categorical, Bernoulli, binomial, Poisson, or negative binomial.

The procedure is to modulate the values of a simulated input by the specified number of standard deviations and recompute the target with the modulated values, without changing the values of the other inputs. The mean change in the target is then taken to be the value of the one-at-a-time sensitivity measure for that input.

For each simulated input  $x_j$  for which the one-at-a-time measure is supported:

1. Define the temporary data matrix  $X' = X$
2. Add the specified number of standard deviations of the input's distribution to each value of  $x_j$  in  $X'$ .
3. Calculate  $y' = F(X')$
4. Calculate  $sa_j = \frac{1}{n} \sum_{i=1}^n (y'_i - y_i)$
5. Repeat Step 2, but now subtracting the specified number of standard deviations from each value of  $x_j$ . Continue with Steps 3 and 4 to obtain the value of  $sa_j$  in this case.

### Contribution to variance measure

The contribution to variance measure uses the method of Sobol (2001) to calculate the total contribution to the variance of a target due to a simulated input. The total contribution to variance, as defined by Sobol, automatically includes interaction effects between the input of interest and the other inputs in the predictive model.

The contribution to variance measure is not supported for targets with an ordinal or nominal measurement level, or for simulated inputs with any of the following distributions: categorical, Bernoulli, binomial, Poisson, or negative binomial.

Let  $X'$  be an additional set of simulated data, in the same form as  $X$  and with the same number of simulated records.

Define the following:

$$f_0 = \frac{1}{n} \sum_{i=1}^n y_i$$

$$D = \frac{1}{n} \sum_{i=1}^n y_i^2 - (f_0)^2$$

For each simulated input  $x_j$  for which the contribution to variance measure is supported, calculate

$$D_{x \setminus x_j} = \frac{1}{n} \sum_{i=1}^n y_i [F(X'_{x_j} + X_{x \setminus x_j})]_i - (f_0)^2$$

where:

- $x \setminus x_j$  denotes the set of all inputs excluding  $x_j$
- $X'_{x_j} + X_{x \setminus x_j}$  is a derived data matrix where the column associated with  $x_j$  is taken from  $X'$  and the remaining columns (for all inputs excluding  $x_j$ ) are taken from  $X$

The total contribution to variance from  $x_j$  is then given by

$$sa_j = \frac{D - D_{x \setminus x_j}}{D}$$

*Note:* When interaction terms are present, the sum of the  $sa_j$  over all simulated inputs for which the contribution of variance is supported, may be greater than 1.

## References

Billar, B., and S. Ghosh. 2006. Multivariate input processes. In: *Handbooks in Operations Research and Management Science: Simulation*, B. L. Nelson, and S. G. Henderson, eds. Amsterdam: Elsevier Science, 123–153.

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# Support Vector Machine (SVM) Algorithms

## Introduction to Support Vector Machine Algorithms

The Support Vector Machine (SVM) is a supervised learning method that generates input-output mapping functions from a set of labeled training data. The mapping function can be either a classification function or a regression function. For classification, nonlinear kernel functions are often used to transform input data to a high-dimensional feature space in which the input data become more separable compared to the original input space. Maximum-margin hyperplanes are then created. The produced model depends on only a subset of the training data near the class boundaries.

Similarly, the model produced by Support Vector Regression ignores any training data that is sufficiently close to the model prediction. (Support Vectors can appear only on the error tube boundary or outside the tube.)

## SVM Algorithm Notation

$x_i$	The $i$ th training sample
$y_i$	The class label for the $i$ th training sample
$l$	The number of training samples
$K(x_i \cdot x_j)$	The kernel function value for the pair of samples $i, j$
$Q(x_i \cdot x_j) = y_i y_j K(x_i \cdot x_j)$	The kernel matrix element at row $i$ and column $j$
$\alpha_i$	Coefficients for training samples (zero for non-support vectors)
$\alpha_i^*$	Coefficients for training samples for support vector regression models
$f(x)$	Decision function
$m$	The number of classes of the training samples
$C$	The upper bound of all variables
$e$	The vector with all elements equal to 1
$sgn(x)$	The sign function: $\begin{cases} 1 & \text{if } x \geq 0 \\ -1 & \text{otherwise} \end{cases}$

## SVM Types

This section describes the types of SVM available, based on the descriptions in the LIBSVM technical report (Chang and Lin, 2003).  $K(x_i \cdot x_j)$  is the kernel function selected by the user. For more information, see the topic “SMO Algorithm” on p. 371.

# Spatial Temporal Prediction Algorithms

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## 1. Introduction

Spatio-temporal statistical analysis has many applications. For example, energy management for buildings or facilities, performance analysis and forecasting for service branches, or public transport planning. In these applications, measurements such as energy usage are often taken over space and time. The key questions here are what factors will affect future observations, what can we do to effect a desired change, or to better manage the system. In order to address these questions, we need to develop statistical techniques which can forecast future values at different locations, and can explicitly model adjustable factors to perform what-if analyses.

However, these analytical needs are not the focus of traditional spatio-temporal statistical research. In traditional statistical research, spatio-temporal analysis is treated just as an extension of spatial analysis and focuses more on looking for patterns in past data rather than forecasting future values. The traditional spatio-temporal research targets different application areas such as environmental research. There are, however, different types of spatio-temporal problems in which time is the key component. We therefore need to treat spatio-temporal analysis as a unique type of problem itself, not an extension to spatial analysis. Moreover, we need to explicitly model these factors to allow for what-if analysis. Although these kinds of problems could be addressed by traditional methods, the emphasis is quite different.

This algorithm assumes a fixed set of spatial locations (either point location or center of an area) and equally spaced time stamps common across locations. It can issue predicted or interpolated values at locations with no response measurements (but with available covariates). We call our model spatio-temporal prediction (STP).

The goal of the STP algorithm is to address the needs for solving the spatio-temporal problems. STP can generate predictions at any location within a 3D space for any future time. It also explicitly models the external factors so we can perform what-if analysis.

### 1.1 Handling of missing data

The algorithm is designed to accommodate missing values in the response variable, as well as in the predictors. We consider an observation at a given time point and location ‘complete’ if all predictors and the response are observed at that time and location. To allow for model fitting in spite of missing data, all of the following conditions must be met:

1. At each location, observations need to be complete for at least one sequence of at least  $L + 2$  consecutive time points.
2. At each location  $s_i$ , for any pair of locations  $s_i, s_j, s_j \neq s_i$ , observations must be complete at *both* locations simultaneously for at least two sequences of  $L + 2$  consecutive time points.

3. Overall, at least  $L$  sequences of at least  $L + 2$  consecutive time points must be present in the data (to allow for estimation of  $\alpha$ ).
4. The total number of complete samples must be at least equal to  $D + L + 2$ , where  $D$  is the number of predictors, including the intercept, and  $L$  the user-specified lag.
5. After removing locations according to the rules above, no more than 5% of the remaining records should be incomplete. As an example, if after removing locations,  $n$  locations and  $m$  time stamps remain, no more than  $n \times m \times .05$  records should be incomplete.

The above conditions should be verified in the following order:

Step 1. Remove locations that do not meet condition 1.

Step 2. Remove locations that violate condition 2 in the following order:

- (a) Let  $\mathcal{J}$  be the set of points that violate condition 2.
- (b) Eliminate from the data set the observation(s) that violate condition 2 for the greatest number of pairs. In case of a tie, remove all observations that are tied.
- (c) Update  $\mathcal{J}$  by removing any observations that now no longer violate Condition 2. That is, remove observation that only violated the condition 2 in a pair with the observations that were removed in Step 2b.
- (d) Iterate steps 2b and 2c until  $\mathcal{J}$  is empty.

Step 3. If after Steps 1 and 2, conditions 3-5 are violated, the model cannot be fit.

## 2 Model

### 2.1 Notation

The following notation is used for the model inputs:

Name	Symbol	Type	Dimensions
Number of time stamps	$m > L$	integer	1
Number of measurement locations	$n \geq 3$	integer	1
Number of prediction grid points	$N$	integer	1
Number of predictors (including intercept)	$D$	integer	1
Index of time stamps	$t \in \{1, \dots, m\}$	integer	1
Spatial coordinates	$s \in \{s_1, \dots, s_n\}; s_j = (u_j, v_j, w_j)'$	vector	$3 \times 1$
Targets observed at location $s$ and time $t$	$Y_t(s)$	scalar	1
Targets observed at location $s$	$Y(s)$	vector	$m \times 1$
Targets observed at time $t$	$Y_t$	vector	$n \times 1$
Predictors observed at location $s$ and time $t$	$X_t(s) = (X_{t,1}(s), \dots, X_{t,D}(s))'$	vector	$D \times 1$
Predictors observed at location $s$	$X(s) = (X_1(s), \dots, X_m(s))'$	matrix	$m \times D$
Predictors observed at time $t$	$X_t = (X_t(s_1), \dots, X_t(s_n))'$	matrix	$n \times D$
Maximum autoregressive time lag	$L > 0$	integer	1
Length of prediction steps	$H > 0$	integer	1

#### Notes

- i. For a predictor that does not vary over space,  $X_{t,d}(s_1) = X_{t,d}(s_2) = \dots = X_{t,d}(s_n)$ ;

ii. For a predictor that does not evolve over time,  $X_{1,d}(s) = X_{2,d}(s) = \dots = X_{m,d}(s)$ .

The following notation is used for model definition and computation:

Name	Symbol	Type	Dimension
Coefficient vector for linear model	$\boldsymbol{\beta} = (\beta_1, \dots, \beta_D)$	vector	$D$
Coefficient vector for AR model	$\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_L)$	vector	$L$
Vector of 1's	$\mathbf{1} = (1, \dots, 1)'$	vector	variable
Kronecker product	$\otimes$	operator	NA

## 2.1 Model structure

$$Y_t(s) = \sum_{d=1}^D \beta_d X_{t,d}(s) + Z_t(s) \quad (1)$$

where  $Z_t(s)$  is mean-zero space-time correlated random process. Users can specify whether an “intercept” term needs to be included in the model. The inference algorithm works with general “continuous” variables, and with or without intercept.

- Autoregressive model, AR( $L$ ) for time autocorrelation (Brockwell and Davis, 2002):

$$Z_t(s) = \sum_{l=1}^L \alpha_l Z_{t-l}(s) + \epsilon_t(s) \quad (2)$$

Note that users need to specify the maximum AR lag  $L$ .

Let  $\epsilon_t = (\epsilon_t(s_1), \dots, \epsilon_t(s_n))'$  be the AR residual vector at time  $t$ . Since the time autocorrelation effect has already been removed,  $\epsilon_{L+1}, \dots, \epsilon_m$  are independent.

- Parametric or nonparametric covariance model for spatial dependence:

$$V(\epsilon_t) = \Sigma_S, t = L + 1, \dots, m \quad (3)$$

where  $\Sigma_S = \{R(s_i, s_j)\}_{i,j=1,\dots,n}$  is a  $n \times n$  covariance matrix of spatial covariance functions  $R(s, s') = Cov(Y_t(s), Y_t(s'))$  at observed locations. Two alternative ways of modeling the spatial covariance function  $R(s_i, s_j)$  are implemented - a *variogram-based parametric* model (Cressie, 1993) and a *Empirical Orthogonal Functions (EOF)-based nonparametric* model (Cohen and Johnes, 1969; Creutin and Obled, 1982).

Note that users can specify which covariance model to be used.

- If a “parametric model” is chosen, the algorithm will automatically test for the goodness-of-fit. If the test suggests a parametric model is not adequate, the algorithm switch to EOF model fitting and issue prediction based on EOF model.
- If a EOF model is chosen, the switching test part will be skipped, and both model fitting and prediction will follow EOF-based algorithm.

Under this model decomposition, the covariance structure for the spatio-temporal process  $Y = (Y'_{L+1}, \dots, Y'_m)'$  is of separable form

$$V(Y) = V(Z) = \Sigma = \Sigma_T \otimes \Sigma_S \quad (4)$$

where  $\Sigma_T = \{\gamma_T(t - t')\}_{t=L+1,\dots,m;t'=L+1,\dots,m}$  is the  $(m - L) \times (m - L)$  AR( $L$ ) covariance

matrix with the autocovariance function.

### 3 Estimation algorithm

This section provides details on the multi-step procedure to fit the STP model (see Figure 1) when the user specifies a “parametric model”. If an “empirical model” is specified, the switching test part will be skipped, and both model fitting and prediction follows EOF-based algorithm.

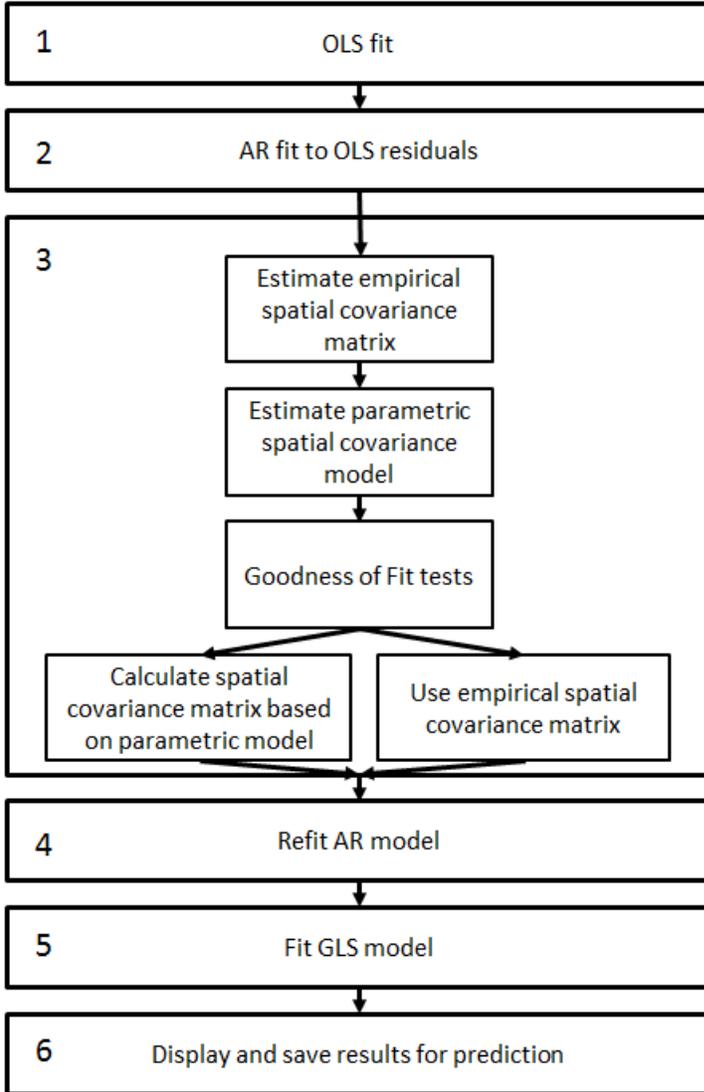


Figure 1. Flowchart of algorithm steps for model fitting when a “parametric model” is specified.

Step 1: Fit regression model by ordinary least squares (OLS) regression using only observations that have no missing values (see Section 3.1).

We first ignore the spatio-temporal dependence in the data and simply estimate the fixed regression part by OLS and obtain the regression residuals  $Z_t(s)$ .

Step 2: Fit autoregressive model using only data without missing values (see Section 3.2).

Ignoring spatial dependence in OLS residuals  $Z_t(s)$ , we estimate autoregressive

coefficients by fitting the regression model (2) and obtain the AR residuals  $\epsilon_t(s)$ .

Step 3: Fit spatial covariance model and test for goodness of fit on data without missing values (see Section 3.3).

We fit a parametric spatial covariance model. We perform two Goodness of Fit tests to decide whether to continue with the parametric covariance model or the empirical covariance matrix.

Step 4: Refit autoregressive model using augmented data (see Section 3.4).

We refit autoregressive model accounting for spatial dependence by generalized least squares (GLS) and obtain improved AR coefficients  $\alpha$ .

Step 5: Refit Regression model using augmented data (see Section 3.5).

We obtain improved regression coefficients  $\beta$  by GLS to account for spatio-temporal correlation in the data.

Step 6: Save the results for use in output and prediction.

### 3.1 Fit regression model

We first ignore the spatio-temporal dependence in the data and simply estimate the fixed regression part by OLS. Assume that out of  $nm$  location-time combinations,  $q$  samples have missing values in either  $X$  or  $Y$ . Let  $Y = (Y'_1, \dots, Y'_m)'$ , a  $(nm - q) \times 1$ -vector and  $X = (X'_1, \dots, X'_m)'$ , a  $(nm - q) \times D$  matrix, such that  $X$  and  $Y$  contain only complete observations, i.e., observations without any missing values. The OLS estimates of the regression coefficients are:

$$\hat{\beta} = (X'X)^{-1}X'Y \quad (5)$$

The residuals are:

$$\hat{Z} = Y - X\hat{\beta}. \quad (6)$$

### 3.2 Fit autoregressive model

We estimate autoregressive coefficients by OLS assuming no spatial correlation and AR(L) as model for time-series autocorrelation,

$$\hat{Z}_t = \alpha_1 \hat{Z}_{t-1} + \dots + \alpha_L \hat{Z}_{t-L} + \epsilon_t, \quad (7)$$

where  $\hat{Z}_t$  is a  $n_t \times 1$  vector. Note that due to the existence of missing values, the number of locations  $n_t$  varies among different time points. Moreover, for each time points  $t$ , only locations with no missing values at  $L + 1$  consecutive time points, i.e.,  $(t, t - 1, \dots, t - L)$  can be used for model fitting, therefore,  $\sum_{t=L+1}^m n_t \leq [n(m - L) - q]$ .

Step 1: Construct  $n_t \times L$  time lag matrix

$$\hat{Z}_{t-lag} = (\hat{Z}_{t-1}, \hat{Z}_{t-2}, \dots, \hat{Z}_{t-L}), t = L + 1, \dots, m \quad (8)$$

Step 2: Let  $\hat{Z}_{lag} = (\hat{Z}'_{L+1-lag}, \dots, \hat{Z}'_{m-lag})'$  and  $\hat{Z}^* = (\hat{Z}'_{L+1}, \dots, \hat{Z}'_m)'$ . Solve the linear system

$$(\hat{Z}'_{lag} \hat{Z}_{lag}) \alpha = \hat{Z}'_{lag} \hat{Z}^* \quad (9)$$

which is equivalent to solving

$$\left( \sum_{t=L+1}^m \hat{Z}'_{t-lag} \hat{Z}_{t-lag} \right) \boldsymbol{\alpha} = \sum_{t=L+1}^m \hat{Z}'_{t-lag} \hat{Z}_t \quad (10)$$

using the sweep operation to find estimate  $\hat{\boldsymbol{\alpha}}$ .

Step 3: Compute the de-autocorrelated AR(L) residuals

$$\hat{\epsilon}_t = \hat{Z}_t - \hat{\alpha}_1 \hat{Z}_{t-1} - \dots - \hat{\alpha}_L \hat{Z}_{t-L}, t = L + 1, \dots, m \quad (11)$$

### 3.3 Fit model and check goodness of fit for spatial covariance structure

We explicitly model the spatial covariance structure among locations, rather than using variogram estimation.

Under the assumption of the model (stationarity, AR-relationship removed), the mean of the residuals is 0 at all locations. We therefore estimate the unadjusted empirical covariances  $s_{ij}$  and correlations  $r_{ij}$  assuming mean 0, i.e.,

$$\mathbf{S} = [s_{ij}]_{i,j=1,\dots,n}, s_{ij} = \frac{1}{t_{ij}} \sum_t \hat{\epsilon}_t(s_i) \hat{\epsilon}_t(s_j) \quad (12)$$

where  $t_{ij}$  is the number of complete residual pairs between locations  $s_i$  and  $s_j$ , and  $t$  indexes these pairs, i.e., the time points for which both  $\hat{\epsilon}_t(s_i)$  and  $\hat{\epsilon}_t(s_j)$  are non-missing.

$$r_{ij} = \frac{s_{ij}}{\sqrt{s_{ii}s_{jj}}} \quad (13)$$

To determine whether to model the spatial covariance structure parametrically or to use the nonparametric EOF model, we perform the following two tests sequentially:

1. Fit parametric model to covariances using the parameter vector  $\boldsymbol{\psi} = (\sigma^2, \theta, \tau^2)$  (Cressie 1993)

$$\text{Cov}(\epsilon_t(s_i), \epsilon_t(s_j); \hat{\boldsymbol{\psi}}) = \begin{cases} \hat{\sigma}^2 \exp(-(h_{ij}/\hat{\theta})^p), & \text{if } h_{ij} > 0; \\ \hat{\sigma}^2 + \hat{\tau}^2, & \text{otherwise.} \end{cases} \quad (14)$$

where  $h_{ij} = \|s_i - s_j\|_2$  is the Euclidean distance between locations  $s_i$  and  $s_j$ . Users need to specify the values for the order parameter  $p$ .

$p \in [1, 2]$  is a user-defined parameter that determines the class of covariance models to be fit.  $p = 1$  corresponds to an exponential covariance model,  $p = 2$  results in a Gaussian covariance model and  $p \in (1, 2)$  belongs to the powered exponential family.

Next, determine if there is a significant decay over space by testing  $H_0: -1/\theta^p \geq 0$ . If we fail to reject  $H_0$ , we conclude that the decay over space is not significant, and EOF estimation will be used. If EOF estimation is used, there is not need to calculate  $\theta$ ,  $\sigma$  or  $\tau$ , as we have concluded that they are invalid descriptions of the covariance matrix. In fact, there may not be valid solutions for these parameters, therefore they should not be

estimated.

2. If the previous test rejects  $H_0$ , test for homogeneity of variances among locations: if homogeneity of variances is rejected, EOF estimation will be used. Otherwise, the parametric covariance model will be used.

### 3.3.1 Fit and test parametric model

- a) Enforce a minimum correlation of +.01: if  $r_{ij} < .01$ , set  $s_{ij} = .01\sqrt{s_{ii}s_{jj}}$  and  $r_{ij} = .01$ .
- b) Let  $\mathbf{s}$  be the vectorized lower triangular of the covariance matrix (excluding the diagonal, i.e., excluding variances),  $\mathbf{r}$  be the vectorized lower triangular of the correlation matrix (excl. diagonal), and  $\mathbf{h}$  the corresponding vector of pairwise distances between the  $n$  locations.  $\mathbf{s}$ ,  $\mathbf{r}$  and  $\mathbf{h}$  are each vectors of length  $n(n-1)/2$ .

Define  $\varphi = -1/\theta^p$ . Fit the linear model  $\ln \mathbf{s} = \ln \sigma^2 + \varphi \mathbf{h}^p$  using a GLS fit:

$$\mathbf{A} = [1, \mathbf{h}^p] \quad (15)$$

$$\mathbf{V}^{-1} = \frac{1}{2} \mathbf{T}(\mathbf{B}^{-1} - c\mathbf{b}\mathbf{b}')\mathbf{T} \quad (16)$$

where  $\mathbf{b} = 2\mathbf{r}^2/(1 - \mathbf{r}^2)$ ,  $\mathbf{r}^2$  is obtained by squaring each element of vector  $\mathbf{r}$ ,  $\mathbf{B}^{-1} = \text{diag}(\mathbf{b})$ , and scalar  $c = 1/(1 + \mathbf{1}'\mathbf{B}^{-1}\mathbf{1})$ . Also, let  $\mathbf{T} = \text{diag}[\sqrt{t_k}]$ ,  $k = 1, \dots, n(n-1)/2$ , where  $t_k$  is the number of pairs of de-autocorrelated residuals in the calculation of the corresponding element  $r_k$  in  $\mathbf{r}$ , i.e., the number of observations pairs that went into calculating  $r_k$ , which may be different for each entry of the covariance matrix, depending on missing values. Note that  $t_k$  corresponds to the vectorized lower triangular of  $[t_{ij}]_{i,j=1,\dots,n}$ , where  $t_{ij}$  are as defined in (12).

Let  $\boldsymbol{\eta} = (\ln \sigma^2, \varphi)$ , the GLS estimator can be calculated as

$$\hat{\boldsymbol{\eta}} = (\mathbf{A}'\mathbf{V}^{-1}\mathbf{A})^{-1} \mathbf{A}'\mathbf{V}^{-1} \ln \mathbf{s}$$

The standard error for  $\hat{\boldsymbol{\eta}}$  will be  $se(\hat{\boldsymbol{\eta}}) = \sqrt{\text{diag}[(\mathbf{A}'\mathbf{V}^{-1}\mathbf{A})^{-1}]}$ .

Calculate the test statistic  $z_1 = \frac{\hat{\varphi}}{se(\hat{\varphi})}$ . If  $z_1 \geq z_{.05}$ , where  $z_{.05}$  is the .05 quantile of the standard normal distribution (or critical value for selected level of significance  $\gamma_1$ ), then all following calculations will be performed using the empirical spatial covariance matrix, i.e.,  $\Sigma_S = \mathbf{S}$ , and the nonparametric EOF model will be used for prediction. Equivalently, a p-value  $p_1$  can be calculated by evaluating the standard Normal cumulative distribution function (CDF) at  $z_1$  (i.e.,  $p_1 = P(Z < z_1)$ ). If  $p_1 \geq \text{level of significance } \gamma_1$ , then all following calculations will be performed using the empirical covariance matrix.

- c) If the previous test does reject  $H_0$  (i.e., we have not yet decided to continue with the empirical covariance matrix), continue to perform the following test: Let  $\mathbf{v} = (s_{11}, s_{22}, \dots, s_{nn})'$  be the  $(n \times 1)$ -vector of location-specific variances. Calculate the weighted mean variance  $\bar{v}$

$$\bar{v} = \mathbf{1}'\mathbf{W}^{-1}\mathbf{v}/(\mathbf{1}'\mathbf{W}^{-1}\mathbf{1}) = \mathbf{1}'\mathbf{W}^{-1}\mathbf{v} / \sum_{i,j} w_{ij}^* \quad (17)$$

where  $\mathbf{W} = [w_{ij}] = [s_{ij}^2/t_{ij}]_{i,j=1,\dots,n}$  is an  $n \times n$  matrix, where  $t_{ij}$  is defined as in (12), and  $\mathbf{W}^{-1} = [w_{ij}^*]_{i,j=1,\dots,n}$ .

Calculate the test statistic  $z_2 = (\mathbf{v} - \bar{\mathbf{v}})' \mathbf{W}^{-1} (\mathbf{v} - \bar{\mathbf{v}})$ . If  $z_2 \geq \chi_{n-1,95}^2$  (or critical value for  $[1 - \text{selected level of significance } \gamma_2]$ ), all following calculations will be performed using the empirical spatial covariance matrix, i.e.,  $\Sigma_S = \mathbf{S}$ , and the nonparametric EOF model will be used for prediction. Equivalently, one may compute a p-value  $p_2$  by evaluating 1 minus the  $\chi_{n-1}^2$  - CDF:  $p_2 = P(\chi_{n-1}^2 > z_2)$ . If  $p_2 < \text{level of significance } \gamma_2$ , then all following calculations will be performed using the empirical spatial covariance matrix.

- d) If the two tests in b) and c) do not indicate a switch to the EOF model, all following calculations will be performed using the parametric covariance model, i.e., the spatial covariance matrix  $\Sigma_S$  is constructed according to (14). Recall that  $\eta = (\ln \sigma^2, -1/\theta^p)$ . The missing parameter  $\tau^2$  is derived as  $\widehat{\tau^2} = \max \left\{ 0, \frac{1}{n} \sum_{i=1,\dots,n} s_{ii} - \exp[\widehat{\ln \sigma^2}] \right\}$ .

### 3.4 Re-fit autoregressive model

We refit the autoregressive model accounting for spatial dependence using GLS with augmented data:

Step 1: Compute the Cholesky factorization  $\Sigma_S = \mathbf{H}_S \mathbf{H}_S'$  and the inverse matrix  $\mathbf{H}_S'$ .

Step 2: Substitute 0 for missing values such that  $\widehat{\mathbf{Z}}_{t-lag,impute}$  is an  $n \times L$  matrix and  $\widehat{\mathbf{Z}}_{t,impute}$  is a vector of length  $n$ .

Step 3: Augment predictor matrix as follows. Let

$$\widehat{\mathbf{Z}}_{lag,impute} = \left( \widehat{\mathbf{Z}}'_{L+1-lag,impute}, \dots, \widehat{\mathbf{Z}}'_{m-lag,impute} \right)' \text{ be a } n(m-L) \times L \text{ matrix and}$$

$$\widehat{\mathbf{Z}}_{impute} = \left( \widehat{\mathbf{Z}}'_{L+1,impute}, \dots, \widehat{\mathbf{Z}}'_{m,impute} \right)' \text{ is a vector of length } n(m-L), \text{ then}$$

$$\widehat{\mathbf{Z}}_{lag,aug} = \left( \widehat{\mathbf{Z}}_{lag,impute}, \dots, \mathbf{I}_{Zmiss} \right)$$

where  $\mathbf{I}_{Zmiss}$  is a  $n(m-L) \times q_Z$  indicator matrix given  $q_Z$  the total number of rows with missing values in either  $\widehat{\mathbf{Z}}^*$  or  $\widehat{\mathbf{Z}}_{lag}$ . If there is a missing value in the  $i$ th row of either  $\widehat{\mathbf{Z}}^*$  or  $\widehat{\mathbf{Z}}_{lag}$ , and if this is the  $j$ th out of all  $q_Z$  rows that have missing values, then the  $j$ th column of  $\mathbf{I}_{Zmiss}$  is all 0 except for the  $i$ th element, which is set to 1.

Step 4: Remove the spatial correlation:  $\widetilde{\mathbf{Z}}_{t-lag,aug} = \mathbf{H}_S^{-1} \widehat{\mathbf{Z}}_{t-lag,aug}$  and  $\widetilde{\mathbf{Z}}_{t,impute} = \mathbf{H}_S^{-1} \widehat{\mathbf{Z}}_{t,impute}$ , where  $\widehat{\mathbf{Z}}_{t-lag,aug}$  are the submatrices of  $\widehat{\mathbf{Z}}_{lag,aug}$  that correspond to the rows of the matrices  $\widehat{\mathbf{Z}}_{t-lag,impute}$ .

Step 5: Use the same computational steps as for the linear system in equation (10) to solve the linear system

$$\left( \sum_{t=L+1}^m \widetilde{\mathbf{Z}}'_{t-lag,aug} \widetilde{\mathbf{Z}}_{t-lag,aug} \right) \boldsymbol{\alpha}_{aug} = \sum_{t=L+1}^m \widetilde{\mathbf{Z}}'_{t-lag,aug} \widetilde{\mathbf{Z}}_{t,impute} \quad (18)$$

where  $\boldsymbol{\alpha}_{aug}$  is a vector of length  $L + q_Z$ , and there are  $L^* + q_Z^*$  non-redundant

parameters in above linear system. The AR coefficient estimate  $\hat{\alpha}$  is the subvector consisting of the first  $L$  elements of  $\hat{\alpha}_{aug}$ , there are  $L^*$  non-redundant parameters in first  $D$  elements of  $\hat{\alpha}_{aug}$ , and  $q_Z^*$  non-redundant parameters in last  $q_Z$  elements of  $\hat{\alpha}_{aug}$ .

### 3.5 Re-fit Regression model

Refit regression model by GLS using augmented data to account for spatio-temporal correlation in the data.

Step 1: Substitute the following for missing values such that  $\mathbf{X}_{impute}$  is a  $nm \times D$  matrix and  $\mathbf{Y}_{impute}$  is a vector of length  $nm$ : at location  $s_i$ , use the mean of  $\mathbf{Y}(s_i)$  and the mean of each predictor in  $\mathbf{X}(s_i)$ .

Step 2: Augment predictor matrix as follows.

$$\mathbf{X}_{aug} = (\mathbf{X}_{impute}, \mathbf{I}_{Xmiss})$$

where  $\mathbf{I}_{Xmiss}$  is a  $nm \times q$  indicator matrix given  $q$  the total number of rows with missing values in either  $\mathbf{X}$  or  $\mathbf{Y}$ . If there is a missing value in  $i$ th row of either  $\mathbf{X}$  or  $\mathbf{Y}$ , and if this is the  $j$ th out of all  $q$  rows that have missing value, then the  $j$ th column of  $\mathbf{I}_{Xmiss}$  is all 0 except for the  $i$ th element, which is 1.

Step 3: Remove the spatial correlation:  $\tilde{\mathbf{X}}_{t,aug} = \mathbf{H}_S^{-1}\mathbf{X}_{t,aug}$  and  $\tilde{\mathbf{Y}}_{t,impute} = \mathbf{H}_S^{-1}\mathbf{Y}_{t,impute}$ .

Step 4: Remove the autocorrelation:

$$\tilde{\mathbf{X}}_{t,aug} = \tilde{\mathbf{X}}_{t,aug} - \hat{\alpha}_1\tilde{\mathbf{X}}_{t-1,aug} - \dots - \hat{\alpha}_L\tilde{\mathbf{X}}_{t-L,aug}, t = L + 1, \dots, m \quad (19)$$

$$\tilde{\mathbf{Y}}_{t,impute} = \tilde{\mathbf{Y}}_{t,impute} - \hat{\alpha}_1\tilde{\mathbf{Y}}_{t-1,impute} - \dots - \hat{\alpha}_L\tilde{\mathbf{Y}}_{t-L,impute}, t = L + 1, \dots, m \quad (20)$$

Step 5: Solve the linear system

$$(\tilde{\mathbf{X}}'_{aug}\tilde{\mathbf{X}}_{aug})\boldsymbol{\beta}_{aug} = \tilde{\mathbf{X}}'_{aug}\tilde{\mathbf{Y}}_{impute} \quad (21)$$

where  $\tilde{\mathbf{Y}}_{impute} = (\tilde{\mathbf{Y}}'_{L+1,impute}, \dots, \tilde{\mathbf{Y}}'_{m,impute})'$ , an  $n(m-L) \times 1$ -vector and  $\tilde{\mathbf{X}}_{aug} = (\tilde{\mathbf{X}}'_{L+1,aug}, \dots, \tilde{\mathbf{X}}'_{m,aug})'$ , a  $n(m-L) \times (D+q)$  matrix,  $\boldsymbol{\beta}_{aug}$  is a vector of length  $D+q$ , and there are  $D^* + q^*$  non-redundant parameters in above linear system. The regression coefficients estimate  $\hat{\boldsymbol{\beta}}$  is the subvector consisting of first  $D$  elements of  $\hat{\boldsymbol{\beta}}_{aug}$ , there are  $D^*$  non-redundant parameters in first  $D$  elements of  $\hat{\boldsymbol{\beta}}_{aug}$ , and  $q^*$  non-redundant parameters in last  $q$  elements of  $\hat{\boldsymbol{\beta}}_{aug}$ .

### 3.6 Statistics to display

#### 3.6.1 Goodness of Fit statistics

We present statistics referring to the three main elements of the model: the mean structure, the spatial covariance structure, and the temporal structure.

##### 1. Goodness of fit mean structure model $\mathbf{X}\boldsymbol{\beta}$ :

Let  $\mathcal{Q}$  be the set of observations  $(Y_t(s), \mathbf{X}_t(s))$  that have missing values in either  $Y_t(s)$  or  $\mathbf{X}_t(s)$ . Note that  $q$  has been defined as the number of observations in  $\mathcal{Q}$ .

Calculate the mean squared error (MSE) and an  $R^2$  statistic based only on complete observations:

$$\text{MSE} = \sum_{\substack{s \in \{s_1, \dots, s_n\}; \\ t=1, \dots, m; \\ Y_t(s) \notin \mathcal{Q}}} (Y_t(s) - \hat{Y}_t(s))^2 / (nm - q - D^*) \quad (22)$$

$$R^2 = \begin{cases} 1 - \frac{\sum_{\substack{s \in \{s_1, \dots, s_n\}; \\ t=1, \dots, m; \\ Y_t(s) \notin \mathcal{Q}}} (Y_t(s) - \hat{Y}_t(s))^2}{\sum_{\substack{s \in \{s_1, \dots, s_n\}; \\ t=1, \dots, m; \\ Y_t(s) \notin \mathcal{Q}}} Y_t(s)^2}, & \text{if there is no intercept} \\ 1 - \frac{\sum_{\substack{s \in \{s_1, \dots, s_n\}; \\ t=1, \dots, m; \\ Y_t(s) \notin \mathcal{Q}}} (Y_t(s) - \hat{Y}_t(s))^2}{\sum_{\substack{s \in \{s_1, \dots, s_n\}; \\ t=1, \dots, m; \\ Y_t(s) \notin \mathcal{Q}}} (Y_t(s) - \bar{Y}_t(s))^2}, & \text{if there is an intercept} \end{cases} \quad (23)$$

where  $\hat{Y}_t(s) = \mathbf{X}'_t(s)\boldsymbol{\beta}$ ,  $D^*$  is the number of non-redundant parameters of re-fitted regression in first  $D$  elements of  $\hat{\boldsymbol{\beta}}_{aug}$ , and  $\bar{Y}_t(s)$  is the mean of  $Y$  only on complete observations. Note that for this calculation the original (untransformed) observations  $\mathbf{Y}$  and covariates  $\mathbf{X}$  are used. Alternatively, we can calculate the adjusted  $R^2$

$$R^2_{adj} = 1 - \frac{nm - q}{nm - q - D^*} (1 - R^2) \quad (24)$$

## 2. Goodness of fit for AR model:

Present  $t$ -tests for AR parameters based on variance estimates in item 3 in Section 3.6.2.

## 3. Goodness of fit of spatial covariance model:

Present the test statistics listed in item 5 in Section 3.6.2.

### 3.6.2 Model and parameter estimates

The following information should be displayed as a summary of the model:

1. Model coefficients  $\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\alpha}}$  obtained in Sections 3.4 and 3.5
2. Standard errors of elements of  $\boldsymbol{\beta}$  based on  $V(\hat{\boldsymbol{\beta}})$ , the covariance matrix of  $\hat{\boldsymbol{\beta}}$ , which is the upper  $D \times D$  submatrix of  $V(\hat{\boldsymbol{\beta}}_{aug})$ :

$$V(\hat{\boldsymbol{\beta}}_{aug}) = \frac{SS_e}{df_e} \times (\tilde{\mathbf{X}}'_{aug} \tilde{\mathbf{X}}_{aug})^{-1} = \frac{SS_e}{df_e} \times \left( \sum_{t=L+1}^m \tilde{\mathbf{X}}'_{t,aug} \tilde{\mathbf{X}}_{t,aug} \right)^{-1} \quad (25)$$

where

- $SS_e = \sum_{i=1}^N (\tilde{\mathbf{Y}}_{impute} - (\tilde{\mathbf{Y}}_{impute})^*)^2 = \tilde{r}_{\tilde{\mathbf{Y}}\tilde{\mathbf{Y}}}(n(m-L) - 1)V(\tilde{\mathbf{Y}}_{impute})$ ,
  - $(\tilde{\mathbf{Y}}_{impute})^*$  is the predicted value based on estimated  $\hat{\boldsymbol{\beta}}$ ,
  - $\tilde{r}_{\tilde{\mathbf{Y}}\tilde{\mathbf{Y}}}$  is corresponding element of  $\tilde{\mathbf{Y}}_{impute}$  in the correlation matrix of re-fitted regression after sweep operation,
  - $n(m-L)$  is number of transformed records used in equation (21) for re-fit regression ,
  - and  $V(\tilde{\mathbf{Y}}_{impute})$  is variance of  $\tilde{\mathbf{Y}}_{impute}$ .
- $df_e = n(m-L) - p$ , and  $p = D^* + q^*$  is the number of non-redundant parameters in re-fitted regression.

Based on these standard errors, t-test statistics and/or p-values may be computed and displayed according to standard definitions and output scheme of linear models (please refer to linear model documentation):

- (a) For each element  $\beta_j$  of  $\hat{\boldsymbol{\beta}}$  and the corresponding  $j$ -th diagonal element of  $V(\hat{\boldsymbol{\beta}})$ ,  $j = 1, \dots, D$ , compute the t-statistic  $t_j = \beta_j / \sqrt{V(\hat{\boldsymbol{\beta}})_{jj}}$
- (b) The p-value corresponding to  $t_j$  is  $2 \times$  the value of the cumulative distribution function of a t-distribution with  $nm - q - D^*$  degrees of freedom, i.e.,  $p_j = 2 \cdot \left( 1 - P(t_{nm-q-D^*} \leq |t_j|) \right)$ .

Note that depending on the implementation of the GLS estimation in Section 3.5,

$(\tilde{\mathbf{X}}'_{aug} \tilde{\mathbf{X}}_{aug})^{-1}$  may have already been computed, in which case this expression does not need to be recalculated.

3. Standard errors of  $\boldsymbol{\alpha}$  based on  $V(\hat{\boldsymbol{\alpha}})$ , the covariance matrix of  $\hat{\boldsymbol{\alpha}}$ , which is the upper  $L \times L$  submatrix of  $V(\hat{\boldsymbol{\alpha}}_{aug})$ :

$$V(\hat{\boldsymbol{\alpha}}_{aug}) = \frac{SS_e^*}{df_e^*} \times \left( \sum_{t=L+1}^m \tilde{\mathbf{Z}}'_{t-lag,aug} \tilde{\mathbf{Z}}_{t-lag,aug} \right)^{-1} \quad (26)$$

where

- $SS_e^* = \sum_{i=1}^N (\tilde{\mathbf{Z}}_{t,impute} - (\tilde{\mathbf{Z}}_{t,impute})^*)^2 = \tilde{r}_{\tilde{\mathbf{Z}}\tilde{\mathbf{Z}}}(n(m-L) - 1)V(\tilde{\mathbf{Z}}_{t,impute})$ ,
  - $(\tilde{\mathbf{Z}}_{t,impute})^*$  is the predicted value based on estimated  $\hat{\boldsymbol{\alpha}}$  and  $\tilde{\mathbf{Z}}_{t-lag,aug}$
  - $\tilde{r}_{\tilde{\mathbf{Z}}\tilde{\mathbf{Z}}}$  is corresponding element of  $\tilde{\mathbf{Z}}_{t,impute}$  in the correlation matrix of re-fitted autoregressive model after sweep operation,
  - $n(m-L)$  is number of transformed records used in equation (18) for re-fit autoregressive,

- and  $V(\tilde{Z}_{t,impute})$  is variance of  $\tilde{Z}_{t,impute}$ .
- $df_e^* = n(m - L) - p_{AR}$ , and  $p_{AR} = L^* + q_Z^*$  is the number of non-redundant parameters in re-fitted autoregressive model.

Based on these standard errors, t-test statistics and/or p-values may be computed and displayed according to standard definitions and output scheme of linear models.

- (a) For each element  $\alpha_j$  of  $\hat{\alpha}$  and the corresponding  $j$ -th diagonal element of  $V(\hat{\alpha})$ ,  $j = 1, \dots, L$ , compute the t-statistic  $t_j = \alpha_j / \sqrt{V(\hat{\alpha})_{jj}}$
  - (b) The p-value corresponding to  $t_j$  is  $2 \times$  the value of the cumulative distribution function of a t-distribution with  $\sum_{t=1}^m n_t - L^*$  degrees of freedom, i.e.,  $p_j = 2 \cdot \left(1 - P(t_{\sum_{t=1}^m n_t - L^*} \leq |t_j|)\right)$ .
4. Indicator of which method has been automatically chosen to model spatial covariances, either empirical covariance (EOF) or parametric variogram model.
  5. Test statistics from goodness of fit tests for parametric model:
    - Test statistic  $z_1$ , p-value  $p_1$ , level of significance  $\gamma_1$  used for automated test for fit of slope parameter
    - Test statistic  $z_2$ , p-value  $p_2$ , level of significance  $\gamma_2$  used for testing homogeneity of variances
  6. Parametric covariance parameters  $\hat{\psi}$  if parametric model has been chosen

### 3.6.3 Tests of effects in Mean Structure Model (Type III)

For each effect specified in the model, type III test matrix  $L$  is constructed and  $H_0: L_i\beta = 0$  is tested. Construction of type III matrix  $L$  as well as generating estimable function (GEF) is based on the generating matrix  $H$ , which is the upper  $D \times D$  submatrix of  $(\tilde{X}'_{aug}\tilde{X}_{aug})^{-1}\tilde{X}'_{aug}\tilde{X}_{aug}$ , such that  $L_i\beta$  is estimable. It involves parameters only for the given effect. For type III analysis,  $L$  does not depend on the order of effects specified in the model. If such a matrix cannot be constructed, the effect is not testable.

Then the  $L$  matrix is then used to construct the test statistic

$$F = \frac{\hat{\beta}'L'(L\Sigma L')^{-1}L\hat{\beta}}{r_c}$$

where

- $\hat{\beta}$  is the subvector of the first  $D$  elements of  $\hat{\beta}_{aug}$  obtained in Step 5 of Section 3.5,
- $r_c = rank(L\Sigma L')$ ,
- $\Sigma$  is the covariance matrix of  $\hat{\beta}$ , which is the upper  $D \times D$  submatrix of  $V(\hat{\beta}_{aug})$  defined in equation (25).

The statistic has an approximate  $F$  distribution. The numerator degrees of freedom  $df1$  is  $r_c$  and the denominator degrees of freedom  $df2$  is  $nm - q - D^*$ , where  $D^*$  is the number of

non-redundant parameters in the first  $D$  parameters of refitted regression model obtained in Section 3.5. Then the p-values can be calculated accordingly.

An additional test also should be computed, which is similar to “corrected model” if there is an intercept or “model” if there is no intercept in ANOVA table in linear regression. Essentially, the null hypothesis is regression parameters (except intercept if there is on) are zeros. The test statistic would be the same as the above F statistic except the L matrix is from GEF. If there is no intercept, the L matrix is the whole GEF. If there is an intercept, the L matrix is GEF without the first row which corresponds to the intercept.

Statistics saved for Test of effects in Mean Structure Model (including corrected model or model):

- $F$  statistics
- $df1$
- $df2$
- $p$ -value

### 3.6.4 Location clustering for spatial structure visualization

Large spatial covariance matrix or correlation matrix are not suitable to demonstrate the relation among the locations. Grouping method, also called community detection or position analysis (Wasserman, 1994), can be used to identify some representative location clusters. To simplify the implementation, hierarchical clustering (Johnson, 1967) is used to detect clusters among locations based on STP model spatial statistics.

Please note location clustering is only supported when empirical nonparametric covariance model is used.

Given a set of  $n$  locations  $\{s_1, \dots, s_n\}$  in STP to be clustered, and their corresponding spatial correlation matrix  $R$ , a  $n*n$  matrix, as the similarity matrix

$$R = [r_{ij}]_{i,j=1,\dots,n}$$

Given similarity threshold  $\alpha$  with default value 0.2, and  $N_C$  with default value 10, the process of location clustering is described in following steps, which is based on the basic process of hierarchical clustering.

Step 1. Initialize the clusters and similarities:

- Assign each location  $s_i$  to a cluster  $C_i$  ( $i = 1, \dots, n$ ). So that for  $n$  locations, the total number of clusters  $n_C = n$  at the beginning, and each cluster has just one location,
- Define the set of clusters:  $C$ ,
- Define similarity matrix

$$R^C = [r_{ij}^C]_{i,j=1,\dots,n}$$

where the similarity  $r_{ij}^C$  between the clusters  $C_i$  and  $C_j$  is the similarity  $r_{ij}$  between location  $s_i$  and  $s_j$ .

Step 2. Find 2 clusters  $C_i$  and  $C_j$  in  $C$  with largest similarity  $\max(r_{ij}^C)$ ,

If  $\max(r_{ij}^C) > \alpha$ :

- Merge  $C_i$  and  $C_j$  into a new cluster  $C_{\langle i,j \rangle}$  to include all locations in  $C_i$  and  $C_j$ ,
- Compute similarities between the new cluster  $C_{\langle i,j \rangle}$  and other clusters  $C_k, k \neq i$  and  $j$

$$r_{\langle i,j \rangle, k}^C = \min(r_{ik}^C, r_{jk}^C)$$

- Update  $C$  by adding  $C_{\langle i,j \rangle}$ , discarding  $C_j$  and  $C_i$ . So  $n_C = n_C - 1$ .
- Update similarity matrix  $R^C$  by adding  $r_{\langle i,j \rangle, k}^C$ , discarding  $r_{ik}^C$  and  $r_{jk}^C$ , go to step 3.

If  $\max(r_{ij}^C) \leq \alpha$ , go to step 4.

Step 3. Repeat step 2.

Step 4. For all the detected clusters with more than 1 location, compute following statistics:

- Cluster size:  $n_{C_i}$  is the number of locations in  $C_i$ ,
- Closeness:

$$d_i = \frac{1}{n_{C_i}(n_{C_i} - 1)/2} \sum r_{kl}, \forall s_k, s_l \in C_i, \text{ and } k \neq l.$$

Step 5. Define clusters for interactive visualization:

- $C_{closeness}$ : The first  $N_C$  clusters sorted by descending closeness  $d_i$ ,
- $C_{size}$ : The first  $N_C$  clusters sorted by descending cluster size  $n_{C_i}$ .

Step 6. Output the union for location cluster visualization:

$$C^* = C_{closeness} \cup C_{size}$$

Statistics saved for spatial structure visualization including:

1. Number of excluded locations during handling of missing data
2. Spatial correlation matrix  $\mathbf{R} = [r_{ij}]_{i,j=1,\dots,n}$
3. Statistics of each output location cluster in  $C^*$ :
  - Closeness  $d_i$
  - Cluster size  $n_{C_i}$
  - Coordinates of locations in this cluster

### 3.7 Results saved for prediction

1. Model coefficients  $\hat{\boldsymbol{\beta}}$ ,  $\hat{\boldsymbol{\alpha}}$  and the covariance estimate  $V(\hat{\boldsymbol{\beta}})$  as defined in (25).
2. Transformed regression residuals and predictors of  $L$  most recent observations for prediction:

$$\check{\mathbf{Z}}_{m-l+1} = \mathbf{H}'_S^{-1} \mathbf{H}_S^{-1} (\mathbf{Y}_{m-l+1, impute} - \mathbf{X}_{m-l+1, aug} \hat{\boldsymbol{\beta}}_{aug}), l = 1, \dots, L \quad (27)$$

$$\check{\mathbf{X}}_{m-l+1, impute} = \mathbf{H}'_S^{-1} \mathbf{H}_S^{-1} \mathbf{X}_{m-l+1, impute}, l = 1, \dots, L \quad (28)$$

3. Indicator of which method has been chosen to model spatial covariances, either empirical

- covariance (EOF) or parametric variogram model.
4. Parametric covariance parameters  $\hat{\psi}$  if parametric model has been chosen.
  5. Coordinates of locations  $s$ .
  6. Number of unique time points used for model build,  $m$ .
  7. Number of records with missing values in the data set used in model building,  $q$ .
  8. Spatial covariance matrix  $\Sigma_S$ .
  9.  $H_S^{-1}$ , inverse of Cholesky factor of spatial covariance matrix.

## 4 Prediction

We perform the following procedure to issue predictions for future time  $m + 1, \dots, m + H$  at prediction locations  $\mathbf{G} = (\mathbf{g}_1, \dots, \mathbf{g}_N)$  using the results saved in the output file (see Figure 2). The input data set format should include location  $\mathbf{G}$ , predictors  $\mathbf{X}$  for  $t = m + 1, \dots, m + H$ .

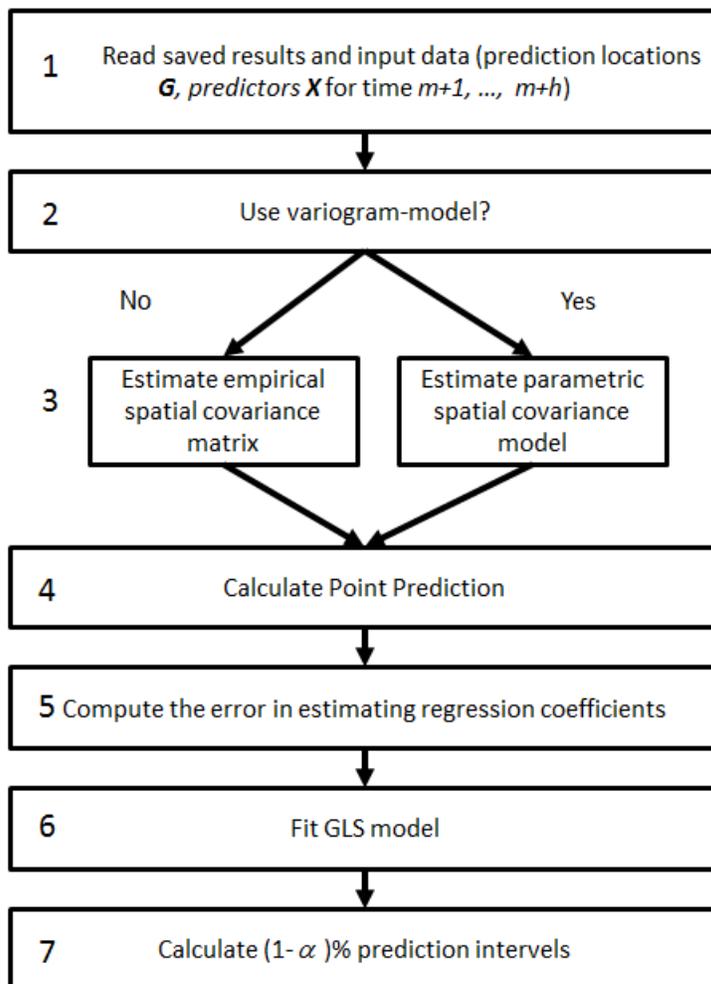


Figure 2. Flowchart of algorithm steps for model prediction

## 4.1 Point prediction

Step 1: Construct the  $N \times n$  spatial covariance matrix to capture the spatial dependence between prediction grids  $\mathbf{g} \in \mathbf{G}$  and original sample locations  $\mathbf{s}$ .

- If variogram-based spatial covariance matrix

$$V_S(\mathbf{g}) = V(\epsilon_t(\mathbf{g})) = \sigma^2 + \tau^2 \quad (29)$$

and

$$\mathbf{C}_S(\mathbf{G}) = \{Cov(\epsilon_t(\mathbf{g}_i), \epsilon_t(\mathbf{s}_j); \hat{\psi})\}_{i=1, \dots, N; j=1, \dots, n} \quad (30)$$

according to (14) for all locations  $\mathbf{g}$  (whether locations were included in the model build or not).

- If EOF-based spatial covariance function is used:

For locations  $\mathbf{g}_i$  that are included in the original sample locations  $\mathbf{s}$ ,  $Cov_{EOF}(\epsilon_t(\mathbf{g}_i), \epsilon_t(\mathbf{s}))$  is equal to the row corresponding to location  $\mathbf{g}_i$  in the empirical covariance matrix  $\Sigma_S$  and  $V_S(\mathbf{g}_i)$  is equal to the empirical variance at that location, i.e., the diagonal element of  $\Sigma_S$  corresponding to that location.

For locations  $\mathbf{g}_i$  that were not included in the model build, calculate the spatial covariance in the following way:

- Perform eigendecomposition on the empirical covariance matrix

$$\mathbf{S} = \mathbf{\Phi} \mathbf{\Lambda} \mathbf{\Phi}'$$

where  $\mathbf{\Phi} = (\phi_1, \dots, \phi_n)$  with  $\Phi_k = (\phi_k(\mathbf{s}_1), \dots, \phi_k(\mathbf{s}_n))'$  is the  $n \times n$  matrix of eigenvectors and  $\mathbf{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_n)$  is the  $n \times n$  matrix of eigenvalues.

- Apply inverse distance weighting (IDW) (Shepard 1968) to interpolate eigenvectors to locations with no observations.

$$\phi_k(\mathbf{g}) = \sum_{i=1}^n \frac{w_i(\mathbf{g}) \phi_k(\mathbf{s}_i)}{\sum_{j=1}^n w_j(\mathbf{g})}, k = 1, \dots, n$$

where

$$w_i(\mathbf{g}) = \frac{1}{\text{dist}(\mathbf{g}, \mathbf{s}_i)^\rho}$$

is an Inverse Distance Weighting (IDW) function with  $\rho \leq d$  for  $d$ -dimensional space and  $\text{dist}(\mathbf{g}, \mathbf{s}_i)$  may be any distance function. As a default value, use Euclidean distance with  $\rho = 2$  and  $\text{dist}(\mathbf{g}, \mathbf{s}_i)^2 = (\mathbf{g} - \mathbf{s}_i)'(\mathbf{g} - \mathbf{s}_i)$ .

- The EOF-based spatial variance-covariance functions are

$$V_S(\mathbf{g}) = V(\epsilon_t(\mathbf{g})) = \sum_{k=1}^n \lambda_n \phi_k^2(\mathbf{g}) \quad (31)$$

and

$$\text{Cov}(\epsilon_t(\mathbf{g}_i), \epsilon_t(\mathbf{s}_j)) = \sum_{k=1}^n \lambda_n \phi_k(\mathbf{g}_i) \phi_k(\mathbf{s}_j) \quad (32)$$

and the corresponding  $N \times n$  spatial covariance matrix

$$\mathbf{C}_S(\mathbf{G}) = \left\{ \text{Cov}_{EOF}(\epsilon_t(\mathbf{g}_i), \epsilon_t(\mathbf{s}_j)) \right\}_{i=1, \dots, N; j=1, \dots, n} \quad (33)$$

Note that under the EOF model, we allow for space-varying variances.

Step 2: Spatial interpolation to prediction locations  $\mathbf{g}$  for the most recent  $L$  time units,  $Z_{m-L+1}, \dots, Z_m$

$$\hat{\mathbf{Z}}_{m-l+1}(\mathbf{G}) = \mathbf{C}_S(\mathbf{G}) \boldsymbol{\Sigma}_S^{-1} \mathbf{Z}_{m-l+1} = \mathbf{C}_S(\mathbf{G}) \check{\mathbf{Z}}_{m-l+1}, l = 1, \dots, L \quad (34)$$

where  $\hat{\mathbf{Z}}_{m-l+1}(\mathbf{G})$  is a vector of length  $N$ .

Step 3: Iteratively forecast for future time  $m+1, \dots, m+H$  at prediction locations  $\mathbf{G}$ .

$$\hat{\mathbf{Z}}_{m+1}(\mathbf{G}) = \hat{\alpha}_1 \hat{\mathbf{Z}}_m(\mathbf{G}) + \dots + \hat{\alpha}_L \hat{\mathbf{Z}}_{m-L+1}(\mathbf{G}) \quad (35)$$

$$\hat{\mathbf{Z}}_{m+2}(\mathbf{G}) = \hat{\alpha}_1 \hat{\mathbf{Z}}_{m+1}(\mathbf{G}) + \dots + \hat{\alpha}_L \hat{\mathbf{Z}}_{m-L+2}(\mathbf{G}) \quad (36)$$

$$\hat{\mathbf{Z}}_{m+H}(\mathbf{G}) = \hat{\alpha}_1 \hat{\mathbf{Z}}_{m+H-1}(\mathbf{G}) + \dots + \hat{\alpha}_L \hat{\mathbf{Z}}_{m+H-L}(\mathbf{G}) \quad (37)$$

where  $\hat{\mathbf{Z}}_{m+h}(\mathbf{G}), h = 1, \dots, H$  are vectors of length  $N$ .

Step 4: Incorporate predicted systematic effect

$$\hat{\mathbf{Y}}_{m+h}(\mathbf{G}) = \hat{\mathbf{Z}}_{m+h}(\mathbf{G}) + X_{m+h}(\mathbf{G}) \hat{\boldsymbol{\beta}}, \quad h = 1, \dots, H \quad (38)$$

where  $\hat{\mathbf{Y}}_{m+h}(\mathbf{G}), h = 1, \dots, H$  are vectors of length  $N$ .

## 4.2 Prediction intervals

Under the assumption of Gaussian Process and known variance components, the prediction error  $\hat{\mathbf{Y}}_{m+h}(\mathbf{g}_i) - Y_{m+h}(\mathbf{g}_i)$  comes from two sources:

- The prediction error that would be incurred even if regression coefficients  $\boldsymbol{\beta}$  were known.
- The error in estimating regression coefficients  $\boldsymbol{\beta}$

The variance of prediction error is thus

$$V[\hat{\mathbf{Y}}_{m+h}(\mathbf{g}_i) - Y_{m+h}(\mathbf{g}_i)] = (\mathbf{X}'_{m+h}(\mathbf{g}_i) - \mathbf{C}'_{m+h}(\mathbf{g}_i) \boldsymbol{\Sigma}^{-1} \mathbf{X}_{impute}) V(\hat{\boldsymbol{\beta}}) (\mathbf{X}'_{m+h}(\mathbf{g}_i) - \mathbf{C}'_{m+h}(\mathbf{g}_i) \boldsymbol{\Sigma}^{-1} \mathbf{X}_{impute})' \quad (39)$$

$$+ V_{m+h}(\mathbf{g}_i) - \mathbf{C}'_{m+h}(\mathbf{g}_i) \boldsymbol{\Sigma}^{-1} \mathbf{C}_{m+h}(\mathbf{g}_i) \quad (40)$$

Expression (39) arises from the variance expression for universal kriging, while (40) is the variance of a predicted random effect with known variance of the random effects

(McCulloch et al. 2008, p.171).

- $C_{m+h}(g_i) = C_T(m+h) \otimes C_S(g_i)$  is the covariance vector of length  $nm$  between the prediction  $Y_{m+h}(g_i)$  and measurements  $Y_1(s), \dots, Y_m(s)$ . Note that  $C_T(m+h) = \{\gamma_T(m+h-t)\}_{t=1, \dots, m}$  is the AR(L) covariance vector of length  $m$  and  $C_S(g_i) = \left\{ \text{Cov}(Y_t(g_i), Y_t(s_j)) \right\}_{j=1, \dots, n}$  is the spatial covariance vector of length  $n$ .
- The  $nm \times nm$  covariance matrix  $\Sigma$  is defined as to  $\Sigma = \Sigma_T \otimes \Sigma_S$  and  $\Sigma_T = \{\gamma_T|t-t'|\}_{t,t'=1, \dots, m}$ . Note that  $\Sigma_S$  is a quantity stored after the model build step.
- $V_{m+h}(g_i) = V(Y_{m+h}(g_i)) = \gamma_T(0)V_S(g_i)$  is the variance of  $Y_{m+h}(g_i)$ .
- Note that expressions (39) and (40) are not computed explicitly, but instead are implemented as described in the following.

### Computational process:

Step 1: Compute the error in estimating regression coefficients  $\beta$  in (39).

For  $l = 1, \dots, L$ , interpolate  $X$  to prediction locations  $g$  for the most recent  $L$  time units

$$\mathbf{P}_{m+1-l}(g_i) = \mathbf{X}'_{m+1-l, \text{impute}} \Sigma_S^{-1} \mathbf{C}_S(g_i) = \check{\mathbf{X}}'_{m+1-l, \text{impute}} \mathbf{C}_S(g_i) \quad (41)$$

where  $\mathbf{P}_{m+1-l}(g_i)$  is a vector of dimension  $D \times 1$ . Define

$$\hat{X}_{m+h-l}(g_i) = \begin{cases} \mathbf{P}_{m+h-l}(g_i), & \text{if } h-l \leq 0; \\ \mathbf{X}_{m+h-l}(g_i), & \text{otherwise.} \end{cases} \quad (42)$$

For  $t = m-L+1, \dots, m$  ( $h \leq l$ ), we only have  $X$  at sample locations  $s$ , so  $\hat{X}_t(g_i) = P_t(g_i)$ , the interpolated values from  $X_t(s)$ ; for  $t > m$  (or  $h > l$ ), we already input  $X$  at prediction locations  $g$ , so there is no need to interpolate and  $\hat{X}_t(g_i) = X_t(g_i)$ .

Then, for  $h = 1, \dots, H$ , recursively compute the  $D \times 1$  vectors  $W_{m+h}(g_i)$

$$W_{m+h}(g_i) = X_{m+h}(g_i) + \sum_{l=1}^L \hat{\alpha}_l (\hat{W}_{m+h-l}(g_i) - \hat{X}_{m+h-l}(g_i)) \quad (43)$$

where

$$\hat{W}_{m+h-l}(g_i) = \begin{cases} 0, & \text{if } h-l \leq 0; \\ W_{m+h-l}(g_i), & \text{otherwise.} \end{cases} \quad (44)$$

The prediction error in estimating  $\beta$ , that is, expression (39) is thus

$$W'_{m+h}(g_i) V(\hat{\beta}) W_{m+h}(g_i) \quad (45)$$

where  $V(\hat{\beta})$  is computed in (25).

Step 2: Compute the prediction error that would be incurred if regression coefficients  $\beta$  were known, i.e., equation (40).

- Compute  $C_T(m+h)$  by AR(L) autocovariance function  $\gamma_T(k)$  (McLeod 1975).

First, compute  $\gamma_T(0), \dots, \gamma_T(L)$  by solving a linear system  $AX = b$ ,

$$\begin{pmatrix} 1 & -\hat{\alpha}_1 & -\hat{\alpha}_2 & \dots & -\hat{\alpha}_{L-1} & -\hat{\alpha}_L \\ -\hat{\alpha}_1 & 1 - \hat{\alpha}_2 & -\hat{\alpha}_3 & \dots & -\hat{\alpha}_L & 0 \\ -\hat{\alpha}_2 & -(\hat{\alpha}_1 + \hat{\alpha}_3) & 1 - \hat{\alpha}_4 & \dots & 0 & 0 \\ -\hat{\alpha}_3 & -(\hat{\alpha}_2 + \hat{\alpha}_4) & -(\hat{\alpha}_1 + \hat{\alpha}_5) & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -\hat{\alpha}_{L-2} & -(\hat{\alpha}_{L-3} + \hat{\alpha}_{L-1}) & -(\hat{\alpha}_{L-4} + \hat{\alpha}_L) & \dots & 0 & 0 \\ -\hat{\alpha}_{L-1} & -(\hat{\alpha}_{L-2} + \hat{\alpha}_L) & -\hat{\alpha}_{L-3} & \dots & 1 & 0 \\ -\hat{\alpha}_L & -\hat{\alpha}_{L-1} & -\hat{\alpha}_{L-2} & \dots & -\hat{\alpha}_1 & 1 \end{pmatrix} \begin{pmatrix} \gamma_T(0) \\ \gamma_T(1) \\ \gamma_T(2) \\ \gamma_T(3) \\ \vdots \\ \gamma_T(L-2) \\ \gamma_T(L-1) \\ \gamma_T(L) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (46)$$

Note that the first element of the vector on the right hand side (the variance of the measurement error) is fixed to be one, to account for the normalization through the spatial variance-covariance structure.

For  $k = L + 1, \dots, m + H - 1$ , recursively compute

$$\gamma_T(k) = \hat{\alpha}_1 \gamma_T(k-1) + \dots + \hat{\alpha}_L \gamma_T(k-L) \quad (47)$$

Remark: To construct the  $(L+1) \times (L+1)$  matrix  $A$ ,

$$A_{ij} = \begin{cases} -[\alpha_{i-1}], & j = 1; i = 1, \dots, L+1 \\ -[\alpha_{i-j}] - [\alpha_{i+j-2}], & j = 2, \dots, L+1; i = 1, \dots, L+1. \end{cases} \quad (48)$$

where

$$[\alpha_k] = \begin{cases} -1, & k = 0; \\ 0, & k < 0 \text{ or } k > L; \\ \hat{\alpha}_k, & 0 < k \leq L. \end{cases} \quad (49)$$

- Compute the approximated factorization of  $\Sigma_T^{-1}$  such that  $R'R \approx \Sigma_T^{-1}$ , where  $R$  is a  $(m-L) \times m$  matrix (follows from Cholesky or Gram-Schmidt orthogonalization, see for example Fuller 1975):

$$R = \begin{pmatrix} -\hat{\alpha}_L & \dots & -\hat{\alpha}_1 & 1 & 0 & 0 & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots \\ \dots & 0 & -\hat{\alpha}_L & \dots & -\hat{\alpha}_1 & 1 & 0 & 0 \\ \dots & \dots & 0 & -\hat{\alpha}_L & \dots & -\hat{\alpha}_1 & 1 & 0 \\ \dots & \dots & \dots & 0 & -\hat{\alpha}_L & \dots & -\hat{\alpha}_1 & 1 \end{pmatrix} \quad (50)$$

- Compute the value of expression (40):

$$\gamma_T(0)V_S(g_i) - (C'_T(m+h) \otimes C'_S(g_i))(R'R \otimes H_S^{-1}H_S^{-1})(C_T(m+h) \otimes C_S(g_i)) \quad (51)$$

where  $C'_S(g_i)$  is a the row of  $C_S(G)$  corresponding to location  $g_i$ .

Step 3: The  $(1 - \alpha\%)$  prediction interval is

$$\hat{Y}_{m+h}(g_i) \pm t_{nm-q-D^*,\alpha/2} \sqrt{V[\hat{Y}_{m+h}(g_i) - Y_{m+h}(g_i)]} \quad (55)$$

where  $V[\hat{Y}_{m+h}(g_i) - Y_{m+h}(g_i)]$  is the sum of equations (39) and (40) as computed in expressions (45) and (51), respectively.  $t_{nm-q-D^*,\alpha/2}$  is defined as  $P(X \leq t_{nm-q-D^*,\alpha/2}) = 1 - \alpha/2$  where  $X$  follows t-distribution with degree freedom  $nm - q - D^*$ . The default value for  $\alpha$  is 0.05.

As final output from the prediction step, point prediction, variances of point predictions and prediction interval (lower and upper bounds) are issued for each specified (location, time).

We remark that to perform what-if-analysis, a set of  $\mathbf{X}$  variables under the new settings need to be provided. Then we re-run the prediction algorithm described in Section 4 to obtain prediction results under adjusted settings.

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### **C-Support Vector Classification (C-SVC)**

Given training vectors  $x_i \in R^l$ ,  $i = 1, \dots, l$ , in two classes, and a vector  $y \in R^l$  such that  $y_i \in \{-1, 1\}$ , C-SVC solves the following dual problem:

$$\min f(\alpha) = \frac{1}{2} \alpha^T Q \alpha - e^T \alpha$$

such that  $0 \leq \alpha_i \leq C$ ,  $i = 1, \dots, l$  and  $y^T \alpha = 0$ , where

$$\alpha = (\alpha_1, \alpha_2, \dots, \alpha_l)^T$$

and  $Q$  is an  $l \times l$  matrix,  $Q(x_i \cdot x_j) = y_i y_j K(x_i \cdot x_j)$

The decision function is

$$\text{sgn} \left( \sum_{i=1}^l y_i \alpha_i K(x_i, x) + b \right)$$

where  $b$  is a constant term.

### **$\varepsilon$ -Support Vector Regression ( $\varepsilon$ -SVR)**

In regression models, we estimate the functional dependence of the dependent (target) variable  $y \in R$  on an  $n$ -dimensional input vector  $\mathbf{x}$ . Thus, unlike classification problems, we deal with real-valued functions and model an  $R^n \rightarrow R^1$  mapping. Given a set of data  $\{(x_1, z_1), \dots, (x_l, z_l)\}$ , such that  $x_i \in R^n$  is an input and  $z_i \in R^1$  is a target output, the dual form of  $\varepsilon$ -Support Vector Regression is

$$\min f(\alpha, \alpha^*) = \frac{1}{2} (\alpha - \alpha^*)^T Q (\alpha - \alpha^*) + \varepsilon \sum_{i=1}^l (\alpha_i + \alpha_i^*) + z_i \sum_{i=1}^l (\alpha_i - \alpha_i^*)$$

such that  $0 \leq \alpha_i$  and  $\alpha_i^* \leq C$  for  $i = 1, \dots, l$ , and

$$\sum_{i=1}^l (\alpha_i - \alpha_i^*) = 0$$

where  $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_l)^T$ ,  $\alpha^* = (\alpha_1^*, \alpha_2^*, \dots, \alpha_l^*)^T$ , and  $Q$  is an  $l \times l$  matrix,  $Q_{ij} = K(x_i \cdot x_j)$

The approximate function is

$$\sum_{i=1}^l (-\alpha_i + \alpha_i^*) K(x_i, x) + b$$

where  $b$  is a constant term.

## Primary Calculations

The primary calculations for building SVM models are described below.

### Solving Quadratic Problems

In order to find the decision function or the approximate function, the quadratic problem must be solved. After the solution is obtained, we can get different coefficients  $\alpha_i$ :

- if  $0 < \alpha_i < C$ , the corresponding training sample is a **free support vector**.
- if  $\alpha_i = C$ , the corresponding training sample is a **boundary support vector**.
- if  $\alpha_i = 0$ , the corresponding training sample is a **non-support vector**, which doesn't affect the classification or regression result.

Free support vectors and boundary support vectors are called **support vectors**.

This document adapts the decomposition method to solve the quadratic problem using second order information (Fan, Chen, and Lin, 2005). In order to solve all the SVM's in a unified framework, we'll introduce a general form for C-SVC and  $\varepsilon$ -SVR.

For  $\varepsilon$ -SVR, we can rewrite the dual form as

$$\min f(\alpha, \alpha^*) = \frac{1}{2} \begin{pmatrix} \alpha \\ \alpha^* \end{pmatrix}^T \begin{pmatrix} Q & -Q \\ -Q & Q \end{pmatrix} \begin{pmatrix} \alpha \\ \alpha^* \end{pmatrix} + \begin{pmatrix} \varepsilon e^T + z^T \\ \varepsilon e^T - z^T \end{pmatrix}^T \begin{pmatrix} \alpha \\ \alpha^* \end{pmatrix}$$

such that  $y^T \begin{pmatrix} \alpha \\ \alpha^* \end{pmatrix} = 0$  and  $0 \leq \alpha_i, \alpha_i^* \leq C$  for  $i = 1, \dots, l$ , where  $y$  is a  $2l \times 1$  vector with  $y_i = 1$  for  $i = 1, \dots, l$  and  $y_i = -1$  for  $i = l+1, \dots, 2l$ .

Given this, the general form is

$$\min f(\alpha) = \frac{1}{2} \alpha^T Q \alpha + p^T \alpha$$

such that  $0 \leq \alpha_i \leq C$  for  $i = 1, \dots, l$ , and  $y^T \alpha = \text{constant}$

	$\alpha$ in $W(\alpha)$	$p^T$	$y^T \alpha = \text{constant}$
C-SVC	$(\alpha_1, \alpha_2, \dots, \alpha_l)^T$	$-e^T$	$y = (y_1, \dots, y_l)^T$ $y^T \alpha = 0$
$\varepsilon$ -SVR	$(\alpha_1, \alpha_2, \dots, \alpha_l, \alpha_1^*, \alpha_2^*, \dots, \alpha_l^*)^T$	$\begin{pmatrix} \varepsilon e^T + z^T \\ \varepsilon e^T - z^T \end{pmatrix}^T$	$y = (1_1, \dots, 1_l, -1_{l+1}, \dots, -1_{2l})^T$ $y^T \alpha = 0$

### The Constant in the Decision Function

After the quadratic programming problem is solved, we get the support vector coefficients in the decision function. We need to compute the constant term in the decision function as well. We introduce two accessory variables  $r_1$  and  $r_2$ :

- For  $y_i = 1$ :

If  $0 < \alpha_i < C$ ,

$$r_1 = \frac{\sum_{0 < \alpha_i < C, y_i = 1} \nabla f(\alpha_i)}{\sum_{0 < \alpha_i < C, y_i = 1} 1}$$

Otherwise,

$$r_1 = \frac{\max_{\alpha_i = C, y_i = 1} \nabla f(\alpha_i) + \min_{\alpha_i = 0, y_i = 1} \nabla f(\alpha_i)}{2}$$

- For  $y_i = -1$ :

If  $0 < \alpha_i < C$ ,

$$r_2 = \frac{\sum_{0 < \alpha_i < C, y_i = -1} \nabla f(\alpha_i)}{\sum_{0 < \alpha_i < C, y_i = -1} 1}$$

Otherwise,

$$r_2 = \frac{\max_{\alpha_i = C, y_i = -1} \nabla f(\alpha_i) + \min_{\alpha_i = 0, y_i = -1} \nabla f(\alpha_i)}{2}$$

After  $r_1$  and  $r_2$  are obtained, calculate  $b = \frac{r_1 + r_2}{2}$

### Variable Scale

For continuous input variables, linearly scale each attribute to  $[-1, 1]$  or  $[0, 1]$ :

$$V^{new} = \frac{V - V_{\min}}{V_{\max} - V_{\min}} (newmax - newmin) + newmin$$

For categorical input fields, if there are  $m$  categories, then use  $(0, 1, 2, \dots, m)$  to represent the categories and scale the values as for continuous input variables.

### Model Building Algorithm

In this section, we provide a fast algorithm to train the SVM. A modified sequential minimal optimization (SMO) algorithm is provided for C-SVC binary and  $\epsilon$ -SVR models. A fast SVM training algorithm based on divide-and-conquer is used for all SVMs.

### SMO Algorithm

Due to the density of the kernel matrix, traditional optimization methods cannot be directly applied to solve for the vector  $\alpha$ . Unlike most optimization methods which update the whole vector  $\alpha$  in each step of an iterative process, the decomposition method modifies a subset of  $\alpha$  per iteration. This subset, denoted as the working set  $B$ , leads to a small sub-problem to be minimized in each iteration. Sequential minimal optimization (SMO) is an extreme example of this approach which restricts  $B$  to have only two elements. In each iteration no optimization algorithm is needed to solve a simple two-variable problem. The key step of SML is the working set selection method, which determines the speed of convergence for the algorithm.

### Kernel functions

The algorithm supports four kernel functions:

Linear function	$K(\mathbf{x}_i \cdot \mathbf{x}_j) = \mathbf{x}_i^T \cdot \mathbf{x}_j$
Polynomial function	$K(\mathbf{x}_i \cdot \mathbf{x}_j) = (\gamma \mathbf{x}_i^T \cdot \mathbf{x}_j + r)^d$
RBF function	$K(\mathbf{x}_i \cdot \mathbf{x}_j) = \exp\left(-\frac{\ \mathbf{x}_i - \mathbf{x}_j\ ^2}{2\sigma^2}\right)$ $= \exp(-\gamma \ \mathbf{x}_i - \mathbf{x}_j\ ^2), \gamma = \frac{1}{2\sigma^2}$
Hyperbolic tangent function	$K(\mathbf{x}_i \cdot \mathbf{x}_j) = \tanh(\gamma \mathbf{x}_i^T \cdot \mathbf{x}_j + r)$ $\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$

### Base Working Set Selection Algorithm

The base selection algorithm derives the selection set  $B = \{i, j\}$  based on  $\tau$ ,  $C$ , the target vector  $y$ , and the selected kernel function  $K(\mathbf{x}_i, \mathbf{x}_j)$ .

Let

$$a_{ij} = K_{ii} + K_{jj} - 2K_{ij}, b_{ij} = -y_i \nabla f(\alpha^k)_i + y_j \nabla f(\alpha^k)_j$$

and

$$\bar{a}_{ts} = \begin{cases} a_{ts} & \text{if } a_{ts} > 0 \\ \tau & \text{otherwise} \end{cases}$$

where  $\tau$  is a small positive number.

Select

$$i \in \arg \max_t \{-y_t \nabla f(\alpha^k)_t | t \in I_{up}(\alpha^k)\},$$

$$j \in \arg \min_t \left\{-\frac{b_{it}^2}{a_{it}} | t \in I_{low}(\alpha^k), -y_t \nabla f(\alpha^k)_t < -y_i \nabla f(\alpha^k)_i\right\}$$

where

$$I_{up}(\alpha) = \{t | \alpha_t < C, y_t = 1 \text{ or } \alpha_t > 0, y_t = -1\}$$

$$I_{low}(\alpha) = \{t | \alpha_t < C, y_t = -1 \text{ or } \alpha_t > 0, y_t = 1\}$$

Return  $B = \{i, j\}$ , where  $\nabla f(\alpha) = Q\alpha + \mathbf{p}$ .

### Shrink Algorithm

In order to speed up the convergence of the algorithm near the end of the iterative process, the decomposition method identifies a possible set  $A$  containing all final free support vectors. Hence, instead of solving the whole problem, the decomposition method works on a smaller problem:

$$\min_{\alpha_A} \frac{1}{2} \alpha_A^T Q_{AA} \alpha_A - (\mathbf{p}_A - Q_{AN} \alpha_N)^T \alpha_A$$

$$\text{s. t. } 0 \leq (\alpha_A)_t \leq C, t = 1, \dots, q$$

$$\mathbf{y}_A^T \alpha_A = \text{const} - \mathbf{y}_N^T \alpha_N$$

where  $N = \{1, 2, \dots, l\} \setminus A$  is the set of shrunken variables.

Afer every  $\min(l, 1000)$  iterations, we try to shrink some variables. During the iterative process  $m(\alpha^k) > M(\alpha^k)$ . Until  $m(\alpha^k) - M(\alpha^k) \leq \epsilon$  is satisfied, we can shrink variables in the following set:

$$\begin{aligned} & \{t | -y_t \nabla f(\alpha_t) > m(\alpha^k), \alpha_t = C, y_t = 1 \text{ or } \alpha_t = 0, y_t = -1\} \cup \\ & \{t | -y_t \nabla f(\alpha_t) < M(\alpha^k), \alpha_t = 0, y_t = 1 \text{ or } \alpha_t = C, y_t = -1\} \end{aligned}$$

Thus the set  $A$  of activated variables is dynamically reduced every  $\min(l, 1000)$  iterations.

- To account for the tendency of the shrinking method to be too aggressive, we reconstruct the gradient when the tolerance reaches

$$m(\alpha^k) \leq M(\alpha^k) + 10\epsilon$$

After reconstructing the gradient, we restore some of the previously shrunken variables based on the relationship

$$\begin{aligned} & \{t | -y_t \nabla f(\alpha_t) \leq m(\alpha^k), \alpha_t = C, y_t = 1 \text{ or } \alpha_t = 0, y_t = -1\} \cup \\ & \{t | -y_t \nabla f(\alpha_t) \geq M(\alpha^k), \alpha_t = 0, y_t = 1 \text{ or } \alpha_t = C, y_t = -1\} \end{aligned}$$

### Gradient Reconstruction

To decrease the cost of reconstruction of the gradient  $\nabla f(\alpha)$ , during the iterations we always keep

$$\bar{G}_i = C \sum_{\alpha_j=C} Q_{ij} i = 1, \dots, l$$

Then for the gradient  $\nabla f(\alpha_i)$ ,  $i \notin A$ , we have

$$\nabla f(\alpha_i) = \sum_{j=1}^l Q_{ij} \alpha_j + p_i = \bar{G}_i + \sum_{0 < \alpha_j < C} Q_{ij} \alpha_j + p_i$$

and for the gradient  $\nabla f(\alpha_i)$ ,  $i \in A$  we have

$$\nabla f(\alpha_i^{k+1}) = \nabla f(\alpha_i^k) + Q_{it} \Delta \alpha_t + Q_{is} \Delta \alpha_s$$

where  $t$  and  $s$  are the working set indices.

### Unbalanced Data Strategy

For some classification problems, the algorithm uses different parameters in the SVM formulation. The differences only affect the procedure for updating  $\alpha^k$ . Different conditions are handled as follows:

For :

Conditions		Update parameters
$y_i \neq y_j$	$\alpha_i - \alpha_j > C_i - C_j$ and $\alpha_i > C_i$	$\alpha_i^{new} = C_i$ $\alpha_j^{new} = C_i - (\alpha_i - \alpha_j)$
	$\alpha_i - \alpha_j \leq C_i - C_j$ and $\alpha_j > C_j$	$\alpha_j^{new} = C_j$ $\alpha_i^{new} = C_j + (\alpha_i - \alpha_j)$
	$\alpha_i - \alpha_j > 0$ and $\alpha_j < 0$	$\alpha_j^{new} = 0$ $\alpha_i^{new} = (\alpha_i - \alpha_j)$
	$\alpha_i - \alpha_j \leq 0$ and $\alpha_i < 0$	$\alpha_i^{new} = 0$ $\alpha_j^{new} = -(\alpha_i - \alpha_j)$
$y_i = y_j$	$\alpha_i + \alpha_j > C_i$ and $\alpha_i > C_i$	$\alpha_i^{new} = C_i$ $\alpha_j^{new} = (\alpha_i + \alpha_j) - C_i$
	$\alpha_i + \alpha_j \leq C_i$ and $\alpha_j < 0$	$\alpha_j^{new} = 0$ $\alpha_i^{new} = (\alpha_i + \alpha_j)$
	$\alpha_i + \alpha_j > C_j$ and $\alpha_j > C_j$	$\alpha_i^{new} = (\alpha_i + \alpha_j) - C_j$ $\alpha_j^{new} = C_j$
	$\alpha_i + \alpha_j \leq C_j$ and $\alpha_i < 0$	$\alpha_i^{new} = 0$ $\alpha_j^{new} = (\alpha_i + \alpha_j)$

**SMO Decomposition**

The following steps are used in the SMO decomposition:

1. Find  $\alpha^1$  as the initial feasible solution, and set  $k = 1$ .
2. If  $\alpha^k$  is a stationary solution, stop.

A feasible solution is stationary if  $m(\alpha) - M(\alpha) \leq \epsilon$ , where

$$m(\alpha) = \max_{i \in I_{up}} \{-y_i \nabla f(\alpha_i)\}$$

$$M(\alpha) = \min_{i \in I_{low}} \{-y_i \nabla f(\alpha_i)\}$$

$$I_{up}(\alpha) = \{t | \alpha_t < C, y_t = 1 \text{ or } \alpha_t > 0, y_t = -1\}$$

$$I_{low}(\alpha) = \{t | \alpha_t < C, y_t = -1 \text{ or } \alpha_t > 0, y_t = 1\}$$

Find a two-element working set  $B = \{i, j\}$  using the working set selection algorithm. (For more information, see the topic “Base Working Set Selection Algorithm” on p. 371.)

3. If the shrink algorithm is being used to speed up convergence, apply the algorithm here. (For more information, see the topic “Shrink Algorithm” on p. 372.)
4. Derive  $\alpha^{k+1}$  as follows:
  - ▶ If  $C_i \neq C_j$ , or if solving a classification problem, use the unbalanced data strategy. (For more information, see the topic “Unbalanced Data Strategy” on p. 373.)
  - ▶ If  $a_{ij} > 0$ , solve the subproblem

$$\min_{\alpha_B} \frac{1}{2} [\alpha_i \quad \alpha_j] \begin{bmatrix} Q_{ii} & Q_{ij} \\ Q_{ji} & Q_{jj} \end{bmatrix} \begin{bmatrix} \alpha_i \\ \alpha_j \end{bmatrix} + \left( -\mathbf{p}_B + Q_{BN} \alpha_N^k \right)^T \begin{bmatrix} \alpha_i \\ \alpha_j \end{bmatrix} + \text{cont}$$

Subject to the constraints

$$\begin{aligned} 0 &\leq \alpha_i, \alpha_j \leq C, \\ y_i \alpha_i + y_j \alpha_j &= -\mathbf{y}_N^T \alpha_N^k \end{aligned}$$

and let

$$\begin{aligned} \alpha_i^{new} &= \alpha_i^{old} + \frac{y_i b_{ij}}{a_{ij}} \\ \alpha_j^{new} &= \alpha_j^{old} - \frac{y_j b_{ij}}{a_{ij}} \end{aligned}$$

- ▶ Otherwise, solve the subproblem

$$\min_{\alpha_B} \frac{1}{2} [\alpha_i \quad \alpha_j] \begin{bmatrix} Q_{ii} & Q_{ij} \\ Q_{ji} & Q_{jj} \end{bmatrix} \begin{bmatrix} \alpha_i \\ \alpha_j \end{bmatrix} + (-\mathbf{p}_B + Q_{BN}\alpha_N^k)^T \begin{bmatrix} \alpha_i \\ \alpha_j \end{bmatrix} + \frac{\tau - a_{ij}}{4} \left( (\alpha_i - \alpha_i^k)^2 + (\alpha_j - \alpha_j^k)^2 \right)$$

subject to the same constraints described above, where  $\tau$  is a small positive number and  $N = \{1, 2, \dots, l\} \setminus B$ , and let

$$\alpha_i^{new} = \alpha_i^{old} + \frac{y_i b_{ij}}{\tau}$$

$$\alpha_j^{new} = \alpha_j^{old} - \frac{y_j b_{ij}}{\tau}$$

Finally, set  $\alpha_B^{k+1}$  to be the optimal point of the subproblem.

Set  $\alpha_N^{k+1} = \alpha_N^k$ , set  $k = k + 1$ , and go to step 2.

### Fast SVM Training

For binary SVM models, the dense kernel matrix cannot be stored in memory when the number of training samples  $l$  is large. Rather than using the standard decomposition algorithm which depends on a cache strategy to compute the kernel matrix, a divide-and-conquer approach is used, dividing the original problem into a set of small subproblems that can be solved by the SMO algorithm (Dong, Suen, and Krzyzak, 2005). For each subproblem, the kernel matrix can be stored in a kernel cache defined as part of contiguous memory. The size of the kernel matrix should be large enough to hold all the support vectors in the whole training set and small enough to satisfy the memory constraint. Since the kernel matrix for the subproblem is completely cached, each element of the kernel matrix needs to be evaluated only once and must be calculated using a fast method.

There are two steps in the fast SVM training algorithm:

- ▶ Parallel optimization
- ▶ Fast sequential optimization

These steps are described in more detail below.

### Parallel Optimization

Since the kernel matrix  $\mathbf{Q}$  is symmetric and semi-positive definite, its block diagonal matrices are semi-positive definite, and can be written as

$$Q_{diag} = \begin{bmatrix} Q_1 & & & \\ & Q_2 & & \\ & & \ddots & \\ & & & Q_k \end{bmatrix}$$

where  $l_i \times l_i$  matrices  $Q_i, i = 1, \dots, k, \sum_i^k l_i = l$  are block diagonal. Then we obtain  $k$  optimization subproblems as described in “Base Working Set Selection Algorithm” on p. 371. All the subproblems are optimized using the SMO decomposition algorithm in parallel. After this parallel optimization, most non-support vectors will be removed from the training set. Then a new training set can be obtained by collecting support vectors from the sub-problems. Although the size of the new training set is much smaller than that of the original one, the memory may not be large enough to store the kernel matrix, especially when dealing with a large dataset. Therefore a fast sequential optimization technique is used.

### **Fast Sequential Optimization**

The technique for fast sequential optimization works by iteratively optimizing subsets of the problem. Initially, the training set is shuffled, all  $\alpha_i, i = 1, \dots, l$  are set to zero, and a subset  $\text{Sub} \subseteq S$  is selected from the training set  $S$ . The size of the subset  $d$  is set ( $d \leq l$ ).

Optimization proceeds as follows:

- ▶ Apply the SMO algorithm to optimize a subproblem in  $\text{Sub}$  with kernel caching, and update  $\alpha_i$  and the kernel matrix. For more information, see the topic “SMO Algorithm” on p. 371.
- ▶ Select a new subset using the queue subset method. The size of the subset is chosen to be large enough to contain all support vectors in the training set but small enough to satisfy the memory constraint. For more information, see the topic “Queue Method for Subset Selection” on p. 376.
- ▶ Return to step 1 unless any of the following stopping conditions is true:
  - $|\Delta SV| < 20$  and (Number of learned samples)  $> l$
  - $SV \geq (d - 1)$
  - (Number of learned samples)  $> T \cdot l$

where  $|\Delta SV|$  is the change in number of support vectors between two successive subsets,  $l$  is the size of the new training set, and  $T (> 1.0)$  is a user-defined maximum number of loops through the data allowed.

### **Queue Method for Subset Selection**

The **queue method** selects subsets of the training set that can be trained by fast sequential optimization. For more information, see the topic “Fast Sequential Optimization” on p. 376..

The method is initialized by setting the subset to contain the first  $d$  records in the training data and the queue  $\mathbf{Q}_S$  to contain all the remaining records, and computing the kernel matrix for the subset.

Once initialized, subset selection proceeds as follows: each non-support vector in the subset is added to the end of the queue, and replaced in the subset with the record at the front of the queue (which is consequently removed from the queue). When all non-support vectors have been replaced, the subset is returned for optimization. On the next iteration, the same process is applied, starting with the subset and the queue in the same state they were in at the end of the last iteration.

### Blank Handling

All records with missing values for any input or output field are excluded from the estimation of the model.

### Model Nugget/Scoring

The SVM Model Nugget generates predictions and predicted probabilities for output classes. Predictions are based on the category with the highest predicted probability for each record.

To choose a predicted value, posterior probabilities are approximated using a sigmoid function(Platt, 2000). The approximation used is

$$P(y = 1|x) \approx P_{A,B}(x) = \frac{1}{1 + \exp(Af(x) + B)}$$

The optimal parameters  $A$  and  $B$  are the estimated by solving the following regularized maximum likelihood problem with a set of labeled examples  $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_l, y_l)$ ,  $\mathbf{x} \in \mathbf{R}^n$ ,  $y \in \{+1, -1\}$ , and  $N_+$  is the number of positive examples and  $N_-$  is the number of negative examples:

$$\min_{z=(A,B)} F(z) = -\sum_{i=1}^l (t_i \log(p_i) + (1 - t_i) \log(1 - p_i))$$

$$p_i = P_{A,B}(x_i) \text{ and } t_i = \begin{cases} \frac{N_++1}{N_++2} & \text{if } y_i = +1 \\ \frac{1}{N_-+2} & \text{if } y_i = -1 \end{cases}, i = 1, \dots, l$$

$$\nabla F(z) = \begin{bmatrix} \sum_{i=1}^l f_i (t_i - p_i) \\ \sum_{i=1}^l (t_i - p_i) \end{bmatrix}$$

$$H(z) = \nabla^2 F(z) = \begin{bmatrix} \sum_{i=1}^l f_i^2 p_i (1 - p_i) & \sum_{i=1}^l f_i p_i (1 - p_i) \\ \sum_{i=1}^l f_i p_i (1 - p_i) & \sum_{i=1}^l p_i (1 - p_i) \end{bmatrix}$$

### Blank Handling

Records with missing values for any input field cannot be scored and are assigned a predicted value and probability value(s) of \$null\$.



# Temporal Causal Modeling Algorithms

---

## 1. Introduction

Forecasting and prediction are important tasks in real world applications that involve decision making. In such applications, it is important to go beyond discovering statistical correlations and unravel the key variables that influence the behaviors of other variables using an algebraic approach. Many real world data, such as stock price data, are temporal in nature; that is, the values of a set of variables depend on the values of another set of variables at several time points in the past. Temporal causal modeling, or TCM, refers to a suite of methods that attempt to discover key temporal relationships in time series data. This chapter describes a particular method to discover temporal relationships using a combination of Granger causality and regression algorithms for variable selection. Although this treatment strives to be self-contained, a minimal set of papers describing the design principles behind the method can be found in [Lozano et al., 2011, Lozano et al., 2009, Arnold et al., 2007]<sup>1</sup>.

The rest of the chapter is organized as follows. Section 2 lays the groundwork for the TCM algorithm (notation and brief history) and explains the greedy orthogonal matching pursuit (GOMP) [Lozano et al., 2011] algorithm that is used. Section 3 describes the techniques used to fit and forecast time series and compute approximated forecasting intervals. Section 4 describes scenario analysis, which refers to a capability of the TCM product to “play-out” the repercussions of artificially setting the value of a time series. Section 5 describes the detection of outliers, and Section 6 discusses how potential causes for outliers can be established using root cause analysis.

## 2. Model

Introduced by Clive Granger [Granger, 1980], Granger causality in time series is based on the intuition that a cause should necessarily precede its effect, and that if time series  $a$  causally affects time series  $b$ , then the past values of  $a$  should be useful in predicting the future values of  $a$ . More specifically, time series  $a$  is said to “Granger cause” time series  $b$  if the accuracy of regressing for  $b$  in terms of past values of both  $a$  and  $b$  is statistically significantly better than regressing just with past values of  $b$ . If the time series have  $T$  time points and are denoted by  $\{a_t\}_{t=1}^T$  and  $\{b_t\}_{t=1}^T$ , then the following regressions are performed:

$$b_t \approx \sum_{j=1}^L \alpha_j a_{t-j} + \sum_{j=1}^L \beta_j b_{t-j} \quad (1)$$

$$b_t \approx \sum_{j=1}^L \beta_j b_{t-j} \quad (2)$$

Here  $L$  is the number of lags; that is, the value of  $b$  at time  $t$  can only be determined by values of other time series at times  $\{t-1, t-2, \dots, t-L\}$ . If Equation (1) is statistically more significant (using some test for significance) than Equation (2), then  $a$  is deemed to Granger cause  $b$ .

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<sup>1</sup> The methods described in this chapter are particularly useful for under-determined systems, where the number of time series ( $n$ ) far exceeds the number of samples ( $m$ ); that is  $n \gg m$ . Although these methods function for both over-determined ( $m \gg n$ ) and fully-determined ( $n == m$ ) systems, there are other approaches to pursue for such systems.

## 2.1 Graphical Granger Modeling

The classical definition of Granger causality is defined for a pair of time series. In the real world, we are interested in finding not one, but *all* the significant time series that influence the target time series. In order to accomplish this, we use group greedy ( $\ell_0$ ) regression algorithms with variable selection (see Section 2.3). An important feature of our TCM algorithm is that it groups influencer/predictor variables; that is, we are interested in predicting whether time series  $a$  as a whole –  $\{a_{t-1}, a_{t-2}, \dots, a_{t-L}\}$  – has influence over time series  $b$ . Such grouping is a more natural interpretation of causality and also helps sparsify the solution set. For example, without such grouping we may select the time-lagged series  $a_{t-2}$  to model  $b_t$  but not select any other value of  $a$ , which increases the number of choices for variable selection  $L$ -fold, where  $L$  is the number of lags that is allowed.

## 2.2 Notation

The following notation is used throughout this chapter unless otherwise stated:

Table 1: Notation

Notation	Type	Description
$\mathcal{N}$	—	Set of natural numbers
$\mathcal{R}$	—	Set of real numbers
$\backslash$	—	Regression solve operator
$ \cdot $	$\mathcal{N}$	Size operator
$\ \cdot\ _2$	$\mathcal{R}$	$\ell_2$ norm of a vector, i.e., $\ \mathbf{z}\ _2 = \sqrt{\sum_i z_i^2}$
$m$	$\mathcal{N}$	Number of time points
$n$	$\mathcal{N}$	Number of time series
$L$	$\mathcal{N}$	Number of lags for each target, $L < m$
$\mathbf{X}$	$\mathcal{R}^{m \times n}$	Design matrix of input series
$\mathbf{y}$	$\mathcal{R}^{m \times 1}$	Target series vector
$G$	$G: \mathcal{R}^{m \times n} \times J \times L \rightarrow \mathcal{R}^{(m-L) \times  J L}$ $J = \{j_1, j_2, \dots\}, 1 \leq j_k \leq n$	Computes lag matrix for the set of column indices in $J$
$M$	$M: \mathcal{R}^{m \times k} \rightarrow \mathcal{R}^{k \times 1}$	Computes means for $k$ series
$S$	$S: \mathcal{R}^{m \times k} \rightarrow \mathcal{R}^{k \times 1}$	Computes standard deviations for $k$ series
$\epsilon$	$\mathcal{R}$	Tolerance value for stopping criterion
$K^*$	$\mathcal{N}$	Max number of predictors selected or maximum number of iterations
$K$	$\mathcal{N}$	Actual number of predictors selected for a target series $\mathbf{y}$
$\hat{\boldsymbol{\beta}}^*$	$\mathcal{R}^{k \times 1}, 0 \leq k \leq KL$	Estimated coefficients for predictors on the transformed scale

In this section, we introduce the algorithm that is used to construct the temporal causal model. The list of symbols used in the rest of this chapter is summarized in Table 1. Most of the symbols are self-explanatory; however, the function  $G$ , which stands for grouping, requires some additional explanation.  $G$  is a function that takes a matrix ( $\mathcal{R}^{m \times n}$ ), a set of column indices  $J$ , and a lag value  $L$  and constructs a lag matrix that has  $(m - L)$  rows and  $(|J|L)$  columns. Basically, for every column index  $j \in J$ ,  $G$  constructs a  $(m - L) \times L$  lag matrix by carefully unrolling the  $j^{\text{th}}$  column of the input matrix. An example of  $G$ 's action is shown below:

## Temporal Causal Modeling Algorithms

$$G \left( \mathbf{X} = \begin{bmatrix} a_1 & b_1 & c_1 & d_1 \\ a_2 & b_2 & c_2 & d_2 \\ a_3 & b_3 & c_3 & d_3 \\ a_4 & b_4 & c_4 & d_4 \\ a_5 & b_5 & c_5 & d_5 \end{bmatrix}, J = \{1\}, L = 2 \right) \rightarrow \begin{bmatrix} a_2 & a_1 \\ a_3 & a_2 \\ a_4 & a_3 \end{bmatrix}$$

In this example, the input matrix  $\mathbf{X} \in \mathcal{R}^{5 \times 4}$  has 4 time series ( $n = 4$ ) and five time points per time series ( $m = 5$ ). The lag matrix associated with the time series in column 1, when  $L$  (lag) is 2, is produced by invoking  $G(\mathbf{X}, \{1\}, 2)$ . Note that the lag matrix consists of the lag-1 vector of  $\mathbf{X}$  as the first column, the lag-2 vector as the second column, up to the lag- $L$  vector as the  $L^{\text{th}}$  column. Similarly, the functions  $(M, S)$  accept any input matrix and compute the mean and the standard deviation, respectively, of the matrix's columns. For purposes of numerical stability, and to increase interpretability during modeling, columns of the lagged matrix are both centered by the column means and scaled by the column standard deviations<sup>2</sup>. On the other hand, the target  $\mathbf{y}$  is *only centered*. An example of mean centering and scaling for the lagged matrices is shown below:

$$\left( \begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \\ a_3 & b_3 \end{bmatrix} \right) \rightarrow \begin{bmatrix} \frac{a_1 - a_\mu}{a_\sigma} & \frac{b_1 - b_\mu}{b_\sigma} \\ \frac{a_2 - a_\mu}{a_\sigma} & \frac{b_2 - b_\mu}{b_\sigma} \\ \frac{a_3 - a_\mu}{a_\sigma} & \frac{b_3 - b_\mu}{b_\sigma} \end{bmatrix}$$

Here,  $(a_\mu, a_\sigma)$  and  $(b_\mu, b_\sigma)$  are the means and standard deviations of the first and the second columns,  $(a, b)$  respectively.

## 2.3 Group Orthogonal Matching Pursuit (GOMP)

### Algorithm 1: GOMP

**Input:**  $\mathbf{X}, \mathbf{y}, G, M, S, L, \epsilon, K^*, J_{sel}^0, \tilde{J}_{sel}$ .

**Output:**  $J_{sel}, \hat{\boldsymbol{\beta}}^*$ .

- 1  $\mathbf{X}_{aug}^0 = G(\mathbf{X}, J_{sel}^0, L)$ ;
- 2 for  $i \in [1, (m - L)]$  do  $\mathbf{X}_{aug}^0(i, :) = \frac{\mathbf{X}_{aug}^0(i, :) - M(\mathbf{X}_{aug}^0)^T}{S(\mathbf{X}_{aug}^0)^T}$ ;
- 3  $\hat{\boldsymbol{\beta}}^{*0} = \mathbf{X}_{aug}^0 \setminus (\mathbf{y} - M(\mathbf{y}))$ ;
- 4  $\mathbf{r}^0 = \mathbf{y} - M(\mathbf{y}) - \mathbf{X}_{aug}^0 \hat{\boldsymbol{\beta}}^{*0}$ ;
- 5 if any redundant series are found, delete them in  $J_{sel}^0$ ;
- 6 if  $(|J_{sel}^0| \geq K^*)$ , then  $J_{sel}^0 = J_{sel}^0(1:K^*)$ , update  $\hat{\boldsymbol{\beta}}^{*0}$ , return  $J_{sel}^0, \hat{\boldsymbol{\beta}}^{*0}$  and stop;
- 7 otherwise update  $\hat{\boldsymbol{\beta}}^{*0}$  and  $\mathbf{r}^0$ ;
- 8 for  $k \in 1, 2, 3 \dots (K^* - |J_{sel}^0|)$  do
- 9  $j^k = \operatorname{argmin}(\mathbf{X}, \mathbf{r}^{k-1}, G, M, S, L, \epsilon, J_{sel}^0, \tilde{J}_{sel})$ ;
- 10 if  $j^k = -1$ , return  $J_{sel}^{(k-1)}$  and  $\hat{\boldsymbol{\beta}}^{*(k-1)}$  and stop;
- 11  $\mathbf{X}_{aug}^k = G(\mathbf{X}, J_{sel}^{k-1} \cup j^k, L)$ ;

<sup>2</sup> Although each column of the lagged matrix has a different mean and standard deviation, due to the structure of these columns, it is possible to compute the mean and the standard deviation of the time series itself and use those to center and scale the lagged columns.

## Temporal Causal Modeling Algorithms

```

12   for  $i \in [1, (m - L)]$  do
13      $\mathbf{X}_{aug}^k(i, :) = \frac{\mathbf{X}_{aug}^k(i, :) - M(\mathbf{X}_{aug}^k)^T}{S(\mathbf{X}_{aug}^k)^T}$ ;
14      $\hat{\boldsymbol{\beta}}^{*k} = \mathbf{X}_{aug}^k \setminus (\mathbf{y} - M(\mathbf{y}))$ ;
15      $\mathbf{r}^k = \mathbf{y} - M(\mathbf{y}) - \mathbf{X}_{aug}^k \hat{\boldsymbol{\beta}}^{*k}$ ;
16      $J_{sel}^k = J_{sel}^{k-1} \cup j^k$ ;
17     if  $\|\mathbf{r}^k\|_2 \leq \epsilon$ , break;
18   return  $J_{sel}^k, \hat{\boldsymbol{\beta}}^{*k}$ .

```

We begin by describing Algorithm 1: GOMP, which will be used to establish causality of time-series data. This algorithm receives the variables  $\mathbf{X}, \mathbf{y}, G, M, S, L, \epsilon, K^*$  (described in Table 1) as input. Briefly,  $\mathbf{y} \in \mathcal{R}^{(m-L) \times 1}$  is a target vector for which we want to establish the Granger causality (note that we have excluded the first  $L$  values of  $\mathbf{y}$ ). In contrast,  $\mathbf{X} \in \mathcal{R}^{m \times n}$  is the input *unlagged* time series data.  $L$  is the number of lags for each predictor in each target series,  $K^*$  is the maximum number of predictors to be selected per-target, and  $\epsilon$  determines whether a new predictor needs to be added. In addition,  $G, M$  and  $S$  are grouping, centering, and scaling functions which have been described in Section 2.2.  $J_{sel}^0$  is the set of pre-selected predictor indices for  $\mathbf{y}$ , and always contains the lagged  $\mathbf{y}$ .  $J_{sel}$  is the set of forbidden predictors, if any, for  $\mathbf{y}$ . If there are no forbidden predictors, then  $J_{sel} \sim = \emptyset$ . Given these, the goal is to greedily find predictors that solve the system  $\mathbf{X}\boldsymbol{\beta} = \mathbf{y}$  subject to sparsity constraints.

The greedy algorithm approximates an  $\ell_0$ -sparse solution by iteratively choosing the best predictor for addition at each iteration. We use superscripts to denote the iteration number in Algorithm 1. For example,  $J_{sel}^0$  represents the initial values of  $J_{sel}$  at the 0<sup>th</sup> iteration (before the actual iteration starts). The first part of the algorithm (lines 1 – 4) constructs and solves a linear system consisting of the predictors in  $J_{sel}^0$  to obtain  $\boldsymbol{\beta}^{*0}$ , the coefficient vector for predictors on the transformed scale. At the end of this first part, we have  $\mathbf{r}^0$ , the initial residual. Then check whether there are redundant predictor series in  $J_{sel}^0$ . If yes, then delete them. If the number of predictor series in the (updated)  $J_{sel}^0$  is equal to or larger than the maximum number of iterations (i.e.,  $|J_{sel}^0| \geq K^*$ ) then keep the first  $K^*$  predictor series in  $J_{sel}^0$ , update  $\boldsymbol{\beta}^{*0}$ , return  $J_{sel}^0$  and  $\boldsymbol{\beta}^{*0}$ , and stop the process (line 6); otherwise (i.e.,  $|J_{sel}^0| < K^*$ ), update  $\boldsymbol{\beta}^{*0}$  and  $\mathbf{r}^0$  (line 7) if any redundant predictor series were deleted. Then start the iterative process to add one predictor series at a time (line 8). The first step in predictor selection (line 9) consists of an **argmin** function that systematically goes over each eligible predictor and evaluates its goodness (see Algorithm 2). This step is the performance critical portion of the algorithm and can be searched in parallel. At the end of the step,  $j^k$ , the index corresponding to the best predictor is available. However, if no suitable predictor is found in the **argmin** function (i.e.,  $j^k = -1$ ), then return  $J_{sel}^{k-1}$  and  $\boldsymbol{\beta}^{*(k-1)}$  and stop (line 10). The next part (lines 11 – 14) re-estimates the model coefficients by adding  $j^k$  to the model. Line 15 updates the residual,  $\mathbf{r}^k$ , for this model and line 16 adds  $j^k$  to the model. Finally, if the  $\ell_2$  norm of the current residuals is equal to or smaller than the tolerance value (i.e.,  $(\|\mathbf{r}^k\|_2 \leq \epsilon)$ ), then the iterative process is terminated.

Note that if the tolerance  $\epsilon$  is achieved by adding  $j^k$ , then no new iterations are required and the iterative process is terminated. Thus the actual number of predictors selected,  $K$ , can be less than the maximum number of iterations, (i.e.,  $K \leq K^*$ ). However, if the tolerance  $\epsilon$  is set very small, then it is highly unlikely that such a situation will happen.

### Algorithm 2: argmin

---

**Input:**  $\mathbf{X}, \mathbf{r}, G, M, S, L, \epsilon_2, K^*, J_{sel}^0, J_{sel} \sim$ .

**Output:**  $j_{sel}$ : Selected group index.

```

1   $cost = \|\mathbf{r}\|_2^2, j_{sel} = -1;$ 
2  for  $j \in 1, 2, 3 \dots n$  do
3    if  $j \in J_{sel} \parallel j \in \tilde{J}_{sel}$  continue;
4     $\mathbf{X}_{G_j} = G(\mathbf{X}, j, L);$ 
5    for  $i \in [1, (m - L)]$  do  $\mathbf{X}_{G_j}(i, :) = \frac{\mathbf{X}_{G_j}(i, :) - M(\mathbf{X}_{G_j})^T}{S(\mathbf{X}_{G_j})^T};$ 
6     $\hat{\boldsymbol{\beta}}_j = \mathbf{X}_{G_j} \setminus \mathbf{r};$ 
7     $\mathbf{r}_j = \mathbf{r} - (\mathbf{X}_{G_j} \hat{\boldsymbol{\beta}}_j)_{G_j};$ 
8    if  $\|\mathbf{r}_j\|_2^2 < (cost - \epsilon_2)$ , then  $(cost, j_{sel}) = (\|\mathbf{r}_j\|_2^2, j);$ 
9  return  $j_{sel}$ .
```

The implementation of the **argmin** function (line 8, Algorithm 1) is shown in Algorithm 2. The algorithm first assigns the initial cost to be the square of the  $\ell_2$  norm of the current residuals, and the selected group index to be  $-1$  (line 1). Then it loops over each series group, first checking if the time series being considered for addition ( $j$ ) has already been added to the solution  $J_{sel}$  or if it is a forbidden predictor (line 3). If the current group ( $j$ ) is not yet selected, the lagged transformed matrix corresponding to this time series ( $\mathbf{X}_{G_j}$ ) is constructed using the  $G, M$  and  $S$  functions (lines 4 and 5). After grouping and transforming  $\mathbf{X}_{G_j}$ , the residual ( $\mathbf{r}_j$ ) corresponding to the candidate time series  $j$  is computed by first regressing  $\mathbf{r}$  on  $\mathbf{X}_{G_j}$  (line 6), and then computing the residual (line 7). Finally, the current time series is selected as the leading candidate if the square of the  $\ell_2$  norm of its residual ( $\mathbf{r}_j$ ) is lower than the previous estimate minus a threshold value,  $\epsilon_2$ . Including such a threshold value prevents selecting an (almost) identical series.

The loop in Algorithm 2 (line 2) can be thought of as iterating over all candidate series. For each candidate series, the following computations are carried out: (1) a filter is applied in line 3 to ensure that it is a valid candidate; (2) lines 4 and 5 map the current candidate to the transformed matrix ( $\mathbf{X}_{G_j}$ ) that represents the lag matrix to be used; (3) lines 6 and 7 evaluate the goodness of the current candidate by first solving a dense linear system and then computing the residual; (4) line 8 applies a predicate to check if the current candidate series is better than previously evaluated candidates. Notice that the predicate (line 8) is associative and commutative; therefore, Algorithm 2 can be parallelized by dividing the iteration space ( $[1, n]$ ) into chunks and executing each chunk in parallel. To get the globally best group, it is sufficient to *reduce* the groups that were selected by each parallel instance in a tree-like fashion by applying the predicate in line 8.

## 2.4 Selecting $L$

Both Algorithms 1 and 2 accept  $L$  as an input parameter which can be specified by user. If  $L$  is not explicitly specified then the following heuristic approach can be used to determine  $L$  based on  $m$  (# of time points) and  $s$  (periodicity or seasonal length):

- (1) If  $s > 1$  and  $m \geq 4s$ , then  $L = \min(s, 20)$ .
- (2) If  $s = 1$  or  $m < 4s$ , then  $L = 5$ .

## 2.5 AR(L) Model

Out of the  $n$  series in the data, some series may be used as predictors only, so no TCM models are built for them. However, if they are selected as predictors for some target series, then simple models need to be built for them in order to do forecasting. For example, suppose that time series 1 is a selected predictor for time series 2, but there is no model built for time series 1. While a model for time series 1 is not needed in order to forecast time series 2 at time  $(t + 1)$  (where  $t$  is the latest time in the data), forecasts for time  $(t + 2)$  require values of time series 1 for time  $(t + 1)$ , which then requires a model for time series 1.

Hence, for each predictor-only series, a simple auto-regressive (AR) model is built using the same lag,  $L$ , as used for the target series. This model, called an AR( $L$ ) model, can be constructed using Algorithm 1 by specifying  $J_{sel}^0$  to be the target itself and setting the maximum number of predictors to be 1.

## 2.6 Post-estimation steps

Algorithm 1 selects the best predictors (time series) to model a target series  $\mathbf{y}$ . Without loss of generality, we assume that the model for  $\mathbf{y}$  is  $\mathbf{y} = \bar{\mathbf{y}} + \mathbf{X}_G^* \hat{\boldsymbol{\beta}}^* + \mathbf{r} = \hat{\mathbf{y}} + \mathbf{r}$ , where  $\mathbf{X}_G^*$  is the selected predictor series matrix with the lagged terms on the transformed scale,  $\hat{\boldsymbol{\beta}}^*$  is the estimated standardized coefficient vector, and  $\mathbf{r} = \mathbf{y} - \hat{\mathbf{y}}$  is the residual vector.

However, this is not the end of modeling. Several post processing steps are needed in order to complete the modeling process for  $\mathbf{y}$ . The steps include three parts: (1) coefficients and statistics inference; (2) tests of model effects; (3) model quality measures.

### 2.6.1 Coefficients and statistical inference

The results of Algorithm 1 include  $\hat{\boldsymbol{\beta}}^*$  and  $(\mathbf{X}^{*T} \mathbf{X}^*)^-$  (by solving the linear system from Cholesky decomposition), where superscript T means the transpose of a matrix or vector, and  $(\mathbf{z})^-$  is a generalized inverse of the  $\mathbf{z}$  matrix. Based on these quantities, the first step is to compute coefficient estimates, their standard errors, and statistical inference on the original scale.

Table 2: Additional notation

Notation	Description
$K$	Actual number of predictors selected (including target itself) for $\mathbf{y}$ , i.e., $K =  J_{sel} $ .
$p$	Number of coefficient estimates in $\hat{\boldsymbol{\beta}}^*$ , i.e., $p = K \times L$
$p^c$	Number of non-redundant coefficient estimates in $\hat{\boldsymbol{\beta}}^*$ , $p^c \leq p$
$\mathbf{X}_G^*$	Selected predictor series matrix with lagged terms on the transformed scale. This is an $(m - L) \times p$ matrix as $\mathbf{X}_G^* = [\mathbf{X}_{G_1}^*, \dots, \mathbf{X}_{G_K}^*]$ with $\mathbf{X}_{G_j}^* = G(\mathbf{X}^*, j, L) = [\mathbf{X}_{G_{j1}}^*, \dots, \mathbf{X}_{G_{jL}}^*]$ (an $(m - L) \times L$ matrix).
$\mathbf{X}_G$	Selected predictor series matrix on the original scale. This is an $(m - L) \times (p + 1)$ matrix as $\mathbf{X}_G = [\mathbf{1}, \mathbf{X}_{G_1}, \dots, \mathbf{X}_{G_K}] = [\mathbf{1}, \mathbf{X}_{G_{11}}, \dots, \mathbf{X}_{G_{1L}}, \dots, \mathbf{X}_{G_{K1}}, \dots, \mathbf{X}_{G_{KL}}]$ , where $\mathbf{1}$ is a column vector of 1's corresponding to an intercept.
$\hat{\boldsymbol{\beta}}$	Unstandardized coefficient estimates vector (corresponding to $\mathbf{X}_G$ ), which is a $(p + 1) \times$

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	1 vector. The first element, $\hat{\beta}_0$ , is the intercept estimate.
$\hat{\sigma}^2$	Estimated variance of the model based on residuals.
$\Sigma^*$	Covariance matrix of standardized coefficient estimates on the transformed scale, i.e., $\Sigma^* = \hat{\sigma}^2(\mathbf{X}_G^{*\top}\mathbf{X}_G^*)^{-}$ . The $j^{\text{th}}$ diagonal element is $\hat{\sigma}_{\hat{\beta}_j^*}^2$ and its square root, $\hat{\sigma}_{\hat{\beta}_j^*}$ , is the standard error of the $j^{\text{th}}$ standardized coefficient estimate.
$\Sigma$	Covariance matrix of unstandardized coefficient estimates on the original scale. The $j^{\text{th}}$ diagonal element is $\hat{\sigma}_{\hat{\beta}_j}^2$ and its square root, $\hat{\sigma}_{\hat{\beta}_j}$ , is the standard error of the $j^{\text{th}}$ unstandardized coefficient estimate.
$\mathbf{M}$	Centering vector of $\mathbf{X}$ , i.e., $\mathbf{M} = [M_1, \dots, M_p]^T$ , where $M_j = M(\mathbf{X}_j)$ is the mean of $\mathbf{X}_j$ .
$\mathbf{S}$	Scaling matrix of $\mathbf{X}$ , i.e., $\mathbf{S} = \text{diag}[S_1, \dots, S_p]$ , where $S_j = S(\mathbf{X}_j)$ is the standard deviation of $\mathbf{X}_j$ .
$\mathbf{A}$	Transformation matrix of $\mathbf{X}$ to $\mathbf{X}^*$ , i.e., $\mathbf{A} = \begin{bmatrix} -\mathbf{M}^T\mathbf{S}^{-1} \\ \mathbf{S}^{-1} \end{bmatrix}$ , which is a $(p+1) \times p$ vector. Note that $\mathbf{X}_G^* = \mathbf{X}_G\mathbf{A}$ .

The relationship between  $\hat{\boldsymbol{\beta}}$  and  $\hat{\boldsymbol{\beta}}^*$  is  $\hat{\boldsymbol{\beta}} = \mathbf{A}\hat{\boldsymbol{\beta}}^* + [\bar{y}, 0, \dots, 0]^T$  and the relationship between  $\Sigma$  and  $\Sigma^*$  is  $\Sigma = \mathbf{A}\Sigma^*\mathbf{A}^T$ . The relevant statistics are computed as follows:

- **Unstandardized coefficient estimates**

$$\hat{\beta}_j = S_j^{-1}\hat{\beta}_j^*, \quad j = 1, \dots, p \quad (3)$$

$$\hat{\beta}_0 = \bar{y} - \mathbf{M}^T\mathbf{S}^{-1}\hat{\boldsymbol{\beta}}^* \quad (4)$$

- **Standard errors of unstandardized coefficient estimates**

$$\hat{\sigma}_{\hat{\beta}_j} = \frac{\hat{\sigma}_{\hat{\beta}_j^*}}{S_j}, \quad j = 1, \dots, p \quad (5)$$

$$\hat{\sigma}_{\hat{\beta}_0} = \text{sqr}t \left( \begin{bmatrix} M_1 \\ S_1 \\ \vdots \\ M_p \\ S_p \end{bmatrix} \Sigma^* \begin{bmatrix} M_1 \\ S_1 \\ \vdots \\ M_p \\ S_p \end{bmatrix} \right) \quad (6)$$

where  $\Sigma^* = \hat{\sigma}^2(\mathbf{X}_G^{*\top}\mathbf{X}_G^*)^{-}$  and  $\hat{\sigma}^2 = SS_e/df_e$  with  $SS_e = \|\mathbf{y} - \hat{\mathbf{y}}\|_2^2 = \sum_{t=1}^{t=(m-L)} (y_t - \hat{y}_t)^2$  and  $df_e = m - L - p^c - 1$ .

- **t-statistics for coefficient estimates**

$$t_j = \frac{\hat{\beta}_j}{\hat{\sigma}_{\hat{\beta}_j}}, \quad j = 0, 1, \dots, p, \quad (7)$$

which follows an asymptotic  $t$  distribution with  $df_e$  degrees of freedom. Then the  $p$ -value is computed as

$$p_{t_j} = 2 \times \left(1 - \text{prob}(t_{df_e} \leq |t_j|)\right) \quad (8)$$

- **100(1 -  $\alpha$ )% confidence internals**

$$\hat{\beta}_j \pm \hat{\sigma}_{\hat{\beta}_j} \times t_{\alpha/2, df_e} \quad (9)$$

where  $\alpha$  is the significance level and  $t_{\alpha/2, df_e}$  is the  $100(1 - \alpha/2)^{\text{th}}$  percentile of the  $t$  distribution with  $df_e$  degrees of freedom.

## 2.6.2 Tests of model effects

For each selected predictor series for  $\mathbf{y}$ , there are  $L$  lagged columns associated with it. The columns can be grouped together, considered as an effect, and tested with a null hypothesis of zero for all coefficients. This is similar to the test of a categorical effect with all dummy variables in a (generalized) linear model setting. Only type III tests are conducted here. For each selected predictor series  $\mathbf{X}_{G,i}$ , the type III test matrix  $\mathbf{L}_i$  is constructed and  $H_0 : \mathbf{L}_i \boldsymbol{\beta} = \mathbf{0}$  is tested based on an F-statistic.

- **F-statistics for effects**

$$F_i = \frac{\hat{\boldsymbol{\beta}}^T \mathbf{L}_i^T (\mathbf{L}_i \boldsymbol{\Sigma} \mathbf{L}_i^T)^{-1} \mathbf{L}_i \hat{\boldsymbol{\beta}}}{r_i} \quad (10)$$

where  $r_i = \text{rank}(\mathbf{L}_i \boldsymbol{\Sigma} \mathbf{L}_i^T)$ . The statistic follows an approximate  $F$  distribution with the numerator degrees of freedom  $r_i$  and the denominator degrees of freedom  $df_e$ . Then the  $p$ -value is computed as follows:

$$p_{F_i} = 1 - \text{prob}(F_{r_i, df_e} \leq |F_i|) \quad (11)$$

## 2.6.3 Model quality measures

In addition to statistical inferences, the goodness of the model can be evaluated. The following model quality measures are provided:

- **Root Mean Squared Error (RMSE)**

$$RMSE = \sqrt{MSE} = \sqrt{\frac{SS_e}{df_e}} \quad (12)$$

Note that  $RMSE = \hat{\sigma}$ .

- **Root Mean Squared Percentage Error (RMSPE)**

$$RMSPE = \sqrt{MSPE} = \sqrt{\frac{\sum_{t=L+1}^m \left(\frac{y_t - \hat{y}_t}{y_t}\right)^2}{(m-L)}} \quad (13)$$

- **R squared**

$$R^2 = 1 - \frac{\sum_{t=1}^{t=(m-L)} (y_t - \hat{y}_t)^2}{\sum_{t=1}^{t=(m-L)} (y_t - \bar{y})^2} = 1 - \frac{SS_e}{SS_t} \quad (14)$$

- **Bayesian Information Criterion (BIC)**

$$BIC = (m - L) \ln \left( \frac{SS_e}{(m-L)} \right) + ((p^c + 1) \ln(m - L)) \quad (15)$$

- **Akaike Information Criterion (AIC)**

$$AIC = (m - L) \ln \left( \frac{SS_e}{(m-L)} \right) + 2(p^c + 1) \quad (15')$$

### 3. Scoring

Once the models  $(\hat{\beta}, J_{sel})$  for all the required targets ( $\mathbf{y}$ ) are built and post-estimation statistics are computed, the next task is to use these models to do scoring. There are two types of scoring: (1) fit: in-sample prediction for the past and current values of the target series; (2) forecast: out-of-sample prediction for future values of the target series.

#### 3.1 Fit

Without loss of generality, we assume  $\mathbf{X}$  and  $\mathbf{X}_G$  are the selected predictor series matrices without lagged terms and with lagged terms, respectively; and  $\hat{\beta}$  is the coefficient estimates vector for the target  $\mathbf{y}$ , so  $\mathbf{X} = [\mathbf{X}_1, \dots, \mathbf{X}_K]$ ,  $\mathbf{X}_G = [\mathbf{1}, \mathbf{X}_{G_{11}}, \dots, \mathbf{X}_{G_{1L}}, \dots, \mathbf{X}_{G_{K1}}, \dots, \mathbf{X}_{G_{KL}}]$  and  $\hat{\beta} = [\hat{\beta}_0, \hat{\beta}_{11}, \dots, \hat{\beta}_{1L}, \dots, \hat{\beta}_{K1}, \dots, \hat{\beta}_{KL}]^T$ . Given that all series have  $m$  time points, in-sample prediction of  $\mathbf{y}$  is one-step ahead prediction and can be written as

$$\hat{y}_t = \mathbf{X}_{G,t} \hat{\beta} = \hat{\beta}_0 + \sum_{j \in J_{sel}} \sum_{\ell=1}^L \hat{\beta}_{j,\ell} \cdot X_{G_{j,\ell},t} \quad (16)$$

$$= \hat{\beta}_0 + \sum_{j \in J_{sel}} \sum_{\ell=1}^L \hat{\beta}_{j,\ell} \cdot X_{j,t-\ell}; \quad t = L + 1, \dots, m. \quad (17)$$

The corresponding  $100(1 - \alpha)\%$  confidence interval of  $\mathbf{y}$  is

$$[\hat{y}_t - t_{\alpha/2, df_e} \times \hat{\sigma}, \hat{y}_t + t_{\alpha/2, df_e} \times \hat{\sigma}]; \quad t = L + 1, \dots, m. \quad (18)$$

#### 3.2 Forecast

Given that data is available up to time interval  $m$ , the one-step ahead forecast for  $\mathbf{y}$  is

$$\hat{y}_m(1) = \hat{\beta}_0 + \sum_{j \in J_{sel}} \sum_{\ell=1}^L \hat{\beta}_{j,\ell} \cdot X_{j,m+1-\ell} \quad (19)$$

The  $h$ -step ahead forecast for  $\mathbf{y}$  is

$$\hat{y}_m(h) = \hat{\beta}_0 + \sum_{j \in J_{sel}} \sum_{\ell=1}^L \hat{\beta}_{j,\ell} \cdot \hat{X}_{j,m+h-\ell} \quad (20)$$

where

$$\hat{X}_{j,m+h-\ell} = \begin{cases} X_{j,m+h-\ell}, & h \leq \ell \\ \hat{X}_{j,m}(h-\ell), & h > \ell \end{cases}$$

Thus, forecasting the value of  $y_{m+2}$  requires us to first forecast the values of all the predictors up to time  $(m+1)$ . Forecasting the values of all the predictors up to time  $(m+1)$  requires us to use Equation (19) on all the predictors  $j \in J_{sel}$ . Similarly, to predict the value of  $y_{m+3}$ , we need to forecast the values of predictors  $j \in J_{sel}$  at time  $(m+2)$  by using Equation (20). This task poses a bigger problem; to forecast the values of  $j \in J_{sel}$  at time  $(m+2)$ , we first need to forecast the values of the predictors of  $j \in J_{sel}$  at time  $(m+1)$ . That is, as we increasingly look into the future, we need to forecast more and more values to determine the value of  $y_{m+h}$ .

### 3.3 Approximated forecasting variances and intervals

In this subsection, we outline how forecasting variances and intervals can be computed for TCM models. We start by using the following representation for the linear model built by TCM for target  $y_{m+h}$ :

$$y_{m+h} = \hat{\beta}_0 + \sum_{j \in J_{sel}} \sum_{\ell=1}^L \hat{\beta}_{j,\ell} \cdot X_{j,m+h-\ell} + \varepsilon_{m+h} \quad (21)$$

where  $\varepsilon_{m+h} \sim N(0, \sigma^2)$  and  $\sigma^2$  is estimated as  $\hat{\sigma}^2$  (computed in Section 2.6.1). Please note that we don't include parameter estimation error when defining forecasting error in TCM.

The forecasting error at  $m+1$  is defined as the difference between  $y_{m+1}$  and  $\hat{y}_m(1)$ , which can be written as

$$e_{y,m}(1) = y_{m+1} - \hat{y}_m(1) = \varepsilon_{m+1} \quad (22)$$

The forecasting variance for one-step ahead forecasts is computed as  $\hat{\sigma}^2$ . For multi-step ahead forecasts, the forecasting error at  $m+h$  is

$$e_{y,m}(h) = y_{m+h} - \hat{y}_m(h) = \sum_{j \in J_{sel}} \sum_{\ell=1}^L \hat{\beta}_{j,\ell} \cdot e_{X_j,m}(h-\ell) + \varepsilon_{m+h} \quad (23)$$

where  $e_{X_j,m}(h-\ell) = X_{j,m+h-\ell} - \hat{X}_{j,m}(h-\ell)$  and  $e_{X_j,m}(h-\ell) = 0$  if  $h \leq \ell$ .

In general,  $e_{X_j,m}(1), \dots, e_{X_j,m}(h-\ell)$  are not independent of each other. The larger the  $h$  is, the more complex the dependence is. In addition,  $e_{X_j,m}(h-\ell)$  and  $e_{X_i,m}(h-\ell)$  might not be independent for  $j, i \in J_{sel}$ . In order to fully consider the dependence, we need to write all time series in vector autoregressive (VAR) format. Since we assume the number of series  $n$  is usually large, the parameter matrix, which is an  $n \times n$  matrix, might be too large to handle in computation of the forecasting variances. Therefore, we make the assumption that all forecasting error terms in Equation (23),  $e_{X_j,m}(h-\ell), j \in J_{sel}, \ell = 1, \dots, L$ , are independent, so it is easier to compute the forecasting variances.

Based on the above independence assumption, the approximated variance of the forecasting error,  $e_{y,m}(h)$ , is

$$\hat{\sigma}_{e_{y,m},h}^2 = \sum_{j \in J_{sel}} \sum_{\ell=1}^L \hat{\beta}_{j,\ell}^2 \hat{\sigma}_{e_{X_j,m},h-\ell}^2 + \hat{\sigma}^2 \quad (24)$$

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where  $\hat{\sigma}_{e_{X_j, m, h-\ell}}^2$  is the variance of the forecasting error in the series  $X_j$  at  $m + h - \ell$ .

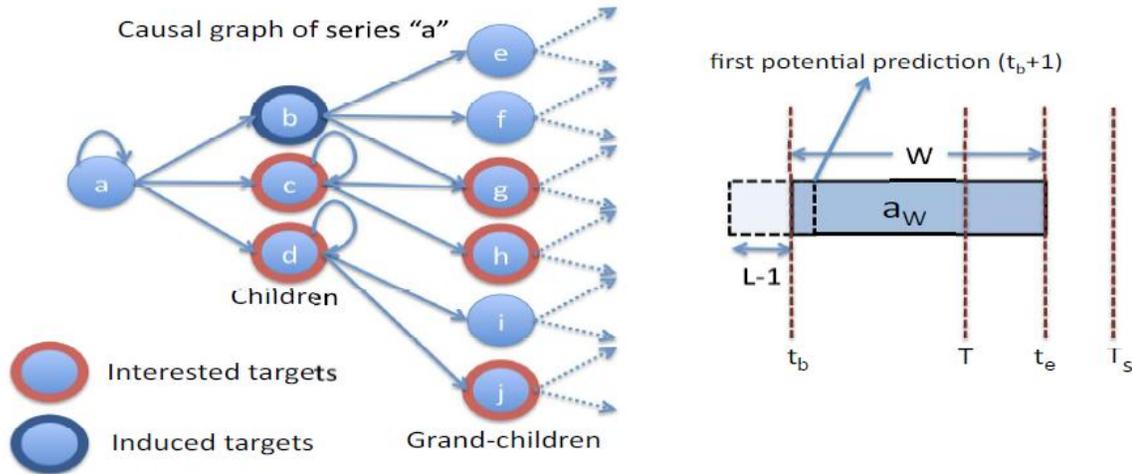
Then the corresponding  $100(1 - \alpha)\%$  approximated forecasting interval of  $y_{m+h}$  can be expressed as

$$\left[ \hat{y}_m(h) - t_{\alpha/2, df_e} \times \hat{\sigma}_{e_{y, m, h}}, \hat{y}_m(h) + t_{\alpha/2, df_e} \times \hat{\sigma}_{e_{y, m, h}} \right] \quad (25)$$

## 4. Scenario analysis

Scenario analysis refers to a capability of TCM to “play-out” the repercussions of artificially setting the value of a time series. A scenario is the set of forecasts that are generated by substituting the values of a *root* time series by a vector of substitute values, as illustrated in Figure 1.

Figure 1: Causal graph of a root time series and the specification of the vector of substitute values



During scenario analysis, we specify the targets that we want to analyze as a response to changes in the values of the root series (“a” in Figure 1), along with the time window. In Figure 1, we are interested in the behavior of time series “c”, “d”, “g”, “h”, and “j” *only*. The rest of the time series are ignored. The figure also depicts the vector  $\mathbf{a}_W$  of values for “a” that should be used instead of the observed or predicted values of “a”. The values  $(t_b, t_e, T, T_s)$  specify the beginning and end of the replacement values for the root series, the current time, and the farthest time for analysis, respectively.

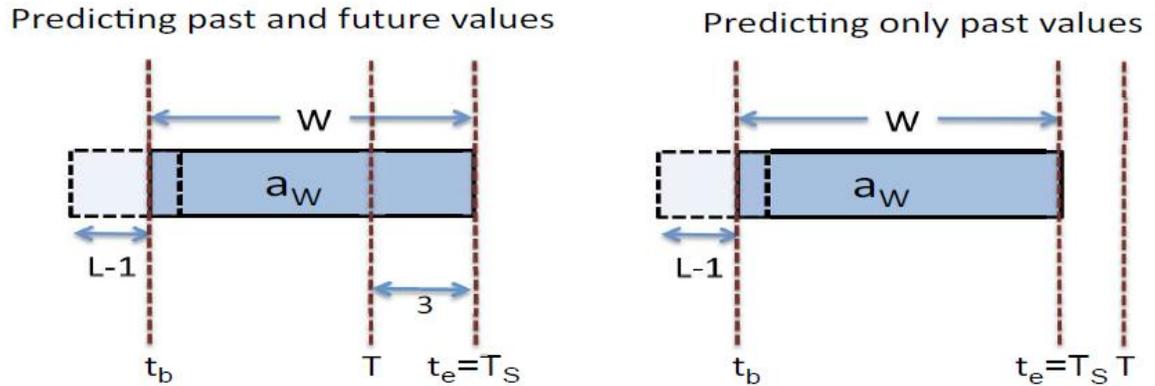
The partial Granger causal graph of time series “a” is shown in Figure 1. That is, “a” is the parent of itself, “b”, “c”, and “d”. Similarly, it is the grand-parent of “e”, “f”, “g”, “h”, “i”, and “j”. Further descendents are possible, but only two generations suffice for the sake of explanation. Figure 1 also displays the specification of the vector  $\mathbf{a}_W$ , of length  $W$ , that contains the replacement values of the root series. In the example shown in the figure,  $\mathbf{a}_W$  starts at time  $t_b < T$ , where  $T$  is the current time, and ends at  $t_e > T$ , which is in the future. We are also given  $T_s$ , the last time point ( $t_e \leq T_s$ ) for which we want to perform scenario analysis on the target variables. Finally, we are given a set of time series for which the scenario predictions are carried out. In the figure, these are “c”, “d”, “g”, “h”, and “j”, which are marked with a thick red border. Since “b” is required to model “g”, “b” is marked with a thick blue border to signify that it is an induced target. Given this information, the goal of scenario analysis is to forecast the

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values of the target time series (“c”, “d”, “g”, “h”, and “j”) up to time  $T_s$ , based on the values of the root time series  $\mathbf{a}_W$ .

Notice that we have to predict values of targets up to time  $T_s$ , where  $T_s$  can be  $> (T + 1)$  or  $\leq (T + 1)$ . When  $T_s = (T + 2)$ , we need to compute the values of the predictors of the target time series at time  $(T + 1)$ . Similarly, when  $T_s = (T + 3)$ , we need to compute the values of the predictors’ predictors at time  $(T + 1)$  and the values of the predictors at time  $(T + 2)$  before predicting the values of the target time series at time  $(T + 3)$ .

Figure 2: Scenarios with and without predicting future values



The left-hand panel in Figure 2 depicts a scenario where the values of ancestors of targets of interest also have to be predicted. In this particular case,  $T_s = (T + 3)$  and therefore it is necessary to predict the values of the predictors of the targets at  $(T + 1)$  and  $(T + 2)$ , and values of the predictors’ predictors at time  $(T + 1)$ . The right-hand panel depicts a scenario where the entire period of prediction is earlier than the current time  $T$  (i.e.,  $T_s < T$ ). In this case, all the values of the predictors and their ancestors are readily available.

### Determining $\mathbf{a}_W$

In the discussion above, we have neglected the issue of  $\mathbf{a}_W$ , the substitute values for time series “a”, which is the root time series. For purposes of scenario analysis, it is sufficient to consider that  $\mathbf{a}_W$  is readily available. In a typical use case for scenario analysis,  $\mathbf{a}_W$  will come from the values specified by the user’s direct input, although its values could also come as input from a calling meta-process (as is the case with the use of scenario analysis as a sub-procedure in root cause analysis, as shown in Section 6).

### Caveat on scenario analysis

It is possible to carry out scenario analysis for a time period that is entirely in the future; that is  $t_b > T$ . However, forecasting errors in the remaining predictors may make such scenario analysis inherently low-precision. That is, if  $\theta = t_b - T$  and  $t_b > T$ , then the precision of scenario analysis decreases with an increase in  $\theta$ .

## 4.1 SA, the scenario analysis algorithm

### Input:

The inputs to SA are: (1)  $\mathbf{r}$ : the root time series; (2)  $\mathbf{r}_W$ : the vector of replacement values for time series  $\mathbf{r}$ ; (3)  $(t_b, t_e, T, T_s)$ : the beginning and end time for the modified values of  $\mathbf{r}$ , the current time, and the last time point for

## Temporal Causal Modeling Algorithms

which target values need to be predicted, respectively; (4)  $D$ : a set of descendant target time series of interest along with their relation to  $\mathbf{r}$  (which may be input as the Granger causal graph,  $G$ ). Notice that the length of  $\mathbf{r}_W$  is  $t_e - t_b + 1$  and  $t_e \leq T_s$ . Furthermore, it is erroneous to have a target  $\mathbf{d} \in D$ , where  $\mathbf{r}$  is not an ancestor of  $\mathbf{d}$ .

### Output:

For each  $\mathbf{d}$  in  $D$ , we output a vector  $\mathbf{d}_{sa}$  containing values that pertain to the scenario analysis of these time series and the corresponding confidence intervals (when  $T_s \leq T$ ) or approximated forecasting intervals (when  $T_s > T$ ). Please note that the time period for the children series in  $D$  is  $[t_b + 1, T_s]$ , for the grand-children series is  $[t_b + 2, T_s]$ , etc.

### Preparation:

To prepare for SA, we first calculate the closure on the set of targets  $D^*$  that need to be predicted, which is determined by the relationship between  $\mathbf{r}$  and each of the targets in  $D$ . Essentially,  $D^*$  is computed by iteratively looking at the path from each  $\mathbf{d} \in D$  and adding all those intermediate nodes that are ancestors of  $\mathbf{d}$  and are also descendants of  $\mathbf{r}$ . In the example shown in Figure 1, the time series “b” is itself not of primary interest, but since it is a parent of “g”, which is of interest, “b” is also added as a target of interest to the set {“c”, “d”, “g”, “h”, “j”}.

Next, we compute  $M$ , the set of models that need to be included in order to perform scenario analysis on  $D^*$ . Obviously,  $M$  contains the models for each of the series in  $D^*$ , i.e.,  $D^* \subset M$ ; however, depending on the time span of the scenario analysis, additional models of some time series might have to be brought in (see Figure 2). Basically, depending on how far ahead  $T_s$  is from  $T$ , we may need to compute the values of the ancestors (other than  $\mathbf{r}$ ) of the targets of interest at time points  $(T + 1), \dots, (T_s - 1)$ . That is, the set  $\{M - D^*\}$  (which may be  $\emptyset$ ) contains all series that are needed for scenario analysis and are not descendants of  $\mathbf{r}$ .

At the end of the preparation phase we have  $D^*$  and  $M$ , which allows us to predict all the time series of interest.

### Computation:

The computation in scenario analysis is exactly that of scoring the values of a set of time series (see Section 3). For each target in  $D^*$ , we have a range of time points for which we need to fit/forecast values. For example, for immediate children of the root (“c”, “d”, and the induced child “b” in Figure 1), this range is  $[t_b + 1, T_s]$ . Similarly, for grand-children (“g”, “h”, and “j” in Figure 1), this range is  $[t_b + 2, T_s]$ . Using the models in  $M$  and substituted values  $\mathbf{r}_W$  for  $\mathbf{r}$ , this task can be carried out.

## 5. Outlier detection

One of the advantages of building TCM models is the ability to detect model-based outliers. Outliers can be defined in several ways. For now, we shall define an outlier in a time series to be a value that strays too far from its expected (fitted) value based on the TCM models. The detection process is based on the normal distribution assumption for series  $\mathbf{y}$ . Consider the value of a time series  $\mathbf{y}$  at time  $t$ . Let  $y_t$  and  $\hat{y}_t$  be the observed and expected values of  $\mathbf{y}$  at time  $t$ , respectively; and  $\hat{\sigma}^2$  be the variance of  $\mathbf{y}$  from the TCM model (based on residuals). Given these inputs, we call  $y_t$  an outlier if the likelihood of  $y_t$  when modeled as a normal random variable with mean  $\hat{y}_t$  and variance  $\hat{\sigma}^2$  is below a particular threshold.

**Input:**

The inputs to OD (outlier detection) are: (1)  $y_t, \forall t$ ; (2)  $\hat{y}_t, \forall t$ ; (3)  $\hat{\sigma}^2$ ; (4) the outlier threshold value  $\kappa \in (0,1]$  (the default is 0.95).

**Computation:**

- a) Under the assumption that the observed value  $y_t$  is a normal random variable with mean  $\hat{y}_t$  and variance  $\hat{\sigma}^2$ , compute the square score at time  $t$  as

$$s_{sqr,t} = \frac{(y_t - \hat{y}_t)^2}{\hat{\sigma}^2} \quad (26)$$

- b) Compute the outlier probability as

$$p_{sqr,t} = \text{prob}(\chi_1^2 \leq s_{sqr,t}) \quad (27)$$

where  $\chi_1^2$  is a random variable with a chi-squared distribution with 1 degree of freedom.

- c) Flag  $y_t$  as an outlier if  $p_{sqr,t} \geq \kappa$ .

**Output:**

The output to OD for series  $\mathbf{y}$  is a set of time points with their corresponding outlier probabilities.

## 6. Outlier root cause analysis

In Section 5, we saw how to detect outliers. The next logical step is to find the likely causes for a time series whose value has been flagged as an outlier. Outlier root cause analysis refers to the capability to explore the Granger causal graph in order to analyse the key/root values that resulted in the outlier under question. To formalize this notion, consider a time series  $\mathbf{y}$ , whose observed value at time  $t$  (that is,  $y_t$ ) has been flagged as an outlier due to its abnormal deviation from its expected value  $\hat{y}_t$ . The goal of outlier root cause analysis (*ORCA*) is to output the set of time series  $\mathcal{A}$  that can be considered as root causes of the anomalous value of  $y_t$ . The idea is that setting the values of time series in the predictor set  $\mathbf{X}$  to their normal/expected values, instead of their observed values, will bring the outlying  $y_t$  back to normal. The normal value of  $y_t$  is unknown so we specify it with the expected value of  $\mathbf{y}$  at time  $t$  as predicted by  $\mathbf{y}$ 's univariate model, which is an  $\text{AR}(L)$  model, and denoted as  $\tilde{y}_t$ .

The result of *ORCA* has the following objective function with a constraint as follows:

$$\arg \max_{x \in \mathcal{A}_y} |\hat{y}_t - \tilde{y}_t| - |\hat{y}_{t|x=\hat{x}} - \tilde{y}_t| \quad (28)$$

$$\text{s. t. } |\hat{y}_t - \tilde{y}_t| \geq |\hat{y}_{t|x=\hat{x}} - \tilde{y}_t|$$

where  $\mathcal{A}_y$  corresponds to the set of ancestors of  $\mathbf{y}$  according to the Granger causal graph  $G$ . The quantity  $\hat{y}_{t|x=\hat{x}}$  should be interpreted as the likely predicted value of  $y$  at time  $t$  had the value of its ancestor  $x$  been set to its expected value of  $\hat{x}$ . We see that Equation (28) is made up of two parts: (1) the portion  $|\hat{y}_t - \tilde{y}_t|$ , which is the

degree of “outlier-ness” of  $y$  at  $t$  as predicted by the “Granger model”, where the outlier-ness is judged based on what is expected from the history of  $y$ ; (2) the portion  $|\hat{y}_{t|x=\hat{x}} - \tilde{y}_t|$ , which is the degree of “outlier-ness” of  $y$  at  $t$  as predicted by the “Granger model”, if  $x$  was corrected. In other words, Equation (28) amounts to replacing the observed value  $y_t$  by its “expected” value, given by a simpler, univariate model. Therefore Equation (28) expresses the reduction in the degree of outlier-ness in  $y_t$  brought about by correcting  $x$ .

## 6.1 ORCA, the outlier root cause analysis algorithm

### Input:

The inputs to *ORCA* are: (1)  $y$ , the anomalous time series; (2)  $t$ , the time at which the anomaly was detected; (3)  $y_t$ , the anomalous value; (4)  $\hat{y}_t$ , the expected value of  $y_t$ ; (5)  $k$ , the oldest generation of ancestors to search based on the Granger causal graph,  $G$ .

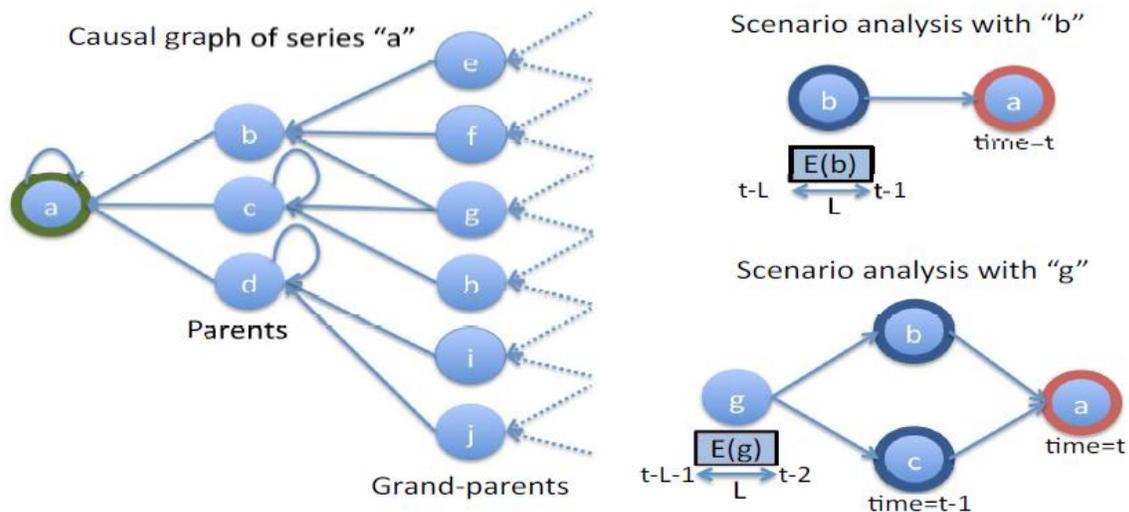
### Output:

*ORCA* outputs the set of root causes  $\mathcal{A}$  of the anomaly in  $y_t$ , where each  $x \in \mathcal{A}$  maximizes the objective function in Equation (28) by the same amount.

### Preparation:

To prepare for *ORCA*, we first compute  $\mathcal{A}_y$ , the set of ancestors that need to be examined as the potential root causes of the anomaly in  $y_t$ .

Figure 3: Outlier root cause analysis for a time series



In the example shown in Figure 3, assuming that  $y = "a"$  and  $k = 2$ , then  $\mathcal{A}_y = \{ "b", "c", "d", "e", "f", "g", "h", "i", "j" \}$ .  $\mathcal{A}_y$  can be computed by performing a reverse breadth-first search from  $y$  to  $k$  levels.

Second, each potential root cause  $x \in \mathcal{A}_y$  is prepped for scenario analysis by computing the vector of substitute values of  $x$  to be used during scenario analysis. Note that the length of this substitute vector is  $L$ , the lag. For

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example, consider  $\mathbf{b}_L$ , the substitute for time series “b” in Figure 3. As “b” is a parent of “a”, we need to compute the fits of “b” from  $(t - L)$  to  $(t - 1)$ . On the other hand, as “g” is a grand-parent of “a”,  $\mathbf{g}_L$  contains the fits for “g” from the time  $(t - L - 1)$  to  $(t - 2)$  (see Section 3.1 for computation of fits). Please note that this approach assumes that any anomalies are purely in “b” (the parent series) or “g” (the grandparent series). In particular, it is assumed that anomalies in “b” are not caused by values in the grandparent series, including anomalous values in the grandparent series.

Third, for each potential root cause  $\mathbf{x} \in \mathcal{A}_y$ , scenario analysis is carried out (see Section 4) using the substitute values computed in the previous step. For the example in Figure 3, scenario analysis is called for series “b” with the parameters ( $\mathbf{r} = \mathbf{b}, \mathbf{r}_W = \mathbf{b}_L, t_b = (t - L), t_e = (t - 1), T = t, D = \{\mathbf{a}\}, T_s = t$ ). And the result of scenario analysis is  $\hat{y}_{t|x=\hat{x}}$ .

### Computation:

The process of *ORCA* is as follows:

- Initialize  $\mathcal{A}$ , the set of potential root causes for  $y_t$ , to  $\emptyset$ .  
Initialize  $obj_{max}$ , the maximum objective function value, to 0.
- Suppose there are  $J$  series in  $\mathcal{A}_y, \mathbf{x}_1, \dots, \mathbf{x}_J$ .  
For each  $\mathbf{x}_j, j \in 1, \dots, J$ , compute  $obj_j = |\hat{y}_t - \tilde{y}_t| - |\hat{y}_{t|x_j=\hat{x}_j} - \tilde{y}_t|$ .  
If  $obj_j \geq obj_{max}$ , set  $obj_{max} = obj_j$  and store  $\mathbf{x}_j$  in  $\mathcal{A}$ .

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# Time Series Algorithms

The Time Series node builds univariate exponential smoothing, ARIMA (Autoregressive Integrated Moving Average), and transfer function (TF) models for time series, and produces forecasts. The procedure includes an Expert Modeler that identifies and estimates an appropriate model for each dependent variable series. Alternatively, you can specify a custom model.

This algorithm is designed with help from professor Ruey Tsay at The University of Chicago.

## Notation

The following notation is used throughout this chapter unless otherwise stated:

$Y_t$ ( $t=1, 2, \dots, n$ )	Univariate time series under investigation.
$n$	Total number of observations.
$\hat{Y}_t(k)$	Model-estimated $k$ -step ahead forecast at time $t$ for series $Y$ .
$S$	The seasonal length.

## Models

The Time Series node estimates exponential smoothing models and ARIMA/TF models.

### Exponential Smoothing Models

The following notation is specific to exponential smoothing models:

$\alpha$	Level smoothing weight
$\gamma$	Trend smoothing weight
$\phi$	Damped trend smoothing weight
$\delta$	Season smoothing weight

#### Simple Exponential Smoothing

Simple exponential smoothing has a single level parameter and can be described by the following equations:

$$L(t) = \begin{cases} \alpha Y(t) + (1 - \alpha)L(t - 1), & \text{if } Y(t) \text{ is not missing} \\ L(t - 1), & \text{else} \end{cases}$$

$$\hat{Y}_t(k) = L(t)$$

It is functionally equivalent to an ARIMA(0,1,1) process.

### **Brown's Exponential Smoothing**

Brown's exponential smoothing has level and trend parameters and can be described by the following equations:

$$L(t) = \begin{cases} \alpha Y(t) + (1 - \alpha)L(t-1), & \text{if } Y(t) \text{ is not missing} \\ L(t-1) + T(t-1), & \text{else} \end{cases}$$

$$T(t) = \begin{cases} \alpha(L(t) - L(t-1)) + (1 - \alpha)T(t-1), & \text{if } Y(t) \text{ is not missing} \\ T(t-1), & \text{else} \end{cases}$$

$$\hat{Y}_t(k) = L(t) + ((k-1) + \alpha^{-1})T(t)$$

It is functionally equivalent to an ARIMA(0,2,2) with restriction among MA parameters.

### **Holt's Exponential Smoothing**

Holt's exponential smoothing has level and trend parameters and can be described by the following equations:

$$L(t) = \begin{cases} \alpha Y(t) + (1 - \alpha)(L(t-1) + T(t-1)), & \text{if } Y(t) \text{ is not missing} \\ L(t-1) + T(t-1), & \text{else} \end{cases}$$

$$T(t) = \begin{cases} \gamma(L(t) - L(t-1)) + (1 - \gamma)T(t-1), & \text{if } Y(t) \text{ is not missing} \\ T(t-1), & \text{else} \end{cases}$$

$$\hat{Y}_t(k) = L(t) + kT(t)$$

It is functionally equivalent to an ARIMA(0,2,2).

### **Damped-Trend Exponential Smoothing**

Damped-Trend exponential smoothing has level and damped trend parameters and can be described by the following equations:

$$L(t) = \begin{cases} \alpha Y(t) + (1 - \alpha)(L(t-1) + \varphi T(t-1)), & \text{if } Y(t) \text{ is not missing} \\ L(t-1) + \varphi T(t-1), & \text{else} \end{cases}$$

$$T(t) = \begin{cases} \gamma(L(t) - L(t-1)) + (1 - \gamma)\varphi T(t-1), & \text{if } Y(t) \text{ is not missing} \\ \varphi T(t-1), & \text{else} \end{cases}$$

$$\hat{Y}_t(k) = L(t) + \sum_{i=1}^k \phi^i T(t)$$

It is functionally equivalent to an ARIMA(1,1,2).

### Simple Seasonal Exponential Smoothing

Simple seasonal exponential smoothing has level and season parameters and can be described by the following equations:

$$L(t) = \begin{cases} \alpha(Y(t) - S(t-s)) + (1-\alpha)L(t-1), & \text{if } Y(t) \text{ is not missing} \\ L(t-1), & \text{else} \end{cases}$$

$$S(t) = \begin{cases} \delta(Y(t) - L(t)) + (1-\delta)S(t-s), & \text{if } Y(t) \text{ is not missing} \\ S(t-s) & \text{else} \end{cases}$$

$$\hat{Y}_t(k) = L(t) + S(t+k-s)$$

It is functionally equivalent to an ARIMA(0,1,(1,s,s+1))(0,1,0) with restrictions among MA parameters.

### Winters' Additive Exponential Smoothing

Winters' additive exponential smoothing has level, trend, and season parameters and can be described by the following equations:

$$L(t) = \begin{cases} \alpha(Y(t) - S(t-s)) + (1-\alpha)(L(t-1) + T(t-1)), & \text{if } Y(t) \text{ is not missing} \\ L(t-1) + T(t-1), & \text{else} \end{cases}$$

$$T(t) = \begin{cases} \gamma(L(t) - L(t-1)) + (1-\gamma)T(t-1), & \text{if } Y(t) \text{ is not missing} \\ T(t-1), & \text{else} \end{cases}$$

$$S(t) = \begin{cases} \delta(Y(t) - L(t)) + (1-\delta)S(t-s), & \text{if } Y(t) \text{ is not missing} \\ S(t-s) & \text{else} \end{cases}$$

$$\hat{Y}_t(k) = L(t) + kT(t) + S(t+k-s)$$

It is functionally equivalent to an ARIMA(0,1,s+1)(0,1,0) with restrictions among MA parameters.

### Winters' Multiplicative Exponential Smoothing

Winters' multiplicative exponential smoothing has level, trend and season parameters and can be described by the following equations:

$$L(t) = \begin{cases} \alpha(Y(t)/S(t-s)) + (1-\alpha)(L(t-1) + T(t-1)), & \text{if } Y(t) \text{ is not missing} \\ L(t-1) + T(t-1), & \text{else} \end{cases}$$

$$T(t) = \begin{cases} \gamma(L(t) - L(t-1)) + (1-\gamma)T(t-1), & \text{if } Y(t) \text{ is not missing} \\ T(t-1), & \text{else} \end{cases}$$

$$S(t) = \begin{cases} \delta(Y(t)/L(t)) + (1-\delta)S(t-s), & \text{if } Y(t) \text{ is not missing} \\ S(t-s) & \text{else} \end{cases}$$

$$\hat{Y}_t(k) = (L(t) + kT(t))S(t+k-s)$$

There is no equivalent ARIMA model.

### Estimation and Forecasting of Exponential Smoothing

The sum of squares of the one-step ahead prediction error,  $\sum (Y_t - \hat{Y}_{t-1}(1))^2$ , is minimized to optimize the smoothing weights.

### Initialization of Exponential Smoothing

Let  $L$  denote the level,  $T$  the trend and,  $S$ , a vector of length  $s$ , denote the seasonal states. The initial smoothing states are made by back-casting from  $t=n$  to  $t=0$ . Initialization for back-casting is described here.

For all the models  $L = y_n$ .

For all non-seasonal models with trend,  $T$  is the negative of the slope of the line (with intercept) fitted to the data with time as a regressor.

For the simple seasonal model, the elements of  $S$  are seasonal averages minus the sample mean; for example, for monthly data the element corresponding to January will be average of all January values in the sample minus the sample mean.

For the additive Winters' model, fit  $y = \alpha t + \sum_{i=1}^s \beta_i I_i(t)$  to the data where  $t$  is time and  $I_i(t)$  are seasonal dummies. Note that the model does not have an intercept. Then  $T = -\alpha$ , and  $S = \beta - \text{mean}(\beta)$ .

For the multiplicative Winters' model, fit a separate line (with intercept) for each season with time as a regressor. Suppose  $\mu$  is the vector of intercepts and  $\beta$  is the vector of slopes (these vectors will be of length  $s$ ). Then  $T = -\text{mean}(\beta)$  and  $S = (\mu + \beta) / (\text{mean}(\mu) + \text{mean}(\beta))$ .

The initial smoothing states are:

$$L' = L(0)$$

$$T' = -T(0)$$

$$S' = (S(1-s), S(2-s), \dots, S(-1), S(0)) = (S(1), S(2), \dots, S(-1+s), S(0))$$

### ARIMA and Transfer Function Models

The following notation is specific to ARIMA/TF models:

$a_t (t = 1, 2, \dots, n)$	White noise series normally distributed with mean zero and variance $\sigma^2$
$p$	Order of the non-seasonal autoregressive part of the model
$q$	Order of the non-seasonal moving average part of the model
$d$	Order of the non-seasonal differencing
$P$	Order of the seasonal autoregressive part of the model
$Q$	Order of the seasonal moving-average part of the model
$D$	Order of the seasonal differencing

$s$	Seasonality or period of the model
$\phi_p(B)$	AR polynomial of B of order p, $\phi_p(B) = 1 - \varphi_1 B - \varphi_2 B^2 - \dots - \varphi_p B^p$
$\theta_q(B)$	MA polynomial of B of order q, $\theta_q(B) = 1 - \vartheta_1 B - \vartheta_2 B^2 - \dots - \vartheta_q B^q$
$\Phi_P(B^s)$	Seasonal AR polynomial of BS of order P, $\Phi_P(B^s) = 1 - \Phi_1 B^s - \Phi_2 B^{s^2} - \dots - \Phi_P B^{s^P}$
$\Theta_Q(B^s)$	Seasonal MA polynomial of BS of order Q, $\Theta_Q(B^s) = 1 - \Theta_1 B^s - \Theta_2 B^{s^2} - \dots - \Theta_Q B^{s^Q}$
$\Delta$	Differencing operator $\Delta = (1 - B)^d(1 - B^s)^D$
$B$	Backward shift operator with $BY_t = Y_{t-1}$ and $Ba_t = a_{t-1}$
$Z\sigma_t^2$	Prediction variance of $Z_t$
$N\sigma_t^2$	Prediction variance of the noise forecasts

Transfer function (TF) models form a very large class of models, which include univariate ARIMA models as a special case. Suppose  $Y_t$  is the dependent series and, optionally,  $X_{1t}, X_{2t}, \dots, X_{kt}$  are to be used as predictor series in this model. A TF model describing the relationship between the dependent and predictor series has the following form:

$$Z_t = f(Y_t),$$

$$\Delta Z_t = \mu + \sum_{i=1}^k \frac{Num_i}{Den_i} \Delta_i B^{b_i} f_i(X_{it}) + \frac{MA}{AR} a_t.$$

The univariate ARIMA model simply drops the predictors from the TF model; thus, it has the following form:

$$\Delta Z_t = \mu + \frac{MA}{AR} a_t$$

The main features of this model are:

- An initial transformation of the dependent and predictor series,  $f$  and  $f_i$ . This transformation is optional and is applicable only when the dependent series values are positive. Allowed transformations are log and square root. These transformations are sometimes called variance-stabilizing transformations.
- A constant term  $\mu$ .
- The unobserved i.i.d., zero mean, Gaussian error process  $a_t$  with variance  $\sigma^2$ .
- The moving average lag polynomial  $MA = \theta_q(B)\Theta_Q(B^s)$  and the auto-regressive lag polynomial  $AR = \phi_p(B)\Phi_P(B^s)$ .
- The difference/lag operators  $\Delta$  and  $\Delta_i$ .
- A delay term,  $B^{b_i}$ , where  $b_i$  is the order of the delay
- Predictors are assumed given. Their numerator and denominator lag polynomials are of the form:  $Num_i = (\omega_{i0} - \omega_{i1}B - \dots - \omega_{iu}B^u)(1 - \Omega_{i1}B^s - \dots - \Omega_{iv}B^{vs})B^b$  and  $Den_i = (1 - \delta_{i1}B - \dots - \delta_{ir}B^r)(1 - \Delta_{i1}B^s - \dots)$ .
- The “noise” series

$$N_t = \Delta Z_t - \mu - \sum_{i=1}^k \frac{Num_i}{Den_i} \Delta_i B^{b_i} X_{it}$$

is assumed to be a mean zero, stationary ARMA process.

### **Interventions and Events**

Interventions and events are handled like any other predictor; typically they are coded as 0/1 variables, but note that a given intervention variable's exact effect upon the model is determined by the transfer function in front of it.

### **Estimation and Forecasting of ARIMA/TF**

There are two forecasting algorithms available: Conditional Least Squares (CLS) and Exact Least Squares (ELS) or Unconditional Least Squares forecasting (ULS). These two algorithms differ in only one aspect: they forecast the noise process differently. The general steps in the forecasting computations are as follows:

1. Computation of noise process  $N_t$  through the historical period.
2. Forecasting the noise process  $N_t$  up to the forecast horizon. This is one step ahead forecasting during the historical period and multi-step ahead forecasting after that. The differences in CLS and ELS forecasting methodologies surface in this step. The prediction variances of noise forecasts are also computed in this step.
3. Final forecasts are obtained by first adding back to the noise forecasts the contributions of the constant term and the transfer function inputs and then integrating and back-transforming the result. The prediction variances of noise forecasts also may have to be processed to obtain the final prediction variances.

Let  $\hat{N}_t(k)$  and  $\sigma_t^2(k)$  be the  $k$ -step forecast and forecast variance, respectively.

### **Conditional Least Squares (CLS) Method**

$\hat{N}_t(k) = E(N_{t+k} | N_t, N_{t-1}, \dots)$  assuming  $N_t = 0$  for  $t < 0$ .

$$\sigma_t^2(k) = \sigma^2 \sum_{j=0}^{k-1} \psi_j^2$$

where  $\psi_j$  are coefficients of the power series expansion of  $MA / (\Delta \times AR)$ .

Minimize  $S = \Sigma (N_t - \hat{N}_t(1))^2$ .

Missing values are imputed with forecast values of  $N_t$ .

### **Maximum Likelihood (ML) Method (Brockwell and Davis, 1991)**

$\hat{N}_t(k) = E(N_{t+k} | N_t, N_{t-1}, \dots, N_1)$

Maximize likelihood of  $\left\{N_t - \hat{N}_t(1)\right\}_{t=1}^n$ ; that is,

$$L = -\ln(S/n) - (1/n) \sum_{j=1}^n \ln(\eta_j)$$

where  $S = \sum (N_t - \hat{N}_t(1))^2 / \eta_t$ , and  $\sigma_t^2 = \sigma^2 \eta_t$  is the one-step ahead forecast variance.

When missing values are present, a Kalman filter is used to calculate  $\hat{N}_t(k)$ .

### **Error Variance**

$$\hat{\sigma}^2 = S / (n - k)$$

in both methods. Here  $n$  is the number of non-zero residuals and  $k$  is the number of parameters (excluding error variance).

### **Initialization of ARIMA/TF**

A slightly modified Levenberg-Marquardt algorithm is used to optimize the objective function. The modification takes into account the “admissibility” constraints on the parameters. The admissibility constraint requires that the roots of AR and MA polynomials be outside the unit circle and the sum of denominator polynomial parameters be non-zero for each predictor variable. The minimization algorithm requires a starting value to begin its iterative search. All the numerator and denominator polynomial parameters are initialized to zero except the coefficient of the 0th power in the numerator polynomial, which is initialized to the corresponding regression coefficient.

The ARMA parameters are initialized as follows:

Assume that the series  $Y_t$  follows an ARMA(p,q)(P,Q) model with mean 0; that is:

$$Y_t - \varphi_1 Y_{t-1} - \cdots - \varphi_p Y_{t-p} = a_t - \theta_1 a_{t-1} - \cdots - \theta_q a_{t-q}$$

In the following  $c_l$  and  $\rho_l$  represent the  $l$ th lag autocovariance and autocorrelation of  $Y_t$  respectively, and  $\hat{c}_l$  and  $\hat{\rho}_l$  represent their estimates.

### **Non-Seasonal AR Parameters**

For AR parameter initial values, the estimated method is the same as that in appendix A6.2 of (Box, Jenkins, and Reinsel, 1994). Denote the estimates as  $\hat{\varphi}'_1, \dots, \hat{\varphi}'_{p+q}$ .

### **Non-Seasonal MA Parameters**

Let

$$w_t = Y_t - \varphi_1 Y_{t-1} - \cdots - \varphi_p Y_{t-p} = a_t - \theta_1 a_{t-1} - \cdots - \theta_q a_{t-q}$$

The cross covariance

$$\lambda_l = E(w_{t+l}a_t) = E((a_{t+l} - \theta_1 a_{t+l-1} - \dots - \theta_q a_{t+l-q})a_t) = \begin{cases} \sigma_a^2 & l = 0 \\ -\theta_1 \sigma_a^2 & l = 1 \\ \dots & \dots \\ -\theta_q \sigma_a^2 & l = q \\ 0 & l > q \end{cases}$$

Assuming that an AR(p+q) can approximate  $Y_t$ , it follows that:

$$Y_t - \varphi'_1 Y_{t-1} - \dots - \varphi'_p Y_{t-p} - \varphi'_{p+1} Y_{t-p-1} - \dots - \varphi'_{p+q} Y_{t-p-q} = a_t$$

The AR parameters of this model are estimated as above and are denoted as  $\hat{\varphi}'_1, \dots, \hat{\varphi}'_{p+q}$ .

Thus  $\lambda_l$  can be estimated by

$$\begin{aligned} \lambda_l &\approx E\left((Y_{t+l} - \varphi_1 Y_{t+l-1} - \dots - \varphi_p Y_{t+l-p}) (Y_t - \varphi'_1 Y_{t-1} - \dots - \varphi'_{p+q} Y_{t-p-q})\right) \\ &= \left(\rho_l - \sum_{j=1}^{p+q} \varphi_j \rho_{l+j} - \sum_{i=1}^p \varphi_i \rho_{l-i} + \sum_{i=1}^p \sum_{j=1}^{p+q} \varphi_i \varphi_j \rho_{l+j-i}\right) c_0 \end{aligned}$$

And the error variance  $\sigma_a^2$  is approximated by

$$\hat{\sigma}_a^2 = Var\left(-\sum_{j=0}^{p+q} \varphi'_j Y_{t-j}\right) = \sum_{i=0}^{p+q} \sum_{j=0}^{p+q} \varphi'_i \varphi'_j c_{i-j} = c_0 \sum_{i=0}^{p+q} \sum_{j=0}^{p+q} \varphi'_i \varphi'_j \rho_{i-j}$$

with  $\hat{\varphi}'_0 = -1$ .

Then the initial MA parameters are approximated by  $\theta_l = -\lambda_l / \sigma_a^2$  and estimated by

$$\hat{\theta}_l = -\hat{\lambda}_l / \hat{\sigma}_a^2 = \frac{\rho_l - \sum_{j=1}^{p+q} \hat{\varphi}_j \rho_{l+j} - \sum_{i=1}^p \hat{\varphi}_i \rho_{l-i} + \sum_{i=1}^p \sum_{j=1}^{p+q} \hat{\varphi}_i \hat{\varphi}_j \rho_{l+j-i}}{\sum_{i=0}^{p+q} \sum_{j=0}^{p+q} \hat{\varphi}'_i \hat{\varphi}'_j \rho_{i-j}}$$

So  $\hat{\theta}_l$  can be calculated by  $\hat{\varphi}'_j, \hat{\varphi}_i$ , and  $\{\hat{\rho}_l\}_{l=1}^{p+2q}$ . In this procedure, only  $\{\hat{\rho}_l\}_{l=1}^{p+q}$  are used and all other parameters are set to 0.

### Seasonal parameters

For seasonal AR and MA components, the autocorrelations at the seasonal lags in the above equations are used.

### Calculation of the Transfer Function

The transfer function needs to be calculated for each predictor series. For the predictor series  $X_{it}$ , let the transfer function be:

$$V_{it} = \frac{Num_i}{Den_i} \Delta_i B^{b_i} f_i(X_{it})$$

It can be calculated as follows:

1. Calculate  $U_{it} = \Delta_i B^{b_i} f_i(X_{it})$
2. Recursively calculate

$$V_{it} = - \sum_{j=1}^{D_i} Cden_i(j) * V_{it-j} + \sum_{j=0}^{N_i} Cnum_i(j) * U_{it-j}$$

where  $Cden_i(j)$  and  $Cnum_i(j)$  are the coefficients of  $B^j$  in the polynomials  $Den_i$  and  $Num_i$  respectively. Likewise, the summation limits  $D_i$  and  $N_i$  are the maximum degree of  $B^j$  in the polynomials  $Den_i$  and  $Num_i$  respectively.

All missing  $V_{it-j}$  in the first term of  $V_{it}$  are taken to be  $V_{i,-\infty}$  and missing  $U_{it-j}$  in the second term are taken to be  $U_{i,-\infty}$ , where  $U_{i,-\infty}$  is the first non-missing measurement of  $U_{it}$ .  $V_{i,-\infty}$  is given by

$$V_{i,-\infty} = \frac{Num_i(1)}{Den_i(1)} * U_{i,-\infty}$$

where  $Num_i(1)$  and  $Den_i(1)$  are the  $Num_i$  and  $Den_i$  polynomials evaluated at  $B = 1$ .

### **Diagnostic Statistics**

ARIMA/TF diagnostic statistics are based on residuals of the noise process,  $R(t) = N(t) - \hat{N}(t)$ .

### **Ljung-Box Statistic**

$$Q(K) = n(n+2) \sum_{k=1}^K r_k^2 / (n-k)$$

where  $r_k$  is the kth lag ACF of residual.

$Q(K)$  is approximately distributed as  $\chi^2(K-m)$ , where  $m$  is the number of parameters other than the constant term and predictor related-parameters.

## **Outlier Detection in Time Series Analysis**

The observed series may be contaminated by so-called outliers. These outliers may change the mean level of the uncontaminated series. The purpose of outlier detection is to find if there are outliers and what are their locations, types, and magnitudes.

The Time Series node considers seven types of outliers. They are additive outliers (AO), innovational outliers (IO), level shift (LS), temporary (or transient) change (TC), seasonal additive (SA), local trend (LT), and AO patch (AOP).

## Notation

The following notation is specific to outlier detection:

$U(t)$  or  $U_t$       The uncontaminated series, outlier free. It is assumed to be a univariate ARIMA or transfer function model.

## Definitions of Outliers

Types of outliers are defined separately here. In practice any combination of these types can occur in the series under study.

### AO (Additive Outliers)

Assuming that an AO outlier occurs at time  $t=T$ , the observed series can be represented as

$$Y(t) = U(t) + wI_T(t)$$

where  $I_T(t) = \begin{cases} 0 & t \neq T \\ 1 & t = T \end{cases}$  is a pulse function and  $w$  is the deviation from the true  $U(T)$  caused by the outlier.

### IO (Innovational Outliers)

Assuming that an IO outlier occurs at time  $t=T$ , then

$$Y(t) = \mu(t) + \frac{\theta(B)}{\Delta\varphi(B)}(a(t) + wI_T(t))$$

### LS (Level Shift)

Assuming that a LS outlier occurs at time  $t=T$ , then

$$Y(t) = U(t) + wS_T(t)$$

where  $S_T(t) = \frac{1}{1-B}I_T(t) = \begin{cases} 0 & t < T \\ 1 & t \geq T \end{cases}$  is a step function.

### TC (Temporary/Transient Change)

Assuming that a TC outlier occurs at time  $t=T$ , then

$$Y(t) = U(t) + wD_T(t)$$

where  $D_T(t) = \frac{1}{1-\delta B}I_T(t)$ ,  $0 < \delta < 1$  is a damping function.

### SA (Seasonal Additive)

Assuming that a SA outlier occurs at time  $t=T$ , then

$$Y(t) = U(t) + wSS_T(t)$$

where  $SS_T(t) = \frac{1}{1-B^s} I_T(t) = \begin{cases} 1 & t = T + ks, k \geq 0 \\ 0 & o.w. \end{cases}$  is a step seasonal pulse function.

### LT (Local Trend)

Assuming that a LT outlier occurs at time  $t=T$ , then

$$Y(t) = U(t) + wT_T(t)$$

where  $T_T(t) = \frac{1}{(1-B)^2} I_T(t) = \begin{cases} t + 1 - T & t \geq T \\ 0 & o.w. \end{cases}$  is a local trend function.

### AOP (AO patch)

An AO patch is a group of two or more consecutive AO outliers. An AO patch can be described by its starting time and length. Assuming that there is a patch of AO outliers of length  $k$  at time  $t=T$ , the observed series can be represented as

$$Y(t) = U(t) + \sum_{i=1}^k w_i I_{T-1+i}(t)$$

Due to a masking effect, a patch of AO outliers is very difficult to detect when searching for outliers one by one. This is why the AO patch is considered as a separate type from individual AO. For type AO patch, the procedure searches for the whole patch together.

### Summary

For an outlier of type O at time  $t=T$  (except AO patch):

$$Y(t) = \mu(t) + wL_O(B) I_T(t) + \frac{\theta(B)}{\Delta\varphi(B)} a(t)$$

where

$$L_O(B) = \begin{cases} 1 & O = AO \\ 1/(\Delta\pi(B)) & O = IO \\ 1/(1-B) & O = LS \\ 1/(1-\delta B) & O = TC \\ 1/(1-B^s) & O = SA \\ 1/(1-B)^2 & O = LT \end{cases}$$

with  $\pi(B) = \varphi(B)/\theta(B)$ . A general model for incorporating outliers can thus be written as follows:

$$Y(t) = \mu(t) + \sum_{k=1}^M w_k L_{O_k}(B) I_{T_k}(t) + \frac{\theta(B)}{\Delta\varphi(B)} a(t)$$

where  $M$  is the number of outliers.

### **Estimating the Effects of an Outlier**

Suppose that the model and the model parameters are known. Also suppose that the type and location of an outlier are known. Estimation of the magnitude of the outlier and test statistics are as follows.

The results in this section are only used in the intermediate steps of outlier detection procedure. The final estimates of outliers are from the model incorporating all the outliers in which all parameters are jointly estimated.

#### **Non-AO Patch Deterministic Outliers**

For a deterministic outlier of any type at time T (except AO patch), let  $e(t)$  be the residual and  $x(t) = \pi(B) L(B) \Delta I_T(t)$ , so:

$$e(t) = wx(t) + a(t)$$

From residuals  $e(t)$ , the parameters for outliers at time T are estimated by simple linear regression of  $e(t)$  on  $x(t)$ .

For  $j = 1$  (AO), 2 (IO), 3 (LS), 4 (TC), 5 (SA), 6 (LT), define test statistics:

$$\lambda_j(T) = \frac{w_j(T)}{\sqrt{\text{Var}(w_j(T))}}$$

Under the null hypothesis of no outlier,  $\lambda_j(T)$  is distributed as  $N(0,1)$  assuming the model and model parameters are known.

#### **AO Patch Outliers**

For an AO patch of length  $k$  starting at time T, let  $x_i(t; T) = \pi(B) \Delta I_{T+i-1}(t)$  for  $i = 1$  to  $k$ , then

$$e(t) = \sum_{i=1}^k w_i(T) x_i(t; T) + a(t)$$

Multiple linear regression is used to fit this model. Test statistics are defined as:

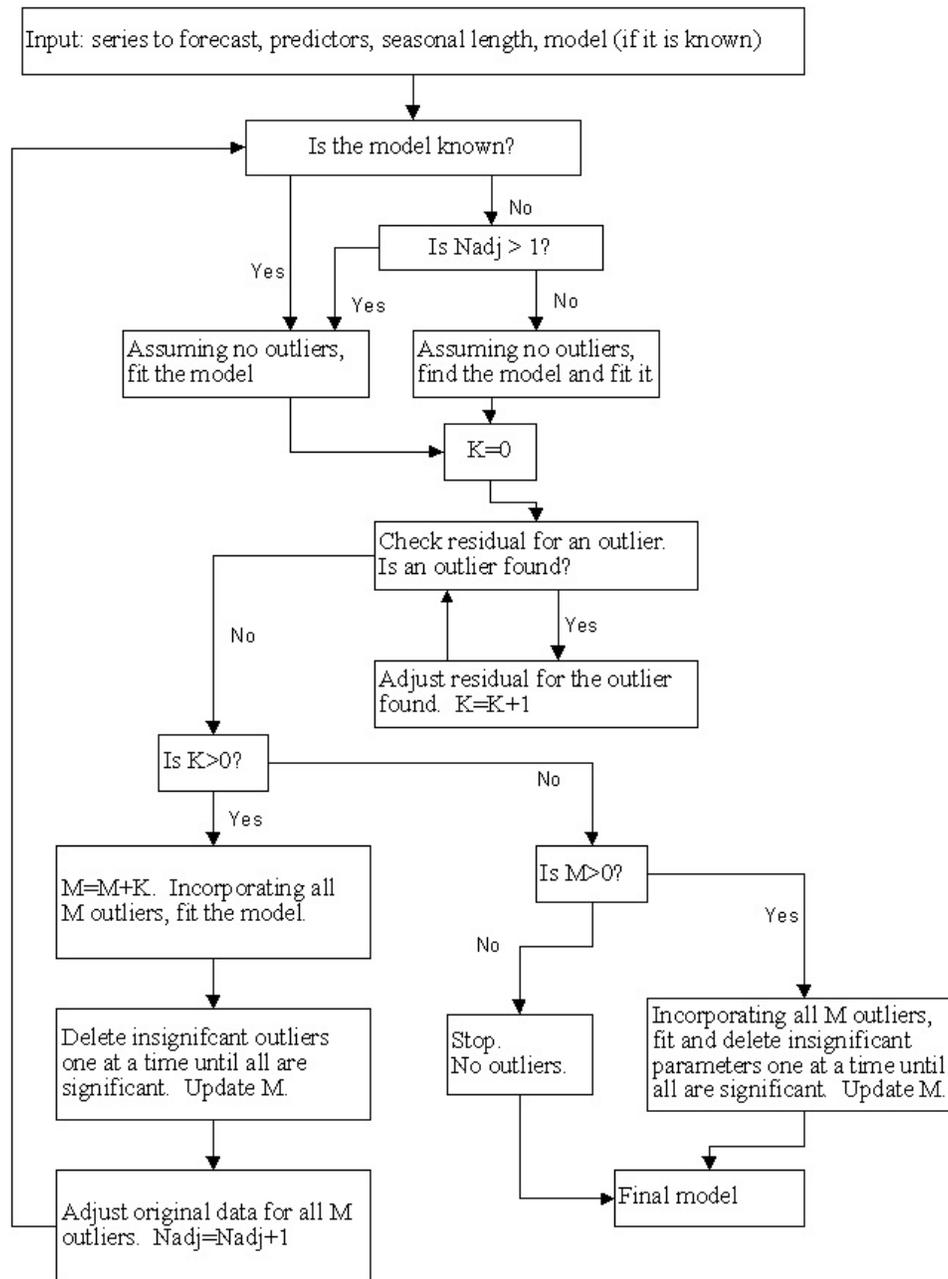
$$\chi^2(T) = \frac{\mathbf{w}'(T)(X_T'X_T)^{-1}\mathbf{w}(T)}{\sigma^2}$$

Assuming the model and model parameters are known,  $\chi^2(T)$  has a Chi-square distribution with  $k$  degrees of freedom under the null hypothesis  $w_1(T) = \dots = w_k(T) = 0$ .

### **Detection of Outliers**

The following flow chart demonstrates how automatic outlier detection works. Let  $M$  be the total number of outliers and  $N_{adj}$  be the number of times the series is adjusted for outliers. At the beginning of the procedure,  $M = 0$  and  $N_{adj} = 0$ .

Figure 35-1



## Goodness-of-Fit Statistics

Goodness-of-fit statistics are based on the original series  $Y(t)$ . Let  $k$  = number of parameters in the model,  $n$  = number of non-missing residuals.

**Mean Squared Error**

$$MSE = \frac{\sum (Y(t) - \hat{Y}(t))^2}{n-k}$$

**Mean Absolute Percent Error**

$$MAPE = \frac{100}{n} \sum \left| (Y(t) - \hat{Y}(t)) / Y(t) \right|$$

**Maximum Absolute Percent Error**

$$MaxAPE = 100 \max \left( \left| (Y(t) - \hat{Y}(t)) / Y(t) \right| \right)$$

**Mean Absolute Error**

$$MAE = \frac{1}{n} \sum |Y(t) - \hat{Y}(t)|$$

**Maximum Absolute Error**

$$MaxAE = \max \left( |Y(t) - \hat{Y}(t)| \right)$$

**Normalized Bayesian Information Criterion**

$$\text{Normalized BIC} = \ln(MSE) + k \frac{\ln(n)}{n}$$

**R-Squared**

$$R^2 = 1 - \frac{\sum (Y(t) - \hat{Y}(t))^2}{\sum (Y(t) - \bar{Y})^2}$$

**Stationary R-Squared**

A similar statistic was used by Harvey (Harvey, 1989).

$$R_S^2 = 1 - \frac{\sum_t (Z(t) - \hat{Z}(t))^2}{\sum_t (\Delta Z(t) - \overline{\Delta Z})^2}$$

where

The sum is over the terms in which both  $Z(t) - \hat{Z}(t)$  and  $\Delta Z(t) - \overline{\Delta Z}$  are not missing.

$\overline{\Delta Z}$  is the simple mean model for the differenced transformed series, which is equivalent to the univariate baseline model ARIMA(0,d,0)(0,D,0).

For the exponential smoothing models currently under consideration, use the differencing orders (corresponding to their equivalent ARIMA models if there is one).

$$d = \begin{cases} 2 & \text{Brown, Holt} \\ 1 & \text{other} \end{cases}, D = \begin{cases} 0 & s = 1 \\ 1 & s > 1 \end{cases}$$

*Note:* Both the stationary and usual R-squared can be negative with range  $(-\infty, 1]$ . A negative R-squared value means that the model under consideration is worse than the baseline model. Zero R-squared means that the model under consideration is as good or bad as the baseline model. Positive R-squared means that the model under consideration is better than the baseline model.

## Expert Modeling

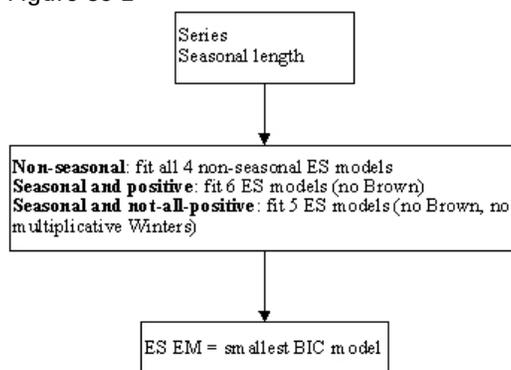
### Univariate Series

Users can let the Expert Modeler select a model for them from:

- All models (default).
- Exponential smoothing models only.
- ARIMA models only.

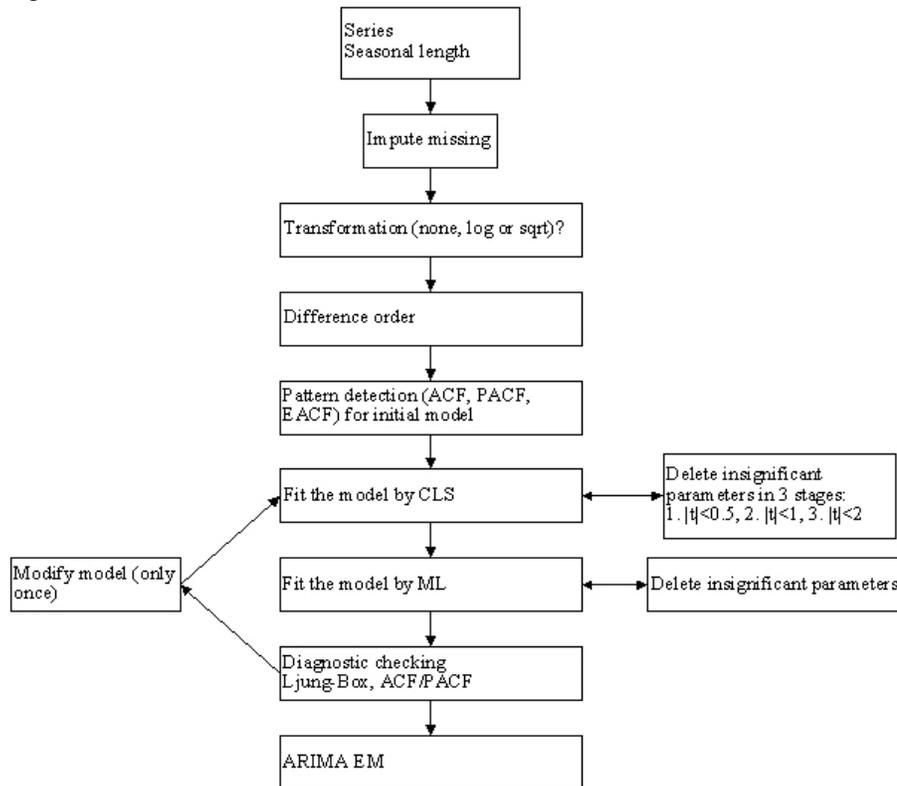
### Exponential Smoothing Expert Model

Figure 35-2



### ARIMA Expert Model

Figure 35-3



*Note:* If  $10 < n < 3s$ , set  $s=1$  to build a non-seasonal model.

### All Models Expert Model

In this case, the Exponential Smoothing and ARIMA expert models are computed, and the model with the smaller normalized BIC is chosen.

*Note:* For short series,  $n < \max(20, 3s)$ , use Exponential Smoothing Expert Model on p. 393.

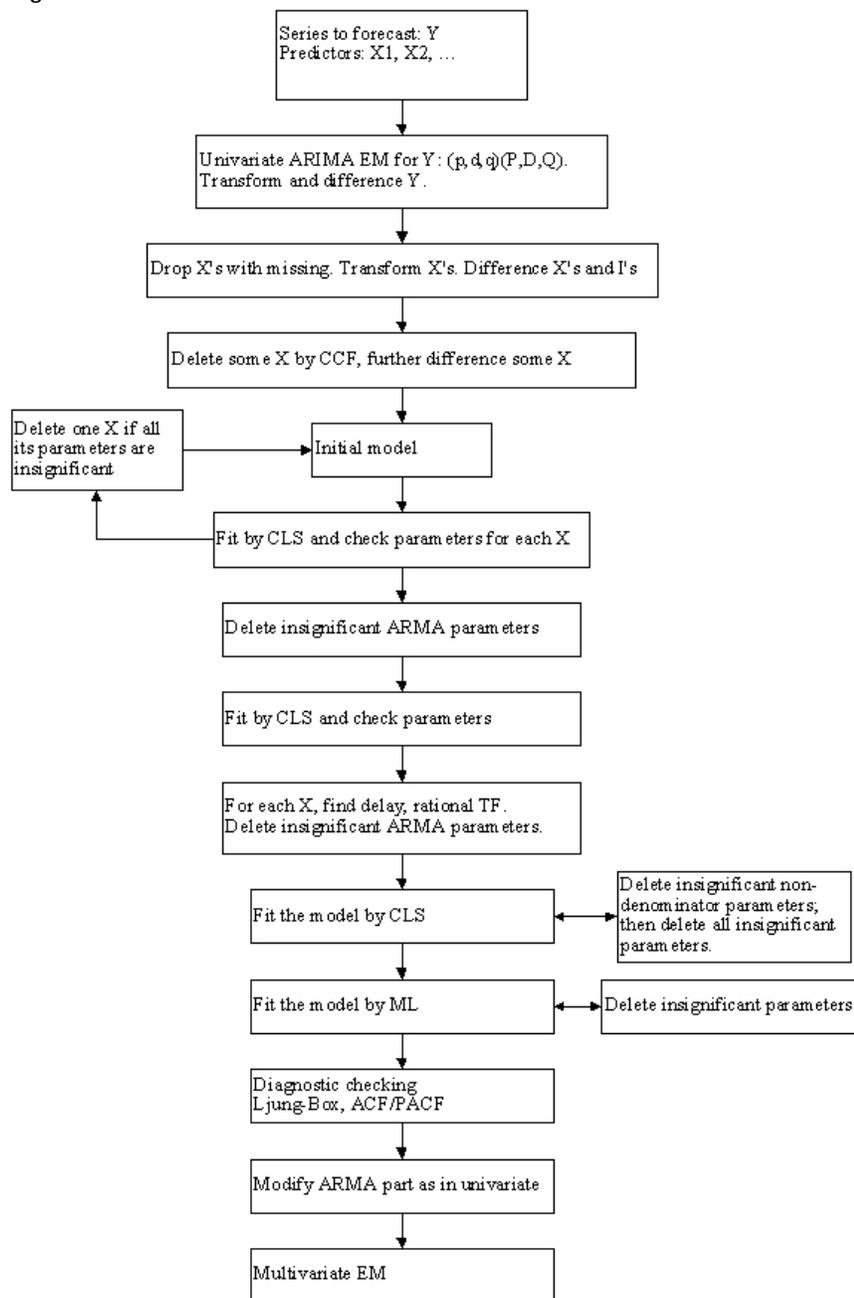
### Multivariate Series

In the multivariate situation, users can let the Expert Modeler select a model for them from:

- All models (default). Note that if the multivariate expert ARIMA model drops all the predictors and ends up with a univariate expert ARIMA model, this univariate expert ARIMA model will be compared with expert exponential smoothing models as before and the Expert Modeler will decide which is the best overall model.
- ARIMA models only.

**Transfer Function Expert Model**

Figure 35-4



Note: For short series,  $n < \max(20, 3s)$ , fit a univariate expert model.

## **Blank Handling**

Generally, any missing values in the series data will be imputed in the Time Intervals node used to prepare the data for time series modeling. If blanks remain in the series data submitted to the modeling node, ARIMA models will attempt to impute values, as described in “Estimation and Forecasting of ARIMA/TF” on p. 384.

Missing values for predictors will result in the field containing the missing values to be excluded from the time series model.

## **Generated Model/Scoring**

Predictions or forecasts for Time Series models are intricately related to the modeling process itself. Forecasting computations are described with the algorithm for the corresponding model type. For information on forecasting in exponential smoothing models, see “Exponential Smoothing Models” on p. 379. For information on forecasting in ARIMA models, see “Estimation and Forecasting of ARIMA/TF” on p. 384.

## **Blank Handling**

Blank handling for the generated model is very similar to that for the modeling node.

If any predictor has missing values within the forecast period, the procedure issues a warning and forecasts as far as it can.

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# ***TwoStep Cluster Algorithms***

## ***Overview***

The TwoStep cluster method is a scalable cluster analysis algorithm designed to handle very large data sets. It can handle both continuous and categorical variables or attributes. It requires only one data pass. It has two steps 1) pre-cluster the cases (or records) into many small sub-clusters; 2) cluster the sub-clusters resulting from pre-cluster step into the desired number of clusters. It can also automatically select the number of clusters.

## ***Model Parameters***

As the name implies, the TwoStep clustering algorithm involves two steps: Pre-clustering and Clustering.

### ***Pre-cluster***

The pre-cluster step uses a sequential clustering approach. It scans the data records one by one and decides if the current record should be merged with the previously formed clusters or starts a new cluster based on the distance criterion (described below).

The procedure is implemented by constructing a modified cluster feature (CF) tree. The CF tree consists of levels of nodes, and each node contains a number of entries. A leaf entry (an entry in the leaf node) represents a final sub-cluster. The non-leaf nodes and their entries are used to guide a new record quickly into a correct leaf node. Each entry is characterized by its CF that consists of the entry's number of records, mean and variance of each range field, and counts for each category of each symbolic field. For each successive record, starting from the root node, it is recursively guided by the closest entry in the node to find the closest child node, and descends along the CF tree. Upon reaching a leaf node, it finds the closest leaf entry in the leaf node. If the record is within a threshold distance of the closest leaf entry, it is absorbed into the leaf entry and the CF of that leaf entry is updated. Otherwise it starts its own leaf entry in the leaf node. If there is no space in the leaf node to create a new leaf entry, the leaf node is split into two. The entries in the original leaf node are divided into two groups using the farthest pair as seeds, and redistributing the remaining entries based on the closeness criterion.

If the CF tree grows beyond allowed maximum size, the CF tree is rebuilt based on the existing CF tree by increasing the threshold distance criterion. The rebuilt CF tree is smaller and hence has space for new input records. This process continues until a complete data pass is finished. For details of CF tree construction, see the BIRCH algorithm (Zhang, Ramakrishnan, and Livny, 1996).

All records falling in the same entry can be collectively represented by the entry's CF. When a new record is added to an entry, the new CF can be computed from this new record and the old CF without knowing the individual records in the entry. These properties of CF make it possible to maintain only the entry CFs, rather than the sets of individual records. Hence the CF-tree is much smaller than the original data and can be stored in memory more efficiently.

Note that the structure of the constructed CF tree may depend on the input order of the cases or records. To minimize the order effect, randomly order the records before building the model.

## Cluster

The cluster step takes sub-clusters (non-outlier sub-clusters if outlier handling is used) resulting from the pre-cluster step as input and then groups them into the desired number of clusters. Since the number of sub-clusters is much less than the number of original records, traditional clustering methods can be used effectively. TwoStep uses an agglomerative hierarchical clustering method, because it works well with the auto-cluster method (see the section on auto-clustering below).

**Hierarchical clustering** refers to a process by which clusters are recursively merged, until at the end of the process only one cluster remains containing all records. The process starts by defining a starting cluster for each of the sub-clusters produced in the pre-cluster step. (For more information, see the topic “Pre-cluster” on p. 397.) All clusters are then compared, and the pair of clusters with the smallest distance between them is selected and merged into a single cluster. After merging, the new set of clusters is compared, the closest pair is merged, and the process repeats until all clusters have been merged. (If you are familiar with the way a decision tree is built, this is a similar process, except in reverse.) Because the clusters are merged recursively in this way, it is easy to compare solutions with different numbers of clusters. To get a five-cluster solution, simply stop merging when there are five clusters left; to get a four-cluster solution, take the five-cluster solution and perform one more merge operation, and so on.

## Distance Measure

The TwoStep clustering method uses a log-likelihood distance measure, to accommodate both symbolic and range fields. It is a probability-based distance. The distance between two clusters is related to the decrease in log-likelihood as they are combined into one cluster. In calculating log-likelihood, normal distributions for range fields and multinomial distributions for symbolic fields are assumed. It also assumes that the fields are independent of each other, and so are the records. The distance between clusters  $i$  and  $j$  is defined as

$$d(i, j) = \xi_i + \xi_j - \xi_{\langle i, j \rangle}$$

where

$$\xi_v = -N_v \left( \sum_{k=1}^{K^A} \frac{1}{2} \log (\hat{\sigma}_k^2 + \hat{\sigma}_{vk}^2) + \sum_{k=1}^{K^B} \hat{E}_{vk} \right)$$

and

$$\hat{E}_{vk} = - \sum_{l=1}^{L_k} \frac{N_{vkl}}{N_v} \log \frac{N_{vkl}}{N_v}$$

In these expressions,

$K^A$  is the number of range type input fields,

$K^B$  is the number of symbolic type input fields,

$L_k$  is the number of categories for the  $k$ th symbolic field,

$N_v$  is the number of records in cluster  $v$ ,

$N_{vkl}$  is the number of records in cluster  $v$  which belongs to the  $l$ th category of the  $k$ th symbolic field,

$\hat{\sigma}_k^2$  is the estimated variance of the  $k$ th continuous variable for all records,

$\hat{\sigma}_{vk}^2$  is the estimated variance of the  $k$ th continuous variable for records in the  $v$ th cluster, and

$\langle i, j \rangle$  is an index representing the cluster formed by combining clusters  $i$  and  $j$ .

If  $\hat{\sigma}_k^2$  is ignored in the expression for  $\zeta_v$ , the distance between clusters  $i$  and  $j$  would be exactly the decrease in log-likelihood when the two clusters are combined. The  $\hat{\sigma}_k^2$  term is added to solve the problem caused by  $\hat{\sigma}_{vk}^2 = 0$ , which would result in the natural logarithm being undefined. (This would occur, for example, when a cluster has only one case.)

### **Number of Clusters (auto-clustering)**

TwoStep can use the hierarchical clustering method in the second step to assess multiple cluster solutions and automatically determine the optimal number of clusters for the input data. A characteristic of hierarchical clustering is that it produces a sequence of partitions in one run: 1, 2, 3, ... clusters. In contrast, a  $k$ -means algorithm would need to run multiple times (one for each specified number of clusters) in order to generate the sequence. To determine the number of clusters automatically, TwoStep uses a two-stage procedure that works well with the hierarchical clustering method. In the first stage, the BIC for each number of clusters within a specified range is calculated and used to find the initial estimate for the number of clusters. The BIC is computed as

$$BIC(J) = -2 \sum_{j=1}^J \xi_j + m_J \log(N)$$

where

$$m_J = J \left\{ 2K^A + \sum_{k=1}^{K^B} (L_K - 1) \right\}$$

and other terms defined as in “Distance Measure”. The ratio of change in BIC at each successive merging relative to the first merging determines the initial estimate. Let  $dBIC(J)$  be the difference in BIC between the model with  $J$  clusters and that with  $(J + 1)$  clusters,  $dBIC(J) = BIC(J) - BIC(J + 1)$ . Then the change ratio for model  $J$  is

$$R_1(J) = \frac{dBIC(J)}{dBIC(1)}$$

If  $dBIC(1) < 0$ , then the number of clusters is set to 1 (and the second stage is omitted). Otherwise, the initial estimate for number of clusters  $k$  is the smallest number for which  $R_1(J) < 0.04$

In the second stage, the initial estimate is refined by finding the largest relative increase in distance between the two closest clusters in each hierarchical clustering stage. This is done as follows:

- ▶ Starting with the model  $C_k$  indicated by the BIC criterion, take the ratio of minimum inter-cluster distance for that model and the next larger model  $C_{k+1}$ , that is, the previous model in the hierarchical clustering procedure,

$$R_2(k) = \frac{d_{\min}(C_k)}{d_{\min}(C_{k+1})}$$

where  $C_k$  is the cluster model containing  $k$  clusters and  $d_{\min}(C)$  is the minimum inter-cluster distance for cluster model  $C$ .

- ▶ Now from model  $C_{k-1}$ , compute the same ratio with the following model  $C_k$ , as above. Repeat for each subsequent model until you have the ratio  $R_2(2)$ .
- ▶ Compare the two largest  $R_2$  ratios; if the largest is more that 1.15 times the second largest, then select the model with the largest  $R_2$  ratio as the optimal number of clusters; otherwise, from those two models with the largest  $R_2$  values, select the one with the larger number of clusters as the optimal model.

## Blank Handling

The TwoStep cluster node does not support blanks. Records containing blanks, nulls, or missing values of any kind are excluded from model building.

## Effect of Options

### Outlier Handling

An optional outlier-handling step is implemented in the algorithm in the process of building the CF tree. Outliers are considered as data records that do not fit well into any cluster. We consider data records in a leaf entry as outliers if the number of records in the entry is less than a certain fraction (25% by default) of the size of the largest leaf entry in the CF tree. Before rebuilding the CF tree, the procedure checks for potential outliers and sets them aside. After rebuilding the CF tree, the procedure checks to see if these outliers can fit in without increasing the tree size. At the end of CF tree building, small entries that cannot fit in are outliers.

## **Generated Model/Scoring**

### **Predicted Values**

When scoring a record with a TwoStep Cluster generated model, the record is assigned to the cluster to which it is closest. The distance between the record and each cluster is calculated, and the cluster with the smallest distance is selected as the closest, and that cluster is assigned as the predicted value for the record. Distance is calculated in a similar manner to that used during model building, considering the record to be scored as a “cluster” with only one record. For more information, see the topic “Distance Measure” on p. 398.

If outlier handling was enabled during model building, the distance between the record and the closest cluster is compared to a threshold  $C = \log(V)$ , where

$$V = \prod_k R_k \prod_m L_m.$$

where  $R_k$  is the range of the  $k$ th numeric field and  $L_m$  is number of categories for the  $m$ th symbolic field.

If the distance from the nearest cluster is smaller than  $C$ , assign that cluster as the predicted value for the record. If the distance is greater than  $C$ , assign the record as an outlier.

### **Blank Handling**

As with model building, records containing blanks are not handled by the model, and are assigned a predicted value of \$null\$.



# TwoStep-AS Cluster Algorithms

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## 1. Introduction

Clustering technique is widely used by retail and consumer product companies who need to learn more about their customers in order to apply 1-to-1 marketing strategies. By means of clustering technique, customers are partitioned into groups by their buying habits, gender, age, income level, etc., and retail and consumer product companies can tailor their marketing and product development strategy to each customer group.

Traditional clustering algorithms can broadly be classified into partitional clustering and hierarchical clustering. Partitional clustering algorithms divide data cases into clusters by optimizing certain criterion function. A well-known representative of this class is the  $k$ -means clustering. Hierarchical clustering algorithms proceed by stages producing a sequence of partitions in which each partition is nested into the next partition in the sequence. Hierarchical clustering can be agglomerative and divisive. Agglomerative clustering starts with a singleton cluster (for example, a cluster that contains one data case only) and proceeds by successively merging the clusters at each stage. On the contrary, divisive clustering starts with one single cluster that contains all data cases and proceeds by successively separating the cluster into smaller clusters. Notice that no initial values are needed for hierarchical clustering.

However, traditional clustering algorithms do not adequately address the problem of large datasets. This is where the two-step clustering method can be helpful (see ref. [1][2]). This method first performs a pre-clustering step by scanning the entire dataset and storing the dense regions of data cases in terms of summary statistics called cluster features. The cluster features are stored in memory in a data structure called the CF-tree. Then an agglomerative hierarchical clustering algorithm is applied to cluster the set of cluster features. Since the set of cluster features is much smaller than the original dataset, the hierarchical clustering can perform well in terms of speed. Notice that the CF-tree is incremental in the sense that it does not require the whole dataset in advance and only scans the dataset once.

One essential element in the clustering algorithms above is the distance measure that reflects the relative similarity or dissimilarity of the clusters. *Chiu et al* proposed a new distance measure that enables clustering on data sets in which the features are of mixed types. The features can be continuous, nominal, categorical, or count. This distance measure is derived from a probabilistic model in the way that the distance is equivalent to the decrease in log-likelihood value as a result of merging two clusters. In the following, the new distance measure will be used in both the CF-tree growth and the clustering process, unless otherwise stated.

In this chapter, we extend the two-step clustering method into the distributed setting, specifically under the map-reduce framework. In addition to generating a clustering solution, we also provide mechanisms for selecting the most relevant features for clustering given data, as well as detecting rare outlier points. Moreover, we provide an enhanced set of evaluation and diagnostic features enabling insight, interactivity, and an improved overall user experience as required by the Analytic Catalyst application.

The chapter is organized as follows. We first declare some general notes about algorithms, development, etc. Then we define the notations used in the document. Operations for data pre-processing are introduced in section 4. In section 5, we briefly describe the data and the measures such as distance, tightness, and so on. In section 6, 7, and 8, we present the key algorithms used in model building, including CF-tree growth, Hierarchical Agglomerative Clustering (HAC), and determination of the

number of clusters, respectively. Section 9 describes the entire solution of distributed clustering on Hadoop. Section 10 describes how to score new cases (to assign cluster memberships). Finally, Section 11 includes various measures used for model evaluation and model diagnostics. Insights and interestingness are also derived.

## 2. Notes

- To create CF-trees efficiently, we assume that operations within a main memory environment (for example, RAM) is efficient, and the size of the main memory can be allocated or controlled by user.
- We assume that the data is randomly partitioned. If this assumption is not allowed, sequential partition can still be applied. But note that the clustering result can be impacted, particularly if the data is ordered in some special way.
- CE is implemented in the Analytic Framework.

## 3. Notations

The following notations are used throughout this chapter unless otherwise stated:

$R$	Number of data partitions/splits.
$N_j$	Number of cases in cluster $C_j$ .
$N_{jk}$	Number of cases in cluster $C_j$ which have non-missing values in the $k$ th feature.
$K$	Number of features used for clustering.
$x_i = (x_{i1}, \dots, x_{iK})$	The $i$ th data case. $x_i$ is a $K$ -dimensional vector.
$x_{ik}^A, k = 1, \dots, K^A$	Value of the $k$ th continuous feature of the $i$ th data case $x_i$ . There are $K^A$ number of continuous features.
$x_{ik}^B, k = 1, \dots, K^B$	Value of the $k$ th categorical feature of the $i$ th data case $x_i$ . There are $K^B$ number of categorical features.
$L_k, k = 1, \dots, K^B$	Number of categories of the $k$ th categorical feature in the entire data.
$N_{jkl}, k = 1, \dots, K^B, l = 1, \dots, L_k$	Number of cases in cluster $C_j$ whose $k$ th categorical feature takes the $l$ th category.
$s_{jk}, k = 1, \dots, K^A$	Sum of values of the $k$ th continuous feature in cluster $C_j$ .
$s_{jk}^2, k = 1, \dots, K^A$	Sum of squared values of the $k$ th continuous feature in cluster $C_j$ .
$d(j, s)$	Distance between clusters $C_j$ and $C_s$ .
$C_{<j,s>}$	Cluster formed by combining clusters $C_j$ and $C_s$ .

## 4. Data Pre-processing

Data pre-processing includes the following transformations:

- Trailing blanks are trimmed
- Date/time features are transformed into continuous ones
- Normalize continuous features
- Category values of a categorical feature are mapped into integer. As such, the expression " $x_{ik}^B = l$ " indicates that the  $k$ th categorical feature of the  $i$ th case takes the  $l$ th category.
- System/user missing and invalid values are all considered as missing.

- Cases with missing values in all features are discarded.

## 5. Data and Measures

Let  $x_i$  be the  $i$ th data case. Denote  $I_j$  as the index set of cluster  $C_j$ ,  $I_j = \{i: x_i \in C_j\}$ . Let  $K = K^A + K^B$  be the total number of features in which  $K^A$  of them are continuous and  $K^B$  are categorical. Without loss of generality, write  $x_i$  as

$$x_i = (x_{i1}, \dots, x_{iK}) = (x_{i1}^A, \dots, x_{iK^A}^A, x_{i1}^B, \dots, x_{iK^B}^B) \quad (1)$$

where  $x_{ik}^A$  is the value of the  $k$ th continuous feature,  $k = 1, \dots, K^A$ , and  $x_{ik}^B$  is the value of the  $k$ th categorical feature,  $k = 1, \dots, K^B$ . Express  $x_{ik}^B$  as a vector  $(x_{ik1}^B, \dots, x_{ikL_k}^B)$  of  $L_k$  values in which each entry is either zero or one:

$$x_{ikl}^B = \begin{cases} 1, & \text{if } x_{ik}^B \text{ takes the } l\text{th category} \\ 0, & \text{otherwise} \end{cases} \quad (2)$$

### 5.1. Cluster Feature of a Cluster

The cluster feature (sufficient statistics set)  $CF_j$  of a cluster  $C_j$  is a collection of statistics that summarizes the characteristics of a cluster. A possible set  $CF_j$  is given as

$$CF_j = \{N_j, \vec{N}_j, s_j, s_j^2, N_j^B\} \quad (3)$$

where  $N_j$  is the number of data cases in cluster  $C_j$ ,  $\vec{N}_j = (N_{jk}, \dots, N_{jK^A}, N_{j1}^B, \dots, N_{jK^B}^B)$  is a  $K$ -dimensional vector; the  $k$ th entry is the number of data cases in cluster  $C_j$  which have non-missing values in the  $k$ th feature.  $s_j = (s_{j1}, \dots, s_{jK^A})$  is a  $K^A$ -dimensional vector; the  $k$ th entry is the sum of the non-missing values of the  $k$ th continuous feature in cluster  $C_j$ , i.e.

$$s_{jk} = \sum_{i \in I_j} x_{ik}^A \quad (4)$$

for  $k = 1, \dots, K^A$ . Similarly,  $s_j^2 = (s_{j1}^2, \dots, s_{jK^A}^2)$  is a  $K^A$ -dimensional vector such that the  $k$ th entry is the sum of squared non-missing values of the  $k$ th continuous feature in cluster  $C_j$ , i.e.

$$s_{jk}^2 = \sum_{i \in I_j} (x_{ik}^A)^2 \quad (5)$$

for  $k = 1, \dots, K^A$ .

Similarly,  $N_j^B = (N_{j1}^B, \dots, N_{jK^B}^B)$  is a  $\sum_{k=1}^{K^B} (L_k - 1)$ -dimensional vector where the  $k$ th sub-vector  $N_{jk}^B$  is  $(L_k - 1)$  dimensional, given by

$$N_{jk}^B = (N_{jk1}, \dots, N_{jk(L_k-1)}) \quad (6)$$

for  $k = 1, \dots, K^B$ . The  $l$ th entry  $N_{jkl}$  represents the total number of cases in cluster  $C_j$  whose  $k$ th categorical feature takes the  $l$ th category,  $l = 1, \dots, L_k - 1$ , i.e.

$$N_{jkl} = \sum_{i \in I_j} x_{ikl}^B. \quad (7)$$

## 5.2. Updating Cluster Feature when Merging Two Clusters

When two clusters  $C_j$  and  $C_s$  are said to merge, it simply means that the two corresponding sets of data points are merged together to form a union. In this case, the  $CF_{\langle j,s \rangle}$  for the merged cluster  $C_{\langle j,s \rangle}$  can be calculated by simply adding the corresponding elements in  $CF_j$  and  $CF_s$ , that is,

$$CF_{\langle j,s \rangle} = \{N_j + N_s, \bar{N}_j + \bar{N}_s, s_j + s_s, s_j^2 + s_s^2, N_j^B + N_s^B\}. \quad (8)$$

## 5.3. Tightness of a Cluster

The interpretation of tightness of a cluster is that the smaller of the value of tightness, the less variation of the data cases within the cluster. In CE, there are two tightness measures, and they will be used depending on the specified distance measure, log-likelihood distance or Euclidean distance.

### 5.3.1. Tightness based on Log-likelihood Distance

The tightness  $\hat{\eta}_j$  of a cluster  $C_j$  can be defined as average negative log-likelihood function of the cluster evaluated at the maximum likelihood estimates of the model parameters. See Ref. 1 for statistical reasoning for definition.

The tightness  $\hat{\eta}_j$  of a cluster  $C_j$  is given by

$$\hat{\eta}_j = \frac{1}{2} \sum_{k=1}^{K^A} \ln \left( 1 + \frac{\hat{\sigma}_{jk}^2}{\Delta_k} \right) + \sum_{k=1}^{K^B} \hat{E}_{jk} \quad (9)$$

where  $\hat{\sigma}_{jk}^2$  is the maximum likelihood variance estimate of the  $k$ th continuous feature in cluster  $C_j$ .

$$\hat{\sigma}_{jk}^2 = \frac{s_{jk}^2 - N_{jk}(\hat{\mu}_{jk})^2}{N_{jk}} \quad (10)$$

in which  $\hat{\mu}_{jk}$  is the sample mean,

$$\hat{\mu}_{jk} = \frac{s_{jk}}{N_{jk}}. \quad (11)$$

$\hat{E}_{jk}$  is the entropy of the  $k$ th categorical feature in cluster  $C_j$ ,

$$\hat{E}_{jk} = - \sum_{l=1}^{L_k} \hat{q}_{jkl} \ln \hat{q}_{jkl} \quad (12)$$

in which  $\hat{q}_{jkl}$  is the portion of data cases in cluster  $C_j$  whose  $k$ th categorical feature takes the  $l$ th category,

$$\hat{q}_{jkl} = \frac{N_{jkl}}{N_{jk}}. \quad (13)$$

Finally,  $\Delta_k$  is appositve scalar which is added to handle the degenerating conditions and balance the contributions between a continuous feature and a categorical one. The default value of  $\Delta_k$  is 0.01.

To handle missing values, the definition of tightness assumes that the distribution of missing values is the same as for the observed non-missing points in the cluster.

Moreover, the following assumption is always applied:

$$x \ln(x) = 0, \text{ if } x = 0. \quad (14)$$

### 5.3.2. Tightness based on Euclidean Distance

The tightness  $\tilde{\eta}_j$  of a cluster  $C_j$  can be defined as the average Euclidean distance from member cases to the center/centroid of the cluster.

The tightness  $\tilde{\eta}_j$  of a cluster  $C_j$  is given by

$$\tilde{\eta}_j = \sqrt{\frac{\sum_{k=1}^K s_{jk}^2 - N_{jk}(\hat{\mu}_{jk})^2}{N_{jk}}}. \quad (15)$$

Notice that if any feature in cluster  $C_j$  has all missing values, the feature will not be used in the computation.

## 5.4. Distance Measures between Two Clusters

Suppose clusters  $C_j$  and  $C_s$  are merged to form a new cluster  $C_{<j,s>}$  that consists of the union of all data cases in  $C_j$  and  $C_s$ . Two distance measures are available.

### 5.4.1. Log-likelihood Distance

The distance between  $C_j$  and  $C_s$  can be captured by observing the corresponding decrease in log-likelihood as the result of combining  $C_j$  and  $C_s$  to form  $C_{<j,s>}$ .

The distance measure between two clusters  $C_j$  and  $C_s$  is defined as

$$d(j, s) = \sum_{k=1}^{K^A+K^B} d_k(j, s) = \xi_j + \xi_s - \xi_{<j,s>} \quad (16)$$

where

$$\xi_j = -\frac{1}{2} \sum_{k=1}^{K^A} N_{jk} \ln(\hat{\sigma}_{jk}^2 + \Delta_k) - \sum_{k=1}^{K^B} N'_{jk} \hat{E}_{jk} \quad (17)$$

and

$$d_k(j, s) = \begin{cases} \{-N_{jk} \ln(\hat{\sigma}_{jk}^2 + \Delta_k) - N_{sk} \ln(\hat{\sigma}_{sk}^2 + \Delta_k) + N_{<j,s>k} \ln(\hat{\sigma}_{<j,s>k}^2 + \Delta_k)\} / 2, & \text{if feature } k \text{ is continuous} \\ -N'_{jk} \hat{E}_{jk} - N'_{sk} \hat{E}_{sk} + N'_{<j,s>k} \hat{E}_{<j,s>k}, & \text{if feature } k \text{ is categorical} \end{cases} \quad (18)$$

Note that since  $\tilde{\xi}_{\langle j,s \rangle}$  can be calculated by using the statistics in  $CF_{\langle j,s \rangle}$ , the distance can be calculated by first updating the  $CF_{\langle j,s \rangle}$  of the merged cluster  $C_{\langle j,s \rangle}$ .

To handle missing values, the definition of distance assumes that the contribution of missing values equals zero.

### 5.4.2. Euclidean Distance

The Euclidean distance can only be applied if all features are continuous.

The distance between two cases is clearly defined. The distance between two clusters is here defined by the Euclidean distance between the two cluster centers. A cluster center is defined as the vector of cluster means of each feature.

Suppose the centers/centroids of clusters  $C_j$  and  $C_s$  are  $(\hat{\mu}_{j1}, \dots, \hat{\mu}_{jK})$  and  $(\hat{\mu}_{s1}, \dots, \hat{\mu}_{sK})$  respectively, then

$$d(j, s) = \sqrt{\sum_{k=1}^K d_k^2(j, s)} = \sqrt{\sum_{k=1}^K (\hat{\mu}_{jk} - \hat{\mu}_{sk})^2} \quad (19)$$

where

$$d_k(j, s) = |\hat{\mu}_{jk} - \hat{\mu}_{sk}|. \quad (20)$$

Again, any feature in cluster  $C_j$  with all missing values will not be used in the computation.

## 6. CF-Tree Building

CF-tree is a very compact summary of dataset in the way that each entry (leaf entry) in the leaf node is a sub-cluster which absorbs the data cases that are close together, as measured by the tightness index  $\tilde{\eta}$  and controlled by a specific threshold value  $T$ . CF-tree is built dynamically as new data case is inserted, it is used to guide to a new insertion into the correct sub-cluster for clustering purposes.

CF-tree is a height-balanced tree with four parameters:

1. The branching factor  $B$  for the non-leaf nodes. It is the maximum number of entries that a non-leaf node can hold. A non-leaf entry is of the form  $[CF_i, child_i], i = 1, \dots, B$ , in which  $child_i$  is a pointer to its  $i$ th child node and  $CF_i$  is the cluster feature of the sub-cluster represented by this child.
2. The branching factor  $L$  for the leaf nodes. It is the maximum number of entries that a leaf node can hold. A leaf entry is similar to a non-leaf entry except that it does not have a pointer. It is of the form  $[CF_i], i = 1, \dots, L$ .
3. The threshold parameter  $T$  that controls the tightness  $\tilde{\eta}$  of any leaf entries. That is, all leaf entries in a leaf node must satisfy a threshold requirement that the tightness has to be less than  $T$ , i.e.  $\tilde{\eta} \leq T$ .
4. Maximum tree height  $H$ .

In addition, each leaf node has two pointers: “*prev*” and “*next*” which are used to chain all leaf nodes together for efficient scanning.

Figure 1 illustrates a CF-tree of branching factors  $B = 2$ ,  $L = 3$ , and  $H = 1$ .

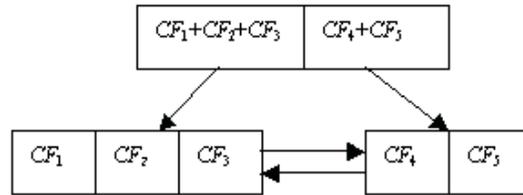


Figure 1. Example of a CF-tree.

## 6.1. Inserting a Single Case or a Sub-cluster into a CF-Tree

The procedure for inserting a data case or a sub-cluster (abbrev. “*Ent*”) into a CF-tree is as follows.

Step 1. Identify the appropriate leaf node.

Starting from the root node, recursively descend the CF-tree by choosing the closest child node according to the distance measure  $d$ .

Step 2. Modify the leaf node.

Upon reaching a leaf node, find the closest leaf entry  $[CF_i]$ , say, and see if *Ent* can be absorbed into  $[CF_i]$  without violating the threshold requirement  $\tilde{\eta} \leq T$ . If so, update the CF information in  $[CF_i]$  to reflect the absorbing action. If not, add a new entry for *Ent* to the leaf. If there is space on the leaf for this new entry to fit in, then we are done. Otherwise, split the leaf node by choosing the farthest pair of entries as seeds, and redistribute the remaining entries based on the closest criteria.

Step 3. Modify the path to the leaf node.

After inserting *Ent* into a leaf node, update the CF information for each non-leaf entry on the path to the leaf node. If there is no leaf split, then only the corresponding CF information is needed to update to reflect the absorbing of *Ent*. If a leaf split happens, then it is necessary to insert a new non-leaf entry into the parent node in order to describe the newly created leaf. If the parent has space for this entry, at all higher levels, only the CF information is needed to update to reflect the absorbing of *Ent*. In general, however, the parent node has to split as well, and so on up to the root node. If the root node is split, the tree height increases by one.

Notice that the growth of CF-tree is sensitive to case order. If the same data case is inserted twice but at different time, the two copies might be entered into two distinct leaf entries. It is possible that two sub-clusters that should be in one cluster are split across nodes. Similarly, it is also possible that two sub-clusters that should not be in one cluster are kept together in the same node.

## 6.2. Threshold Heuristic

In building the CF-tree, the algorithm starts with an initial threshold value (default is 0). Then it scans the data cases and inserts into the tree. If the main memory runs out before data scanning is finished, the threshold value is increased to rebuild a new smaller CF-tree, by re-inserting the leaf entries of the old tree into the new one. After the old leaf entries have been re-inserted, data scanning is resumed from the case at which it was interrupted. The following strategy is used to update the threshold values.

Suppose that at step  $i$ , the CF-tree of the threshold  $T_i$  is too big for the main memory after  $N_i$  data cases in the data have been scanned, and an estimate of the next (larger) threshold  $T_{i+1}$  is needed to rebuild a new smaller CF-tree.

Specifically, we find the first two closest entries whose tightness is greater than the current threshold, and take it as the next threshold value. However, searching the closest entries can be tedious. So we follow BIRCH's heuristic to traverse along a path from the root to the most crowded leaf that has the most entries and find the pair of leaf entries that satisfies the condition.

### 6.3. Rebuilding CF-Tree

When the CF-tree size exceeds the size of the main memory, or the CF-tree height is larger than  $H$ , the CF-tree is rebuilt to a smaller one by increasing the tightness threshold.

Assume that within each node of CF-tree  $t_i$ , the entries are labeled contiguously from 0 to  $n_k - 1$ , where  $n_k$  is the number of entries in that node. Then a path from an entry in the root (level 1) to a leaf node (level  $h$ ) can be uniquely represented by  $(i_1, i_2, \dots, i_{h-1})$ , where  $i_j, j = 1, \dots, h - 1$ , is the label of the  $j$ th level entry on that path. So naturally, path  $(i_1^{(1)}, i_2^{(1)}, \dots, i_{h-1}^{(1)})$  is before (or  $<$ ) path  $(i_1^{(2)}, i_2^{(2)}, \dots, i_{h-1}^{(2)})$  if  $i_1^{(1)} = i_1^{(2)}, \dots, i_{j-1}^{(1)} = i_{j-1}^{(2)}$ , and  $i_j^{(1)} < i_j^{(2)}$  for  $0 \leq j \leq h - 1$ . It is obvious that each leaf node corresponds to a path, since we are dealing with tree structure, and we will just use "path" and "leaf node" interchangeably from now on.

With the natural path order defined above, it scans and frees the old tree, path by path, and at the same time creates the new tree path by path. The procedure is as follows.

- Step 1. Let the new tree start with NULL and OldCurrentPath be initially the leftmost path in the old tree.
- Step 2. Create the corresponding NewCurrentPath in the new tree.  
Copy the nodes along OldCurrentPath in the old tree into the new tree as the (current) rightmost path; call this NewCurrentPath
- Step 3. Insert leaf entries in OldCurrentPath to the new tree.  
With the new threshold, each leaf entry in OldCurrentPath is tested against the new tree to see if it can either be absorbed by an existing leaf entry, or fit in as a new leaf entry without splitting, in the NewClosestPath that is found top-down with the closest criteria in the new tree. If yes and NewClosestPath is before NewCurrentPath, then it is inserted to NewClosestPath, and deleted from the leaf node in NewCurrentPath.
- Step 4. Free space in OldCurrentPath and NewCurrentPath.  
Once all leaf entries in OldCurrentPath are processed, the nodes along OldCurrentPath can be deleted from the old tree. It is also likely that some nodes along NewCurrentPath are empty because leaf entries that originally corresponded to this path have been "pushed forward." In this case, the empty nodes can be deleted from the new tree.
- Step 5. Process the next path in the old tree.  
OldCurrentPath is set to the next path in the old tree if there still exists one, and go to step 2.

### 6.4. Delayed-Split Option

If the CF-tree that resulted by inserting a data case is too big for the main memory, it may be possible that some other data cases in the data can still fit in the current CF-tree without causing a split on any node in the CF-tree (thus the size of the current tree remains the same and can still be in the main memory).

Similarly, if the CF-tree resulted by inserting a data case exceeds the maximum height, it may be possible that some other data cases in the data can still fit in the current CF-tree without increasing the tree height.

Once any of the two conditions happens, such cases are written out to disk (with  $S_1$  amount of disk space put aside for this purpose) and data scanning continues until the disk space runs out as well. The advantage of this approach is that more data cases can fit into the tree before a new tree is rebuilt. Figure 2 illustrates the control flow of delayed-split option.

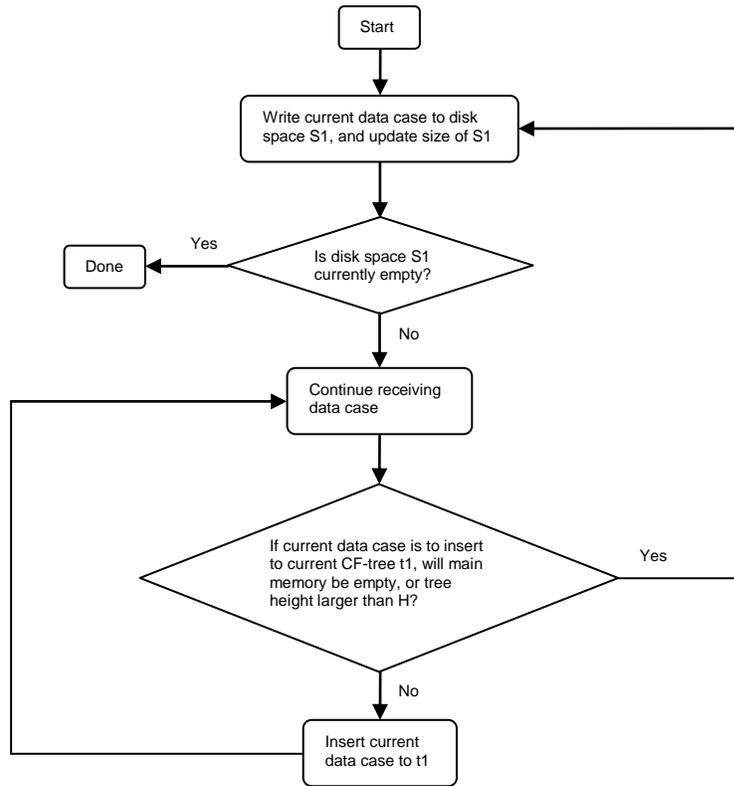


Figure 2. Control flow of delayed-split option.

## 6.5. Outlier-Handling Option

Outlier is defined as leaf entry (sub-cluster) of low density, which contains less than  $N_{min}$  (default 10) cases.

Similar to the delayed-split option, some disk space  $S_2$  is allocated for handling outliers. When the current CF-tree is too big for the main memory, some leaf entries are treated as potential outliers (based on the definition of outlier) and are written out to disk. The others are used to rebuild the CF-tree. Figure 3 shows the control flow of the outlier-handling option.

Implementation notes:

- The size of any outlier leaf entry should also be less than 20% of the maximal size of leaf entries.
- The CF-tree  $t1$  should be updated once any leaf entry is written to disk space  $S_2$ .

- Outliers identified here are local candidates, and they will be analyzed further in later steps, where the final outliers will be determined.

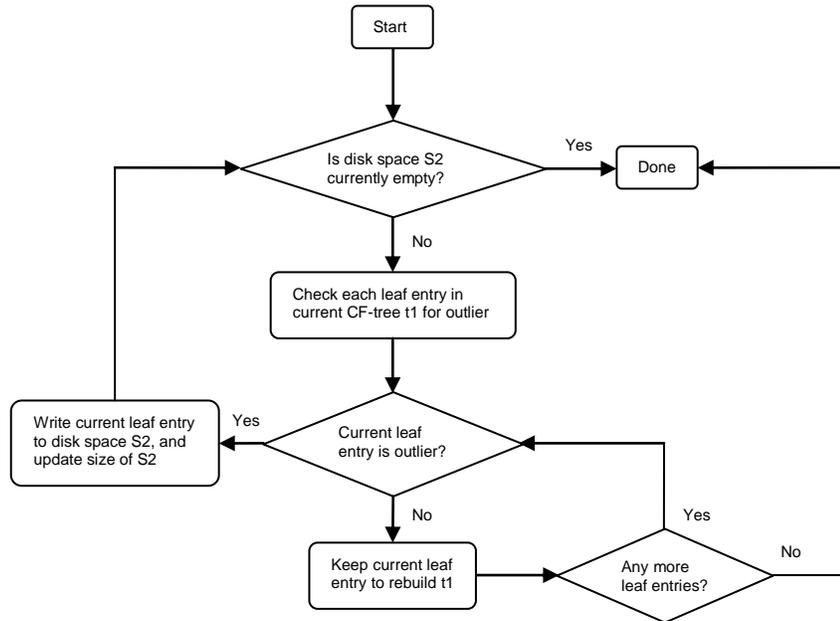


Figure 3. Control flow of outlier-handling option.

## 6.6. Overview of CF-Tree Building

Figure 4 provides an overview of building a CF-tree for the whole algorithm. Initially a threshold value is set, data is scanned, and the CF-tree is built dynamically. When the main memory runs out, or the tree height is larger than the maximum height before the whole data is scanned, the algorithm performs the delayed-split option, outlier-handling option, and the tree rebuilding step to rebuild a new smaller CF-tree that can fit into the main memory. The process continues until all cases in the data are processed. When all data is scanned, cases in disk space  $S_1$  are absorbed and entries in disk space  $S_2$  are scanned again to verify if they are indeed outliers.

Implementation notes:

- When all data is scanned, all cases in disk space  $S_1$  will be inserted into the tree. This may result in rebuilding the tree if necessary.

The following table shows the parameters involved in CF-tree building and their default values.

Parameter	Default value
Assigned main memory ( $M$ )	80*1024 bytes (TBD)
Assigned disk space for outlier-handling ( $S_2$ )	20% of $M$

Assigned disk space for delayed-split ( $S_1$ )	10% of $M$
Adjustment constant to the tightness and distance measures, $\Delta_k, k = 1, \dots, K^A$	0.01
Distance measure (Log-likelihood/Euclidean)	Log-likelihood
Initial threshold value ( $T$ )	0
Branching factor ( $B$ )	8
Branching factor ( $L$ )	8
Maximum tree height ( $H$ )	3
Delayed-split option (on/off)	On
Outlier-handling option (on/off)	On
Outlier definition ( $N_{min}$ )	Leaf entry which contains less than $N_{min}$ cases, default 10

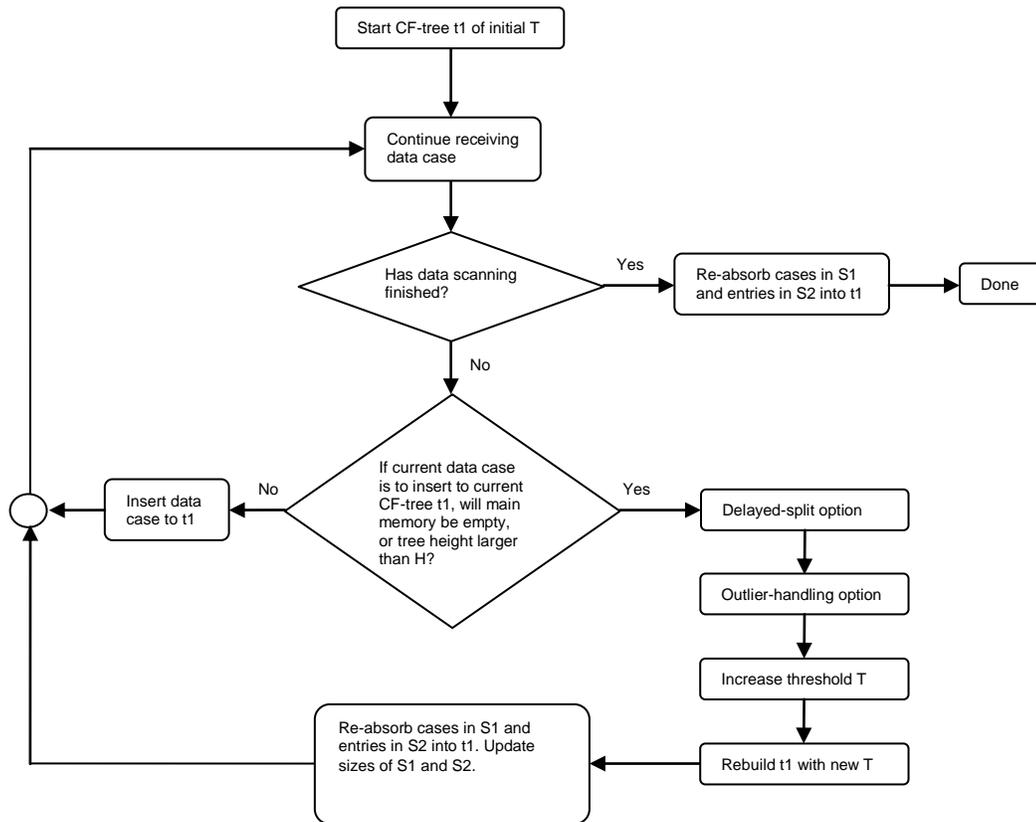


Figure 4. Control flow of CF-tree building.

## 7. Hierarchical Agglomerative Clustering

Hierarchical Agglomerative Clustering (HAC) proceeds by steps producing a sequence of partitions in which each partition is nested into the next partition in the sequence. See ref. [3] for details.

HAC can be implemented using two methods, as described below.

## 7.1. Matrix Based HAC

Suppose that matrix based HAC starts with  $J_0$  clusters. At each subsequent step, a pair of clusters is chosen. The two clusters  $C_j$  and  $C_s$  in the pair are closest together in terms of the distance measure  $d(j, s)$ . A new cluster  $C_{<j,s>}$  is formed to replace one of the clusters in the pair,  $C_j$ , say. This new cluster contains all data cases in  $C_j$  and  $C_s$ . The other cluster  $C_s$  is discarded. Hence the number of clusters is reduced by one at each step. The process stops when the desired number of clusters  $J_1$  is reached. Since the distance measure between any two clusters that are not involved in the merge does not change, the algorithm is designed to update the distance measures between the new cluster and the other clusters efficiently.

The procedure of matrix based HAC is as follows.

```

Step 1. For  $j = 1, \dots, J_0 - 1, \{$ 
    Compute  $d(j, s)$  for  $s = j + 1, \dots, J_0$ ;
    Find  $\delta_j = \min_{s=j+1, \dots, J_0} d(j, s)$  and  $s_j = \arg \min_{s=j+1, \dots, J_0} d(j, s)$ ;
}
Find  $\delta_* = \min_{j=1, \dots, J_0-1} \delta_j$  and  $j_* = \arg \min_{j=1, \dots, J_0-1} \delta_j$ , the closest pair is  $\langle j_*, s_{j_*} \rangle$ ;
Step 2. For  $J = J_0 - 1, \dots, J_1, \{$ 
    Merge the closest pair  $\langle j_*, s_{j_*} \rangle$ , and replace  $C_{j_*}$  by  $C_{\langle j_*, s_{j_*} \rangle}$ ;
    For  $j = 1, \dots, j_* - 1, \{$ 
        If  $s_j = s_{j_*}$ , recompute all distances  $d(j, s)$ ,  $s = j + 1, \dots, J$ , and update  $\delta_j$  and  $s_j$ ;
        If  $s_j \neq s_{j_*}, \{$ 
            Compute  $d = d(j, j_*)$ ;
            If  $d < \delta_j$ , update  $\delta_j = d$  and  $s_j = j_*$ ;
            If  $d = \delta_j$ , no change;
            If  $d > \delta_j$  and  $s_j = j_*$ ,
                Recompute all distances  $d(j, s)$ ,  $s = j + 1, \dots, J$ , and update  $\delta_j$  and  $s_j$ ;
            If  $d > \delta_j$  and  $s_j \neq j_*$ , no change;
        }
    }
}
For  $j = j_*$ , recompute all distances  $d(j, s)$ ,  $s = j + 1, \dots, J$ , and update  $\delta_j$  and  $s_j$ ;
For  $j = j_* + 1, \dots, s_{j_*} - 1, \{$ 
    If  $s_j = s_{j_*}$ , recompute all distances  $d(j, s)$ ,  $s = j + 1, \dots, J$ , and update  $\delta_j$  and  $s_j$ ;
    If  $s_j \neq s_{j_*}$ , no change;
}
For  $j = s_{j_*} + 1, \dots, J$ , no change;
Erase  $C_{s_{j_*}}$ ;
Find  $\delta_* = \min_{j=1, \dots, J} \delta_j$  and  $j_* = \arg \min_{j=1, \dots, J} \delta_j$ , the closest pair is  $\langle j_*, s_{j_*} \rangle$ ;
}

```

Implementation notes:

- In order to reduce the memory requirement, it is not necessary to create an actual distance matrix when determining the closest clusters.
- If the Euclidean distance is used, the ward measure will be used to find the closest clusters. We just replace the distance measure  $d(j, s)$  by  $\frac{N_j N_s}{N_j + N_s} d^2(j, s)$ . This also applies below for CF-tree based HAC.

## 7.2. CF-tree Based HAC

Suppose that CF-tree based HAC starts with  $K_0$  CF-trees  $T_{CF}^k, k = 1, \dots, K_0$  which contain  $J_0$  leaf entries  $C_i, i = 1, \dots, J_0$ . Let  $l(C_i)$  be the index of the CF-tree which contains the leaf entry  $C_i$ . For convenience, suppose  $C_s > C_j$  if  $l(C_s) > l(C_j)$ .

At each subsequent step, a pair of leaf entries is chosen. The two leaf entries  $C_j$  and  $C_s$  in the pair are closest together in terms of the distance measure  $d(j, s)$ . A new leaf entry  $C_{<j,s>}$  is formed to replace one of the leaf entries in the pair,  $C_j$ , say. This new leaf entry contains all data cases in  $C_j$  and  $C_s$ . The other leaf entry  $C_s$  is discarded. Hence the number of leaf entries is reduced by one at each step. Meanwhile, the involved CF-trees will be updated accordingly. The process stops when the desired number of leaf entries  $J_1$  is reached. The output is the set of updated CF-trees, whose leaf entries indicate the produced clusters.

The procedure of CF-tree based HAC is as follows.

Step 1. For  $j = 1, \dots, J_0 - 1, \{$   
  Find the closest leaf entry  $C_{s^k}$  in each CF-tree  $T_{CF}^k$  for  $k = l(C_j), \dots, K_0$ , following the involved tree structure;  
  Find  $\delta_j = \min_{s^k > j, k=l(C_j), \dots, K_0} d(j, s^k)$  and  $s_j = \arg \min_{s^k > j, k=l(C_j), \dots, K_0} d(j, s^k);$   
 $\}$   
  Find  $\delta_* = \min_{j=1, \dots, J_0-1} \delta_j$  and  $j_* = \arg \min_{j=1, \dots, J_0-1} \delta_j$ , the closest pair is  $\langle j_*, s_{j_*} \rangle;$   
Step 2. For  $J = J_0 - 1, \dots, J_1, \{$   
  Merge the closest pair  $\langle j_*, s_{j_*} \rangle$ , update CF-tree  $T_{CF}^{l(C_{j_*})}$  by the new leaf entry  $C_{\langle j_*, s_{j_*} \rangle}$ , and remove the leaf entry  $C_{s_{j_*}}$  from CF-tree  $T_{CF}^{l(C_{s_{j_*}})}$ ;  
  For  $j = 1, \dots, j_* - 1, \{$   
    If  $s_j = s_{j_*}, \{$   
      Find the closest leaf entry  $C_{s^k}$  in each CF-tree  $T_{CF}^k$  for  $k = l(C_j), \dots, K_0;$   
      Find  $\delta_j = \min_{s^k > j, k=l(C_j), \dots, K_0} d(j, s^k)$  and  $s_j = \arg \min_{s^k > j, k=l(C_j), \dots, K_0} d(j, s^k);$   
     $\}$   
    If  $s_j \neq s_{j_*}, \{$   
      Compute  $d = d(j, j_*);$   
      If  $d < \delta_j$ , update  $\delta_j = d$  and  $s_j = j_*;$   
      If  $d = \delta_j$ , no change;  
      If  $d > \delta_j$  and  $s_j = j_*, \{$   
        Find the closest leaf entry  $C_{s^k}$  in each CF-tree  $T_{CF}^k$  for  $k = l(C_j), \dots, K_0;$   
        Find  $\delta_j = \min_{s^k > j, k=l(C_j), \dots, K_0} d(j, s^k)$  and  $s_j = \arg \min_{s^k > j, k=l(C_j), \dots, K_0} d(j, s^k);$   
       $\}$   
      If  $d > \delta_j$  and  $s_j \neq j_*$ , no change;  
     $\}$   
   $\}$   
  For  $j = j_*, \{$   
    Find the closest leaf entry  $C_{s^k}$  in each CF-tree  $T_{CF}^k$  for  $k = l(C_j), \dots, K_0;$   
    Find  $\delta_j = \min_{s^k > j, k=l(C_j), \dots, K_0} d(j, s^k)$  and  $s_j = \arg \min_{s^k > j, k=l(C_j), \dots, K_0} d(j, s^k);$   
   $\}$   
  For  $j = j_* + 1, \dots, s_{j_*} - 1, \{$   
    If  $s_j = s_{j_*}, \{$

```

    Find the closest leaf entry  $C_{s^k}$  in each CF-tree  $T_{CF}^k$  for  $k = l(C_j), \dots, K_0$ ;
    Find  $\delta_j = \min_{s^k > j, k=l(C_j), \dots, K_0} d(j, s^k)$  and  $s_j = \arg \min_{s^k > j, k=l(C_j), \dots, K_0} d(j, s^k)$ ;
  }
  If  $s_j \neq s_{j^*}$ , no change;
}
For  $j = s_{j^*} + 1, \dots, J$ , no change;
Find  $\delta_* = \min_{j=1, \dots, J} \delta_j$  and  $j_* = \arg \min_{j=1, \dots, J} \delta_j$ , the closest pair is  $\langle j_*, s_{j_*} \rangle$ ;
}

```

Step 3. Export updated non-empty CF-trees;

Clearly, CF-tree based HAC is very similar to matrix based HAC. The only difference is that CF-tree based HAC takes advantage of CF-tree structures to efficiently find the closest pair, rather than checking all possible pairs as in matrix based HAC.

## 8. Determination of the Number of Clusters

Assume that the hierarchical clustering method has been used to produce 1, 2 ... clusters already. We consider the following two criterion indices in order to find the appropriate number of final clusters.

Bayesian Information Criterion (BIC):

$$\text{BIC}(J) = -2 \sum_{j=1}^J \tilde{\xi}_j + m_j \ln(N), \quad (23)$$

where  $N$  is the total number of cases in all the  $J$  clusters,

$$m_j = J \left\{ 2K^A + \sum_{k=1}^{K^B} (L_k - 1) \right\}. \quad (24)$$

Akaike Information Criterion (AIC):

$$\text{AIC}(J) = -2 \sum_{j=1}^J \tilde{\xi}_j + 2m_j. \quad (25)$$

Let  $I(J)$  be the criterion index (BIC or AIC) of  $J$  clusters,  $d(J)$  be the distance measure between the two clusters merged in merging  $J + 1$  clusters to  $J$  clusters, and  $J_C$  be the total number of sub-clusters from which to determine the appropriate number of final clusters.

Users can supply the range for the number of clusters  $[J_{min}, J_{max}]$  in which they believe the “true” number of clusters should lie. Notice that if  $J_C < J_{max}$ , reset  $J_{max} = J_C$ .

The following four methods are proposed:

### Method 1. Finding the number of clusters by information convergence.

Let  $\Delta I(J) = I(J) - I(J + 1)$ , where  $I(J)$  can be either  $\text{BIC}(J)$  or  $\text{AIC}(J)$  depending on user's choice.

If  $\Delta I(1) \leq 0$ ,  $J_I = J_{min}$ . Else, let  $R_1(J) = \Delta I(J) / \Delta I(1)$ ;

Let  $J_I$  be the smallest  $J$  in  $[J_{min}, J_{max} - 1]$  which satisfies  $R_1(J) < 0.1$ . If none  $J$  satisfies the condition, let  $J_I = J_{max}$ .

**Method 2. Finding the number of cluster by the largest distance jump.**

To report  $J_d = 1 + \arg \max_{J \in [J_{min}-1, J_{max}-1]} (d(J)/d(J + 1))$  as the number of clusters.

**Method 3. Finding the number of clusters by combining distance jump and information convergence aggressively**

The process goes as follows:

- a) Let  $R_2(J) = d(J)/d(J + 1)$ .
- b) Let  $J_1$  be the largest  $J$  in  $[J_{min}, J_I - 1]$  which satisfies  $R_1(J) > 0.3$ . If none  $J$  satisfies the condition, let  $J_1 = J_{min} - 1$ .
- c) Calculate  $R_2(J)$  for  $J$  in  $[J_1, J_I - 1]$ . Suppose that the max and the second max of  $R_2(J)$  occurred at  $m_1$  and  $m_2$ .
- d) If  $\frac{R_2(m_1)}{R_2(m_2)} > 1.3$ , report  $1 + m_1$  as the cluster number.
- e) Otherwise, report  $1 + \text{MIN}(m_1, m_2)$ .

**Method 4. Finding the number of clusters by combining distance jump and information convergence conservatively**

This method performs the same steps from a) to d) in method 3. But in step e), method 4 reports  $1 + \text{MAX}(m_1, m_2)$ .

By default, method 3 is used with BIC as the information criterion.

## 9. Overview of the Entire Clustering Solution

Figure 5 illustrates the overview of the entire clustering solution.

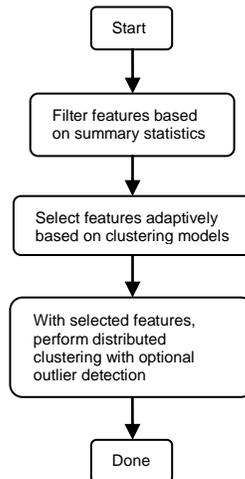


Figure 5. Control flow of the entire clustering solution.

## 9.1. Feature Selection

### 9.1.1. Feature Filtering

Based on the summary statistics produced by DE, CE will perform an initial analysis and determine the features that are not useful for making the clustering solution. Specifically, the following features will be excluded.

#	Rule	Status	Comment
1	Frequency/analysis weight features	Required	
2	Identity features	Required	
3	Constant features	Required	
4	The percentage of missing values in any feature is larger than $\delta$ (default 70%)	Required	
5	The distribution of the categories of a categorical feature is extremely imbalanced, that is $RMSSE > \delta$ (default 0.7)	Discarded	The statistic of $RMSSE$ is the effect size for one sample chi-square test.
6	One category makes up the overwhelming majority of total population above a given percentage threshold $\delta$ (default 95%)	Required	
7	The number of categories of a categorical feature is larger than $\delta$ (default 24)	Required	
8	There are categories of a categorical feature with extremely high or low frequency, that is, the outlier strength is larger than $\delta$ (default 3)	Discarded	
9	The absolute coefficient of variation of a continuous feature is smaller than $\delta$ (default 0.05)	Required	

The remaining features will be saved for adaptive feature selection in the next step.

### 9.1.2. Adaptive Feature Selection

Adaptive feature selection selects the most important features for the final clustering solution. Specifically, it performs the following steps.

- Step 1. Divide the distributed data into data splits.
- Step 2. Build a local CF-tree on each data split.
- Step 3. Distribute local CF-trees into multiple computing units. A unique key is assigned to each CF-tree.
- Step 4. On each computing unit, start with all available features:
  - a. Perform matrix based HAC with all features on the leaf entries to get an approximate clustering solution,  $S_0$ . Suppose there are  $J^*$  final clusters.
  - b. Compute importance for the set of all features.
  - c. Let  $S^* = S_0$  and  $I_{ref}$  be the information criteria of  $S_0$ .
  - d. Remove features with non-positive importance as many as possible, and update  $S^*$  and  $I_{ref}$ .
  - e. Repeat to do the follows:
    - i. Select the most unimportant feature from remaining features which are not checked.
    - ii. Perform matrix based HAC with remaining features (not including the selected one) on the leaf entries to get a new approximate clustering solution,  $S_1$ , with the fixed number of  $J^*$  clusters.

- iii. If the information criteria of  $S1$  plus the information of all discarded features determined by  $S1$  is lower than  $I_{ref}$ , then remove the selected feature, and let  $S^* = S1$ .
  - iv. Continue to check the next feature.
  - f. Select the set of features corresponding to  $S^*$ .
- Step 5. Pour together all the sets of features produced by different computing units. Discard any feature if its occurring frequency is less than  $R * \beta$  (default  $\beta = 50\%$ ). The remaining features will be used to build the final clustering solution.

The process described above can be implemented in parallel using one map-reduce job under the Hadoop framework, as illustrated in Figure 6. See appendix A for details the map-reduce implementation.

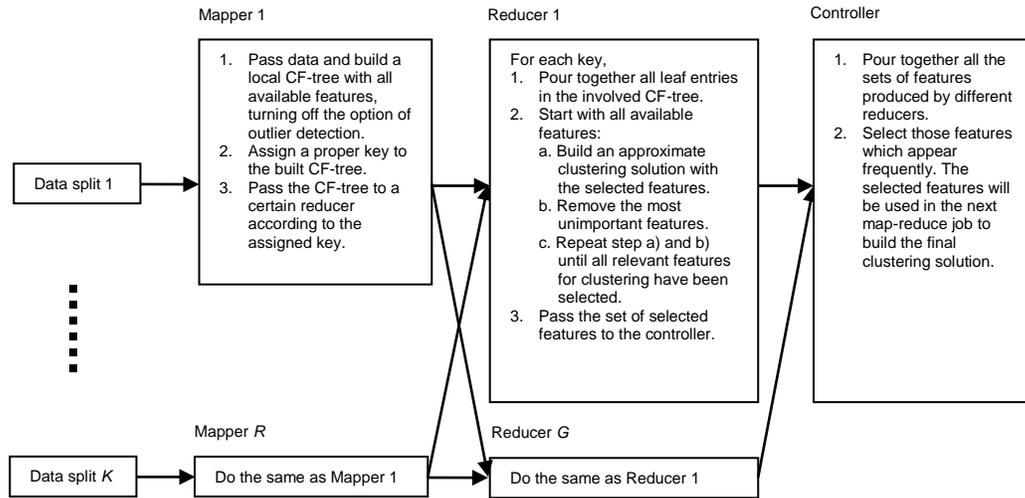


Figure 6. One map-reduce job for feature selection.

Implementation notes:

- In default, the information based feature importance is used for the log-likelihood distance measure, and the effect size based feature importance is for the Euclidean distance.
- If no features are selected, just report all features.

## 9.2. Distributed Clustering

The Clustering Engine (CE) can identify clusters from distributed data with high performance and accuracy. Specifically, it performs the following steps:

- Step 1. Divide the distributed data into data splits.
- Step 2. Build a local CF-tree on each data split.
- Step 3. Distribute local CF-trees into multiple computing units. Note that multiple CF-trees may be distributed to the same computing unit.
- Step 4. On each computing unit, with all CF-entries in the involved CF-trees, perform a series of CF-tree based HACs, and get a specified number of sub-clusters.

Step 5. Pour together all the sub-clusters produced by different computing unit, and perform matrix based HAC to get the final clusters.  
 The number of final clusters is determined automatically or using a fixed one depending on the settings.

The process described above can be implemented in parallel using one map-reduce job under the Hadoop framework, as illustrated in Figure 7. See appendix B for details of the map-reduce implementation.

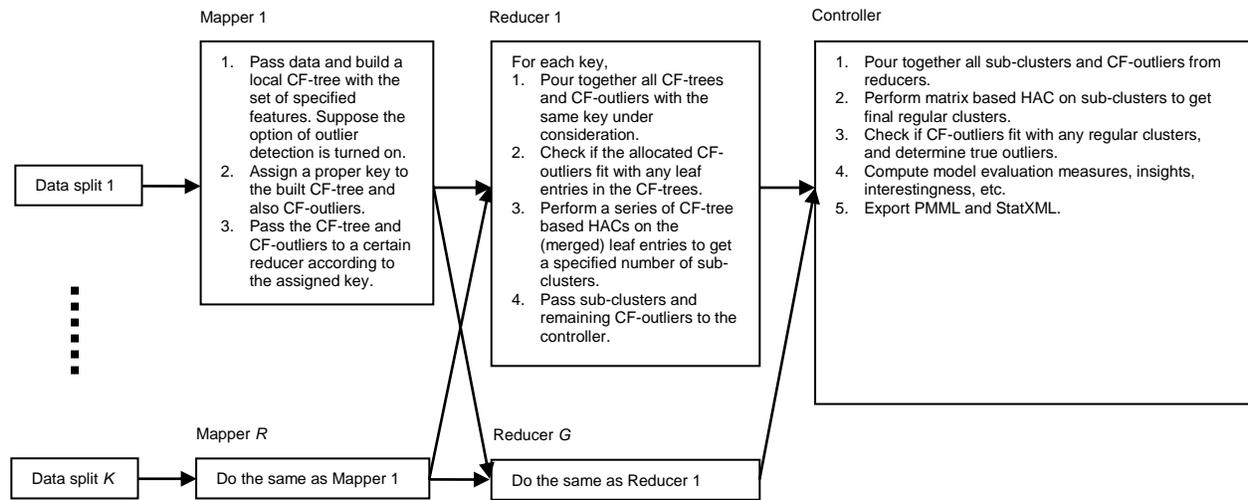


Figure 7. One map-reduce job for distributed clustering with outlier deletion.

Implementation notes:

- The number of computing units is  $Q = \lceil \min(R * S / D_1, D_2 / C_{min}) \rceil$ , (28)  
 where  $D_1$  (default 50,000) is the number of data points which are suitable to perform CF-tree based HAC,  $D_2$  (default 5,000) is the number of data points which are suitable to perform matrix based HAC,  $C_{min}$  is the minimal number of sub-clusters produced by each computing unit, and  $S$  is the maximal number of leaf entries, i.e.  $B^H * L$ , in a single CF-tree.
- The number of sub-clusters produced by each computing unit is  $J_1 = \lceil \min(R * S, D_2) / Q \rceil$ . (29)

### 9.3. Distributed Outlier Detection

Outlier detection in the Clustering Engine will be based and will build upon the outlier handling method described previously in section 6. It is also extended to the distributed setting with the following steps:

- Step 1. On each data split, perform the following:
- 1) Generate local candidate outliers according to the method described in section 6.
  - 2) Distribute the local candidate outliers together with the associated CF-tree to a certain computing unit.
- Step 2. Each computing unit is allocated with a set of candidate outliers and also a set of CF-trees containing regular leaf entries. For each member in the set of candidate outliers, it will be merged with the closest regular leaf entry only if the merging does not break the maximal tightness threshold among the involved CF-trees. Note that we will pass the CF-trees in order to enhance the performance of finding the closest regular leaf entry.
- Step 3. Pour together all the remaining candidate outliers and sub-clusters produced by computing machines. Do the following:
- 1) Perform matrix based HAC on sub-clusters, and get the final regular clusters.
  - 2) Keep only candidate outliers whose distance from the closest regular cluster to the center of the outlier candidate is greater than the corresponding cluster distance threshold  $D_t(j)$
  - 3) Merge the rest of candidate outliers with the corresponding closest regular clusters and update the distance threshold for each regular cluster.
  - 4) For each remaining outlier cluster, compute its outlier strength.
  - 5) Sort remaining outlier clusters according to outlier strength in descending order, and get the minimum outlier strength for the top P (default 5%) percent of outliers, and use it as an outlier threshold in scoring.
  - 6) Export a specified number of the most extreme outlier clusters (default 20), along with the following measures for each cluster: cluster size, outlier strength, probabilities of belonging to each regular cluster.

Outlier strength of a cluster  $C_s$  is computed as

$$O(s) = \sum_{j=1}^J \frac{\tilde{d}(j,s)}{D_t(j)} p(j|s), \quad (30)$$

where  $D_t(j)$  is the distance threshold of cluster  $C_j$ , which is the maximum distance from cluster  $C_j$  to each center of its starting sub-clusters in matrix based HAC,  $\tilde{d}(j, s)$  is the distance from cluster  $C_j$  to the center of cluster  $C_s$ , and  $p(j|s)$  is the probability of cluster  $C_s$  belonging to cluster  $C_j$ , that is

$$p(j|s) = \frac{\exp(-\tilde{d}(j,s))}{\sum_{j=1}^J \exp(-\tilde{d}(j,s))}. \quad (31)$$

Notice that the distance between the cluster center and a cluster  $C_j$  is computed by considering the center of cluster  $C_s$  as a singleton cluster  $C_{s'}$ . The cluster center herein is defined as the mean for a continuous feature, while being the mode for a categorical feature.

## 10. Cluster Membership Assignment

### 10.1. Without Outlier-Handling

Assign a case to the closest cluster according to the distance measure. Meanwhile, produce the probabilities of the case belonging to each regular cluster.

## 10.2. With Outlier-Handling

### 10.2.1. Legacy Method

#### Log-likelihood distance

Assume outliers follow a uniform distribution. Calculate both the log-likelihood resulting from assigning a case to a noise cluster and that resulting from assigning it to the closest non-noise cluster. The case is then assigned to the cluster which leads to the larger log-likelihood. This is equivalent to assigning a case to its closest non-noise cluster if the distance between them is smaller than a critical value  $C = \ln(\prod_k R_k \prod_m L_m)$ , where  $\prod_k R_k$  is the product of ranges of continuous fields, and  $\prod_m L_m$  is the product of category numbers of categorical fields. Otherwise, designate it as an outlier.

#### Euclidean distance

Assign a case to its closest non-noise cluster if the Euclidean distance between them is smaller than a critical value  $C = 2 \sqrt{\frac{1}{JK_A} \sum_{j=1}^J \sum_{k=1}^{K_A} \hat{\sigma}_{jk}^2}$ . Otherwise, designate it as an outlier.

### 10.2.2. New Method

When scoring a new case, we compute the outlier strength of the case. If the computed outlier strength is greater than the outlier threshold, then the case is an outlier and otherwise belongs to the closest cluster. Meanwhile, the probabilities of the case belonging to each regular cluster are produced.

Alternatively, users can specify a customized outlier threshold (3, for example) rather than using the one found from the data.

## 11. Clustering Model Evaluation

Clustering model evaluation enables users to understand the identified cluster structure, and also to learn useful insights and interestingness derived from the clustering solution.

Note that clustering model evaluation can be done using cluster features and also the hierarchical dendrogram when forming the clustering solution.

### 11.1. Across-Cluster Feature Importance

Across-cluster feature importance indicates how influential a feature is in building the clustering solution. This measure is very useful for users to understand the clusters in their data. Moreover, it helps for feature selection, as described in section 12.2.

Across-cluster feature importance can be defined using two methods.

#### 11.1.1. Information Criterion Based Method

If BIC is used as the information criterion, the importance of feature  $k$  is

$$\text{Importance}_k = \frac{\text{BIC}_k^0 - \text{BIC}_k}{\text{diff}_k^{\max}}, \quad (32)$$

where

$$\text{BIC}_k^0 = \begin{cases} N_k \ln(\hat{\sigma}_k^2 + \Delta_k) + 2 \ln(N), & \text{if feature } k \text{ is continuous} \\ 2N'_k \hat{E}_k + (L_k - 1) \ln(N), & \text{if feature } k \text{ is categorical} \end{cases}$$

$$\text{BIC}_k = \begin{cases} \sum_{j=1}^J N_{jk} \ln(\hat{\sigma}_{jk}^2 + \Delta_k) + 2J \ln(N), & \text{if feature } k \text{ is continuous} \\ 2 \sum_{j=1}^J N'_{jk} \hat{E}_{jk} + J(L_k - 1) \ln(N), & \text{if feature } k \text{ is categorical} \end{cases}$$

$$\text{diff}_k^{\max} = \max_k(\text{BIC}_k^0 - \text{BIC}_k),$$

and  $N_k, N'_k$  is the total valid count of feature  $k$  in the data,  $\hat{\sigma}_k^2$  is the grand variance, and  $\hat{E}_k$  is the grand entropy.

Notice that the information measure for the overall population has been decomposed as

$$\text{BIC}^0 = \sum_{k=1}^{K^A + K^B} \text{BIC}_k^0.$$

While if AIC is used, across-cluster importance is

$$\text{Importance}_k = \frac{\text{AIC}_k^0 - \text{AIC}_k}{\text{diff}_k^{\max}}, \quad (33)$$

where

$$\text{AIC}_k^0 = \begin{cases} N_k \ln(\hat{\sigma}_k^2 + \Delta_k) + 4, & \text{if feature } k \text{ is continuous} \\ 2N'_k \hat{E}_k + 2(L_k - 1), & \text{if feature } k \text{ is categorical} \end{cases}$$

$$\text{AIC}_k = \begin{cases} \sum_{j=1}^J N_{jk} \ln(\hat{\sigma}_{jk}^2 + \Delta_k) + 4J, & \text{if feature } k \text{ is continuous} \\ 2 \sum_{j=1}^J N'_{jk} \hat{E}_{jk} + 2J(L_k - 1), & \text{if feature } k \text{ is categorical} \end{cases}$$

$$\text{diff}_k^{\max} = \max_k(\text{AIC}_k^0 - \text{AIC}_k).$$

Notice that, if the importance computed as above is negative, set it as zero. This also applies in the following.

Notice that the importance of a feature will be zero if the information difference corresponding to the feature is negative. This applies for all the calculations of information-based importance.

### 11.1.2. Effect Size Based Method

This method is similar to that used for defining association interestingness for bivariate variables. See ref. 6 for details.

### Categorical Feature

For a categorical feature  $k$ , compute Pearson chi-square test statistic

$$\chi_p^2 = \sum_{l=1}^{L_k} \sum_{j=1}^J \frac{(N_{jkl} - E_{jkl})^2}{E_{jkl}}, \quad (34)$$

where

$$E_{jkl} = \frac{N_{jk} \cdot N_{\cdot kl}}{N_{\cdot k}}, \quad (35)$$

and

$$N_{jk} = \sum_{l=1}^{L_k} N_{jkl}, \quad (36)$$

$$N_{\cdot kl} = \sum_{j=1}^J N_{jkl}, \quad (37)$$

$$N_{\cdot k} = \sum_{l=1}^{L_k} \sum_{j=1}^J N_{jkl}. \quad (38)$$

The p-value is computed as

$$p_{value} = \text{Prob}\{\chi^2 > \chi_p^2\}, \quad (39)$$

in which  $\chi^2$  is a random variable that follows a chi-square distribution with freedom degree of  $(J - 1)(L_k - 1)$ . Note that categories with  $N_{jk} = 0$  or  $N_{\cdot kl} = 0$  will be excluded when computing the statistic and degrees of freedom.

The effect size, Cramer's V, is

$$E_s = \left( \frac{\chi_p^2}{N_{\cdot k} \cdot (q-1)} \right)^{1/2}, \quad (40)$$

where

$$q = \min(J, L_k). \quad (41)$$

The importance of feature  $k$  is produced by the following mapping function

$$\text{Importance}_k = \begin{cases} 0, & p_{value} \geq sig. \\ \text{MonotoneCubicInterpolation}(S_t, I_t, E_s), & p_{value} < sig. \end{cases} \quad (42)$$

where  $sig.$  is significance level (default 0.05),  $S_t$  is a set of threshold values to assess effect size (default  $S_t = \{0.0, 0.2, 0.6, 1.0\}$ ),  $I_t$  is a set of corresponding thresholds of importance (default  $I_t = \{0.00, 0.33, 0.67, 1.00\}$ ), and  $\text{MonotoneCubicInterpolation}(\cdot)$  is a monotone cubic interpolation mapping function between  $S_t$  and  $I_t$ .

### Continuous Feature

For a continuous feature  $k$ , compute F test statistic

$$F = \frac{SSR/(J-1)}{SSE/(N_k-J)} \quad (43)$$

where

$$SSR = \sum_{j=1}^J N_{jk} (\hat{\mu}_{jk} - \hat{\mu}_k)^2, \quad (44)$$

$$SSE = \sum_{j=1}^J N_{jk} \hat{\sigma}_{jk}^2, \quad (45)$$

$$N_k = \sum_{j=1}^J N_{jk}, \quad (46)$$

$$\hat{\mu}_k = \frac{\sum_{j=1}^J N_{jk} \hat{\mu}_{jk}}{N_k}. \quad (47)$$

The F statistic is undefined if the denominator equals zero. Accordingly, the  $p$ -value is calculated as

$$p_{value} = \begin{cases} \text{undefined,} & \text{if both the numerator and denominator of } F \text{ are zero;} \\ 0, & \text{else if the denominator of } F \text{ is zero;} \\ \text{Prob}\{F(J-1, N_k-J) > F\}, & \text{else.} \end{cases} \quad (48)$$

in which  $F(J-1, N_k-J)$  is a random variable that follows a  $F$ -distribution with degrees of freedom  $J-1$  and  $N_k-J$ .

The effect size, Eta square, is

$$E_s = 1 - \frac{\sum_{j=1}^J N_{jk} \hat{\sigma}_{jk}^2}{N_k \hat{\sigma}_k^2}, \quad (49)$$

where

$$\hat{\sigma}_k^2 = \frac{\sum_{j=1}^J s_{jk}^2 - N_k \hat{\mu}_k^2}{N_k}. \quad (50)$$

The importance of feature  $k$  is produced using the same mapping function as (42), and default  $S_t = \{0.0, 0.04, 0.36, 1.0\}$ .

## 11.2. Within-Cluster Feature Importance

Within-cluster feature importance indicates how influential a feature is in forming a cluster. Similar to across-cluster feature importance, within-cluster feature importance can also be defined using two methods.

### 11.2.1. Information Criterion Based Method

If BIC is used as the information criterion, the importance of feature  $k$  within cluster  $C_j$  ( $j = 1, \dots, J$ ) is

$$\text{Importance}_{k,j} = \frac{\text{BIC}_k^0 - \text{BIC}_{k,j}}{\text{diff}_{K,j}^{\max}}, \quad (51)$$

where

$$\text{BIC}_{k,j} = \begin{cases} N_{jk} \ln(\hat{\sigma}_{jk}^2 + \Delta_k) + N_{j^c k} \ln(\hat{\sigma}_{j^c k}^2 + \Delta_k) + 2 * 2 \ln(N), & \text{if feature } k \text{ is continuous} \\ 2N'_{jk} \hat{E}_{jk} + 2N'_{j^c k} \hat{E}_{j^c k} + 2 * (L_k - 1) \ln(N), & \text{if feature } k \text{ is categorical} \end{cases} \quad (52)$$

$$\text{diff}_{K,j}^{\max} = \max_k (\text{BIC}_k^0 - \text{BIC}_{k,j}). \quad (53)$$

Notice that  $j^c$  represents the complement set of  $j$  in  $J$ .

If AIC is used as the information criterion, the importance of feature  $k$  within cluster  $C_j$  ( $j = 1, \dots, J$ ) is

$$\text{Importance}_{k,j} = \frac{\text{AIC}_k^0 - \text{AIC}_{k,j}}{\text{diff}_{K,j}^{\max}}, \quad (54)$$

where

$$\text{AIC}_{k,j} = \begin{cases} N_{jk} \ln(\hat{\sigma}_{jk}^2 + \Delta_k) + N_{j^c k} \ln(\hat{\sigma}_{j^c k}^2 + \Delta_k) + 4 * 2, & \text{if feature } k \text{ is continuous} \\ 2N'_{jk} \hat{E}_{jk} + 2N'_{j^c k} \hat{E}_{j^c k} + 2 * 2(L_k - 1), & \text{if feature } k \text{ is categorical} \end{cases} \quad (55)$$

$$\text{diff}_{K,j}^{\max} = \max_k (\text{AIC}_k^0 - \text{AIC}_{k,j}). \quad (56)$$

### 11.2.2. Effect Size Based Method

Within-cluster importance is defined by comparing the distribution of the feature within a cluster with the overall distribution.

#### Categorical Feature

For cluster  $C_j$  ( $j = 1, \dots, J$ ) and a categorical feature  $k$ , compute Pearson chi-square test statistic

$$\chi_p^2 = \sum_{l=1}^{L_k} \frac{(N_{jkl} - E_{jkl})^2}{E_{jkl}}, \quad (57)$$

where

$$E_{jkl} = \frac{N_{jk} \cdot N_{\cdot kl}}{N_{\cdot k}}. \quad (58)$$

The p-value is computed as

$$p_{value} = \text{Prob}\{\chi^2 > \chi_p^2\}, \quad (59)$$

in which  $\chi^2$  is a random variable that follows a chi-square distribution with freedom degree of  $L_k - 1$ . Note that importance for feature  $k$  within cluster  $C_j$  will be undefined if  $N_{jk}$  equals zero.

The effect size is

$$E_s = \left( \frac{\chi_p^2}{N_{jk}(L_k-1)} \right)^{\frac{1}{2}}. \quad (60)$$

The importance of feature  $k$  within cluster  $C_j$  is produced using the same mapping function as (42), and default  $S_t = \{0.0, 0.2, 0.6, 1.0\}$ .

### Continuous Feature

For cluster  $C_j$  ( $j = 1, \dots, J$ ) and a continuous feature  $k$ , compute t test statistic

$$t = \frac{\hat{\mu}_{jk} - \hat{\mu}_k}{s_d / \sqrt{N_{jk}}}, \quad (61)$$

where

$$s_d = \sqrt{\frac{N_{jk}}{N_{jk}-1} \hat{\sigma}_{jk}^2}. \quad (62)$$

The  $p$ -value is calculated as

$$p_{value} = \begin{cases} \text{undefined,} & \text{if both the numerator and denominator of } t \text{ are zero;} \\ 0, & \text{else if the denominator of } t \text{ is zero;} \\ 1 - \text{Prob}\{|T(N_{jk} - 1)| \leq |t|\}, & \text{else.} \end{cases} \quad (63)$$

in which  $T(N_{jk} - 1)$  is a random variable that follows a  $t$ -distribution with degrees of freedom  $N_{jk} - 1$ .

The effect size is

$$E_s = \frac{|\hat{\mu}_{jk} - \hat{\mu}_k|}{s_d}. \quad (64)$$

The importance of feature  $k$  within cluster  $C_j$  is produced using the same mapping function as (42), and default  $S_t = \{0.0, 0.2, 0.6, 1.0\}$ .

## 11.3. Clustering Model Goodness

Clustering model goodness indicates the quality of a clustering solution. This measure will be computed for the final clustering solution, and it will also be computed for approximate clustering solutions during the process of adaptive feature selection.

Suppose there are  $J$  regular clusters, denoted as  $C_1, \dots, C_J$ . Let  $l(i)$  be the regular cluster label assigned to sub-cluster  $i$ .

Then for each sub-cluster  $i$ , the Silhouette coefficient is computed approximately as

$$S_i = \frac{\Omega - \Phi}{\max(\Phi, \Omega)}, \quad (65)$$

where

$\Phi$  is the weighted average distance from the center of sub-cluster  $i$  to the center of every other sub-cluster assigned to the same regular cluster, that is,

$$\Phi = \frac{\sum_{s \neq i \text{ and } l(s)=l(i)} N_s d(i,s)}{\sum_{s \neq i \text{ and } l(s)=l(i)} N_s}, \quad (66)$$

$\Omega$  is the minimal average distance from the center of sub-cluster  $i$  to the center of sub-clusters in a different regular cluster among all different regular clusters, that is,

$$\Omega = \min \left\{ \frac{\sum_{l(s)=C_j} N_s d(i,s)}{\sum_{l(s)=C_j} N_s} \mid j = 1, \dots, J \text{ and } C_j \neq l(i) \right\}. \quad (67)$$

Clustering model goodness is defined as the weighted average Silhouette coefficient over all starting sub-clusters in the final stage of regular HAC, that is,

$$Goodness = \frac{\sum_j N_j S_j}{\sum_j N_j}. \quad (68)$$

The average Silhouette coefficient ranges between -1 (indicating a very poor model) and +1 (indicating an excellent model). As found by Kaufman and Rousseeuw (1990), average Silhouette greater than 0.5 indicates reasonable partitioning of data; lower than 0.2 means that data does not exhibit cluster structure. In this regard, we can use the following function to map *Goodness* into an interestingness score:

$$Interestingness(Goodness) = MonotoneCubicInterpolation(S_t, I_t, Goodness), \quad (69)$$

where  $S_t = \{-1.0, 0.2, 0.5, 1.0\}$ , and  $I_t = \{0.0, 0.0, 0.5, 1.0\}$ .

Implementation notes:

- Please refer to section 9.3 for the definition of cluster center and also for the calculation of distance.
- When there is only a single sub-cluster in the regular cluster, let  $\Phi$  be the tightness of the sub-cluster.

## 11.4. Special Clusters

With the clustering solution, we can find special clusters, which could be regular clusters with high quality, extreme outlier clusters, and so on.

### 11.4.1. Regular Cluster Ranking

To select the most useful or interesting regular clusters, we can rank them according to any of the measures described below.

#### Cluster tightness

Cluster tightness is given by equation (9) or (15).

Cluster tightness is not scale-free, and it is a measure of cluster cohesion.

#### Cluster importance

Cluster importance indicates the quality of the regular cluster in the clustering solution. A higher importance value means a better quality of the regular cluster.

If BIC is used as the information criterion, the importance for regular cluster  $C_j$  is

$$\text{Importance}_j = \frac{\text{BIC}^0 - \text{BIC}_j}{\text{diff}_j^{\max}}, \quad (70)$$

where

$$\text{BIC}_j = \sum_{k=1}^{K^A+K^B} \text{BIC}_{k,j},$$

$$\text{BIC}^0 = \sum_{k=1}^{K^A+K^B} \text{BIC}_k^0,$$

$$\text{diff}_j^{\max} = \max_j(\text{BIC}^0 - \text{BIC}_j).$$

If AIC is used as the information criterion, the importance for regular cluster  $C_j$  is

$$\text{Importance}_j = \frac{\text{AIC}^0 - \text{AIC}_j}{\text{diff}_j^{\max}}, \quad (71)$$

where

$$\text{AIC}_j = \sum_{k=1}^{K^A+K^B} \text{AIC}_{k,j},$$

$$\text{AIC}^0 = \sum_{k=1}^{K^A+K^B} \text{AIC}_k^0,$$

$$\text{diff}_j^{\max} = \max_j(\text{AIC}^0 - \text{AIC}_j).$$

Cluster importance is scale-free, and in some sense it is a normalized measure of cluster cohesion.

#### Cluster goodness

The goodness measure for regular cluster  $C_j$  is defined as the weighted average Silhouette coefficient over all starting sub-clusters in regular cluster  $C_j$ , that is,

$$Goodness_j = \frac{\sum_{l(i)=c_j} N_i S_i}{\sum_{l(i)=c_j} N_i}. \quad (72)$$

We can also map  $Goodness_j$  into an interestingness score using equation (69).

Cluster goodness is also scale-free, and it is a measure of balancing cluster cohesion and cluster separation.

### 11.4.2. Outlier Clusters Ranking

For each outlier cluster, we have the following measures: cluster size, outlier strength. Each of the measures can be used to rank outlier clusters, so as to find the most interesting ones.

### 11.4.3. Outlier Clusters Grouping

Outlier clusters can be grouped by the nearest regular cluster, using probability values.

## Appendix A. Map-Reduce Job for Feature Selection

### Mapper

Each mapper will handle one data split and use it to build a local CF-tree. The local CF-tree is assigned with a unique key. Notice that if the option of outlier handling is turned on, outliers will not be passed to reducers in case of feature selection.

Let  $T_{CF}^{(r)}(key_r)$  be the CF-tree with the key of  $key_r$  on data split  $r$  ( $r = 1, \dots, R$ ).

The map function is as follows.

<b>Inputs:</b>	
- Data split $r$	// $r = 1, \dots, R$
- $key_r$	// $r = 1, \dots, R$
<Parameter settings>	
- MainMemory	// Default 80*1024 bytes
- OutlierHandling	// {on, off}, default on
- OutlierHandlingDiskSpace	// Default 20% of MainMemory
- OutlierQualification	// Default 10 cases
- DelayedSplit	// {on, off}, default on
- DelayedSplitDiskSpace	// Default 10% of MainMemory
- Adjustment	// Default 0.01
- DistanceMeasure	// {Log-likelihood, Euclidean}, default // Log-likelihood
- InitialThreshold	// Default 0
- NonLeafNodeBranchingFactor	// Default 8
- LeafNodeBranchingFactor	// Default 8
- MaxTreeHeight	// Default 3
<b>Outputs:</b>	
- $T_{CF}^{(r)}(key_r)$	
<b>Procedure:</b>	
1. Build a CF-tree on data split $r$ based on specified features and settings;	
2. Assign $key_r$ to the CF-tree;	
3. Export $T_{CF}^{(r)}(key_r)$ ;	

### Reducer

Each reducer can handle several keys. For each key, it first pours together all CF-trees which have the same key. Then it builds approximate clustering solutions iteratively in order to find the most influential features. The selected features will be passed to the controller.

Let  $F^*(key_r)$  be the set of features produced for the key of  $key_r$ ,  $r = 1, \dots, R$ .

The reduce function for each key is as follows.

<b>Inputs:</b>
----------------

```

-  $T_{CF}^{(r)}(key_r)$ 

<Parameter settings>
- Adjustment // Default 0.01
- DistanceMeasure // {Log-likelihood, Euclidean}, default Log-likelihood
- AutoClustering // {on, off}, default on
- MaximumClusterNumber // Default 15
- MinimumClusterNumber // Default 2
- FixedClusterNumber // Default 5
- ClusteringCriterion // {BIC, AIC}, default BIC
- AutoClusteringMethod // {information criterion, distance jump, maximum, minimum}, default minimum

```

**Outputs:**

```

-  $F^*(key_r)$ 

```

**Procedure:**

1. Let  $F(key_r)$  be the set of all available features;
2. With all leaf entries in CF-tree  $T_{CF}^{(r)}(key_r)$  and using features  $F(key_r)$ , perform matrix based HAC to get an approximate cluster solution  $S_0$ . Suppose the number of approximate final clusters is  $J^*$ , which is determined automatically or using a fixed one depending on the settings;  
Compute importance for each feature in  $F(key_r)$ ;  
*// Importance values should not be truncated*  
Compute  $I(S_0)$ , the information criterion of  $S_0$ ;
3. Let  $F^*(key_r) = F(key_r)$  and  $I_{ref} = I(S_0)$ ;  
Find  $F_\alpha(key_r)$ , the set of features in  $F(key_r)$  with non-positive importance;  
Let  $\tilde{F}(key_r) = F(key_r) - F_\alpha(key_r)$ ;
4. With all leaf entries in CF-tree  $T_{CF}^{(r)}(key_r)$  and using features  $\tilde{F}(key_r)$ , perform matrix based HAC to get a new solution  $S_1$  with fixed  $J^*$ ;  
Compute  $I(S_1)$ , the information criterion of  $S_1$ ;  
Compute the information of all discarded features  $I(F(key_r) - \tilde{F}(key_r))$ , determined by  $S_1$ , as  $\sum_{k \in F(key_r) - \tilde{F}(key_r)} BIC_k$ , or  $\sum_{k \in F(key_r) - \tilde{F}(key_r)} AIC_k$ , depending on the setting, where
$$BIC_k = \begin{cases} \sum_{j=1}^J N_{jk} \ln(\hat{\sigma}_{jk}^2 + \Delta_k) + 2J \ln(N), & \text{if feature } k \text{ is continuous} \\ 2 \sum_{j=1}^J N'_{jk} \hat{E}_{jk} + J(L_k - 1) \ln(N), & \text{if feature } k \text{ is categorical} \end{cases}$$

$$AIC_k = \begin{cases} \sum_{j=1}^J N_{jk} \ln(\hat{\sigma}_{jk}^2 + \Delta_k) + 4J, & \text{if feature } k \text{ is continuous} \\ 2 \sum_{j=1}^J N'_{jk} \hat{E}_{jk} + 2J(L_k - 1), & \text{if feature } k \text{ is categorical} \end{cases}$$
*// Though the discarded features are not used to build  $S_1$ , their statistics are still available in CFs of final clusters in  $S_1$ .*
5. While  $(I(S_1) + I(F(key_r) - \tilde{F}(key_r))) > I_{ref}$  {  
Find the most important feature  $k$  in  $F_\alpha(key_r)$ ;  
Let  $\tilde{F}(key_r) = \tilde{F}(key_r) + \{k\}$ , and  $F_\alpha(key_r) = F_\alpha(key_r) - \{k\}$ ;  
With all leaf entries in CF-tree  $T_{CF}^{(r)}(key_r)$  and using features  $\tilde{F}(key_r)$ , perform matrix based HAC to get a new solution  $S_1$  with fixed  $J^*$ ;  
Compute  $I(S_1)$ , the information criterion of  $S_1$ ;  
Compute  $I(F(key_r) - \tilde{F}(key_r))$ , the information of all discarded features;  
}  
Let  $F^*(key_r) = \tilde{F}(key_r)$  and  $I_{ref} = I(S_1) + I(F(key_r) - \tilde{F}(key_r))$ ;
6. While  $(\tilde{F}(key_r)$  is not empty) {  
Find the most unimportant feature  $k$  in  $\tilde{F}(key_r)$ ;

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```

Let  $\tilde{F}(key_r) = \tilde{F}(key_r) - \{k\}$ ;
If  $(F(key_r) - F_\alpha(key_r) - \{k\})$  is empty, break;
With all leaf entries in CF-tree  $T_{CF}^{(r)}(key_r)$  and using features
 $F(key_r) - F_\alpha(key_r) - \{k\}$ , perform matrix based HAC to get a new solution S1
with fixed  $J^*$ ;
Compute  $I(S1)$ , the information criterion of S1;
Compute  $I(F_\alpha(key_r) + \{k\})$ , the information of all discarded features;
If  $(I(S1) + I(F_\alpha(key_r) + \{k\})) \leq I_{ref}$  {
    Let  $F^*(key_r) = F^*(key_r) - \{k\}$ ;
    Let  $F_\alpha(key_r) = F_\alpha(key_r) + \{k\}$ ;
    Let  $I_{ref} = I(S1) + I(F_\alpha(key_r) + \{k\})$ ;
    Let  $\tilde{F}(key_r) = \tilde{F}(key_r) - \{k\}$ ;
}
}
7. Export  $F^*(key_r)$ ;

```

## Controller

The controller pours together all sets of features produced by reducers, and selects those features which appear frequently. The selected features will be used in the next map-reduce job to build the final clustering solution.

The controller runs the following procedure.

<b>Inputs:</b>	
<Parameter settings>	
- MinFrequency	// Default 50%
<b>Outputs:</b>	
- $F^*$	// Set of selected features
<b>Procedure:</b>	
1. Let $\beta = \text{MinFrequency}$ , and $F^*$ be empty;	
2. Launch a map-reduce job, and get $F^*(key_r)$ , for $r = 1, \dots, R$ from the reducers;	
3. Compute $F = \bigcup_{r=1}^R F^*(key_r)$ ;	
4. For each feature in $F$ ,	
If the occurring frequency is larger than $R * \beta$ , add the feature into $F^*$ ;	
5. Export $F^*$ ;	

## Appendix B. Map-Reduce Job for Distributed Clustering

### Mapper

Each mapper will handle one data split and use it to build a local CF-tree.

Local outlier candidates and the local CF-tree will be distributed to a certain reducer. This is achieved by assigning them a key, which is randomly selected from the key set  $\{key_1, \dots, key_Q\}$ . The number of keys  $Q$  is computed by equation (28).

For convenience, in the following we call leaf entries as pre-clusters. Let  $T_{CF}^{(r)}(key_i)$  and  $S_{out}^{(r)}(key_i)$  be the CF-tree and the set of outliers, respectively, with the key of  $key_i$  ( $i = 1, \dots, Q$ ), on data split  $r$  ( $r = 1, \dots, R$ ).

The map function is as follows.

<b>Inputs:</b>	
- Data split $r$	// $r = 1, \dots, R$
- $key_i$	// $i = 1, \dots, Q$
<Parameter settings>	
- MainMemory	// Default 80*1024 bytes
- OutlierHandling	// {on, off}, default on
- OutlierHandlingDiskSpace	// Default 20% of MainMemory
- OutlierQualification	// Default 10 cases
- DelayedSplit	// {on, off}, default on
- DelayedSplitDiskSpace	// Default 10% of MainMemory
- Adjustment	// Default 0.01
- DistanceMeasure	// {Log-likelihood, Euclidean}, default // Log-likelihood
- InitialThreshold	// Default 0
- NonLeafNodeBranchingFactor	// Default 8
- LeafNodeBranchingFactor	// Default 8
- MaxTreeHeight	// Default 3
<b>Outputs:</b>	
- $T^{(r)}(key_i)$	// Tightness threshold
- $T_{CF}^{(r)}(key_i)$	
- $S_{out}^{(r)}(key_i)$	
<b>Procedure:</b>	
1. Build a CF-tree on data split $r$ based on specified features and settings;	
2. If (DelayedSplit='on'),	
Absorb cases in disk space $S_1$ with tree rebuilding if necessary;	
2. If (OutlierHandling='on'), {	
Absorb entries in disk space $S_2$ without tree rebuilding;	
Check the final CF-tree for outliers;	
Mark the identified outliers and remaining entries in disk space $S_2$ as	
local outlier candidates;	
}	
3. Assign $key_i$ to the CF-tree and the set of outlier candidates;	
4. Export $T^{(r)}(key_i)$ , $T_{CF}^{(r)}(key_i)$ , and $S_{out}^{(r)}(key_i)$ ;	

## Reducer

Each reducer can handle several keys. For each key, it first pours together all CF-trees which have the same key. Then with all leaf entries in the involved CF-trees, it performs a series of CF-tree based HACs to get a specified number of sub-clusters. Finally, the sub-clusters are passed to the controller. The number of sub-clusters produced for each key is computed by equation (29).

Let  $\Omega(key_i)$  be the set of data split indices  $r$  whose key is  $key_i$ ,  $S_{sub}(key_i)$  and  $S_{out}(key_i)$  be the set of sub-clusters and the set of outliers, respectively, produced for the key of  $key_i$ ,  $i = 1, \dots, Q$ .

The reduce function for each key is as follows.

### Inputs:

- $T^{(r)}(key_i)$ ,  $r \in \Omega(key_i)$
  - $T_{CF}^{(r)}(key_i)$ ,  $r \in \Omega(key_i)$
  - $S_{out}^{(r)}(key_i)$ ,  $r \in \Omega(key_i)$
- <Parameter settings>
- OutlierHandling // {on, off}, default on
  - Adjustment // Default 0.01
  - DistanceMeasure // {Log-likelihood, Euclidean}, default Log-likelihood
  - NumSubClusters // Number of sub-clusters produced for each key
  - MinSubClusters // Minimum sub-clusters produced for each key // default 500
  - MaximumDataPoitsCFHAC // Maximum data points for HAC, default 50,000

### Outputs:

- $S_{sub}(key_i)$
- $S_{out}(key_i)$

### Procedure:

1. Let  $J_1 = \text{NumSubClusters}$ ,  $C_{min} = \text{MinSubClusters}$ , and  $D_1 = \text{MaximumDataPoitsCFHAC}$ ;
  2. Compute  $T(key_i) = \max\{T^{(r)}(key_i) | r \in \Omega(key_i)\}$ ;
  3. Compute  $S_{CF}(key_i) = \{T_{CF}^{(r)}(key_i) | r \in \Omega(key_i)\}$ ;
  4. If OutlierHandling is 'on', {
    - Compute  $S_{out}(key_i) = \cup_{r \in \Omega(key_i)} S_{out}^{(r)}(key_i)$ ;
    - For each member in  $S_{out}(key_i)$ , {
      - Find the closest leaf entry in the set of CF-trees  $S_{CF}(key_i)$ ;
      - If the closest leaf entry can absorb the outlier member without violating the threshold requirement  $T(key_i)$ , then merge them, and update  $S_{out}(key_i)$  and the involved CF-tree;
  5. Let  $c_1$  be the total number of leaf entries in  $S_{CF}(key_i)$ ;
- While  $c_1 > D_1$ , {
- Divide the set of CF-trees  $S_{CF}(key_i)$  randomly into  $c_2$  groups, where  $c_2 = \lfloor c_1/D_1 \rfloor$ ;
  - For each group which has a larger number of leaf entries than  $c_3$ , perform CF-tree based HAC to get  $c_3$  leaf entries, where  $c_3 = \lfloor \max(D_1/c_2, C_{min}) \rfloor$ ;
  - Update  $S_{CF}(key_i)$  with new CF-trees produced in the above step;
  - Compute the total number of remaining leaf entries  $c_1$ ;

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- ```
}
6. With the set of CF-trees  $S_{CF}(key_i)$ , perform CF-tree based HAC to get a set of  $J_1$ 
   sub-clusters, i.e.  $S_{sub}(key_i)$ ;
7. Export  $S_{sub}(key_i)$  and  $S_{out}(key_i)$ ;
```

### Controller

The controller pours together all sub-clusters produced by reducers, and performs matrix based HAC to get the final clusters. It identifies outlier clusters as well if the option of outlier handling is turned on. Moreover, it computes model evaluation measures, and derives insights and interestingness from the clustering results.

The controller runs the following procedure.

#### Inputs:

```
<Parameter settings>
- MainMemory // Default 80*1024 bytes
- OutlierHandling // {on, off}, default on
- OutlierHandlingDiskSpace // Default 20% of MainMemory
- OutlierQualification // Default 10 cases
- ExtremeOutlierClusters // Default 20
- DelayedSplit // {on, off}, default on
- DelayedSplitDiskSpace // Default 10% of MainMemory
- Adjustment // Default 0.01
- DistanceMeasure // {Log-likelihood, Euclidean}, default
// Log-likelihood
- InitialThreshold // Default 0
- NonLeafNodeBranchingFactor // Default 8
- LeafNodeBranchingFactor // Default 8
- MaximumTreeHeight // Default 3
- AutoClustering // {on, off}, default on
- MaximumClusterNumber // Default 15
- MinimumClusterNumber // Default 2
- FixedClusterNumber // Default 5
- ClusteringCriterion // {BIC, AIC}, default BIC
- AutoClusteringMethod // {information criterion, distance jump,
// maximum, minimum}, default minimum
- MinSubClusters // Minimum sub-clusters produced for each key,
// default 500
- MaxDataPoitsCFHAC // Maximum data points for CF-tree based HAC,
// default 50,000
- MaxDataPoitsMatrixHAC // Maximum data points for matrix based HAC,
// default 5,000
```

#### Outputs:

- PMML
- StatXML

#### Procedure:

1. Let  $C_{min} = \text{MinSubClusters}$ ,  $D_1 = \text{MaximumDataPoitsCFHAC}$ , and  $D_2 = \text{MaximumDataPoitsMatrixHAC}$ ;
2. Compute the number of keys

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```
NumKeys =  $Q = \lfloor \min(R * S / D_1, D_2 / C_{min}) \rfloor$ ;  
// Each mapper is assigned a key which is selected randomly from the  $Q$  keys  
3. Compute the number of sub-clusters produced for each key  
   NumSubClusters =  $\lfloor \min(R * S, D_2) / Q \rfloor$ ;  
4. Launch a map-reduce job, and get  $S_{sub}(key_i)$  and  $S_{out}(key_i)$ , for  $i = 1, \dots, Q$ ;  
5. Compute  $S_{sub} = \bigcup_{i=1}^Q S_{sub}(key_i)$ ;  
6. Perform matrix based HAC on  $S_{sub}$  to get the set of final regular clusters  $S_{sub}^*$ ,  
   where the number of final clusters is determined automatically or using a  
   fixed one depending on the settings;  
7. If OutlierHandling is 'on', perform the steps from 2) to 7) in Step 3 in  
   section 9.3;  
8. Compute model evaluation measures, insights, and interestingness;  
9. Export the clustering model in PMML, and other statistics in StatXML;
```

### Implementation notes:

- The general procedure of the controller consists of both the controller procedure in appendix A and that in appendix B.

## Appendix C. Procedure for MonotoneCubicInterpolation()

$$f(x) = \text{MonotoneCubicInterpolation}(S_t, I_t, x),$$

where

$x$  is the input statistic that characterizes fields or field pairs in particular aspects (for example, distribution), association strength, etc. Its value range must be bounded below, and it must have a monotonically increasing relationship with the interestingness score threshold values. If the two conditions are not met, a conversion (e.g.  $x = -x'$  or  $x = |x|$ , etc) should be carried out.

$S_t$  is a set of distinct threshold values for the input statistics, which have been accepted and commonly used by expert users to interpret the statistics. The positive infinity ( $+\infty$ ) is included if the input statistic is not bounded from above.

$I_t$  is a set of distinct threshold values for the interestingness scores that  $S_t$  corresponds to. The threshold values must be between 0 and 1.

The size of  $S_t$  and  $I_t$  must be the same. There are at least two values in  $S_t$  excluding positive infinity ( $+\infty$ ).

### Pre-processing

Let  $\{x_k\} = \text{sorted}(S_t)$  such that  $x_1 < \dots < x_n$ , where  $n$  is the number of values in  $S_t$ .

Let  $\{y\} = \text{sorted}(I_t)$  such that  $y_1 < \dots < y_n$ .

**Condition A: There are more than two threshold values for input statistics, and they are all finite numbers**

### Preparing for cubic interpolation

The following steps should be taken for preparing a cubic interpolation function construction.

Step 1, compute the slopes of the secant lines between successive points.

$$\Delta_k = \frac{y_{k+1} - y_k}{x_{k+1} - x_k}$$

for  $k = 1, \dots, n - 1$ .

Step 2, Initialize the tangents at every data point as the average of the secants,

$$m_k = \frac{\Delta_{k-1} + \Delta_k}{2}$$

for  $k = 2, \dots, n - 1$ ; these may be updated in further steps. For the endpoints, use one-sided differences:  $m_1 = \Delta_1$  and  $m_n = \Delta_{n-1}$ .

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Step 3, let  $\alpha_k = m_k / \Delta_k$  and  $\beta_k = m_{k+1} / \Delta_k$  for  $k = 1, \dots, n - 1$ .

If  $\alpha$  or  $\beta$  are computed to be zero, then the input data points are not strictly monotone. In such cases, piecewise monotone curves can still be generated by choosing  $m_k = m_{k+1} = 0$ , although global strict monotonicity is not possible.

Step 4, update  $\mathbf{m}_k$

If  $\alpha^2 + \beta^2 > 9$ , then set  $m_k = \tau_k \alpha_k \Delta_k$  and  $m_{k+1} = \tau_k \beta_k \Delta_k$  where  $\tau_k = \frac{3}{\sqrt{\alpha^2 + \beta^2}}$ .

Note:

1. Only one pass of the algorithm is required.
2. For  $k = 1, \dots, n - 1$ , if  $\Delta_k = 0$  (if two successive  $y_k = y_{k+1}$  are equal), then set  $m_k = m_{k+1} = 0$ , as the spline connecting these points must be flat to preserve monotonicity. Ignore step 3 and 4 for those  $k$ .

### Cubic interpolation

After the preprocessing, evaluation of the interpolated spline is equivalent to cubic Hermite spline, using the data  $x_k, y_k$ , and  $m_k$  for  $k = 1, \dots, n$ .

To evaluate  $x$  in the range  $[x_k, x_{k+1}]$  for  $k = 1, \dots, n-1$ , calculate

$$h = x_{k+1} - x_k \text{ and } t = \frac{x - x_k}{h}$$

then the interpolant is

$$f(x) = y_k h_{00}(t) + h * m_k h_{10}(t) + y_{k+1} h_{01}(t) + h * m_{k+1} h_{11}(t)$$

where  $h_{ii}(t)$  are the basis functions for the cubic Hermite spline.

$h_{00}(t)$	$2t^3 - 3t^2 + 1$
$h_{10}(t)$	$t^3 - 2t^2 + t$
$h_{01}(t)$	$-2t^3 + 3t^2$
$h_{11}(t)$	$t^3 - t^2$

### Condition B: There are two threshold values for input statistics

As we have clarified in the beginning that there are at least two values in  $S_t$  excluding positive infinity  $(+\infty)$ , they must be both finite numbers when there are only two threshold values.

In this case the mapping function is a straight line connecting  $(x_1, y_1)$  and  $(x_2, y_2)$ .

$$f(x) = y_1 + (y_2 - y_1) \frac{x - x_1}{x_2 - x_1}$$

**Condition C: Threshold values include infinity**

Note that there are at least two values in  $S_t$  excluding positive infinity ( $+\infty$ ). Take the last three statistic threshold values and threshold values for the interestingness scores from the sorted lists, we have three pairs of data  $(x_{n-2}, y_{n-2})$ ,  $(x_{n-1}, y_{n-1})$  and  $(+\infty, y_n)$ .

An exponential function

$$f(x) = a - be^{-cx}$$

can be defined by the pairs, where

$$\begin{aligned} a &= y_n \\ b &= \sqrt{(x_{n-1} - x_{n-2}) \frac{(y_n - y_{n-2})^{x_{n-1}}}{(y_n - y_{n-1})^{x_{n-2}}}} \\ c &= \frac{1}{x_{n-1} - x_{n-2}} \ln \frac{y_n - y_{n-2}}{y_n - y_{n-1}} \end{aligned}$$

If  $n = 3$ , which means there are only two distinct values in  $S_t$  excluding positive infinity ( $+\infty$ ), the exponential function is employed for evaluating  $x$  in the range  $[x_1, +\infty)$ .

Otherwise, the exponential function is for evaluating  $x$  in the range  $[x_{n-1}, +\infty)$ . To evaluate  $x$  in the range  $[x_1, x_{n-1})$ , use procedures under "condition A: There are more than two threshold values for input statistics, and they are all finite numbers" with data set  $\{x_1, \dots, x_{n'}\}$  and  $\{y_1, \dots, y_{n'}\}$  where  $n' = n - 1$ . To insure a smooth transition to the exponential function, the tangent  $m_{n'}$  at data point  $x_{n'}$  is given as

$$m_{n'} = \left. \frac{d(a - be^{-cx})}{dx} \right|_{x=x_{n'}} = bce^{-cx_{n'}}$$

again

$$\begin{aligned} a &= y_n \\ b &= \sqrt{(x_{n-1} - x_{n-2}) \frac{(y_n - y_{n-2})^{x_{n-1}}}{(y_n - y_{n-1})^{x_{n-2}}}} \\ c &= \frac{1}{x_{n-1} - x_{n-2}} \ln \frac{y_n - y_{n-2}}{y_n - y_{n-1}} \end{aligned}$$

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