TIBCO® Spotfire® DecisionSite® 9.1.1 Statistics - User's Manual

Important Information

SOME TIBCO SOFTWARE EMBEDS OR BUNDLES OTHER TIBCO SOFTWARE. USE OF SUCH EMBEDDED OR BUNDLED TIBCO SOFTWARE IS SOLELY TO ENABLE THE FUNCTIONALITY (OR PROVIDE LIMITED ADD-ON FUNCTIONALITY) OF THE LICENSED TIBCO SOFTWARE. THE EMBEDDED OR BUNDLED SOFTWARE IS NOT LICENSED TO BE USED OR ACCESSED BY ANY OTHER TIBCO SOFTWARE OR FOR ANY OTHER PURPOSE.

USE OF TIBCO SOFTWARE AND THIS DOCUMENT IS SUBJECT TO THE TERMS AND CONDITIONS OF A LICENSE AGREEMENT FOUND IN EITHER A SEPARATELY EXECUTED SOFTWARE LICENSE AGREEMENT, OR, IF THERE IS NO SUCH SEPARATE AGREEMENT, THE CLICKWRAP END USER LICENSE AGREEMENT WHICH IS DISPLAYED DURING DOWNLOAD OR INSTALLATION OF THE SOFTWARE (AND WHICH IS DUPLICATED IN TIBCO BUSINESSWORKS CONCEPTS). USE OF THIS DOCUMENT IS SUBJECT TO THOSE TERMS AND CONDITIONS, AND YOUR USE HEREOF SHALL CONSTITUTE ACCEPTANCE OF AND AN AGREEMENT TO BE BOUND BY THE SAME.

This product includes software licensed under the Common Public License. The source code for such software licensed under the Common Public License is available upon request to TIBCO and additionally may be obtained from http://wtl.sourceforge.net/.

TIBCO, Spotfire, and Spotfire DecisionSite are either registered trademarks or trademarks of TIBCO Software Inc. and/or subsidiaries of TIBCO Software Inc. in the United States and/or other countries. All other product and company names and marks mentioned in this document are the property of their respective owners and are mentioned for identification purposes only. This software may be available on multiple operating systems. However, not all operating system platforms for a specific software version are released at the same time. Please see the readme.txt file for the availability of this software version on a specific operating system platform.

THIS DOCUMENT IS PROVIDED “AS IS” WITHOUT WARRANTY OF ANY KIND, EITHER EXPRESS OR IMPLIED, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE, OR NON-INFRINGEMENT. THIS DOCUMENT COULD INCLUDE TECHNICAL INACCURACIES OR TYPOGRAPHICAL ERRORS. CHANGES ARE PERIODICALLY ADDED TO THE INFORMATION HEREIN; THESE CHANGES WILL BE INCORPORATED IN NEW EDITIONS OF THIS DOCUMENT. TIBCO SOFTWARE INC. MAY MAKE IMPROVEMENTS AND/OR CHANGES IN THE PRODUCT(S) AND/OR THE PROGRAM(S) DESCRIBED IN THIS DOCUMENT AT ANY TIME.

TIBCO Spotfire DecisionSite is covered by U.S. Patent No. 6,014,661 and U.S. Patent No. 7, 216,116. Other patent(s) pending.

TIBCO Software Inc. Confidential Information

Table of Contents

1 Column Normalization

1.1 Column Normalization Overview

The Column Normalization tool can be used to standardize the values in selected columns using a number of different normalization methods. For example, this can be useful if you plan to perform a clustering later on.

1.2 Using Column Normalization

1.2.1 Normalizing Values in Selected Columns

► To normalize columns:

1. Select **Data** > **Column Normalization...**.
   Response: The Column Normalization dialog is displayed.
2. Select the **Value columns** that you want to normalize.
   Comment: For multiple selection, press **Ctrl** and click on the desired columns or click one column and drag to select the following ones.
3. Click a radio button to select whether to work on **All records** or **Selected records**.
4. Select a method to **Replace empty values with** from the drop-down list.
5. Select a **Normalization method** from the drop-down list.
6. Select the **Overwrite previously added columns** check box to overwrite columns earlier added by this tool.
7. Click **OK**.
   Response: The Column Normalization dialog is closed and the normalized columns either replace the old columns or are added to the data set, depending on your selection in the Overwrite check box.

Tip: You can also use the Column Normalization tool to replace empty values in columns without performing any normalization.

1.2.2 Replacing Empty Values in Columns

If *No normalization* is selected as normalization method in the Column Normalization tool, you can replace empty values in a data set with either a constant, averaged or interpolated values. See Details on Interpolation for more information on how the interpolation option works for row interpolation.

► To replace empty values in existing columns:

1. Select **Data** > **Column Normalization...**.
   Response: The Column Normalization dialog is displayed.
2. Select the **Value columns** in which you want to replace the empty values.
   Comment: For multiple selection, press **Ctrl** and click on the desired columns or click one column and drag to select the following ones.
3. Click a radio button to select whether to work on **All records** or **Selected records**.
4. Select a method to **Replace empty values with** from the drop-down list.
5. Select **No normalization** as the **Normalization method**.
6. Select the **Overwrite previously added columns** check box to overwrite columns created by this tool.
7. Click **OK**.

Response: The Column Normalization dialog is closed and data is added to the previously empty fields of the columns in the data set according to the selected replacement method.

1.2.3 Details on Interpolation

Empty values in the data set can be replaced with either a constant, averaged or interpolated values. The row interpolation of the Column Normalization tool works like this:

If the first value is empty it is replaced with the first non-empty numerical value in the order the columns were entered.

If the last value is empty it is replaced with the previous non-empty numerical value in the order the columns were entered.

If an empty value is found between non-empty numerical values, the values are calculated as the linear interpolation.

If all values in a row are empty, they will be replaced by zero.

Example:

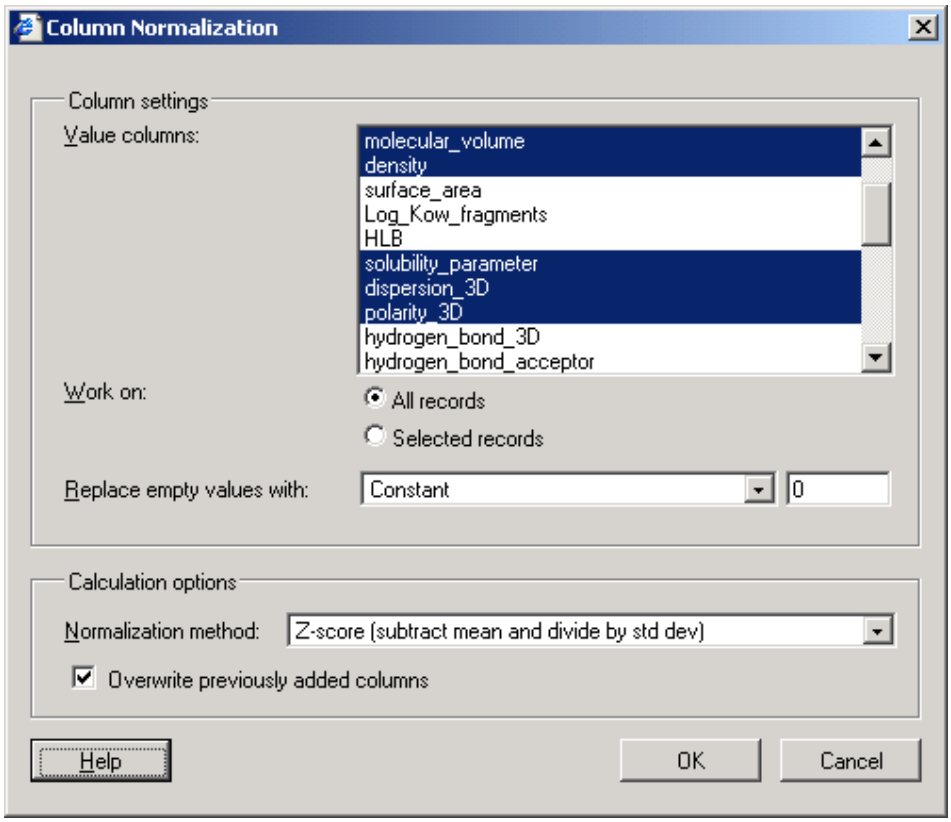
A	C	B	D
null	2	3	4
null	null	3	4
1	null	3	4
1	null	null	4
1	2	null	4
1	2	3	null
null	null	null	null

Becomes:

A	C	B	D
2	2	3	4
3	3	3	4
1	2	3	4
1	2	3	4
1	2	3	4
1	2	3	3
0	0	0	0

1.3 User Interface

1.3.1 Column Normalization Dialog



Option	Description
Value columns	The data columns you want to normalize. Click a column name in the list to select it. To select more than one column, press **Ctrl** and click on the column names in the list.
Work on: All records	All records in the value columns are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Replace empty values with	Defines how empty values in the data set should be replaced. From the drop-down list, select a method. **Note: Empty value** leaves the value empty as before. **Constant** allows you to replace the empty values by any constant (type a number in the text box). **Row average** replaces the value by the average value of the entire row. **Row interpolation** sets the missing value to the interpolated value between the two neighboring values in the row (see Details on interpolation for more information). Similarly, **Column average** and **Column interpolation** return the average/interpolation of the corresponding column values.
Normalization method	The method to use for the normalization. For more information about the available methods, see the methods overview. The option **No**

	normalization gives you the opportunity to replace empty values in a column.
Overwrite previously added columns	Select this check box if you want to replace any previously added columns from the Column Normalization tool. Clear the check box if you wish to keep the old columns. Normalized columns will have the same name as the ones they are based on, followed by "(normalized)". If several sets of normalized columns are saved, they will also be followed by an index number, (1), etc.

► To reach the Column Normalization dialog:

Select **Data** > **Column Normalization...**.

1.4 Theory and Methods

1.4.1 Column Normalization Methods Overview

The following normalization methods are available in the Column Normalization tool:

- Z-score calculation
- Divide by standard deviation
- Scale between 0 and 1

1.4.2 Column Normalization - Z-score

Assume that there are *n* records with seven variables, A, B, C, D, E, F and G, in the data view. We use variable E as an example in the expressions. The remaining variables are normalized in the same way.

The normalized value of e_i for variable E in the ith record is calculated as

$$\text{Normalized}(e_i) = \frac{e_i - \bar{E}}{\text{std}(E)}$$

where

$$\text{std}(E) = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(e_i - \bar{E})^2}$$

$$\bar{E} = \frac{1}{n}\sum_{i=1}^{n} e_i$$

If all values for variable E are identical — so that the standard deviation of E (std(*E*)) is equal to zero — then all values for variable E are set to zero.

1.4.3 Column Normalization - Divide by Standard Deviation

Assume that there are *n* records with seven variables, A, B, C, D, E, F and G, in the data view. We use variable E as an example in the expressions. The remaining variables are normalized in the same way.

The normalized value of e_i for variable E in the ith record is calculated as

$$\text{Normalized}(e_i) = \frac{e_i}{\text{std}(E)}$$

where

$$\text{std}(E) = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}\left(e_i - \bar{E}\right)^2}$$

$$\bar{E} = \frac{1}{n}\sum_{i=1}^{n} e_i$$

If all values for variable E are identical — so that the standard deviation of E (std(*E*)) is equal to zero — then all values for variable E are left unchanged.

1.4.4 Column Normalization - Scale Between 0 and 1

Assume that there are *n* records with seven variables, A, B, C, D, E, F and G, in the data view. We use variable E as an example in the expressions. The remaining variables are normalized in the same way.

The normalized value of e_i for variable E in the ith record is calculated as

$$\text{Normalized}\left(e_i\right) = \frac{e_i - E_{\min}}{E_{\max} - E_{\min}}$$

where

$E_{\min}$ = the minimum value for variable E

$E_{\max}$ = the maximum value for variable E

If all values for variable E are identical, so that $E_{\min}$ is equal to $E_{\max}$, then all values for variable E are set to zero.

2 Row Summarization

2.1 Row Summarization Overview

The Row Summarization tool allows you to combine values from multiple samples into a single column. Measures such as the average, median and standard deviation etc. of groups of columns can be calculated. This can be used to summarize all experimental data or to generate replicate averages and variability for subsets of the data. The resulting columns can be used in subsequent analyses.

2.2 Using Row Summarization

2.2.1 Performing a Row Summarization

The Row Summarization tool allows you to combine values from multiple samples into a single column.

► To use the Row Summarization tool:

1. Select **Data** > **Row Summarization...**.

   Response: The Row Summarization dialog is displayed.
2. Move the desired value columns from **Available columns** to suitable groups in the **Grouped value columns** list.

   Comment: For example, to create a column containing the average per row of the values in two old columns, first make sure that there is just one group in the Grouped value columns list. Then click to select the two columns in the Available columns list and click on **Add >>** to move the columns to the selected group. Several groups can be summarized at the same time. The tool requires that each group has at least two columns.
3. Select a group and click on **Rename Group** to edit the group name.

   Comment: The names of the result columns will be the group names followed by the chosen comparison measure within parentheses. Therefore, using meaningful group names will prove valuable when interpreting the results later on.
4. Click a radio button to select whether to work on **All records** or **Selected records**.
5. Select a method to **Replace empty values with** from the drop-down list.
6. Select a **Summarization measure** from the list box.

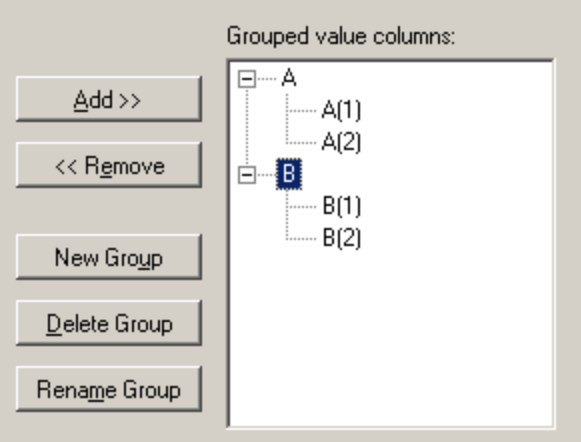
   Comment: For a mathematical description of the different measures, see Statistical measures.
7. Click **OK**.

   Response: New result columns are added to the data set. An annotation may also be added.

2.2.2 Row Summarization Example

If you have performed multiple experiments on a number of different subjects and want to use the average values of the measurements in your following data analyses, you can quickly create new columns using the Row Summarization tool:

ID:	A 1st value	A 2nd value	B 1st value	B 2nd value
Subject 1	0.5	0.6	20	18
Subject 2	1.0	0.8	25	27
Subject 3	0.25	0.15	42	44

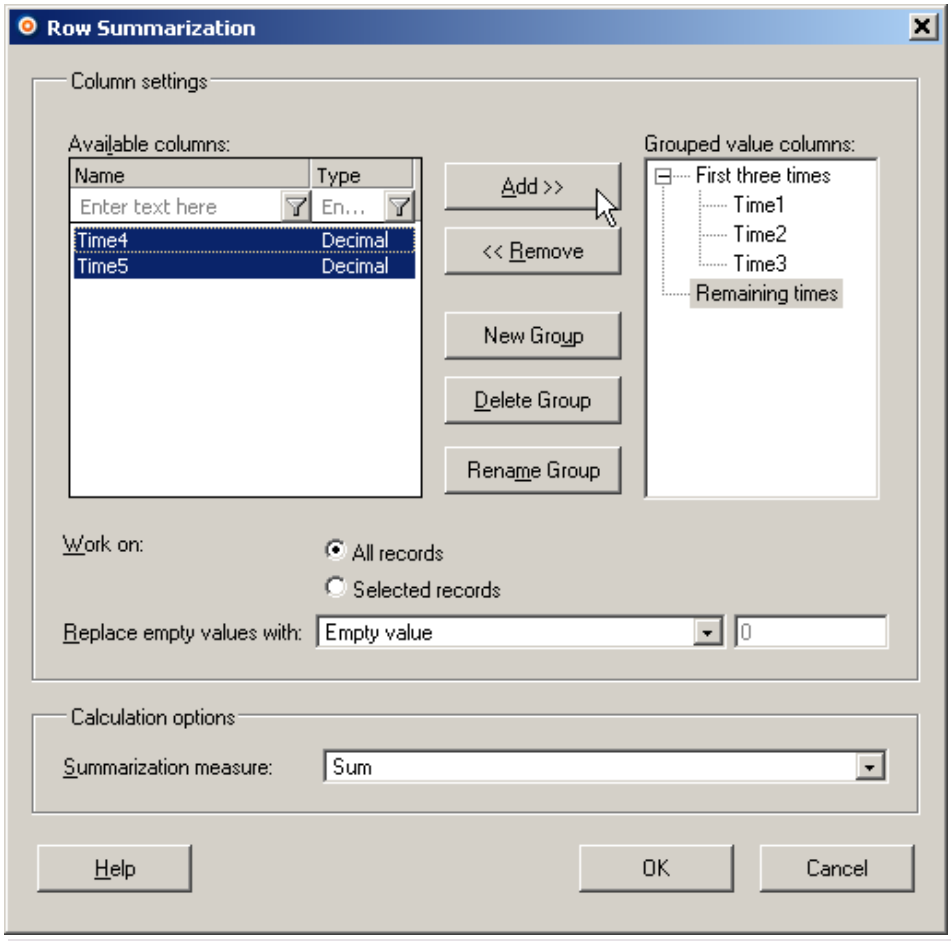


By performing a row summarization using Average as the summary measure and naming the Grouped value columns groups *A* and *B*, the new columns A (Average) and B (Average) are added to the data set:

ID:	A 1st value	A 2nd value	B 1st value	B 2nd value	A (Average)	B (Average)
Subject 1	0.5	0.6	20	18	0.55	19
Subject 2	1.0	0.8	25	27	0.9	26
Subject 3	0.25	0.15	42	44	0.2	43

2.3 User Interface

2.3.1 Row Summarization Dialog



Option	Description
Available columns	The data columns that you can use in the calculation. Click a column name in the list to select it, then click **Add >>** to move it to the selected group in the Grouped value columns list. To select more than one column, press **Ctrl** and click the column names in the list, then click Add >>. You can choose from any column that contains decimal numbers or integers. **Note:** You can right-click on the Name header to get a pop-up menu where you can select other attributes you would like to be visible.
Enter text here 	If you have a data set with many columns, you can right-click on the header of the columns in the Available columns list box and select **Show Search Field** from the pop-up menu. This will display a search field where you can type a search string and limit the number of items in the list. It is possible to use the wildcard characters * and ? in the search.
Grouped value columns	Displays the groups on which the calculation is performed. You can add, delete or rename groups from the field by

	clicking on the corresponding buttons to the left of the field. You move value columns between the fields using the Add >> and << Remove buttons.
Add >>	Moves selected columns from the Available columns field to a selected group in the Grouped value columns field. Click to select the desired columns and the group that you want to add the columns to, then click on Add >>.
<< Remove	Removes all columns from a selected group and brings them back to the Available columns field. If a single column is selected in the Grouped value columns field, it will be removed from the group, while all other columns remain in the group.
New Group	Adds a new group to the Grouped value columns field.
Delete Group	Deletes a selected group from the Grouped value columns field. If the group contained any value columns they are moved back to the Available columns field.
Rename Group	Opens the Edit Group Name dialog, where you can change the name of the selected group. The names of the result columns from a row summarization will be the group names followed by the selected summarization measure within parenthesis. Therefore, using meaningful group names will prove valuable in the interpretation of the results later on.
Work on: All records	All records in the value columns are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Replace empty values with	Defines how empty values in the data set should be replaced. **Empty value** simply ignores empty values. **Constant** allows you to replace the empty values by any constant (type a number in the text box). **Row average** replaces the value by the average value of the entire row. **Row interpolation** sets the missing value to the interpolated value between the two neighboring values in the row.
Summarization measure	The measure to present in the new columns: Min, Median, Max, Sum, Average, Standard deviation or sample Variance. For a mathematical description of the different measures, see Statistical measures.

► To reach the Row Summarization dialog:

Select **Data** > **Row Summarization...**.

3 Hierarchical Clustering

3.1 Hierarchical Clustering Overview

The Hierarchical Clustering tool groups records and arranges them in a dendrogram (a tree graph) based on the similarity between them.

3.2 Using Hierarchical Clustering

3.2.1 Initiating a Hierarchical Clustering

► To start a clustering:

1. Select **Data > Clustering > Hierarchical Clustering...**.
   Response: The Hierarchical Clustering dialog is displayed.
2. Select the value columns on which to base the clustering from the **Available columns** list and click **Add >>**.
   Comment: For multiple selection, press **Ctrl** and click on the desired columns in the Available columns list. Then click Add >> to move the selected columns to the Selected columns list. You can sort the columns in the list alphabetically by clicking on the Name bar.
3. Click a radio button to select whether to work on **All records** or **Selected records**.
4. Select a method to **Replace empty values with** from the drop-down list.
5. Select which **Clustering method** to use for calculating the similarity between clusters.
   Comment: Click for information about available clustering methods.
6. Select which **Similarity measure** to use in the calculations.
   Comment: Click for information about available similarity measures.
7. Select which **Ordering function** to use for displaying the results.
   Comment: Click for information about available ordering functions.
8. Type a new **Column name** in the text box or use the default name.
   Comment: Select the **Overwrite** check box if you want to overwrite a previously added column using the same name. Clear the check box to keep old columns.
9. Select the **Calculate column dendrogram** check box if you want to create a column dendrogram.
10. Click **OK**.
    Response: The Hierarchical Clustering dialog is closed and the clustering is started. The result is displayed according to your settings in the dialog.

3.2.2 Hierarchical Clustering on Keys

A *structure key* is a string that lists the substructures which form a compound. Clustering on keys, then means grouping compounds with similar sets of substructures.

Clustering on keys is based only on the values within the key column, and not all the columns. The key column should contain comma separated string values for all or some of the records in the data set.

The procedure below only shows you how to cluster records based on a specific key column.

► To cluster on keys:

1. If you have not already done it, you should first import the keys that you want to cluster on into Spotfire DecisionSite.

2. Select **Data > Clustering > Hierarchical Clustering on Keys...**.
   Response: The Hierarchical Clustering on Keys dialog is displayed.
3. Select the **Key column** on which to base the calculations.
   Comment: The key column could be any string column in the data set.
4. Click a radio button to select whether to work on **All records** or **Selected records**.
5. Select which **Clustering method** to use for calculating the similarity between clusters.
   Comment: Click for information about available clustering methods.
6. Select which **Similarity measure** to use in the calculations.
   Comment: Click for information about available similarity measures.
7. Select which **Ordering function** to use for displaying the results.
   Comment: Click for information about available ordering functions.
8. Type a new **Column name** in the text box or use the default name.
   Comment: Select the **Overwrite** check box if you want to overwrite a previously added column using the same name. Clear the check box to keep old columns.
9. Click **OK**.
   Response: The *Hierarchical Clustering on Keys* dialog is closed and the clustering is started. A heat map and a row dendrogram visualization is created and information about the clustering is added to the visualization as an annotation.

3.2.3 Adding a Column from Hierarchical Clustering

The ordering column which is added to the data set upon performing a hierarchical clustering is used only to display the row dendrogram and to connect it to the heat map. In order to compare the hierarchical clustering results to those of a K-means clustering, you must first add a clustering column to your data set.

A clustering column contains information about which cluster each record belongs to, and can be used to create a trellis plot.

► To add a clustering column:

1. Perform a hierarchical clustering and locate the Row dendrogram which can be found to the left of the heat map.
   Comment: For more information on how to create the row dendrogram, see Initiating a hierarchical clustering.
2. If the cluster line is not visible (a dotted red line in the row dendrogram), right-click and select **View > Cluster scale** from the pop-up menu to display it.
   Comment: The cluster line will enable you to see how many clusters you are selecting in the dendrogram.
3. Click on the red circle on the cluster slider above the dendrogram and drag it to control how many clusters you want to include in the data column. You can also use the left and right keyboard arrow keys to step through the different number of clusters.
   Response: All clusters for the current position on the cluster slider are shown as small, red circles in the dendrogram.
   Comment: If you position the red circle at its rightmost position on the cluster slider, you get one cluster for each record. If you position it at its leftmost position, you get a single cluster that includes all records. The number of clusters is displayed as a ToolTip which is shown when clicking and holding the left mouse-button on the red circle on the cluster slider.
4. Select **Add Cluster Column** from the row dendrogram menu.
   Response: A column with information about which cluster each record belongs to, is added to the data set.
   Comment: Records in the data set that are not included in the row dendrogram will have empty values in the new clustering column.

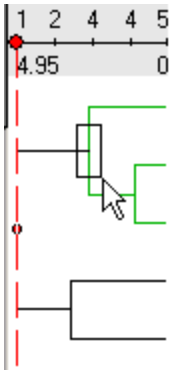
Tip: You can also click on the **Add Clustering Column** button, , to add a clustering column from the last row dendrogram.

3.2.4 Marking and Activating Nodes in the Dendrogram

Marking nodes

To mark a node, click just outside it and drag to enclose the node within the frame that appears and then release. You can also press **Ctrl** and click on the node to mark it. To mark more than one node, press **Ctrl** and click on all the nodes you want to mark. To unmark all nodes, drag to select an area outside the dendrogram.

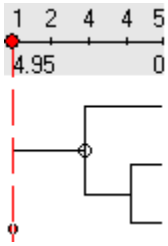
When you mark a node or a number of nodes, the marked parts of the dendrogram are shaded in the color used for marked records, by default green as shown below. The corresponding records are also marked in the heat map and other visualizations.



Note: It is only possible to mark nodes in the row dendrogram, not in the column dendrogram.

Activating nodes

To activate a node, click on it in the dendrogram. The node gets a black ring around it. Only one node can be active at a time. The node remains active until another node is activated. It is possible to zoom in on the active node in the dendrogram by selecting **Zoom to Active** from the Hierarchical Clustering menu or from the dendrogram pop-up menu.



Highlighting nodes

Highlighting nodes in the dendrogram does not have any effect on the visualizations.

3.2.5 Zooming in the Dendrogram

You can zoom to a subtree in the row dendrogram, either by using the visualization zoom bar or the **Zoom to Active** command in the pop-up menu. The pop-up menu is brought up by right-clicking in the dendrogram.

Double-clicking on a node will give the same results as the Zoom to Active command. Double-clicking a white surface in the dendrogram (no node) will take back the zooming one step, unlike the Reset Zoom command which takes you all the way back to the original zooming position.

The dendrogram can also be shown in log scale. This only affects the display of the dendrogram. The numbers in the cluster slider are not transformed into log values. Select **View > Log Scale** from the pop-up menu to view the dendrogram this way.

3.2.6 Resizing the Dendrogram

It is possible to adjust how much of the space in the visualization will be occupied by the dendrogram. This can be especially useful if the heat map contains a single column and the dendrogram structure is complex.

► To resize the dendrogram:

First click on the dendrogram to make sure it is in focus. Then, press **Ctrl** and use the left or right arrow key on the keyboard to make the dendrogram slimmer or wider.
Comment: You cannot make the dendrogram or the heat map completely disappear by resizing them in the visualization.

3.2.7 Exporting a Dendrogram

Note: The Hierarchical Clustering tool allows the dendrograms to be saved with the Analysis. However, it is also possible to export the dendrograms separately and import them again via the Hierarchical Clustering: Dendrogram Import dialog.

► To export a dendrogram:

1. Perform a hierarchical clustering.
   Comment: For more information, see Initiating a hierarchical clustering.
2. Locate the dendrogram(s) in the created heat map visualization.
3. Select **Export > Row Dendrogram** or **Column Dendrogram** from the menu in the top left of the heat map visualization.
   Comment: The command **Export > Column Dendrogram** is only available if you selected to create a column dendrogram during the calculation.
   Response: A Save As dialog is displayed.
4. Type a **File name** and save the file as a DND file.
   Comment: The entire tree structure is saved even if only part of it is visible at the moment of saving.

Tip: To save the dendrogram and heat map as an image, use one of the Reporting tools of Spotfire DecisionSite: PowerPoint® Presentation, Word Presentation or Export as Web Page.

3.2.8 Importing a Dendrogram

Note: The Hierarchical Clustering tool allows the dendrograms to be saved with the Analysis. However, it is still possible to save the dendrograms separately and import them again via the Hierarchical Clustering: Dendrogram Import dialog.

► To import a saved dendrogram:

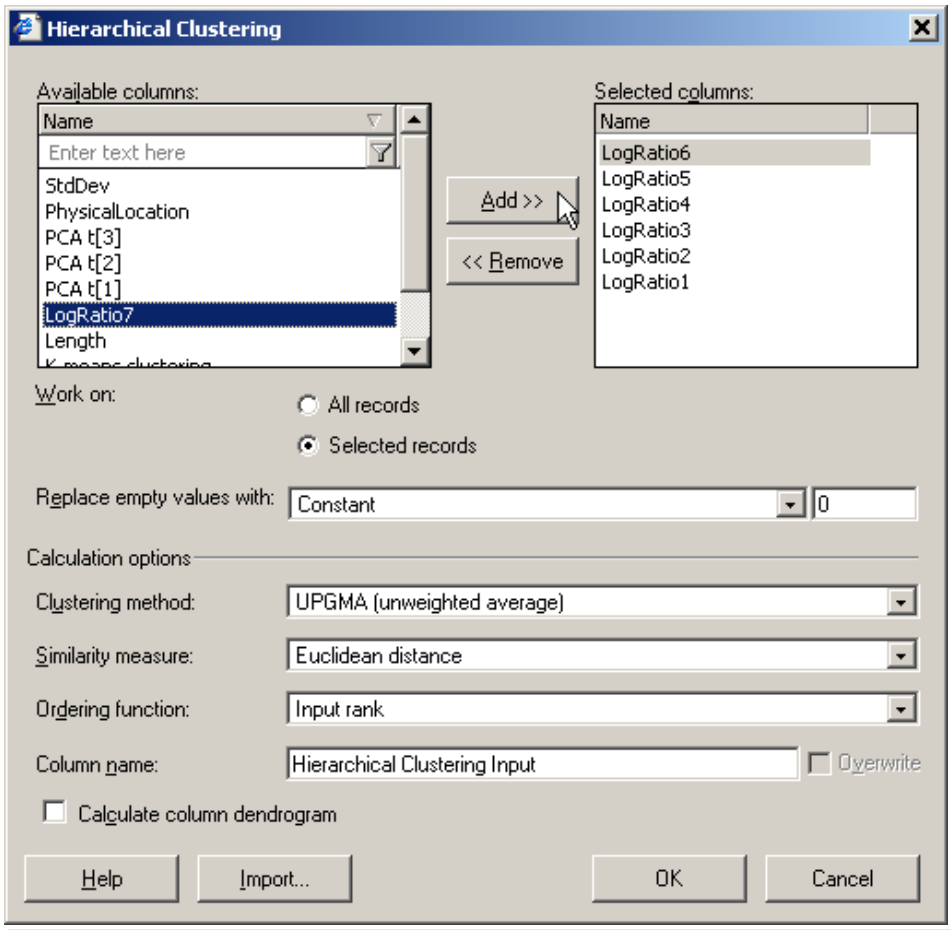
1. Select **Data > Clustering > Hierarchical Clustering...**.
   Response: The Hierarchical Clustering dialog is displayed.
2. Click **Import...**.
   Response: The Hierarchical Clustering: Dendrogram Import dialog is displayed.
3. Click the **Browse...** button by the **Row dendrogram** field.
   Response: An Open File dialog is displayed.
4. Locate the previously exported **Row dendrogram** file (*.dnd) and click **Open**.
   Comment: Only dendrograms associated with the active data set can be opened. If there is a column missing in the data set, or if the names of the columns in the data set

have been changed since the dendrogram was saved, an error message will appear and no dendrogram can be displayed.

5. Decide if you want to open a corresponding column dendrogram or not. Browse to locate the **Column dendrogram** file similarly to steps 3-4 above.
6. Type a **Column name** or use the default one.
   Comment: Select the **Overwrite** check box to overwrite a column with the same name in the data set.
7. Click **OK**.
   Comment: The column containing the hierarchical clustering order of the dendrogram is added to the data set. A heat map visualization is created with the dendrogram(s) displayed on the side(s).

3.3 User Interface

3.3.1 Hierarchical Clustering Dialog



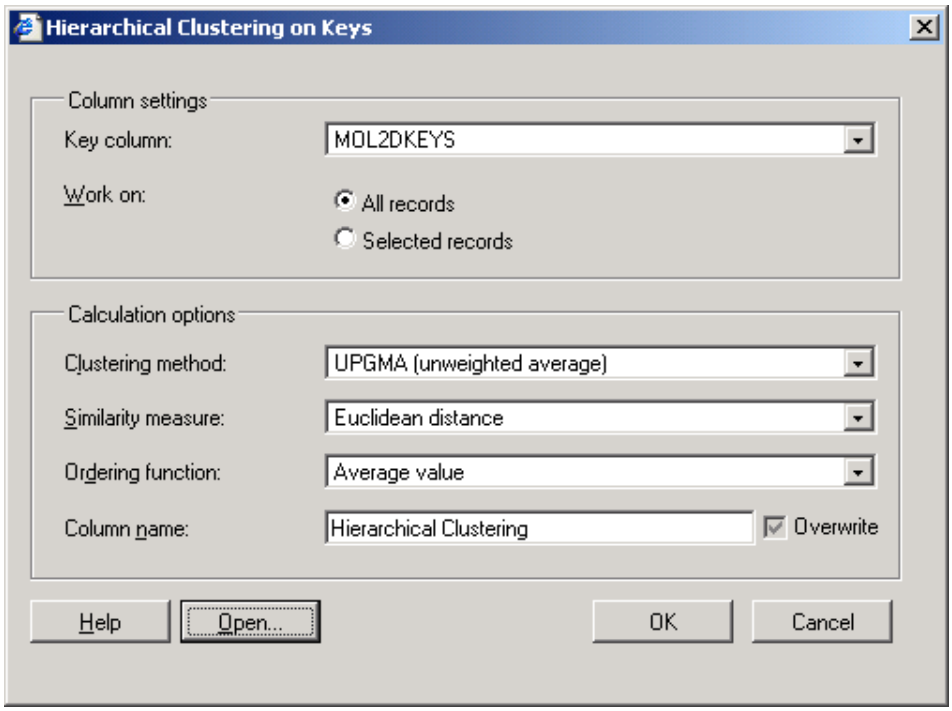
Option	Description
Available columns	Displays all available data columns on which you can perform a clustering. Click a column name in the list and click **Add >>** to move it to the Selected columns list. To select more than one column, press **Ctrl** and click the column names in the list, then click Add >>. You can choose from all columns that contain real numbers or integers. **Note:** You can right-click on the Name header to get a pop-up menu

	where you can select other attributes you would like to be visible.
Enter text here 	If you have a data set with many columns, you can right-click on the header of the columns in the Available columns list box and select **Show Search Field** from the pop-up menu. This will display a search field where you can type a search string and limit the number of items in the list. It is possible to use the wildcard characters * and ? in the search.
Selected columns	Displays the currently selected data columns on which you want to perform a clustering.
Add >>	Adds the highlighted data column to the list of selected columns.
<< Remove	Removes the highlighted data column from the list of selected columns and places them back in the list of available columns.
Work on: All records	All records in the value columns are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Replace empty values with	Defines how empty values in the data set should be replaced in the clustering. **Constant** allows you to replace the empty values by any constant (type a number in the text box). **Row average** replaces the value by the average value of the entire row. **Row interpolation** sets the missing value to the interpolated value between the two neighboring values in the row. **Column average** returns the average of the corresponding column values.
Clustering method	The clustering method to use for calculating the similarity between clusters. Click here for a description of the available methods.
Similarity measure	The similarity measure to use for the clustering. Click here for a description of the available similarity measures.
Ordering function	The ordering function to use for the clustering. Click here for a description of the available ordering functions.
Column name	The name of the new columns containing the results from the hierarchical clustering.
Overwrite	Select this check box if you want to replace a previously added column and plot (with the same name as the one typed in the Column name text box) when you add a new column. Clear the check box if you wish to keep the old column and plot.
Calculate column dendrogram	Select this check box to calculate a column dendrogram during the clustering.
Import...	Opens the Hierarchical Clustering: Dendrogram Import dialog where you can import row and column dendrogram files.

► To reach the Hierarchical Clustering dialog:

Select **Data** > **Clustering** > **Hierarchical Clustering...**.

3.3.2 Hierarchical Clustering on Keys Dialog

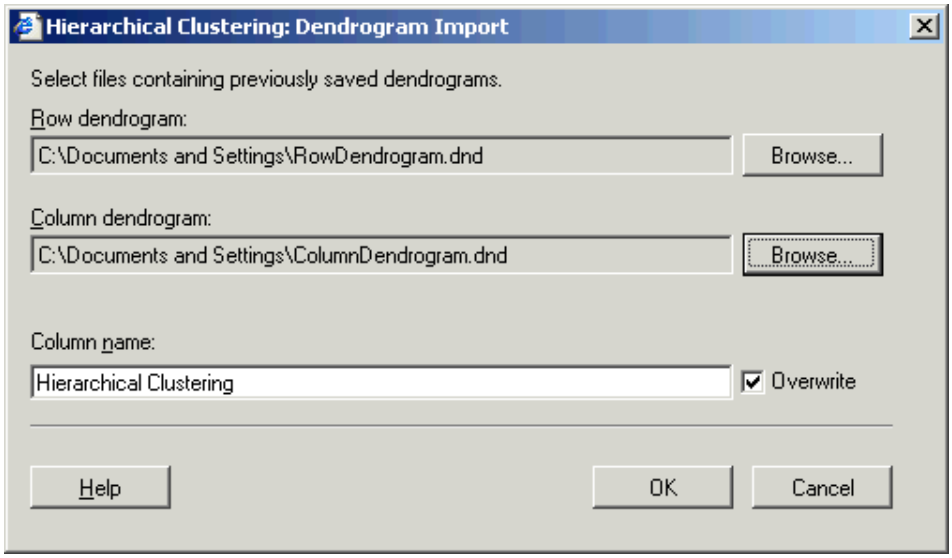


Option	Description
Key column	The data column on which to base the calculations. The key column should contain comma separated string values for all or some of the records in the data set.
Work on: All records	All records in the value columns are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Clustering method	The clustering method to use for calculating the similarity between clusters. Click here for a description of the available methods.
Similarity measure	The similarity measure to use for the clustering. Click here for a description of the available similarity measures.
Ordering function	The ordering function to use for the clustering. Click here for a description of the available ordering functions.
Column name	The name of the new columns containing the results from the hierarchical clustering.
Overwrite	Select this check box if you want to replace a previously added column and plot (with the same name as the one typed in the Column name text box) when you add a new column. Clear the check box if you wish to keep the old column and plot.
Open...	Opens the Hierarchical Clustering: Dendrogram Import dialog where you can open row dendrogram files. Column dendrograms are not available when you are clustering on keys.

► To reach the Hierarchical Clustering on Keys dialog:

Select **Data** > **Clustering** > **Hierarchical Clustering...**.

3.3.3 Hierarchical Clustering Dendrogram Import Dialog



Option	Description
Row dendrogram	Click on the **Browse...** button to display an Open File dialog, where you can select the row dendrogram to open. Only row dendrograms directly associated with the open data set can be opened.
Column dendrogram	Click on the corresponding **Browse...** button to display an Open File dialog, where you can select the column dendrogram to open. The column dendrogram option is not available when you are accessing this dialog from the Hierarchical Clustering on Keys dialog.
Column name	The name of the new columns containing the results from the hierarchical clustering.
Overwrite	Select this check box if you want to replace a previously added column (with the same name as the one typed in the Column name text box) when you add a new column. Clear the check box if you wish to keep the old column.

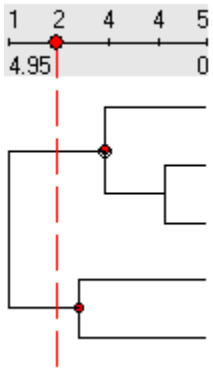
► To reach the Hierarchical Clustering: Dendrogram Import dialog:

1. Select **Data** > **Clustering** > **Hierarchical Clustering...**.
2. Click on the **Open...** button in the lower left part of the dialog to display the **Hierarchical Clustering: Dendrogram Import** dialog.

3.3.4 The Row Dendrogram

The row dendrogram shows the similarity between rows and shows which nodes each record belongs to as a result of the clustering. An example of part of a row dendrogram is shown below.

The vertical axis of the row dendrogram consists of the individual records, and the horizontal axis represents the clustering level.

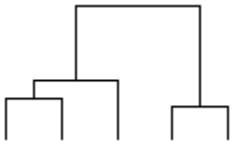


The individual records in the clustered data set are represented by the rightmost nodes in the row dendrogram. Each remaining node in the dendrogram represents a cluster of all records that lie to the right of it in the dendrogram. The leftmost node in the dendrogram is thus a cluster that contains all records.

The row dendrogram is automatically displayed next to the heat map which is created upon clustering. It can, however, be hidden or displayed by selecting **View > Row dendrogram** from the Hierarchical Clustering menu.

3.3.5 The Column Dendrogram

The column dendrogram is drawn in the same way as the row dendrogram but shows the similarity between the variables (the selected value columns). The variables in the clustered data set are represented by the nodes at the lowest part of the column dendrogram.



To display the column dendrogram (if one has been calculated), select **View > Column Dendrogram** from the Hierarchical Clustering menu. The column dendrogram can only be displayed if it has been calculated (select this in the Hierarchical Clustering dialog).

Restricted functionality

The column dendrogram offers less interactivity than the row dendrogram. You cannot add the results from the column dendrogram to the data set and so you cannot create visualizations based on it. There is no cluster slider above the column dendrogram, no cluster line and no horizontal zooming.

3.3.6 Row Dendrogram Menu and Toolbar

Toolbar

The row dendrogram toolbar is located directly above the row dendrogram. The row dendrogram is automatically created upon clustering and it is located to the left of the heat map.

Click on the buttons in the toolbar to activate the corresponding functions.

	Displays the Hierarchical Clustering menu.
	Adds a new column to the data set with information about which cluster each record belongs to. The position of the red circle on the cluster slider above the dendrogram

controls the number of clusters. The column can be used to create a trellis plot of the clusters.

Hierarchical Clustering menu

Option	Description
Zoom to Active	Zooms to the selected subtree so that the active node in the row dendrogram is displayed to the far left of the visualization.
Reset Zoom	Resets the horizontal zooming to its original size so the full width of the row dendrogram is visible.
View >	
> Log Scale	Displays the dendrogram in log scale. Affects only the display of the dendrogram and not the actual numbers of the calculated similarity measures.
> Toolbar	Displays or hides the row dendrogram toolbar. If the toolbar has been hidden, right-click on the row dendrogram and select **View > Toolbar** from the pop-up menu to display it again.
> Cluster Scale	Displays or hides the cluster scale (and cluster line) above the row dendrogram. The cluster scale must be displayed if you want to select the number of clusters to be included in the added cluster column.
> Column Dendrogram	Displays or hides the column dendrogram (if one has been created).
> Row Dendrogram	Displays or hides the row dendrogram.
> Include Empty	Relevant only when you have performed a clustering using selected records. This produces a Hierarchical Clustering (order) column with empty values for all of the remaining records. By marking or clearing the Include Empty option you can determine whether or not to display the records that were not a part of the clustering calculation in the heat map. Obviously, no dendrogram can be displayed for these rows.
Remove Dendrograms	Removes the dendrograms permanently from the visualization.
Add Cluster Column	Adds a new column to the data set with information about which cluster each record belongs to. The position of the red circle on the cluster slider above the dendrogram controls the number of clusters. The column can be used to create a trellis plot of the clusters.
Overwrite	Selects whether or not to overwrite a Hierarchical Clustering (cluster) column, when using the Add cluster column function.
Export >	
> Row Dendrogram	Opens a dialog where you can select a file name and save your row dendrogram.
> Column dendrogram	Opens a dialog where you can select a file name and save your column dendrogram.

Note: The Hierarchical Clustering tool allows the dendrograms to be saved with the Analysis. However, it is still possible to export the dendrograms separately and then import them from within the Hierarchical Clustering: Dendrogram Import dialog.

3.3.7 Dendrogram Pop-up Menus

Right-click in the dendrogram to bring up the pop-up menu.

Row dendrogram pop-up menu:

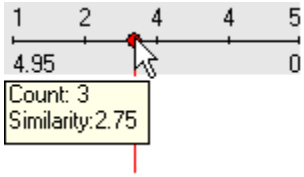
Option	Description
Zoom to Active	Zooms horizontally so that the active node in the row dendrogram is displayed to the far left of the visualization.
Reset Zoom	Resets the horizontal zooming to its original size so the full width of the row dendrogram is visible.
View >	
> Log Scale	Displays the dendrogram in log scale. Affects only the horizontal distances in the dendrogram and not the actual numbers of the calculated similarity measures.
> Toolbar	Displays or hides the row dendrogram toolbar. If the toolbar has been hidden, right-click on the row dendrogram and select **View > Toolbar** from the pop-up menu to display it again.
> Cluster Scale	Displays or hides the cluster scale (and cluster line) above the row dendrogram. The cluster scale must be displayed if you want to select the number of clusters to be included in the added cluster column.
> Column Dendrogram	Displays or hides the column dendrogram (if one has been created).
> Row Dendrogram	Displays or hides the row dendrogram.
> Include Empty	Relevant only when you have performed a clustering using selected records. This produces a Hierarchical Clustering (order) column with empty values for all of the remaining records. By marking or clearing the Include Empty option you can determine whether or not to display the records that were not a part of the clustering calculation in the heat map. Obviously, no dendrogram can be displayed for these rows.
Remove Dendrograms	Removes the dendrograms permanently from the visualization.
Add Cluster Column	Adds a new column to the data set with information about which cluster each record belongs to. The position of the red circle on the cluster slider above the dendrogram controls the number of clusters. The column can be used to create a trellis plot of the clusters.
Overwrite	Selects whether or not to overwrite a Hierarchical Clustering (cluster) column, when using the Add cluster column function.

Column dendrogram pop-up menu:

Option	Description
Zoom to Active	Zooms so that the active node in the column dendrogram is displayed at the top of the visualization.
Reset Zoom	Resets the zooming to its original size so the full width of the row dendrogram is visible.
View >	
> Log Scale	Displays the dendrogram in log scale. Affects only the horizontal distances in the dendrogram and not the actual numbers of the calculated similarity measures.

3.3.8 Cluster Slider in Dendrogram

The scale above the row dendrogram is the cluster slider. The numbers above the scale refer to the number of clusters at different positions in the dendrogram. The numbers below the scale refer to the calculated similarity measures. When you move the cursor over the scale, the number of clusters and the similarity measure at that position are given in a ToolTip.

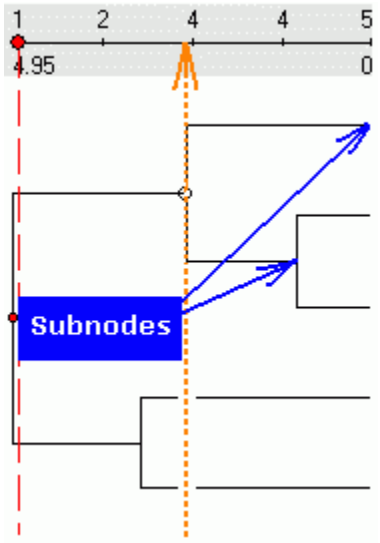


Upper scale

The upper scale assists you in selecting the number of clusters before creating a new clustering column. Click on the red circle on the cluster slider and drag it to the horizontal position you want. The selected clusters are indicated as red circles in the dendrogram. The total number of clusters is shown in a ToolTip as long as you hold down the mouse button.

Lower scale

The lower scale shows the calculated similarity measure in the dendrogram. The position of a node along the scale represents the similarity measure between the two subnodes in that node (there are always exactly two subnodes in each node). In the figure below, the similarity measure between the two subnodes in the active node is indicated by the dotted orange arrow.



The vertical distance has no mathematical meaning in the dendrogram.

Note: There is no cluster slider above the column dendrogram. You cannot create clusters in a column dendrogram and you cannot export information about the column dendrogram as a new column.

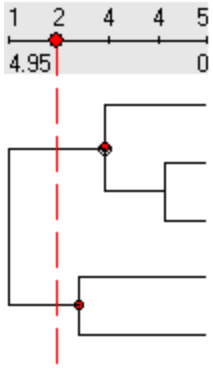
Tip: The cluster slider can also be moved by using the left and right arrows on the keyboard. This increases or decreases the number of clusters in a stepwise fashion.

3.4 Theory and Methods

3.4.1 Hierarchical Clustering Method Overview

Hierarchical clustering arranges objects in a hierarchy with a treelike structure based on the similarity between them.

The graphical representation of the resulting hierarchy is called a dendrogram, or a tree graph. This figure shows a small part of a dendrogram.



In Spotfire DecisionSite, the vertical axis of the dendrogram consists of the individual records and the horizontal axis represents the clustering level. The individual records in the clustered data set are represented by the rightmost nodes in the row dendrogram. Each remaining node in the dendrogram represents a cluster of all records that lie below it to the right in the dendrogram, thus making the leftmost node in the dendrogram a cluster that contains all records.

Misapplication of clustering

Clustering is a very useful data reduction technique. However, it can easily be misapplied. The clustering results are highly affected by your choice of similarity measure and other input

parameters. You should bear this in mind when you evaluate the results. If possible, you should replicate the clustering analysis using different methods. Apply cluster analysis with care and it can serve as a powerful tool for identifying patterns within a data set.

3.4.2 Hierarchical Clustering Algorithm

The algorithm used in the Hierarchical Clustering tool is a hierarchical agglomerative method. This means that the cluster analysis begins with each record in a separate cluster, and in subsequent steps the two clusters that are the most similar are combined to a new aggregate cluster. The number of clusters is thereby reduced by one in each iteration step. Eventually, all records are grouped into one large cluster.

► This is how it works:

1. The similarity between all possible combinations of two records is calculated using a selected similarity measure.
2. Each record is placed in a separate cluster.
3. The two most similar clusters are grouped together and form a new cluster.
4. The similarity between the new cluster and all remaining clusters is recalculated using a selected clustering method.
5. Steps 3 and 4 are repeated until all records eventually end up in one large cluster.

3.4.3 Required Input for Hierarchical Clustering

When you start a clustering you need to specify a number of parameters.

The parameters are set in the Hierarchical Clustering dialog that you reach by selecting **Clustering** > **Hierarchical Clustering** from the **Data** menu.

You need to answer the following questions:

- Which clustering method should be used to calculate the similarity between clusters?
- Which similarity measure should be used to calculate the similarity between records?
- Which ordering function should be used for drawing the dendrogram?

3.4.4 Hierarchical Clustering Ordering Function

The ordering function controls in what vertical order the records (rows) are plotted in the row dendrogram. The two subclusters within a cluster (there are always exactly two subclusters) are weighted and the cluster with the lower weight is placed above the other cluster. The weight can be any one of the following:

- **Input rank** of the records. This is the order of the records during import to DecisionSite.
- **Average value** of the rows. For example, a record *a* with 5 dimensions would have the average $(a_1+a_2+a_3+a_4+a_5)/5$. The average for a record *a* with *k* dimensions is calculated as

$$\bar{a} = \frac{1}{k}\sum_{j=1}^{k} a_j$$

Calculating the weight of a cluster

To calculate the weight w_3 of a new cluster C_3 formed from two subclusters C_1 and C_2 with a weight of $w_1$and w_2, and each containing n_1 and n_2 records, you use the following expression:

$$w_3 = \frac{n_1 \cdot w_1 + n_2 \cdot w_2}{(n_1 + n_2)}$$

3.4.5 Hierarchical Clustering References

Hierarchical clustering

Mirkin, B. (1996) Mathematical Classification and Clustering, Nonconvex Optimization and Its Applications Volume 11, Pardalos, P. and Horst, R., editors, Kluwer Academic Publishers, The Netherlands.

Sneath, P., Sokal, R. R. (1973) Numerical taxonomy, Second Edition, W. H. Freeman, San Francisco.

General information about clustering

Hair, J.F.Jr., Anderson, R.E., Tatham, R.L., Black, W.C. (1995) Multivariate Data Analysis, Fourth Edition, Prentice Hall, Englewood Cliffs, New Jersey.

3.4.6 Similarity Measures

3.4.6.1 Similarity Measures Overview

Spotfire DecisionSite contains several tools which calculate the similarity between different records (e.g., Hierarchical Clustering, K-means Clustering and Profile Search). Calculating similarities can be useful if you want to create lists of similar records which may possibly be treated as a group or if you want to find the record that is most similar to another record. The following similarity measures can be used to calculate the resemblance between records:

- Euclidean distance
- Correlation
- Cosine correlation
- City block distance
- Tanimoto coefficient (only available for Profile Search and Hierarchical Clustering)
- Half square Euclidean distance (only available for Hierarchical Clustering)

Note: When used in clustering, some of the similarity measures may be transformed so that they are always greater than or equal to zero (using 1 – calculated similarity value).

Dimensions

The term *dimension* is used in all similarity measures. The concept of dimension is simple if we are describing the physical position of a point in three dimensional space when the positions on the x, y and z axes refer to the different dimensions of the point. However, the data in a dimension can be of any type. If, for example, you describe a group of people by their height, their age and their nationality, then this is also a three dimensional system. For a record, the number of dimensions is equal to the number of variables in the record.

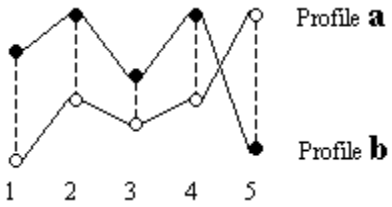
3.4.6.2 Euclidean Distance

The *Euclidean distance* between two profiles, *a* and *b*, with *k* dimensions is calculated as

$$\sqrt{\sum_{j=1}^{k}(a_j - b_j)^2}$$

The Euclidean distance is always greater than or equal to zero. The measurement would be zero for identical profiles and high for profiles that show little similarity.

The figure below shows an example of two profiles called *a* and *b*. Each profile is described by five values. The dotted lines in the figure are the distances (a_1-b_1), (a_2-b_2), (a_3-b_3), (a_4-b_4) and (a_5-b_5) which are entered in the equation above.



3.4.6.3 Correlation

The *Correlation* between two profiles, *a* and *b*, with *k* dimensions is calculated as

$$\frac{\mathrm{cov}(a,b)}{\mathrm{std}(a)\cdot\mathrm{std}(b)}$$

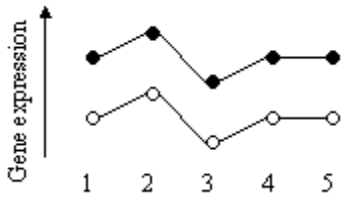
where

$$\mathrm{cov}(a,b)=\frac{1}{k}\sum_{j=1}^{k}(a_j-\bar{a})\cdot(b_j-\bar{b})$$

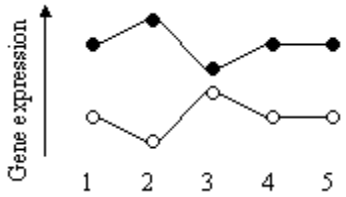
$$\mathrm{std}(a)=\sqrt{\frac{1}{k}\sum_{j=1}^{k}(a_j-\bar{a})^2}$$

$$\bar{a}=\frac{1}{k}\sum_{j=1}^{k}a_j$$

This correlation is called *Pearson Product Momentum Correlation*, simply referred to as *Pearson's correlation* or *Pearson's r*. It ranges from +1 to -1 where +1 is the highest correlation. Complete opposite profiles have correlation -1.



Profiles with identical shape have maximum correlation.



Perfectly mirrored profiles have the maximum negative correlation.

3.4.6.4 Cosine Correlation

The *Cosine correlation* between two profiles, *a* and *b*, with *k* dimensions is calculated as

$$\frac{\sum_{j=1}^{k}a_j\cdot b_j}{\mathrm{norm}(a)\cdot\mathrm{norm}(b)}$$

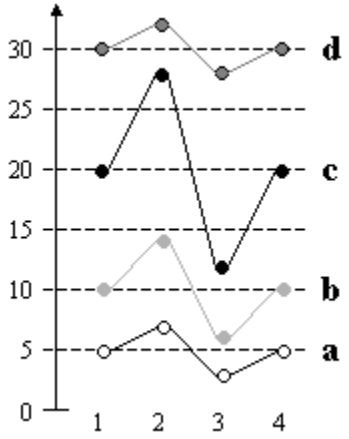
where

$$\mathrm{norm}(a)=\sqrt{\sum_{j=1}^{k}a_j^2}$$

The cosine correlation ranges from +1 to -1 where +1 is the highest correlation. Complete opposite profiles have correlation -1.

Comparison between Cosine correlation and Correlation

The difference between Cosine correlation and Correlation is that the average value is subtracted in Correlation. In the example below, the Cosine correlation will be +1 between any combination of profiles *a*, *b*, and *c*, but it will be slightly less than that between profile *d* and any of the other profiles (+0.974). However, the regular Correlation will be +1 between any of the profiles, including profile *d*.



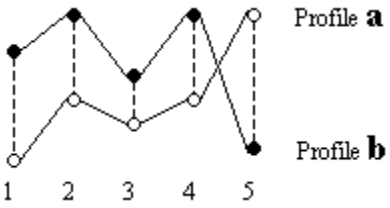
3.4.6.5 City Block Distance

The City block distance between two profiles, *a* and *b*, with *k* dimensions is calculated as

$$\sum_{j=1}^{k} |a_j - b_j|$$

The City Block distance is always greater than or equal to zero. The measurement would be zero for identical profiles and high for profiles that show little similarity.

The figure below shows an example of two profiles called *a* and *b*. Each profile is described by five values. The dotted lines in the figure are the distances (a_1-b_1), (a_2-b_2), (a_3-b_3), (a_4-b_4) and (a_5-b_5) which are entered in the equation above.



In most cases, this similarity measure yields results similar to the Euclidean distance. Note, however, that with City block distance, the effect of a large difference in a single dimension is dampened (since the distances are not squared).

The name *City block distance* (also referred to as *Manhattan distance*) is explained if you consider two points in the xy-plane. The shortest distance between the two points is along the hypotenuse, which is the *Euclidean distance*. The *City block distance* is instead calculated as the distance in x plus the distance in y, which is similar to the way you move in a city (like Manhattan) where you have to move around the buildings instead of going straight through.

3.4.6.6 Tanimoto Coefficient

The *Tanimoto coefficient* between two rows, *a* and *b*, with *k* dimensions is calculated as

$$\frac{\sum_{j=1}^{k} a_j \cdot b_j}{\left(\sum_{j=1}^{k} a_j^2 + \sum_{j=1}^{k} b_j^2 - \sum_{j=1}^{k} a_j \cdot b_j\right)}$$

The Tanimoto similarity measure is only applicable for a binary variable, and for binary variables the Tanimoto coefficient ranges from 0 to +1 (where +1 is the highest similarity).

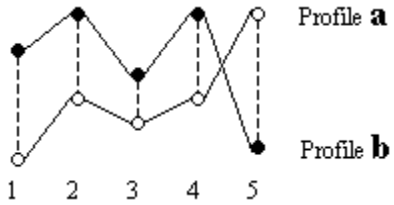
3.4.6.7 Half Square Euclidean Distance

The *Half square Euclidean distance* between two profiles, *a* and *b*, with *k* dimensions is calculated as

$$\frac{1}{2}\sum_{j=1}^{k}\left(a_j - b_j\right)^2$$

The Half square Euclidean distance is always greater than or equal to zero. The measurement would be zero for identical profiles and high for profiles that show little similarity.

The figure below shows an example of two profiles called *a* and *b*. Each profile is described by five values. The dotted lines in the figure are the distances (a_1-b_1), (a_2-b_2), (a_3-b_3), (a_4-b_4) and (a_5-b_5) which are entered in the equation above.



3.4.7 Cluster similarity methods

3.4.7.1 Cluster Similarity Methods

A hierarchical clustering starts by calculating the similarity between all possible combinations of two records using a selected similarity measure. These calculated similarities are then used to derive the similarity between all clusters that are formed from the records during the clustering. You select one of the following clustering methods:

- UPGMA
- WPGMA
- Single linkage
- Complete linkage
- Ward's method

3.4.7.2 UPGMA

UPGMA stands for Unweighted Pair-Group Method with Arithmetic mean.

Assume that there are three clusters called C_1, C_2 and C_3 including n_1, n_2 and n_3 number of records. Clusters C_2 and C_3 are aggregated to form a new single cluster called C_4.

The similarity between cluster C_1 and the new cluster C_4 in the example above is calculated as

$$\mathrm{sim}_{C1,C4} = a \cdot \mathrm{sim}_{C1,C2} + b \cdot \mathrm{sim}_{C1,C3}$$

where

sim = the similarity between the two indexed clusters and

$$a = \frac{n_2}{(n_2 + n_3)}$$

$$b = \frac{n_3}{(n_2 + n_3)}$$

3.4.7.3 WPGMA

WPGMA stands for Weighted Pair-Group Method with Arithmetic mean.

Assume that there are three clusters called C_1, C_2 and C_3 including n_1, n_2 and n_3 number of records. Clusters C_2 and C_3 are aggregated to form a new single cluster called C_4.

The similarity between cluster C_1 and the new cluster C_4 in the example above is calculated as

$$\text{sim}_{C1,C4} = \frac{1}{2}\left(\text{sim}_{C1,C2} + \text{sim}_{C1,C3}\right)$$

where

sim = the similarity between the two indexed clusters.

3.4.7.4 Single Linkage

This method is based on minimum distance. To calculate the similarity between two clusters, each possible combination of two records between the two clusters is compared. The similarity between the clusters is the same as the similarity between the two records in the clusters that are most similar.

3.4.7.5 Complete Linkage

This method is based on maximum distance and can be thought of as the opposite of *Single linkage*. To calculate the similarity between two clusters, each possible combination of two records between the two clusters is compared. The similarity between the two clusters is the same as the similarity between the two records in the clusters that are least similar.

3.4.7.6 Ward's Method

Ward's method means calculating the incremental sum of squares. The similarity measure is automatically set to *Half square Euclidean distance* when using Ward's method. This is not configurable.

Assume that there are three clusters called C_1, C_2 and C_3 including n_1, n_2 and n_3 number of records. Clusters C_2 and C_3 are aggregated to form a new single cluster called C_4.

The similarity between cluster C_1 and the new cluster C_4 in the example above is calculated as

$$\text{sim}_{C1,C4} = a \cdot \text{sim}_{C1,C2} + b \cdot \text{sim}_{C1,C3} - c \cdot \text{sim}_{C2,C3}$$

where

sim = the similarity between the two indexed clusters

$$a = \frac{n_1 + n_2}{(n_1 + n_2 + n_3)}$$

$$b = \frac{n_1 + n_3}{(n_1 + n_2 + n_3)}$$

$$c = \frac{n_1}{(n_1 + n_2 + n_3)}$$

4 Self-Organizing Maps

4.1 Self-Organizing Maps Overview

A Self-Organizing Map (SOM) is a type of clustering algorithm based on neural networks. The algorithm produces a Trellis profile chart, in which similar records appear close to each other, and less similar records appear more distant. From this map it is possible to visually investigate how records are related.

4.2 Using Self-Organizing Maps

4.2.1 Performing Clustering using Self-Organizing Maps

► To perform clustering:

1. Select **Data > Clustering > Self-Organizing Maps...**.
   Response: The Self-Organizing Maps dialog is displayed.
2. Select the value columns on which to base the clustering from the **Available columns** list and click **Add >>**.
   Comment: For multiple selection, press **Ctrl** and click on the desired columns in the Available columns list. Then click Add >> to move the columns to the Selected columns list. You can sort the columns in the list alphabetically by clicking on the Name bar.
3. Click a radio button to select whether to work on **All records** or **Selected records**.
4. Select a method to **Replace empty values with** from the drop-down list.
5. Select a **Normalization method** from the drop-down list.
   Comment: Self Organizing Maps offers three different Normalization methods: Z-score (subtract the mean and divide by standard deviation), Divide by standard deviation, and Scale between 0 and 1. Each of these three methods apply normalization to columns, but not to rows.
6. Enter the **Grid size** width and height.
   Comment: This is the number of separate maps to be calculated. Entering large values gives the map a better resolution, but makes the calculation slower. Entering small values may result in dissimilar records being assigned to the same node.
7. If desired, click **Advanced...** to modify the calculation settings. If you do not want to change the calculation settings, continue to step 14.
8. Select a **Neighborhood function** from the drop-down list.
   Comment: For more information about the available methods, see Neighborhood function.
9. Modify the **Begin radius** and the **End radius** according to your choice.
10. Select a **Learning function**.
    Comment: For more information about the available methods, see Learning function.
11. Modify the **Initial rate**.
    Comment: If you receive the message "Calculation error: Overflow in floating numbers" upon calculation, you may have set the initial training rate too high. Try a lower value.
12. Enter a **Number of training steps** or use the default setting.
13. Click **OK**.
14. Type a new **Column name**, or use the default name.

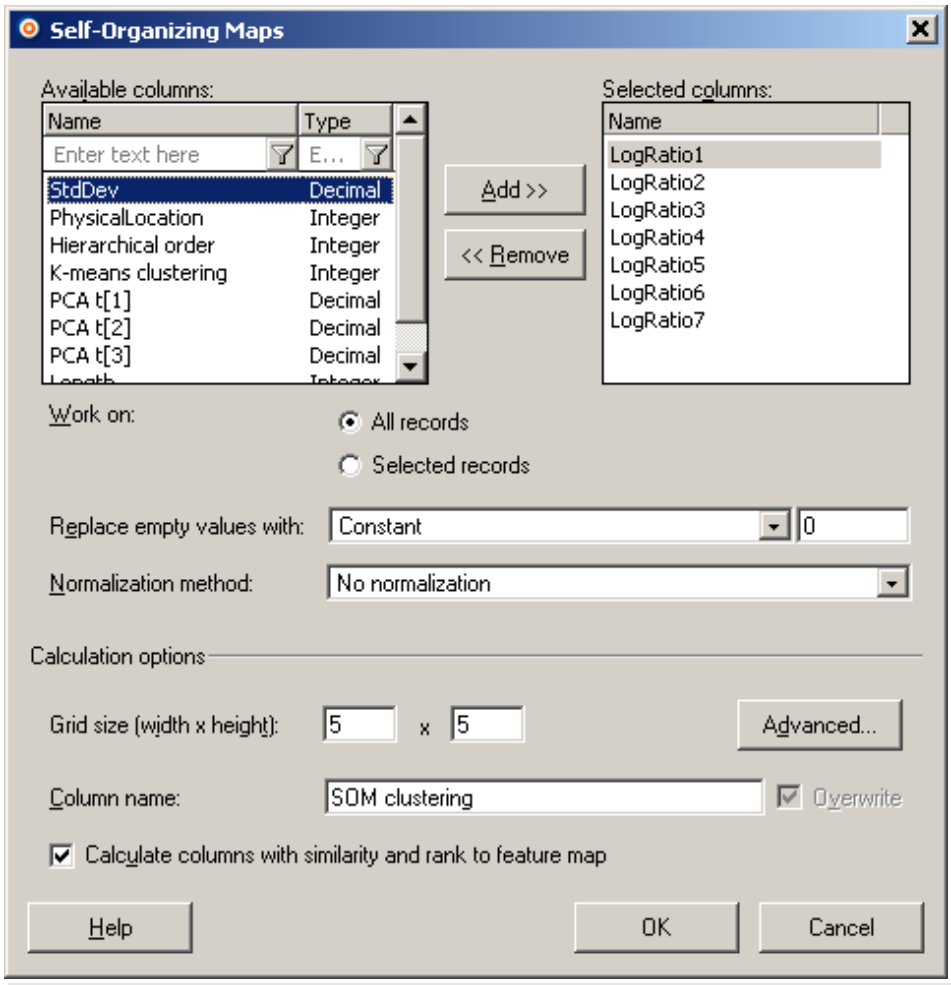
Comment: Select the **Overwrite** check box if you want to overwrite a previously added column with the same name.

15. Select or clear the **Calculate columns with similarity and rank to feature map** check box.
16. Click **OK**.

    Response: The dialog is closed and the algorithm is started. The results of the clustering are added as new data columns to the data set. You see a graphical representation of the result in the trellised profile charts. Each profile chart represents a node in the SOM.

4.3 User Interface

4.3.1 Self-Organizing Maps Dialog



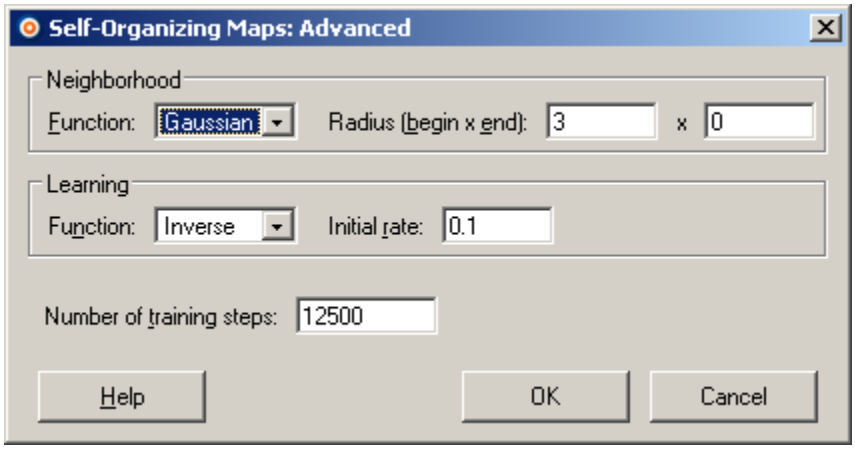
Option	Description
Available columns	Lists all columns available for clustering. Click to select a column to be used in the Self-Organizing Maps, then click Add >>. To select more than one column at a time, press **Ctrl** and click the column names in the list. All numerical columns in the data set are available as value columns. You can sort the columns in the list alphabetically by clicking on the

	Name bar. Click again to reverse sorting and once more to reset the sort order. **Note:** You can right-click on the Name header to get a pop-up menu where you can select other attributes you would like to be visible.
Enter text here 	If you have a data set with many columns, you can right-click on the header of the columns in the Available columns list box and select **Show Search Field** from the pop-up menu. This will display a search field where you can type a search string and limit the number of items in the list. It is possible to use the wildcard characters * and ? in the search.
Selected columns	Lists the selected columns to be used in the calculation.
Add >>	Adds the columns selected in the Available columns list to the Selected columns list.
<< Remove	Removes the selected columns from the Selected columns list.
Work on: All records	All records are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Replace empty values with	Defines how empty values in the data set should be replaced in the clustering. **Constant** allows you to replace the empty values by any constant (type a number in the text box). **Row average** replaces the value by the average value of the entire row. **Row interpolation** sets the missing value to the interpolated value between the two neighboring values in the row. **Column average** replaces the value by the average value of the entire column.
Normalization method	Defines which normalization method to use in the calculation.
Grid size (width x height)	The width and height of the map. Entering large values gives the map a better resolution, but makes the calculation slower. Entering small values may result in dissimilar records being assigned to the same node.
Advanced...	Displays the Self-Organizing Maps: Advanced dialog.
Column name	The main name of the columns added to the data set. The columns identifying the row and column index of the node to which each record has been assigned are appended with (x value) and (y value).
Overwrite	Select the check box to overwrite previously added columns with the same name.
Calculate columns with similarity and rank to feature map	Select this check box to add extra columns to the data set. The first column will contain the rank of the calculated similarity to centroid values. This means that the rank column contains a numbered list where 1 represents the record that is the most similar to its centroid. The name of the added column will be the same as the one entered under Column name, followed by (rank). The second column will contain the calculated similarity of each record to its centroid. The name of the added column will be the same as the one entered under *Column name*, followed by (similarity).

► To reach the Self-Organizing Maps dialog:

Select **Data** > **Clustering** > **Self-Organizing Maps...**.

4.3.2 Self-Organizing Maps Advanced Dialog



Option	Description
Neighborhood Function	The method used to compute how the weight vector of a node should be updated in each iteration. For more information about the available methods, see Neighborhood function.
Radius (begin x end)	The neighborhood radius begin and end values. For more information, see Neighborhood function. The default value of the begin radius is 1/2 of the longer side of the grid. The end radius default value is 0.
Learning Function	The function which controls how learning decreases over time. Usually, the Inverse is more efficient than Linear. For more information about the available methods, see Learning function.
Initial rate	The initial learning-rate, see Learning function. Higher values are recommended for coarse-adjustment and lower values for fine-adjustments. The default value is 0.05. **Tip:** If you receive the message "Calculation error: Overflow in floating numbers" upon calculation, you may have set the initial learning rate too high. Try a lower value.
Number of training steps	The number of iterations of the algorithm. The default value is 500 times the number of nodes in the map.

► To reach the Self-Organizing Maps: Advanced dialog:

1. Select **Data** > **Clustering** > **Self-Organizing Maps...**.
2. Click **Advanced...** in the Self-Organizing Maps dialog.

4.4 Theory and Methods

4.4.1 Self-Organizing Maps Theory Overview

Self-Organizing Maps (SOMs) are a special class of *artificial neural networks* based on *competitive learning*. The algorithm produces a two-dimensional grid, in which similar records appear close to each other, and less similar records appear more distant. From this map it is

possible to visually investigate how records are related. In this sense, SOMs provide a form of clustering.

Misapplication of clustering

Clustering is a very useful data reduction technique. However, it can easily be misapplied. The clustering results are highly affected by your choice of similarity measure and clustering algorithm. You should bear this in mind when you evaluate the results. If possible, you should replicate the clustering analysis using different methods. Apply cluster analysis with care and it can serve as a powerful tool for identifying patterns within a data set.

4.4.2 Self-Organizing Maps Algorithm

The following is a non-mathematical introduction to Self-Organizing Maps (SOMs). For the mathematical details, see Update Formula, and References.

The goal of the algorithm is to distribute records in a two-dimensional grid, such that similar records appear close to each other, and less similar records appear more distant.

► This is how it works:

1. **Initialization**. A two-dimensional rectangular grid is set up. Each node in the grid is assigned an initial weight vector. This vector has the same number of dimensions as the input data.
2. **Sampling**. A record is picked from the data set by random. This record is called the *input vector*.
3. **Similarity matching**. The input vector is compared to the weight vector of each node, and the node whose weight vector is most similar to the input vector is declared the *winner*.
4. **Updating**. The weight vector of each node is modified.

   Comment: Nodes close to the winner (in terms of their position in the grid, not their weight vectors) have their weight vectors modified to approach the input vector, while nodes far from the winner are less affected, or not affected at all. See Update formula.
5. **Iteration**. The algorithm is repeated from step 2.
6. **Best match**. After a number of iterations, the training ends. Each record in the data set is assigned to the node whose weight vector most closely resembles it, using Euclidean distance.
7. **Visualization**. Two new columns are automatically added to the data set, and a Trellis profile chart is created.

   Comment: In the SOM, a node is represented by an X and Y index denoting its position in the grid. After the algorithm has been executed, each record in the data set is given the indices of the node to which it was assigned (see step 6 above). This means that two new columns are added to the data set. The result is visualized as a number of profile charts, trellised by the two new columns such that each chart represents a SOM node and the records assigned to it.

4.4.3 Self-Organizing Maps - Update Formula

The SOM algorithm is an iterative process (see Self-Organizing Maps algorithm). Each time an input vector (a record picked by random from the original data set) has been selected and a winning node appointed, the weight vectors of all the nodes in the grid are updated.

The new weight vector of a node $\mathbf{w}_j$ is given by the equation:

$$\mathbf{w}_j(t+1) = \mathbf{w}_j(t) + a(t) * h_{j,i(x)}(t) * (\mathbf{x}(t) - \mathbf{w}_j(t))$$

where

t	= time, number of iterations so far
a	= learning-rate factor
h	= neighborhood function
x	= input vector (a record from the original data set)
$\mathbf{w}_j$	= weight vector of a node with index j
i(x)	= winning node for input vector **x**

In other words, the new weight vector is given by the old vector plus the product of learning-rate factor, neighborhood function and distance to input vector.

4.4.4 Self-Organizing Maps - Initial Weight Vectors

In the initialization step of the SOM algorithm, each node is assigned an *initial weight vector*. This vector has the same number of dimensions as the input vector, supplying a starting configuration for the SOM.

By default, *linear initialization* is used. Under certain conditions this will fail, and in this case *random initialization* will be used. If so, the algorithm is conducted in two phases: a rough phase and a fine-tune phase.

Linear initialization

Linear initialization creates the most effective starting configuration, reducing the number of iterations needed to reach a meaningful result.

Determine the two eigenvectors of the autocorrelation matrix of the training data x that have the largest eigenvalues, and then let these eigenvectors span a two dimensional linear subspace. A rectangular lattice is defined along this subspace, its centroid coinciding with that of the mean of the x(t), and the main dimensions being the same as the two largest eigenvalues.

Random initialization

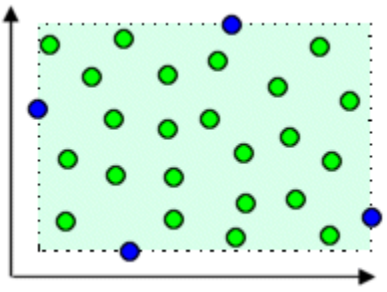
In random initialization, each weight vector **w** is populated with random values, such that for dimension i:

$\mathbf{w}_i = r_i((\max(x_i) - \min(x_i)) + \min(x_i)$

where

w	= weight vector
r	= random value and 0 <= r <= 1
i	= dimension (column)
x	= data set

Less formally, this means that the initial weight vectors are uniformly distributed within a space bounded by the extreme values in the data set:



Random initialization is not considered as effective as linear initialization. This is compensated for by introducing a *rough phase* before the normal training. This means that the first 20% of the assigned training length is carried out with an initial learning rate that is 10 times higher than that which has been defined. The remaining 80% of the training is then carried out with normal parameters.

4.4.5 Self-Organizing Maps - Similarity Matching

In the similarity matching step of the SOM algorithm, a winning node is selected by finding the weight vector most similar to the input vector. Similarity is measured as Euclidean distance.

The winning node i(**x**) is selected using the following formula:

$$i(\mathbf{x}) = \arg\min_j \left\| \mathbf{x}(t) - \mathbf{w}_j \right\|_{j=1}^{j=l}$$

where

t	= time, number of iterations
$\mathbf{w}_j$	= weight vector of a node j
x(t)	= input vector at time t

4.4.6 Self-Organizing Maps - Neighborhood Function

The equation (see Update formula) for calculating how the weight vector of a node is modified in each iteration includes a *neighborhood function*. This function takes into account the Euclidean distance between a node and the winning node, as well as the time passed.

The tool provides two alternatives: the Bubble function and the Gaussian function. Both include a parameter called *effective radius* which varies with time.

Effective Radius

The radius at step *t* is given by:

$$r(t) = r(begin) + \Delta r \cdot t$$

where

$$\Delta r = \frac{r(end) - r(begin)}{k}$$

t	= time, number of iterations so far
k	= training length (set by user)
r(end)	= end radius (set by user)
r(begin)	= initial radius (set by user)

Less formally this means that as the training progresses, the radius goes from the initial value down to the end value.

Bubble neighborhood function

The Bubble function affects all surrounding nodes equally up to a threshold radius. Beyond this radius, nodes are unaffected.

The Bubble function for a node j and a winning node i(x) is defined as follows:

$$h_{j,i(\mathbf{x})} = \begin{cases} 1 & \text{if } d_{i,j} <= r(t) \\ 0 & \end{cases}$$

where

$d_{i,j}$ = Euclidean distance between node and winning node

Gaussian neighborhood function

The Gaussian function is defined as follows:

$$h_{j,i(\mathbf{x})} = -\exp\left(\frac{d^2_{i,j}}{2r(t)}\right)$$

4.4.7 Self-Organizing Maps - Learning Function

The Update formula includes a factor called the *learning-rate factor*. This parameter decreases over time in accordance with a *learning function*. Two options are available: an inverse function, and a linear function (the names describe how learning decreases with time). Which function to use is selected in the Self-Organizing Maps: Advanced dialog.

Both functions initially take the value of the user-specified initial learning-rate. As the training progresses, the functions approach zero.

Inverse learning function

The learning-rate factor at step *t* is given by:

$$\alpha(t) = \alpha(0)\frac{b}{t+b}$$

where

t	= time, number of iterations
b	= training length / 100
$\alpha(0)$	= initial learning-rate (set by user)

Linear learning function

The learning-rate factor at step *t* is given by:

$$a(t) = a(0)\left(1-\left(1-\frac{a(0)}{100}\right)\cdot\frac{t}{trainlen}\right)$$

where

t	= time, number of iterations
trainlen	= training length (set by user)
$\alpha(0)$	= initial learning-rate (set by user)

4.4.8 Map Quality Measures

The quality of the created Self-Organizing Maps can be evaluated based on the mapping precision and the topology preservation. This information is included as a plot annotation after running the tool.

Mapping Precision

The average quantization error is calculated as follows:

$$\varepsilon_q = \frac{1}{N}\sum_{i=1}^{N}\left\|x_i - w_C\right\|$$

where c is the best matching unit for the actual x.

Topology Preservation

The topographic error is calculated as follows:

$$\varepsilon_t = \frac{1}{N}\sum_{i=1}^{N} u(x_k)$$

where u is 1 if the first and second best matching units are not in the near vicinity of each other, otherwise u is 0.

4.4.9 Self-Organizing Maps References

Mirkin, B. (1996) Mathematical Classification and Clustering, Nonconvex Optimization and Its Applications Volume 11, Pardalos, P. and Horst, R., editors, Kluwer Academic Publishers, The Netherlands.

MacQueen, J. (1967). Some methods for classification and analysis of multivariate observations. In Le Cam, L. M. and Neyman, J., editors, Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability. Volume I: Statistics, pages 281-297. University of California Press, Berkeley and Los Angeles, CA.

5 K-means Clustering

5.1 K-means Clustering Overview

K-means clustering is a form of non-hierarchical clustering, which groups records into a defined number of clusters based on their similarity.

5.2 Using K-means Clustering

5.2.1 Performing K-means Clustering

► To initiate a K-means clustering:

1. Select **Data > Clustering > K-means Clustering...**.
   Response: The K-means Clustering dialog is displayed.
2. Select the value columns on which to base the clustering from the **Available columns** list and click **Add >>**.
   Comment: For multiple selection, press **Ctrl** and click on the desired columns in the Available columns list. Then click Add >> to move the columns to the Selected columns list. You can sort the columns in the list alphabetically by clicking on the Name bar.
3. Click a radio button to select whether to work on **All records** or **Selected records**.
4. Select a method to **Replace empty values with** from the drop-down list.
5. Enter the **Maximum number of clusters**.
   Comment: Since empty clusters are discarded at the calculation, the resulting number of clusters may be less than what is specified in this text box.
6. Select a **Cluster initialization** method from the drop-down menu.
   Comment: For more information about the available methods, see Initializing K-means cluster centroids.
7. Select which **Similarity measure** to use for the clustering.
   Comment: Click for information about the available similarity measures.
8. Type a new **Column name** in the text box or use the default name.
   Comment: Select the **Overwrite** check box if you want to overwrite a previously added column with the same name.
9. Click **OK**.
   Response: The K-means Clustering dialog is closed and the clustering is started. You see a graphical representation of the result in the visualizations created. The results of the clustering are added as new data columns to the data set.

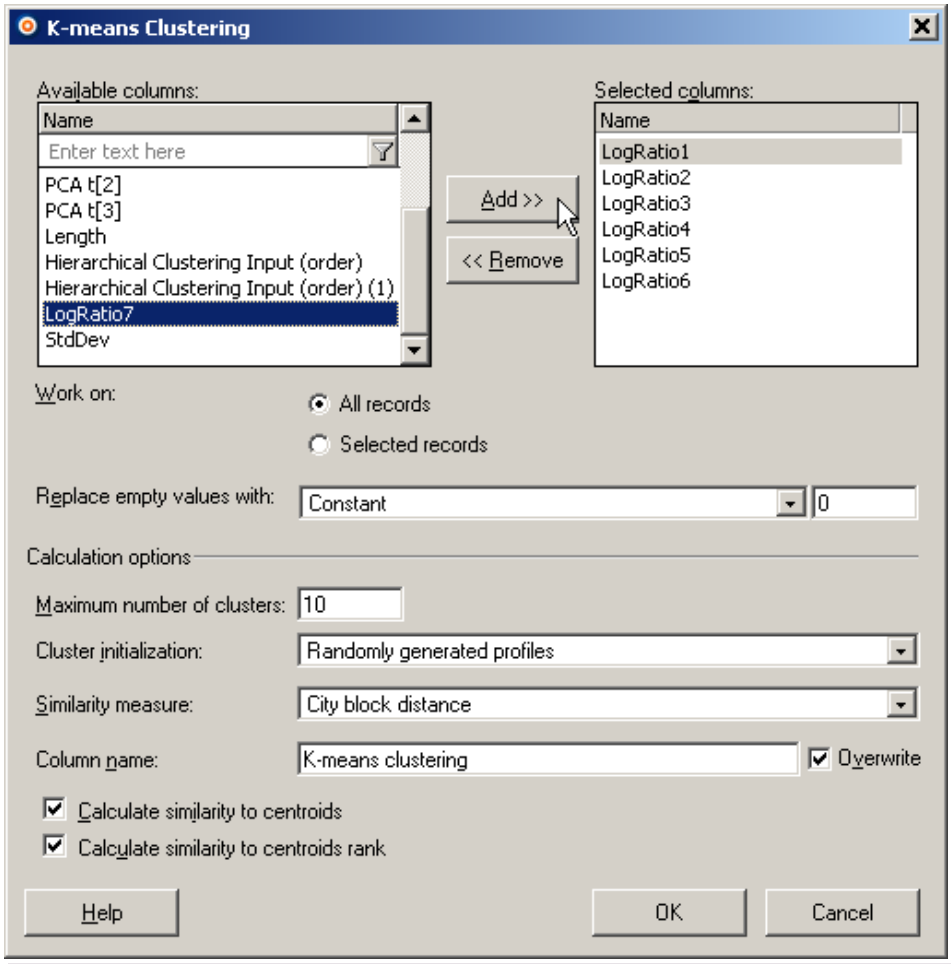
5.2.2 K-means Clustering - Finding Out Cluster Belonging

► To find out which cluster a record belongs to:

1. Perform a K-means clustering.
2. In any visualization (for example, a scatter plot or profile chart), click to activate the record that you are interested in.
3. Look in the Details-on-Demand window and locate the number in the K-means clustering column.

5.3 User Interface

5.3.1 K-means Clustering Dialog



Option	Description
Available columns	Displays all available data columns on which you can perform a clustering. Click a column name in the list and click **Add >>** to add it to the Selected columns list. To select more than one column, press **Ctrl** and click the column names in the list, then click Add >>. You can choose from all columns that contain real numbers or integers. **Note:** You can right-click on the Name header to get a pop-up menu where you can select other attributes you would like to be visible.
Enter text here 	If you have a data set with many columns, you can right-click on the header of the columns in the Available columns list box and select **Show Search Field** from the pop-up menu. This will display a search field where you can type a search string and limit the number of items in the list. It is possible to use the wildcard characters * and ? in the search.
Selected columns	Displays the currently selected data columns on which you want to perform a clustering.
Add >>	Adds the highlighted data column to the list of selected columns.

<< **Remove**	Removes the highlighted data column from the list of selected columns and places them back in the list of available columns.
Work on: All records	All records in the value columns are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Replace empty values with	Defines how empty values in the data set should be replaced in the clustering. **Constant** allows you to replace the empty values by any constant (type a number in the text box). **Row average** replaces the value by the average value of the entire row. **Row interpolation** sets the missing value to the interpolated value between the two neighboring values in the row. **Column average** returns the average of the corresponding column values.
Maximum number of clusters	The maximum number of clusters that you want to calculate (some may turn out empty and will in that case not be displayed).
Cluster initialization	Determines which method to use when initializing the clusters. For more information about the available methods, see Initializing K-means cluster centroids.
Similarity measure	The similarity measure that you want to use for the K-means clustering. For more information about the available measures, see Similarity measures.
Column name	The name for the new columns containing the results from the K-means clustering.
Overwrite	Select this check box if you want to replace a previously added column (with the same name as the one typed in the *Column name* text box) when you add a new column. Clear the check box if you wish to keep the old column.
Calculate similarity to centroids	Select this check box to add an extra column to the data set. This column will contain the calculated similarity of each record to its centroid. The name of the added column will be the same as the one entered under *Column name*, followed by (similarity).
Calculate similarity to centroids rank	Select this check box to add an extra column to the data set. This column will contain the rank of the calculated similarity to centroid values. This means that the rank column contains a numbered list where 1 represents the record that is the most similar to its centroid. The name of the added column will be the same as the one entered under Column name, followed by (rank).
OK	Saves all your settings, launches the K-means clustering calculation and closes the K-means Clustering dialog. A new bar chart visualization is created with the bars colored according to which cluster they belong to. A trellis profile chart visualization is also displayed. Clustering statistics are added as an annotation connected to the visualizations. The clustering statistics contains information about the clustering initialization and results.

► To reach the K-means Clustering dialog:

Select **Data** > **Clustering** > **K-means Clustering...**.

5.4 Theory and Methods

5.4.1 K-means Clustering Method Overview

K-means clustering is a method used for grouping data points into a predetermined number of clusters based on their similarity. Before you start the clustering you must decide how many clusters you want and how the centroids (the center points of these clusters) should be initialized.

K-means clustering is a type of non-hierarchical clustering. It is an iterative process in which each record is assigned to the closest centroid. The centroid for each cluster is then recomputed. These steps are repeated until a steady state has been reached.

Misapplication of clustering

Clustering is a very useful data reduction technique. However, it can easily be misapplied. The clustering results are highly affected by your choice of similarity measure and clustering algorithm. You should bear this in mind when you evaluate the results. If possible, you should replicate the clustering analysis using different methods. Apply cluster analysis with care and it can serve as a powerful tool for identifying patterns within a data set.

5.4.2 K-means Clustering Algorithm

The K-means clustering algorithm is an iterative process. Each record is assigned to the closest centroid. New centroids are calculated for the resulting clusters and the records are reassigned to the closest centroid. The process automatically stops once a steady state has been reached.

► This is how it works:

1. The similarity between each record and all centroids is calculated using a selected similarity measure.
2. All records are assigned to the centroid that is most similar to them.
3. The new centroids for the resulting clusters are calculated according to a method defined by the choice of similarity measure.
4. Steps 1 - 3 are repeated until a steady state is reached, or in other words when no records any longer change cluster between two steps and the centroids no longer vary.

Note: If you are using Data centroid based search then the algorithm is slightly different.

5.4.3 Required Input for K-means Clustering

You have to specify the following before you can start a K-means clustering:

- Which similarity measure should be used?
- How many clusters do you want?
- How should the cluster centroids be initialized?

Similarity measures

Several different similarity measures are available to the K-means clustering tool. Similarity measures express the similarity between records or profiles as numbers and thus make it possible to rank the records according to their similarity. For information about the various measures, go to the section called Similarity measures.

Initializing cluster centroids

When you start a K-means clustering, you have to decide how many clusters you want to use and how the centroids of these clusters should be initialized.

The number of clusters should be based on a reasonable hypothesis of the distribution of the data. If you have too few clusters, you may miss important details and if you have too many clusters, you may end up with many empty clusters or clusters with only one record in them.

Click for information about the available methods for Initializing cluster centroids.

Calculating resulting cluster centroids

The centroids for the resulting clusters from each step in a K-means clustering are calculated differently depending on which similarity measure you use. Click for information about calculating resulting cluster centroids.

5.4.4 Initializing K-means Cluster Centroids

To initiate a K-means clustering, you have to decide which initial centroids to use. The following methods are available:

- Data centroid based search
- Evenly spaced profiles
- Randomly generated profiles
- Randomly selected profiles
- From marked records

Data centroid based search

This method for initializing the centroids uses a slightly different algorithm compared to other methods.

► This is how it works:

1. The first centroid is calculated as the average of all profiles.
2. The similarity between the centroid and all profiles is calculated using a selected similarity measure.
3. The profile that is least similar to the first centroid is picked to be the second centroid.
4. The similarity between the second centroid and all remaining profiles is calculated.
5. The profiles that are more similar to the second centroid than the first centroid are assigned to the second centroid and are then not investigated further.
6. Of the remaining profiles, the profile that is least similar to the first centroid is picked to be the third centroid.
7. Steps 4 through 6 are repeated until the specified number of clusters is reached, or until there are no more profiles left to assign.

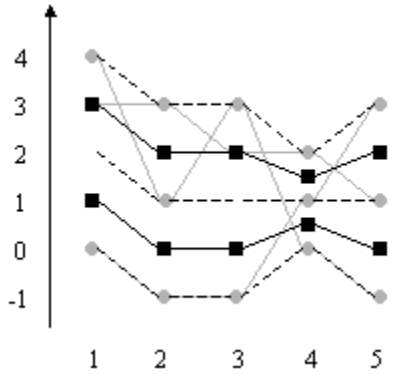
If you run out of profiles before the specified number of clusters has been created, the procedure is automatically repeated but with an adjusted requirement for assigning profiles to the second centroid instead of the first centroid. In the first round, the requirement is that the second centroid must be more similar to the profile than the first centroid. In the second round we sharpen this requirement so that fewer profiles are assigned to the second centroid. If you again run out of profiles before the specified number of clusters has been created, the requirement is again adjusted using the same method.

Evenly spaced profiles

This method generates profiles to be used as centroids that are evenly distributed between the minimum and maximum value for each variable in the profiles in your data set.

The example below shows how the initial centroids are derived. We have a total of three profiles in the data set (the gray circles connected with lines). We have specified that we want

two clusters. The distance between the minimum and maximum value for each variable in the profiles has therefore been divided into two parts (separated by the dashed black lines). The centroids are the average values of each part between the minimum and maximum values (the black squares connected with black lines).

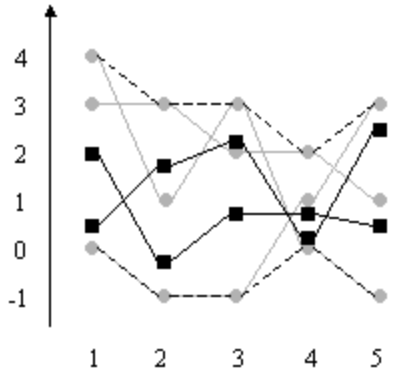


In reality you would have many more than three profiles in your data set, but the example shows the principle of how centroids are derived using the evenly spaced method.

Randomly generated profiles

In this method you generate new profiles to use as centroids from random values based on your data set. Each value in the centroids is randomly selected as any value between the minimum and maximum for each variable in the profiles in your data set.

The example below shows how the initial centroids are derived. We have a total of three profiles in the data set (the gray circles connected with lines). The minimum and maximum values are connected with the dashed black lines. Two examples of randomly generated profiles are shown as the black squares connected with black lines. As can be seen from the figure, each variable in the randomly generated profiles can assume any value between the minimum and maximum value for that variable.



In reality you would have much more than three profiles in your data set, but the example shows the principle of how centroids are randomly generated.

Randomly selected profiles

With this method, you use existing profiles that are randomly selected from your data set as centroids.

From marked records

You import the currently marked profiles in your visualizations and use them as centroids. This option is only available if there are any records marked when starting the tool.

5.4.5 Calculating Resulting K-means Cluster Centroids

After each step in a K-means clustering, the resulting centroid of each cluster is calculated. The centroids are calculated differently depending on the similarity measure used for the clustering.

The new centroid *cnew for* a K-means cluster *C* with *n* records $\{a_i\}_{i=1}^{n}$ and *k* dimensions is calculated as shown below for the various similarity measures.

Correlation

$$c_{new}(C) = c_{new}\left(\left\{\frac{a_i - \bar{a}_i}{\mathrm{std}(a_i)}\right\}_{i=1}^{n}\right) = \left(\frac{1}{n}\sum_{i=1}^{n}\frac{(a_{ij} - \bar{a}_i)}{\mathrm{std}(a_i)}\right)_{j=1}^{k}$$

where

$$\mathrm{std}(a_i) = \sqrt{\frac{1}{k}\sum_{j=1}^{k}(a_{ij} - \bar{a}_i)^2}$$

$$\bar{a}_i = \frac{1}{k}\sum_{j=1}^{k} a_{ij}$$

Cosine correlation

$$c_{new}(C) = c_{new}\left(\left\{\frac{a_i}{\mathrm{norm}(a_i)}\right\}_{i=1}^{n}\right) = \left(\frac{1}{n}\sum_{i=1}^{n}\frac{a_{ij}}{\mathrm{norm}(a_i)}\right)_{j=1}^{k}$$

where

$$\mathrm{norm}(a_i) = \sqrt{\frac{1}{k}\sum_{j=1}^{k} a_{ij}^2}$$

Euclidean distance and City block distance

$$c_{new}(C) = c_{new}\left(\{a_i\}_{i=1}^{n}\right) = \left(\frac{1}{n}\sum_{i=1}^{n} a_{ij}\right)_{j=1}^{k}$$

5.4.6 K-means Clustering References

K-means clustering

Mirkin, B. (1996) Mathematical Classification and Clustering, Nonconvex Optimization and Its Applications Volume 11, Pardalos, P. and Horst, R., editors, Kluwer Academic Publishers, The Netherlands.

MacQueen, J. (1967). Some methods for classification and analysis of multivariate observations. In Le Cam, L. M. and Neyman, J., editors, Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability. Volume I: Statistics, pages 281-297. University of California Press, Berkeley and Los Angeles, CA.

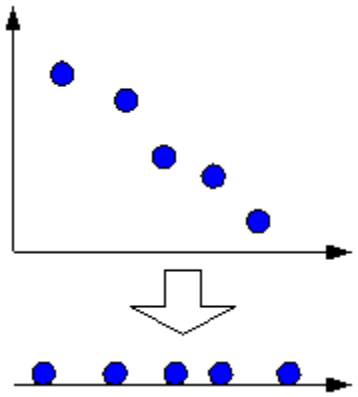
General information about clustering

Hair, J.F.Jr., Anderson, R.E., Tatham, R.L., Black, W.C. (1995) Multivariate Data Analysis, Fourth Edition, Prentice Hall, Englewood Cliffs, New Jersey.

6 Principal Component Analysis

6.1 Principal Component Analysis Overview

Spotfire DecisionSite Statistics provides a simple but powerful data reduction tool called Principal Component Analysis (PCA). The goal of PCA is to reduce the dimensionality of a data set (describe the data set using fewer variables) without significant loss of information.



The PCA algorithm takes a high-dimensional data set as input, and produces a new data set consisting of fewer variables. These variables are linear combinations of the original variables, so it is often possible to ascribe meaning to what they represent.

6.2 Using Principal Component Analysis

6.2.1 Initiating a PCA Calculation

► To initiate a PCA calculation:

1. Select **Data > Clustering > Principal Component Analysis...**.
   Response: The Principal Component Analysis dialog is opened.
2. Select the value columns on which to base the clustering from the **Available columns** list and click **Add >>**.
   Comment: For multiple selection, press **Ctrl** and click on the desired columns in the Available columns list. Then click Add >> to move the columns to the Selected columns list. You can sort the columns in the list alphabetically by clicking on the Name bar.
3. Click a radio button to select whether to work on **All records** or **Selected records**.
4. Select a method to **Replace empty values with** from the drop-down list.
5. Type the number of **Principal components** that you want to calculate.
   Comment: The number of principal components is the number of dimensions to which you wish to reduce the original data. The PCA tool calculates the *n* best components, where *n* is the same as the number of dimensions to which you are projecting.
6. Type a **Column name** for the resulting column or use the default name.
   Comment: Select the **Overwrite** check box to overwrite an old column with the same name.
7. Select whether to create a **2D** or a **3D** scatter plot showing the principal components.
   Comment: Clear the Create Scatter Plot check box if you want to perform the calculation without creating any new visualizations.

8. Decide if you want to **Generate HTML report** or not, by selecting or clearing the check box.

   Comment: The PCA HTML report contains information about the calculation presented as an HTML page.
9. Decide if you want to **Launch DecisionSite with PCA report** or not, by selecting or clearing the check box.

   Response: This launches a new session of DecisionSite containing a plot with the PCA results. For more information on the results, see PCA HTML Report.
10. Click **OK**.

    Response: The principal components are calculated and new columns containing the results are added to the data set. If **Create Scatter Plot** has been selected, a new scatter plot is created according to your settings (2D or 3D). If **Generate HTML report** has been selected, then the PCA Result report is displayed in your default web browser.

6.2.2 Interpreting PCA Results

When the PCA tool is executed, a Principal Component Analysis is performed on the current data set. The result can be regarded as a new data set with fewer variables.

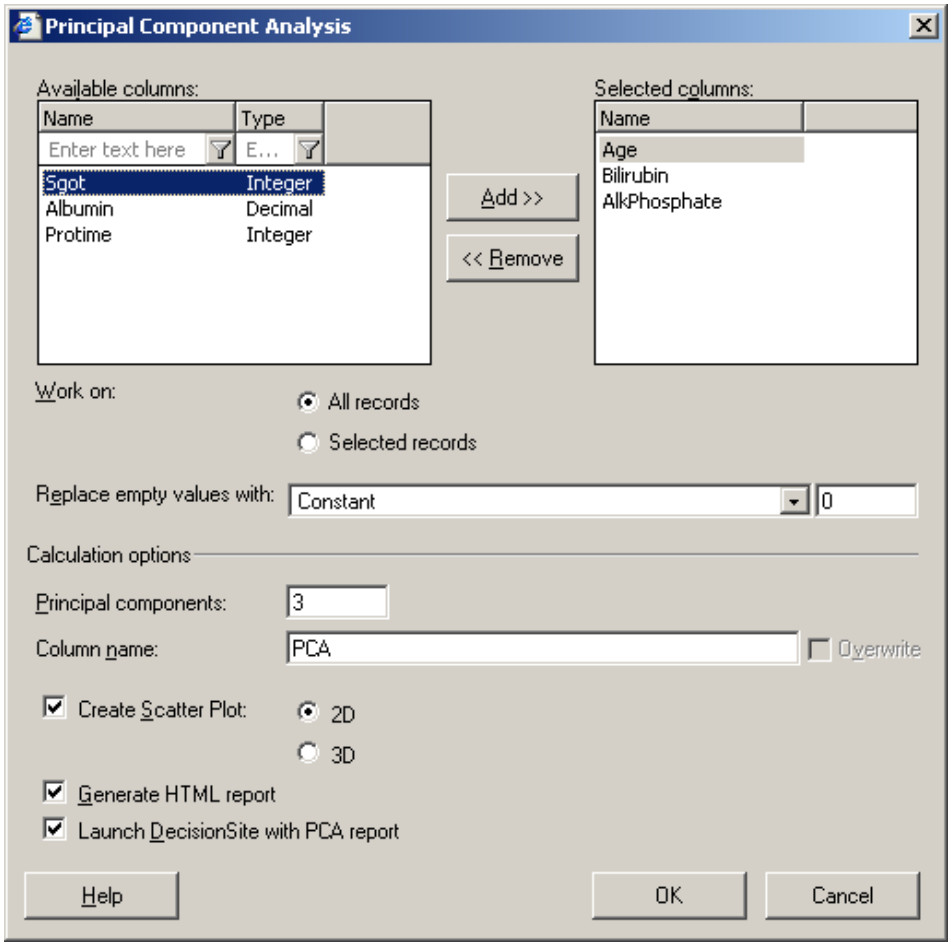
The results of a PCA calculation are often displayed in a scatter plot (scores plot) mapping the principal component score of each projected record. Each point in the plot represents a record in the original data set. The position along a certain axis represents the score of the record on that principal component.

The PCA tool generates one or more principal components depending on the settings in the Principal Component Analysis dialog.

An alternative way of studying the results of PCA is by showing to what extent each original dimension (value column) has contributed to a certain principal component. If desired, you can generate either a new DecisionSite session or a PCA HTML report containing an eigenvector plot where you can directly see which column has contributed the most to a certain principal component.

6.3 User Interface

6.3.1 Principal Component Analysis Dialog



Option	Description
Available columns	Displays all available data columns which you can use in a calculation. Click a column name in the list and click **Add >>** to add it to the Selected columns list. To select more than one column, press **Ctrl** and click the column names in the list, then click Add >>. You can choose from all columns that contain decimal numbers or integers. **Note:** You can right-click on the Name header to get a pop-up menu where you can select other attributes you would like to be visible.
Enter text here 	If you have a data set with many columns, you can right-click on the header of the columns in the Available columns list box and select **Show Search Field** from the pop-up menu. This will display a search field where you can type a search string and limit the number of items in the list. It is possible to use the wildcard characters * and ? in the search.
Selected columns	Displays the currently selected data columns that you want to use in the calculation.
Add >>	Adds the highlighted data column to the list of selected columns.
<< Remove	Removes the highlighted data column from the list of selected columns

	and places them back in the list of available columns.
Work on: All records	All records in the value columns are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Replace empty values with	Defines how empty values in the data set should be replaced. **Constant** allows you to replace the empty values by any constant (type a number in the text box). **Row average** replaces the value by the average value of the entire row. **Row interpolation** sets the missing value to the interpolated value between the two neighboring values in the row. **Column average** returns the average of the corresponding column values.
Principal components	Enter the number of dimensions to which you wish to reduce the original data. This is directly linked to preserved variability. This is also the number of columns that will be exported to the data set.
Column name	The name of the columns containing the results from the principal component analysis.
Overwrite	Select this check box if you want to replace a previously added column (with the same name as the one typed in the **Column name** text box) when you add a new column. Clear the check box if you wish to keep the old column.
Create Scatter Plot	Select whether to create a 2D or 3D plot showing the result of the principal component analysis. Clear the check box if you do not want to create a plot.
Generate HTML report	Select this check box to generate an HTML report with the PCA results. Note that the report is not saved automatically.
Launch DecisionSite with PCA report	Select this check box to start a new DecisionSite session containing a plot with the PCA results. For more information on the results, see PCA HTML Report.

► To reach the Principal Component Analysis dialog:

Select **Data** > **Clustering** > **Principal Component Analysis...**.

6.3.2 PCA HTML Report

The PCA Result report contains all information about the calculation and results. It is displayed as an HTML page in your default web browser. You decide whether or not you want to create a PCA report by selecting or clearing the **Generate HTML report** check box in the Principal Component Analysis dialog.

Note: The PCA Result report is not saved automatically. To keep the report, you have to save it manually.

Option	Description
Number of principal components	The number of components that you selected to project your data to.

Variability preserved	This is directly linked to the number of dimensions to project to (see above). A value of 100% indicates that all variability of the original data is preserved. See also Preserving variability.
Added scored columns	Displays the names of the result columns added to the data set.
Value columns included	Displays the names of the value columns that were included in the calculation.
Eigenvalues	The Eigenvalues table presents the output of the PCA in a numerical format. Each row is associated with a principal component. The columns represent the following: **Principal Component:** Identifies the principal component. **Eigenvalue:** Informally, a measure of the amount of information contained in that component. **Eigenvalue (%):** Displays the eigenvalue as a percentage of the total of all eigenvalues. **Cumulative Eigenvalue (%):** The sum of the eigenvalues of this and previous components, as a percentage of the total of all eigenvalues. The cumulative eigenvalue of the N^{th} principal component is the same as the variability preserved when projecting to N dimensions.
Eigenvalue plot	The Eigenvalues plot, found beside the Eigenvalues table, plots the relative eigenvalue of each principal component, ordered by magnitude. It is useful for rapidly discerning the number of components required for preserving a reasonable amount of variability. A sharp drop followed by a sequence of lower values indicates that the first few components contain a large proportion of the information:
Eigenvectors	These figures indicate to what extent each column in the original data set contributes to each principal component.

6.4 Theory and Methods

6.4.1 PCA Methods Overview

PCA transforms a set of correlated variables into a smaller set of uncorrelated variables called principal components. It is therefore most useful for screening multivariate data in order to

- reduce the dimensionality of the data set
- identify new, meaningful underlying variables
- verify clustering

Reducing dimensionality

Strictly speaking, PCA does not *reduce* dimensionality, but reveals the *true* dimensionality of the original data. Even though *n* variables have been measured, data can sometimes be plotted in less than *n* dimensions without losing any significant information. PCA tells us if this is the case, and which the principal components are.

Identifying new variables

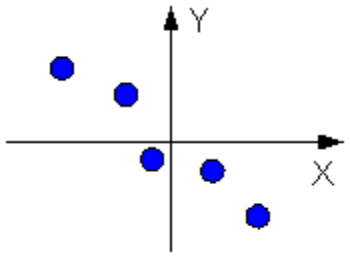
PCA will always identify new variables - principal components. These are linear combinations of the original variables, but are not necessarily *meaningful.* In some cases they can be interpreted as parameters that can be measured experimentally, but usually they cannot. Even so, principal components are often *useful,* for data screening, assumption checking, and cluster verification.

Verifying clustering

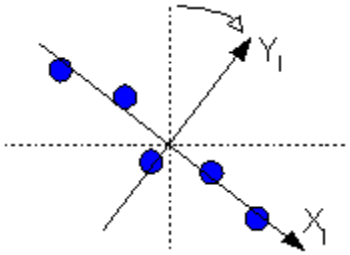
Clustering algorithms are not without drawbacks. Several parameters, such as initial centroid layout and distribution, affect the results of clustering. This means that we need an independent mechanism for evaluating our results. Because we cannot look at a multi-dimensional (> 3D) data set visually, PCA can be used to reduce the dimensionality of the data set. We can then inspect it visually, and see if observable clusters correspond to the structure suggested by the clustering algorithm.

6.4.2 Understanding PCA

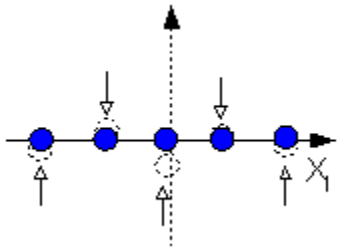
PCA works on the assumption that the data is distributed in such a way that it can be reduced to fewer dimensions. Consider the following:



The data set has two dimensions, and we cannot ignore one axis without losing a lot of important information. However, the data seems to be linear. We therefore rotate the coordinate system so as to maximize variation along one axis:



Seen in reference to the new coordinate system, we have a set of points that vary significantly only along X_I. We can therefore project the points onto this new axis, and ignore the comparatively small variation along Y_I:



The vectors that define the remaining dimensions (in this case only X_I) are what we mean by **principal components**. The position of a point along a given principal component is referred to as its **score.**

This example deals with the trivial case of two dimensions being reduced to one, in which case data reduction is actually redundant. PCA becomes truly useful only with data sets that are comprised of a large number of variables.

6.4.3 PCA Preserving Variability

When performing PCA, we can choose the number of dimensions to project the data to. We want fewer variables than the original data set, but we also want to preserve as much of the

information as possible. The question is how many dimensions to include in order to find a balance between these two requirements.

Total variability

If we add up the variance along each axis in the original data set, we get the **total variability**. Informally, this is an estimate of the amount of information in the data set.

$$V_T = |V_1 + V_2 + \ldots + V_n|$$

When the PCA algorithm rotates the coordinate system, variability remains unchanged. However, when we select a subset of dimensions on which to project the data, we typically reduce the total variability.

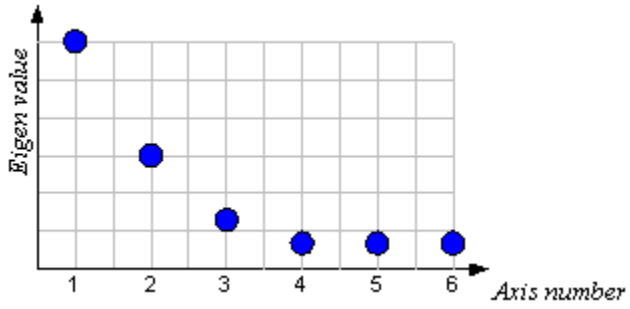
Preserved variability

When a coordinate system has been rotated, the new axes are ranked according to the variance of the data along each new axis (which corresponds to the eigenvalue).

If we choose to project to one dimension, in other words the one with the highest variance, this dimension will correspond to a certain proportion of the total variability, for instance 60%. The second best dimension might contribute another 20%. This adds up to 80% **preserved variability**. By including more dimensions, we can improve this value.

$$V_P = \frac{|V_1 + V_2 + \ldots + V_d|}{VT}$$

Eventually, due to the nature of the PCA algorithm, adding more dimensions will have little or no effect on the preserved variability.



How many dimensions should I use?

It is common to set a limit for the acceptable preserved variability (for example 95%), however, the limit depends largely on the type of data being analyzed. In most cases, it is desirable to reduce the dimensionality to two or three axes, so that these can be investigated visually.

6.4.4 PCA References

For detailed accounts of the PCA methods and algorithms used in the Principal Component Analysis tool, the following book is recommended:

Jolliffe, I., T., Principal Component Analysis, Springer Series in Statistics, New York, Springer-Verlag, 1986.

7 Profile Search

7.1 Profile Search Overview

The Profile Search tool calculates the similarity to a selected profile for all records in the data set and adds the result as a new column. The records are then ranked according to their similarity to the master profile.

You can use an existing record from your data set or create an average profile from several marked records. The built in profile editor makes it possible to edit the master profile.

7.2 Using Profile Search

7.2.1 Initiating a Profile Search

► To initiate a profile search:

1. Click to activate the profile that you want to use as master profile in one of the visualizations or mark a number of profiles on which to base the master profile.

   Comment: You can always edit the active or marked profile to obtain a master profile entirely by your choice.
2. Select **Data** > **Pattern Detection** > **Profile Search...**.

   Response: The Profile Search dialog is opened.
3. Select the value columns on which to base the clustering from the **Available columns** list and click **Add** >>.

   Comment: For multiple selection, press **Ctrl** and click on the desired columns in the Available columns list. Then click Add >> to move the columns to the Selected columns list. You can sort the columns in the list alphabetically by clicking on the Name bar.
4. Click a radio button to select whether to work on **All records** or **Selected records**.
5. Select a method to **Replace empty values with** from the drop-down list.
6. Select whether to use profile from: **Active record** or **Average from marked records**. This is only an option if you have both marked records and an active record to begin with.

   Response: The selected profile is displayed in the profile editor and the name of the profile is displayed to the left above the profile in the editor.

   Comment: You can edit the profile in the editor and type a new name for the edited profile, if desired.
7. Select which **Similarity measure** you want to use for the profile search.

   Comment: Click for information about the available similarity measures.
8. Type a **Column name** for the resulting column or use the default name.

   Comment: Select the **Overwrite** check box to overwrite an old column with the same name.
9. Click **OK**.

   Response: The search is performed using the master profile displayed in the editor, and the results are added to the data set as a new column. A new scatter plot is created displaying the rank vs. the similarity, and an annotation containing information about the calculation settings is added to the visualization.

7.2.2 Changing a Value in a Master Profile

Note: The starting profile does not restrict you in any way. You can easily change or delete existing values in the profile to create any master profile of your choice.

► To change a value in a master profile:

1. Select the profile that you want to edit by activating a record in a visualization.
2. Select **Data** > **Pattern Detection** > **Profile Search...**.

   Response: The Profile Search dialog is opened. The active profile is displayed in the profile editor.
3. Select the value columns on which to base the clustering from the **Available columns** list and click **Add >>**.

   Comment: For multiple selection, press **Ctrl** and click on the desired columns in the Available columns list. Then click Add >> to move the columns to the Selected columns list. You can sort the columns in the list alphabetically by clicking on the Name bar.
4. Click **Edit...**.

   Response: The Profile Search: Edit dialog is opened.
5. Click directly in the editor to activate the variable that you want to change and drag the value to obtain a suitable look on the profile.

   Response: The new value is immediately displayed in the editor.

   Comment: To set a value for a variable with a missing value, select the variable from the Active column list and type a number in the Value text box.
6. Type a **Profile name** in the text box or use the default name.
7. Click **OK**.

   Response: The Profile Search: Edit dialog is closed and the edited profile is shown in the Profile Search dialog. The **Edited** radio button has been selected by default, but you can return to the old profile by clicking Use profile from: **Active record**.

Tip: You can also use the fields below the editor to select an **Active column** in the profile and edit its **Value**.

7.2.3 Removing a Value from Profile Search

► To remove a value from a master profile:

1. Activate the profile that you want to edit in a visualization.
2. Select **Data** > **Pattern Detection** > **Profile Search...**.

   Response: The Profile Search dialog is opened. The active profile is displayed in the profile editor.
3. Click **Edit...**.

   Response: The Profile Search: Edit dialog is opened.
4. Click on the value that you want to remove and press **Delete**.

   Response: The value for the variable is removed in the display.

Tip: You can also use the fields below the editor to select an **Active column** in the profile and remove its **Value** by pressing **Delete**.

7.2.4 Interpreting the Results of Profile Search

When a profile search has been performed, the selected profiles or records in the data set have been ranked according to their similarity to the selected master profile. The value of the selected similarity measure is added to the data set as a new column.

A new scatter plot can be created (optionally) displaying the Similarity plotted against the Similarity rank. This means that the record that is most similar to the master profile will be displayed in the lower, left corner of the visualization.

7.2.5 Adjusting the Scale of the Profile Editor

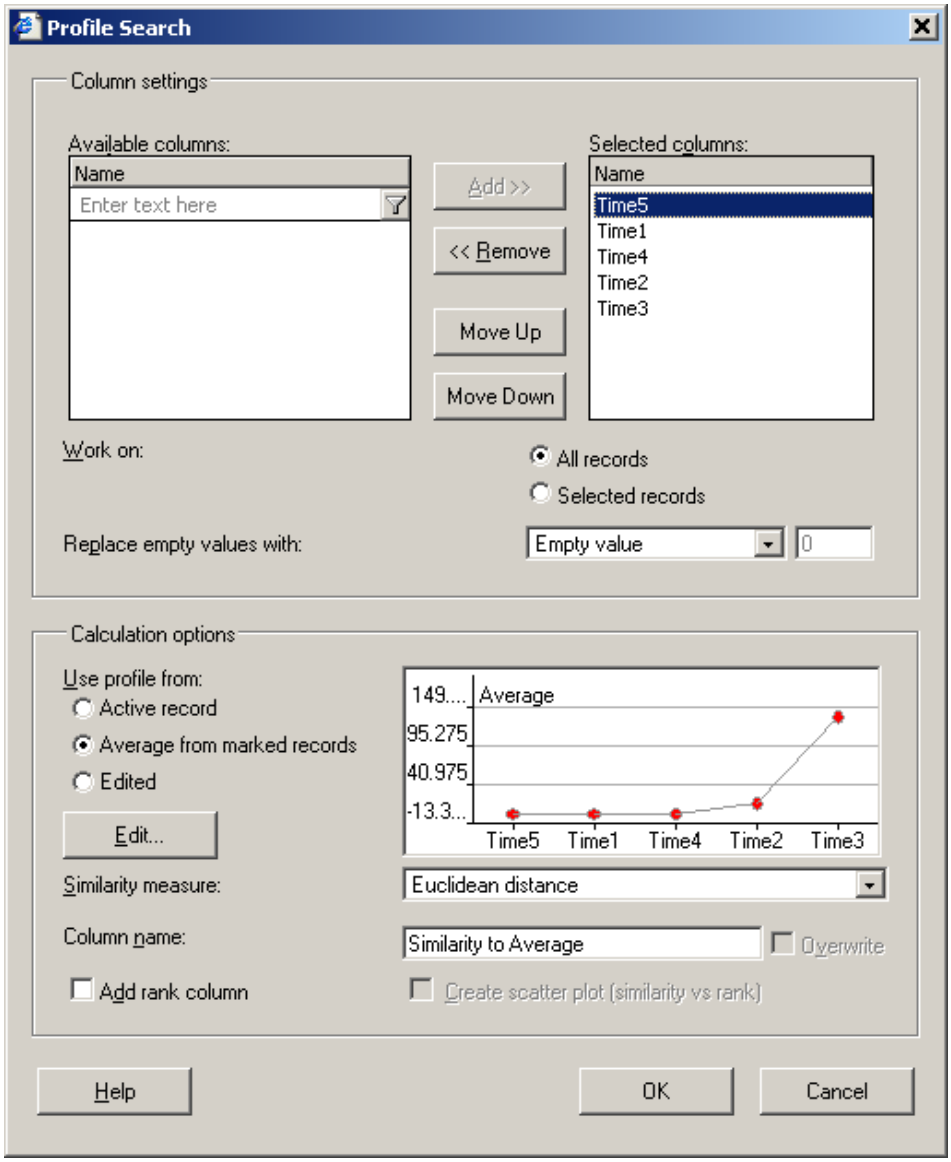
► To adjust the scale of the editor:

1. Click on the **Fit profile to screen** button,  , in the Profile Search: Edit toolbar.
2. Click on the **Reset original profile scale** button,  , to reset the scale.

Tip: You can also select **Fit to screen** or **Reset original scale** from the pop-up menu which is displayed by right-clicking in the edit window.

7.3 User Interface

7.3.1 Profile Search Dialog



Option	Description
Available columns	The data columns that you can include in the search. Click a column name in the list to select it, then click **Add >>** to move it to the Selected columns list. To select more than one column, press **Ctrl** and click the column names in the list. You can choose from any column that contains decimal numbers or integers. **Note:** You can right-click on the Name header to get a pop-up menu where you can select other attributes you would like to be visible.
Enter text here 	If you have a data set with many columns, you can right-click on the header of the columns in the Available columns list box and select **Show Search Field** from the pop-up menu. This will display a search field where you can type a search string and limit the number of items in the

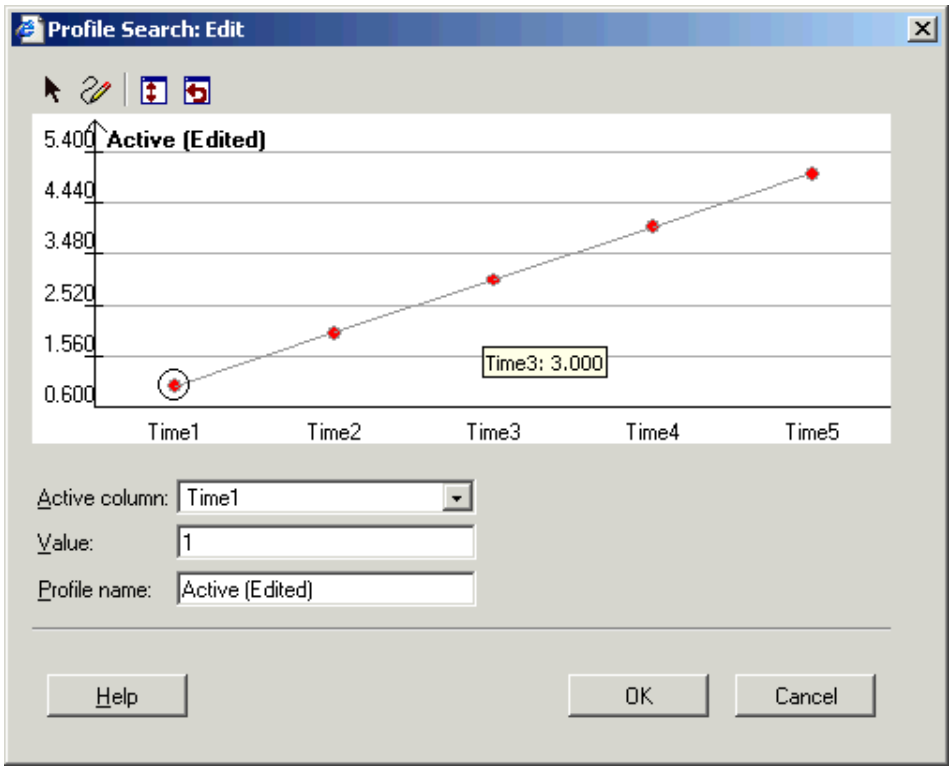
	list. It is possible to use the wildcard characters * and ? in the search.
Selected columns	Displays the currently selected data columns that you want to include in the search.
Add >>	Moves selected columns from the Available columns list to the Selected columns list.
<< Remove	Removes the selected columns and brings them back to the Available columns field.
Move Up	Moves the selected columns up in the Selected columns list and restructures the profile.
Move Down	Moves the selected columns down in the Selected columns list and restructures the profile.
Work on: All records	All records in the value columns are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Replace empty values with	Defines how empty values in the data set should be replaced. **Empty value** calculates the similarity between the two profiles based only on the remaining part of the profile. The result is the same as if the missing value in the profile had been identical with the value for that variable in the master profile. **Constant** allows you to replace the empty values by any constant (type a number in the text box). **Row average** replaces the value by the average value of the entire profile. **Row interpolation** sets the missing value to the interpolated value between the two neighboring values in the profile.
Use profile from: Active record	Click this radio button to use an active record as the master profile.
Use profile from: Average from marked records	Click this radio button to use an average calculated from marked profiles as the master profile.
Use profile from: Edited	Click this radio button to use an edited profile as the master profile.
Edit...	Opens the Profile Search: Edit dialog.
Similarity measure	The similarity measure that you want to use when performing the search.
Column name	The name of the new columns containing the results from the profile search.
Overwrite	Select this check box if you want to replace a previously added column (with the same name as the one typed in the **Column name** text box) when you add a new column. Clear the check box if you wish to keep the old column.
Add rank column	Select this check box to add a column containing the similarity rank to the data set. In this column, the profile that is most similar to the master profile is given the number 1, the second profile is given number 2, etc.

Create scatter plot (similarity vs rank)	A new scatter plot can be created (optionally) displaying the Similarity plotted against the Similarity rank. This means that the record that is most similar to the master profile will be displayed in the lower, left corner of the visualization.

► To reach the Profile Search dialog:

Select **Data** > **Pattern Detection** > **Profile Search...**.

7.3.2 Profile Search Edit Dialog



Edit profile. Allows you to manually edit a single value in the active column by clicking the value and dragging to the desired level.

Free hand drawing. Allows you to manually edit the values in the master profile by clicking and dragging the values using the mouse pointer as a free hand drawing tool.

Fit profile to screen. Automatically adjusts the scale to show the entire profile in the edit window.

Reset original profile scale. Resets the scale to the original value range. Variables outside the range will no longer be visible in the editor.

Option	Description
Active column	Displays all columns available in the profile search.
Value	Displays the value of the active column. To change the value, type a new number in the box.
Profile name	The name of the edited profile. The name is displayed in the top left corner of the editorial window and it is also used in the default column name for the result of the search.

► To reach the Profile Search: Edit dialog:

1. Select **Data** > **Pattern Detection** > **Profile Search...**.
2. Click **Edit...** below the displayed profile.

7.3.3 Profile Search Edit Pop-up Menu

The pop-up menu in the profile search editor includes the following options:

Option	Description
Delete	Deletes the value in the active column from the master profile.
Insert	Inserts a new value in the active column at the point of the right-click. This option is only available if there is a missing value in the master profile.
Fit to screen	Automatically adjusts the scale to show the entire profile in the edit window.
Reset original scale	Resets the scale to the original value range. Variables outside the range will no longer be visible in the editor.

► To reach the Profile Search Edit pop-up menu:

Right-click in the profile editor.

7.4 Theory and Methods

7.4.1 Profile Search Method Overview

In a profile search, all profiles (data points or table rows) are ranked according to their similarity to a master profile. The similarity between each of the profiles and the master profile is calculated using one of the available similarity measures. A new data column with the value of the selected similarity measure for each individual profile is added to the original data set as well as a similarity to master profile rank column.

7.4.2 Required Input for Profile Search

You have to specify the following before you can start a profile search:

- Which master profile do you want to use?
- Which similarity measure should be used?
- Should empty values be excluded from the search?

Master profile

You can use an existing (active) profile as master profile or construct a new master profile as the average of several marked profiles. It is possible to edit the master profile using the built in editor before you start the search.

Similarity measures

The Profile Search tool can use a variety of similarity measures. Similarity measures express the similarity between profiles as numbers, thus making it possible to rank the profiles according to their similarity. For information about the various measures, go to the section Similarity measures.

Excluding empty values

The Profile Search tool can exclude empty values from the calculations. See Excluding empty values for more information.

7.4.3 Excluding Empty Values in Profile Search

The Profile Search tool can exclude empty values from the calculations. When you calculate the similarity between the master profile and a profile that has a missing value, the variable with a missing value is excluded from the comparison. The calculated similarity between the two profiles is then based only on the remaining part of the profile. The result is the same as if the missing value in the profile had been identical with the value for that variable in the master profile.

Similarity measures based on the profile gradient

If you are using a similarity measure that compares the gradients of the profiles, a missing value means that two gradients are excluded from the comparison. If we take an extreme example of a profile where every other value is missing, then there would be no gradients left in the profile to base the comparison on. Since excluding a missing value has the same effect as setting the value of the profile to the same value as in the master profile, the profile in this extreme example would then have the highest possible similarity with the master profile.

Missing values in the master profile

Any missing values in the master profile are always excluded from the search. If, for example, the second variable in the master profile has no value then this variable is always excluded in the comparison with the other profiles, even if you have not specified that you want to exclude empty values.

8 Coincidence Testing

8.1 Coincidence Testing Overview

The Coincidence Testing tool can be used to investigate if values within two columns seem to coincide or not. The results are presented using probability p-values.

8.2 Using Coincidence Testing

8.2.1 Testing if Groups of Identifiers Have Overlap

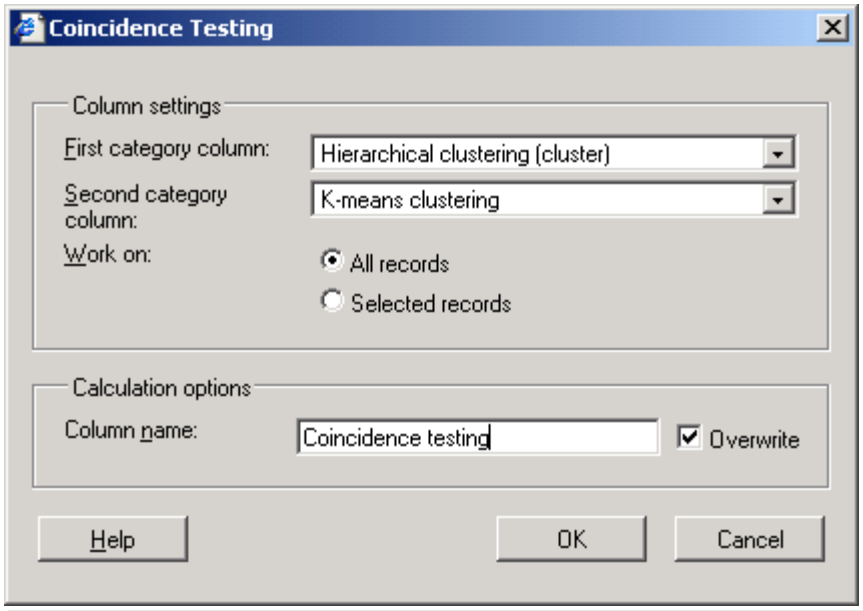
The coincidence testing can be used to assess whether or not different groups of identifiers have a significant overlap. This is useful for comparing different clustering methods.

► To test if similarity is a coincidence:

1. Select **Data > Pattern Detection > Coincidence Testing...**.
   Response: The Coincidence Testing dialog is displayed.
   Note: If you cannot find this tool in the Data menu, you probably need to acquire another license.
2. Select the **First category column**.
   Comment: If you are comparing clustering methods, then choose the results of the first clustering tool here.
3. Select the **Second category column**.
   Comment: If you are comparing clustering methods, then choose the results of the second clustering tool here.
4. Select whether to work on **All records** or **Selected records**.
5. Type a **Column name** for the resulting column or use the default name.
   Comment: Select the **Overwrite** check box to overwrite an old column with the same name.
6. Click **OK**.
   Response: A result column with p-values is added to the data set. An annotation may also be added.

8.3 User Interface

8.3.1 Coincidence Testing Dialog



Option	Description
First category column	The first data column that you want to test.
Second category column	The second data column that you want to test.
Work on: All records	All records in the value columns are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Column name	The name of the new column containing the results from the calculation.
Overwrite	Select this check box if you want to replace a previously added column (with the same name as the one in the Column name text box).

► To reach the Coincidence Testing dialog:

Select **Data** > **Pattern Detection** > **Coincidence Testing...**.

8.4 Theory and Methods

8.4.1 Coincidence Testing Methods Overview

The Coincidence Testing tool calculates the probability of getting an outcome at least as extreme as the particular outcome under the null hypothesis.

Example:

You have performed clustering using two different methods. You want to know how well the two methods agree on the classification of each record. The table below shows the identifiers and cluster classifications for some records. Performing a coincidence test on the two clustering columns produces the Coincidence column:

Identifier	Hierarchical clustering	K-means clustering	Coincidence	Interpretation
A	1	3	0.2	Good match
B	1	3	0.2	Good match
C	1	2	0.95	Worst match
D	2	2	0.2	Good match
E	2	2	0.2	Good match
F	3	1	0.166666...	Best match

The records for which the highest number of cluster classifications is similar will get the lowest p-value in the coincidence test. This means that in this example the "group" with only record F got the best match, but since there was only one record in the "group" this is rather irrelevant. The group with records A and B and the group with records D and E showed quite good matching. C received a low score since the clusterings disagree about the classification.

8.4.2 Description of the Coincidence Testing Algorithm

For any data set loaded into Spotfire DecisionSite, the Coincidence Testing algorithm may be applied to any two columns A and B. The algorithm will calculate a “probability value” (p-value) for each unique pair of values in A and B. The p-values can be used to identify value pairs that are over represented in the data set, i.e., occur more frequently than could be expected by pure chance, assuming no relationship between A and B. This information can be used to discover interesting facts and create hypotheses about the actual relationship between A and B.

The algorithm:

In order to describe the algorithm, the following definitions will be used:

R = number of rows in the data set D

G = number of groups, i.e., unique value pairs, in columns A and B

If the groups are numbered from 1 to G, the following definitions will be used for the group with index i:

K_i = number of rows belonging to group i

M_i = number of rows in D where the A value = the A value in group i

N_i = number of rows in D where the B value = the B value in group i

The p-value for the group with index i can then be calculated as follows:

$P_i = P(X \geq K_i \mid R, N_i, M_i) = \sum P(X = x \mid R, N_i, M_i)$; $x = K_i, ..., \min(N_i, M_i)$

where X is a random variable with a hypergeometric distribution. In probability theory, this distribution describes the number of successes in a sequence of a certain number of draws from a finite population without replacement.

This means that the probability formula can be written as follows:

$$P(X = x \mid R, N_i, M_i) = \binom{N_i}{x} \cdot \binom{R - N_i}{M_i - x} / \binom{R}{M_i}$$

where

$$\binom{n}{k} = \frac{n!}{k!\,(n-k)!} \text{ if } n \geqslant k \geqslant 0$$

$$\binom{n}{k} = 0 \text{ if } k < 0 \text{ or } k > n$$

is the binomial coefficient of n and k.

Example:

Let us consider a data set D which contains information about the country of origin and the number of cylinders for 18 different cars:

Model	Origin	Cylinders
VW 1131	EU	4
Saab 99	EU	4
Chevrolet Impala	USA	8
Pontiac Catalina	USA	8
Plymouth Fury	USA	8
Mercury Monarch	USA	6
Buick Century	USA	6
Audi 100	EU	4
Renault 12	EU	4
Mercedes 280	EU	6
Chevrolet Caprice	USA	8
Oldsmobile Cutlass	USA	8
Peugeot 604	EU	6
Pontiac Lemans	USA	6
Peugeot 504	EU	4
Dodge Colt	USA	4
VW Rabbit	EU	4
Ford Galaxie	USA	8

If we apply the Coincidence Testing algorithm described above to Origin and Cylinders, we find that:

R = 18

G = 5

The 5 groups (unique value pairs for Origin and Cylinders) are:

Group 1: Origin = EU; Cylinders = 4

Group 2: Origin = EU; Cylinders = 6

Group 3: Origin = USA; Cylinders = 4

Group 4: Origin = USA; Cylinders = 6

Group 5: Origin = USA; Cylinders = 8

Furthermore, for group 1 (Origin = EU; Cylinders = 4), we find that:

K1 = 6 (VW 1131, Sabb 99, Audi 100, Renault 12, Peugeot 504, VW Rabbit)

M1 = 8 (number of rows where Origin = EU, regardless of Cylinders)

N1 = 7 (number of rows where Cylinders = 4, regardless of Origin)

The p-value for this group of cars can be calculated as follows:

$P1 = P(X \geq 6 \mid 18, 7, 8) = 0.009049\ldots$

To find the most over represented groups of cars in the data set, we calculate the p-values for all groups and sort the groups by ascending p-value:

P1 = 0.009049…

P5 = 0.011312…

P4 = 0.617647…

P2 = 0.774509…

P3 = 0.999748…

It should be noted that the largest groups are not necessarily the most over represented ones. However, the low p-values for groups 1 and 5 show that, from a statistical point of view, European cars with 4 cylinders and American cars with 8 cylinders are strongly over represented in the data set. This information could perhaps be used to draw further conclusions about the relationship between Origin and Cylinders.

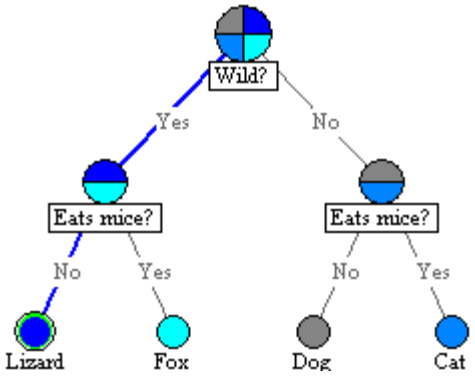
8.4.3 Coincidence Testing References

Tavazoie, S., Hughes, J.D., Campbell, M.J., Cho, R.J., Church, G.M., Systematic determination of genetic network architecture, Nature Genetics, 22 (3), 1999, pp 281-285

9 Decision Tree

9.1 Decision Tree Overview

A decision tree is a way of explaining the behavior of one column (target variable) as a function of other columns (source variables) in a data set.



The output takes the form of a tree structure, where each node represents the subset remaining after a sequence of conditions has been applied. Pie slices represent the distribution of the target variable at that node.

Decision Trees are useful for making predictions and classifying data. In the example described here, we could gather a limited amount of data about animals, produce a decision tree, and then use the rules to categorize other species.

If the source data consisted of historical information on stock market development, we could use it to produce rules for predicting whether to buy or sell shares under various conditions.

9.2 Using Decision Tree

9.2.1 Launching a Decision Tree Analysis

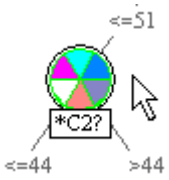
► To launch a Decision Tree analysis:

1. Select **Tools > Decision Tree...**.
   Response: The Decision Tree dialog is opened.
2. Adjust the settings in the Decision Tree dialog, then click **OK** to launch the calculation.
   Response: The algorithm is executed and a decision tree is shown.
3. Analyze the results of the calculation.

9.2.2 Navigating the Decision Tree

Activating a node

By activating a node, the records in that node can be analyzed further in the Detail Display:

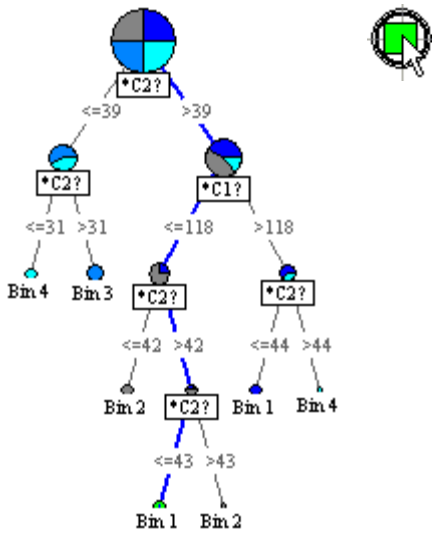


To activate a node in a decision tree, click on a node at the desired level.

Locating individual records

It is possible to investigate where in a tree a particular record occurs. Since each record occurs in several nodes at different levels, the location is expressed as a path leading from the root node to a leaf node.

To locate a record, activate it in a visualization (this is done by clicking on a marker). A blue trail appears in the Decision Tree.



The blue line indicates the nodes which contain the active record.

Identifying node contents in a visualization

To mark records in a visualization based on the contents of a tree node, make sure you have activated a node. Then go to the menu and select **Tree > Mark in Visualization**.

To set the query devices to reflect the contents of a node, first activate a node. Then go to the menu and select **Tree > Update query devices**.

9.2.3 Exporting a Decision Tree Image

Decision Tree allows you to copy the tree as an image bitmap to the clipboard. Exporting a tree this way allows you to add it to a document in another application, for example a web page or a word processing document.

► To copy the Decision Tree image to the clipboard:

1. Create a decision tree.
2. Adjust the appearance of the tree.
3. Select **Tree > Copy image to clipboard** from the Decision Tree menu.

9.2.4 Controlling the Appearance of a Decision Tree

Resizing the tree

- To zoom in or out, click the plus or minus symbols by the  icon. The right and left-hand symbols control width.
- To control font size, click the plus or minus symbols by the **A**-icon.

- To control how size relates to number of records, select **Options...** from the Decision Tree menu. Under **Node size**, select the desired setting.

Collapsing and expanding nodes

- To expand or collapse an individual node, double-click on it.
- To expand or collapse the entire tree, select **Tree > Expand All Nodes** or **Collapse All Nodes**.

9.2.5 Exporting Decision Tree Rules as XML

The rules forming a decision tree can be expressed as XML. Rules exported as XML can be loaded back into Decision Tree to recreate the tree, or to apply the rules to a new data set.

► To export XML:

1. Create a Decision Tree. (See Launching a Decision Tree analysis to see how.)
2. Select **Save** from the Decision Tree menu.
3. In the Save File dialog, select a folder and a file name for the new file.
4. Click **OK**.

9.2.6 Exporting Decision Tree Rules as IF-THEN-ELSE Statements

The rules forming a decision tree can be expressed as a series of nested IF-THEN-ELSE statements.

Rules exported as IF-THEN-ELSE statements are more readable than XML, but cannot be loaded back into Decision Tree to recreate the tree.

► To export IF-THEN-ELSE statements:

1. Create a Decision Tree. (See Launching a Decision Tree analysis to see how.)
2. Select **Options...** from the Decision Tree menu.
3. Under **Generated rules**, select whether to export to a text file, or to open a text editor.
4. Click **OK**.
5. Select **Export Rules > Leading to All Nodes** or **Export Rules > Leading to Marked Nodes**. The latter generates a more compact file.
6. Study the rules in the text editor, or select a file name and a folder for the generated text file.

9.2.7 Using Generated Rules to Classify Data

Rules generated with a Decision Tree analysis can be applied to records where the target variable is unknown. This means using results from one subset to predict values in another subset.

► To predict an unknown target variable:

1. Use the DecisionSite query devices to select a representative subset of data.

   Comment: These are the records Decision Tree will use to generate rules. For example, you could deselect all records with empty values, and use the method described below to create a column of suggested values for these.
2. Select **Tools > Decision Tree...**.

   Response: The Decision Tree dialog is displayed.
3. Select value columns.
4. Select **Work on: Selected records**.

5. Select target column.
6. Click **OK**.
   Response: The decision tree algorithm is executed and a decision tree is shown.
7. Select **Tree > Add New Column** from the Decision Tree menu.
   Response: A new column is added to the data set. This column contains the values predicted by the rules of the Decision Tree.
8. Reset all query devices, so that you can study the whole data set.
9. Analyze the results.
   Comment: For the records that were used as basis for the rules, the new column can be compared to the column that was used as target. If the analysis was successful, the values in these two columns should match (although there might be discrepancies). For records that were not included in the calculation, the new column constitutes suggested values for the target column, based on the generated rules.

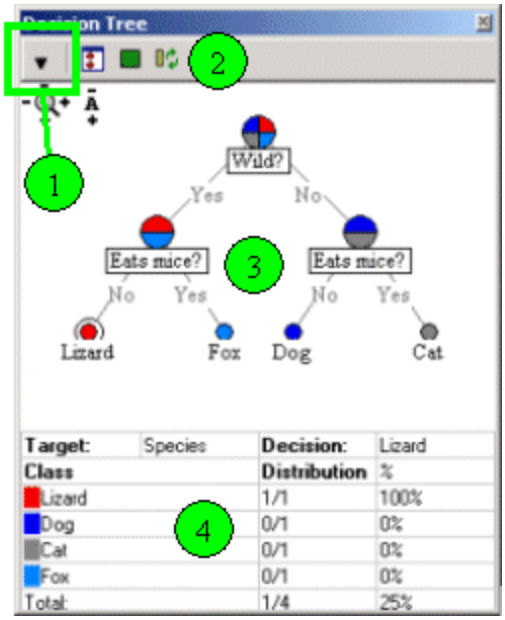
9.2.8 Using Continuous Target Variables

The Decision Tree tool permits only string variables as targets. However, some situations may require numerical variables as targets. A questionnaire, for example, often contains questions of the type "Rate NNN on a scale 1 to 5". Such a variable is categorical, and hence suitable as target in a Decision Tree analysis, but since it is interpreted as numerical when loaded, you will not be able to select it as target in the Decision Tree dialog.

To solve this problem, you can use the conversion function String in the New Column from Expression tool (**Data > New Column > From Expression**) and create a string column that can be used as a target column in the Decision Tree.

9.3 User Interface

9.3.1 Decision Tree User Interface



1. Decision Tree menu


The Decision Tree menu contains all commands required to work with Decision Tree.

2. Decision Tree toolbar

Includes shortcuts for some of the most commonly used commands in the Decision Tree menu.

3. Tree view

The tree view is the graphic representation of the current Decision Tree analysis. The top node represents the whole data set, while the leaf nodes represent groups of records that share the same value in the target column.

4. Detail Display

The detail display presents the distribution of the target variable in the active node.

9.3.2 Decision Tree Menu

The Decision Tree menu is displayed by clicking  and contains all commands necessary for working with Decision Tree.

Option	Description
Tree >	Commands relating to the current tree.
> Fit to Screen	Adjusts the size of the tree to the available surface.
> Mark in Visualization	Marks records in the visualizations according to the contents of the active node in Decision Tree.
> Update Query Devices	Sets the query devices to match the content in the active node.
> Copy Image to Clipboard	Copies the tree image to the clipboard.
> Add New Column	Creates a new column in the data set, containing the classification of the target variable as dictated by the current set of rules.
> Expand All Nodes	Expands all nodes in the tree.
> Collapse All Nodes	Collapses all nodes in the tree.
Options...	Opens the Options dialog.
View >	Commands for toggling the visibility of certain optional information.
> Detail Display	Shows or hides the Detail display at the bottom of the window.
> Decision Information	Shows or hides the decision that is displayed by each node in the tree.
Export Rules >	Exports the current set of rules as a series of nested If-Then-Else statements.
> Leading to Active Node	Exports only the rules leading to the active node.
> Leading to All Nodes	Exports the entire set of rules of the tree.
Open	Opens an XML file with decision tree rules.
Save	Saves the current decision tree rules as an XML file.

Help	Launches the online help system.

9.3.3 Decision Tree Toolbar

This is the Decision Tree toolbar:

Click on the buttons on the toolbar to activate the corresponding functions.

	Displays the Decision Tree menu.
	Adjusts the size of the tree to the available surface.
	Marks records in DecisionSite according to the contents of the active node in Decision Tree.
	Sets the query devices in DecisionSite to match the contents in the active node.

9.3.4 Decision Tree Pop-up Menu

Right-click in the tree to bring up the pop-up menu. The pop-up menu contains commands relevant to the tree, as well as some commonly used functions.

Option	Description
Fit to screen	Adjusts the size of the tree to the available surface.
Mark in visualization	Marks records in the visualizations according to the contents of the active node in Decision Tree.
Update query devices	Sets the query devices to match the content in the active node.
View >	Commands for toggling the visibility of certain optional information.
> **Detail Display**	Shows or hides the Detail display at the bottom of the window.
> **Decision Information**	Shows or hides the decision that is displayed by each node in the tree.
Options…	Opens the Options dialog.

9.3.5 Decision Tree Detail Display

► To show or hide the Detail Display:

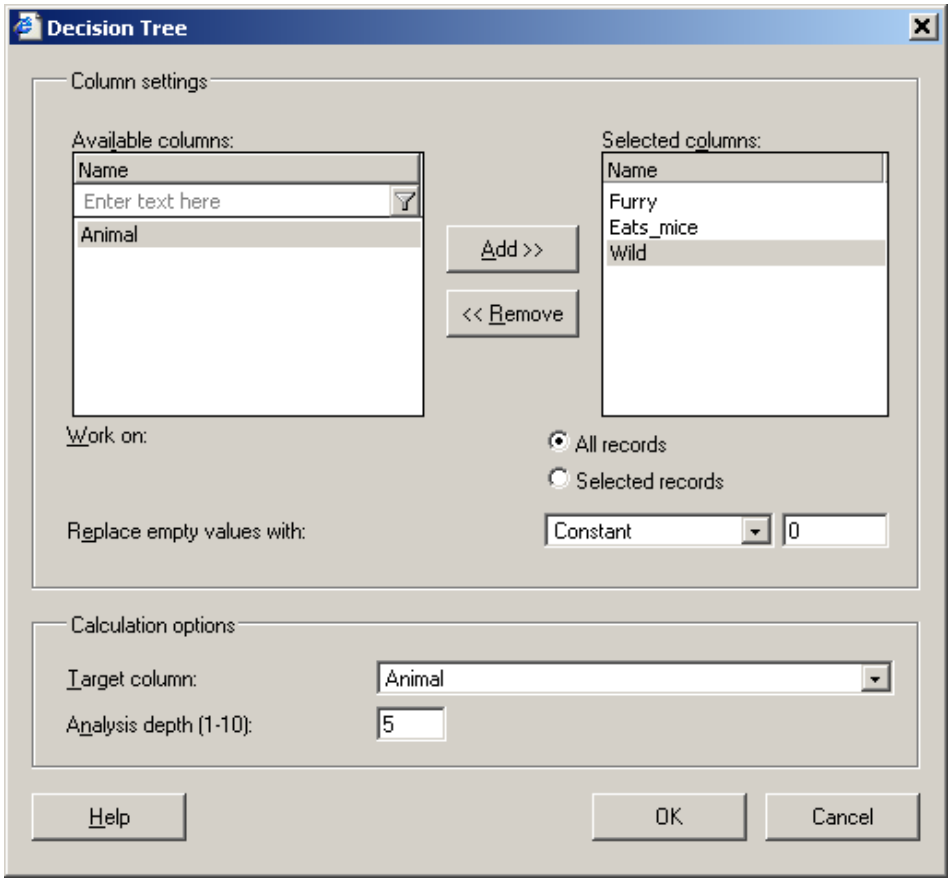
Select **View** > **Detail Display** from the menu.

The Detail Display supplies information on the active node:

Target	The selected target variable.
Decision	The source variable used in the subsequent split.
Class	The possible values of the target variable. The color refers to the color used for that class in the nodes.
Distribution	The frequency of each class in the current node as a fraction of the total

	number of records in the node.
%	As above but as a percentage.
Total	The number of records in the node as a fraction of the total number of records.

9.3.6 Decision Tree Dialog



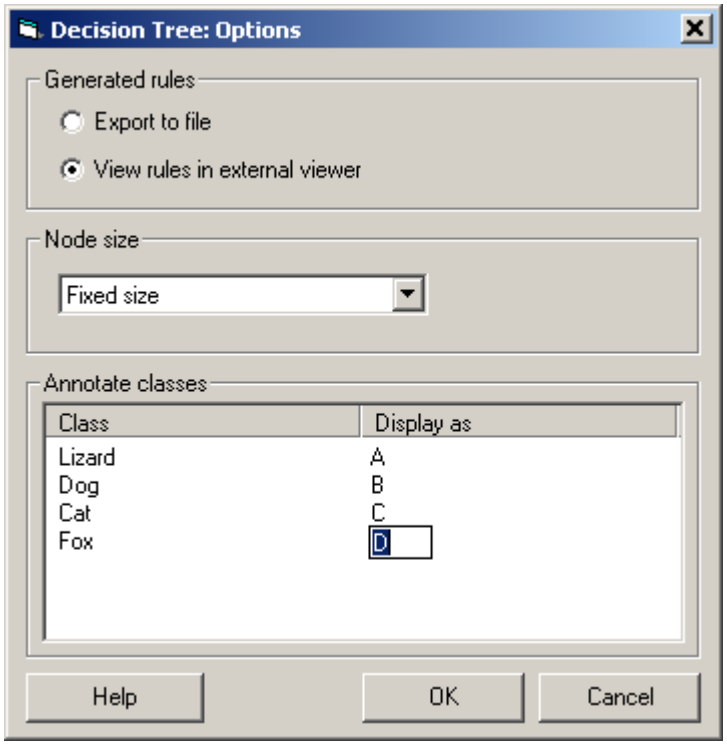
Option	Description
Available columns	Lists all columns on which you can base the decision tree. All the variables that can be important to the decisions should be selected. Click a column name in the list to select it, then click Add >>. To select more than one column, press **Ctrl** and click the column names in the list. You can sort the columns in the list alphabetically by clicking on the Name bar. Click again to reverse sorting and once more to reset the sort order. **Note:** You can right-click on the Name header to get a pop-up menu where you can select other attributes you would like to be visible.
Enter text here 	If you have a data set with many columns, you can right-click on the header of the columns in the Available columns list box and select Show Search Field from the pop-up menu. This will display a search field where you can type a search string and limit the number of items in the list. It is possible to use the wildcard characters * and ? in the search.
Selected columns	Lists the selected source columns to be used in the decision tree.

Add >>	Adds the columns selected in the Available columns list to the Selected columns list.
<< Remove	Removes the selected columns from the Selected columns list.
Work on: All records	All records in the value columns are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Replace empty values with	Defines how empty values in the data set should be treated in the algorithm. From the drop-down list, select a method. **Constant** allows you to replace the empty values by any constant (type a number in the text box). **Row average** replaces the value by the average value of the entire row. **Row interpolation** sets the missing value to the interpolated value between the two neighboring values in the row.
Target column	Here you select the target column of the algorithm. This column should not be included as a selected source column. Only string columns are available.
Analysis depth	Analysis depth means the accuracy with which the algorithm locates the best split for each node. Great depth means high accuracy, but slower execution. Enter a value between 1 and 10, where a high number means high accuracy.

► To reach the Decision Tree dialog:

Select **Tools** > **Decision Tree...**.

9.3.7 Decision Tree: Options Dialog



Option	Description
Generated rules: Export to file	Makes the Export Rules command save rules as a text file.
Generated rules: View rules in external viewer	Makes the Export Rules command launch a text editor for viewing rules.
Node size	Controls how the size of nodes is calculated.
Annotate classes	Edit the class names under **Display as** if you want to change the labels shown on the leaf nodes of the decision tree.

► To reach the Decision Tree: Options dialog:

1. Select **Tools > Decision Tree...**.
2. Click **Menu > Options...** in the Decision Tree window.

9.4 Theory and Methods

9.4.1 Understanding Decision Trees

Decision Trees work on the same principles as the children's game known as "Twenty questions". One participant thinks of something, and the other participants must figure out what by asking a series of questions that can only be answered with *yes* or *no*. (The rules of the game permit "Animal, vegetable or mineral?" as a first question. In this example, we will assume the answer to be "Animal".) The idea is to solve the puzzle with no more than twenty questions, for example:

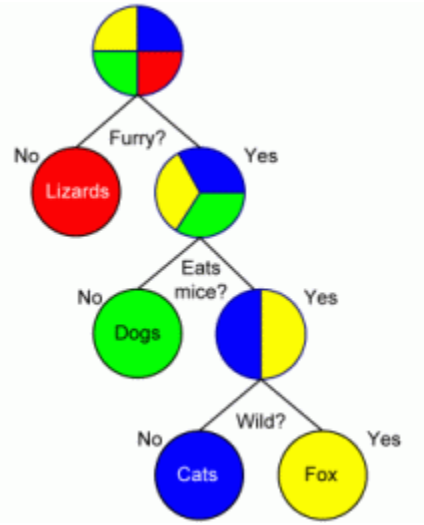
- "Do you have fur?" - "Yes"
- "Do you eat mice?" - "Yes"
- "Are you a wild animal?" - "No"

At this point, the set of possible answers is very limited - almost all creatures that comply to these conditions are cats.

In Decision Tree terminology, we have investigated the three Boolean **source variables** "Furry", "Eats mice" and "Wild animal", to gain information about the **target variable** "Animal". The data set looks like this:

Source	Source	Source	Target
Furry	**Eats mice**	**Wild**	**Animal**
No	No	Yes	Lizard
Yes	No	No	Dog
Yes	Yes	No	Cat
Yes	Yes	Yes	Fox

The Decision Tree corresponding to the game described above looks like this:



However, this is not necessarily the most compact tree that we can build from our data. To produce compact Decision Trees, Spotfire DecisionSite uses an algorithm designed to select rules (questions) that maximize information gain at each level. This means that we know more about the target variable the further down the tree we move, and that the tree becomes as small as possible. Also, the algorithm can handle not only Boolean source variables as in the example, but all common data types.

9.4.2 The Decision Tree Algorithm

When generating decision trees, Spotfire DecisionSite uses a modified version of an algorithm called **C4.5**. It is based on the **information gain ratio criterion**, which essentially ensures that the amount of information gained about a target variable is maximized at each split.

► The algorithm works as follows:

1. The whole data set is designated to the root node.
2. If the node is homogeneous in terms of the target variable (that is, if all records in the subset have the same value for the target variable), the node becomes a leaf node.

   Otherwise, for each source variable:

- If it is continuous, the algorithm tests each value in the set. It selects the value which, when used as threshold value in a split, produces the highest information gain ratio. This type of split always produces exactly two child nodes.
- If it is discrete, each value or bin (a group of distinct values that somehow belong together) is given a child node, and the information gain ratio is computed based on this split.

  Step 2 produces a list of potential information gain ratios, one for each source variable. The split which produces the highest information gain ratio is selected, and the actual split is performed, producing two or more subsets (child nodes).

3. Step 2 is repeated recursively for each child node.

9.4.3 Details of Information Gain Ratio

The following abbreviations are used:

S	= a set of cases
C_i	= case i in a set of cases
X	= a test

Frequency

The frequency of a class C_i in a set of cases S is denoted

$$freq(C_i, S)$$

and refers to the number of cases in S that belong to class C_i.

Norm

The norm of a set of cases S is denoted

$$norm(S) = |S|$$

and refers to the total number of cases in S.

Information

The information stored in a set of cases S is

$$info(S) = -\sum_{i=1}^{k} \frac{freq(C_i, S)}{|S|} \times log_2\left(\frac{freq(C_i, S)}{|S|}\right)$$

which is measured in bits.

Information after test

The information after a set of cases T has been partitioned by a test X

$$info_X(T) = \sum_{i=1}^{n} \frac{|T_i|}{|T|} \times info(T_i)$$

where n is the number of possible outcomes of the test.

Gain

The information gain

$$gain(X) = info(T) - info_X(T)$$

is the amount of information that is gained when the set T is partitioned by test X.

Split information

The split information

$$split\ info(X) = -\sum_{i=1}^{n} \frac{|T_i|}{|T|} \times log_2\left(\frac{|T_i|}{|T|}\right)$$

is a measure of the potential information generated by partitioning T into n subsets.

Gain ratio

The gain ratio,

$$gain\ ratio(X) = \frac{gain(X)}{split\ info(X)}$$

is the proportion of information generated by the split by the test X that is useful, i.e., helpful for classification.

Reference

For detailed accounts of the data processing methods and algorithms used in Spotfire DecisionSite, the following book is recommended:

Quinlan, J.,R., *C4.5: Programs for Machine Learning*, The Morgan Kaufmann series in machine learning. San Mateo, Calif., Morgan Kaufmann Publishers, 1993.

10 Box Plot

10.1 Box Plot Overview

Box plots are graphical tools to visualize key statistical measures, such as median, mean and quartiles. The measures are always based on the records currently selected in the DecisionSite visualizations (using the query devices, for example). Box Plots are persistent. If you save your Analysis with a Box Plot open, the Box Plot and its settings is stored as a part of the Analysis. When the Analysis is reopened, the Box Plot is opened as well.

A single box plot can be used to represent all the data. It is also possible to visualize separate statistics for subsets by selecting a column for the X-axis.

10.2 Using Box Plot

10.2.1 Initiating Box Plots

► To perform a Box Plot analysis:

1. Select **Tools** > **Statistics** > **Box Plot**.
   Response: A new window with a box plot is displayed.
2. Use the Y-axis selector to select the column you want to analyze.
3. If desired, select a column for representation on the X-axis. This should be a column with few unique values.
   Response: A separate box plot for each unique value in the category column (X-axis) is displayed.
4. Analyze the results.

10.2.2 Displaying the Statistics Table

► To show or hide the statistics table:

1. Click on 

and select **Properties**.
   Response: The Box Plot: Properties dialog is displayed.
2. In the **Available measures** list box, click to select the measures that you want to display in the table.
   Comment: For multiple selection press **Ctrl** and click on the desired measures, or use the mouse to draw a rectangle around them.
3. Click **Add** >>.
   Response: The selected measures are added to the **Measures in table** list box.
4. If desired, click on a measure and then click **Move Up** or **Move Down** to rearrange the order of the measures in the table.
5. Select the **Format** that should be used to present the results.
   Comment: Choose from General, Fixed or Scientific.
6. Select the number of significant **Digits/Decimals** to be displayed.
7. When you are finished with all settings in the Box Plot: Properties dialog, click **OK**.
   Response: The dialog is closed and the visualization has been updated according to your new settings. The settings are saved from session to session.

10.2.3 Showing Comparison Circles

► To show or hide the comparison circles in the box plot:

1. Click on Menu and select **Properties**.
   Response: The Box Plot: Properties dialog is displayed.
2. Select the **Show comparison circles** check box in the lower part of the dialog.
   Response: The comparison circles are immediately shown to the right of the box plots.
3. If desired, change the **Alpha level**.
   Comment: This is the level at which groups can be considered significantly different.
4. When you are finished with all settings in the Box Plot: Properties dialog, click **OK**.
   Response: The dialog is closed and the visualization has been updated according to your new settings.

Highlight a comparison circle by highlighting its box plot or vice versa. The highlighted comparison circle is colored red. If a comparison circle has already been activated, highlighting it will instead color the circle blue.

Activate a comparison circle by clicking on it, or by clicking on the box plot to go with the specific circle. The activated comparison circle is colored in a bold green. A green, filled dot labels the active box plot. Comparison circles corresponding to groups that are not significantly different from the active one will also be colored green and unfilled dots will be present under their corresponding box plots.

Tip: You can resize the area containing the comparison circles by placing the mouse pointer over the vertical line separating the circles from the box plots and dragging the handle to the desired position.

10.2.4 Showing Mean and Median

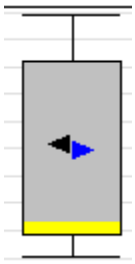
► To show or hide the symbols for mean and median in the box plot:

1. Click on Menu and select **Properties**.
   Response: The Box Plot: Properties dialog is displayed.
2. Select the **Show mean** and/or **Show median** check box in the lower part of the dialog.
   Response: The changes are immediately shown in the box plot visualization. The mean is indicated with a black arrow and the median is indicated with a blue arrow.
3. When you are finished with all settings in the Box Plot: Properties dialog, click **OK**.
   Response: The dialog is closed and the visualization has been updated according to your new settings.

10.2.5 Showing Confidence Interval in Box Plots

► To show or hide the 95% confidence interval in the box plot:

1. Click on Menu and select **Properties**.
   Response: The Box Plot: Properties dialog is displayed.
2. Select the **Show 95% confidence interval** check box in the lower part of the dialog.
   Response: The interval is immediately shown in the box plot visualization.
3. When you are finished with all settings in the Box Plot: Properties dialog, click **OK**.
   Response: The dialog is closed and the visualization has been updated according to your new settings.

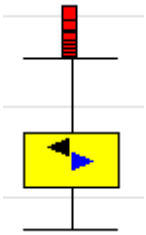


10.2.6 Jittering in Box Plots

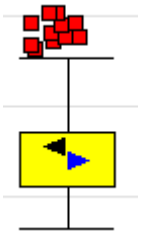
Jittering is used to displace markers horizontally by a random distance, so that overlapping markers are revealed.

Example:

Before jittering:
Difficult to see the number of outside values.



After jittering:
Eleven outside values are visible.



► To jitter outside values:

1. Click on Menu and select **Properties**.
   Response: The Box Plot: Properties dialog is displayed.
2. Move the **Outside values jitter level** slider to a suitable level of jittering.
   Response: The outside values in the visualization are immediately jittered, thus making it possible for you to test how much jittering you want before closing the dialog.
3. When you are finished with all settings in the Box Plot:Properties dialog, click **OK**.
   Response: The dialog is closed and the visualization has been updated according to your new settings.

10.2.7 Zooming Box Plots

► To zoom box plots horizontally:

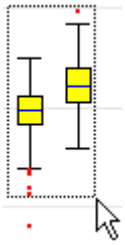
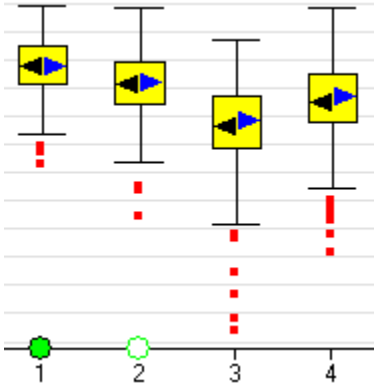
Drag the yellow bar beneath the box plots to select which box plots to display. The statistics table and comparison circles will be equally updated to reflect your selection. There will be no zooming in any other visualizations outside the box plot window.

► To zoom box plots vertically:

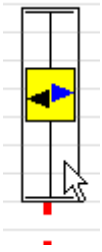
Drag the yellow bar at the left of the box plots to zoom vertically.

10.2.8 Marking, Activating and Highlighting in Box Plots

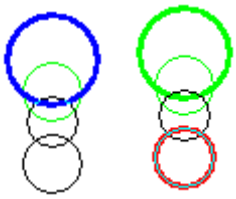
The Box Plot tool allows you to mark, activate and highlight records in much the same way as a bar chart visualization. See also How to mark, activate and highlight.

Do this in a Box Plot...	...which corresponds to the following in the comparison circles...	...and this happens in all visualizations
Mark a range of values. This may include outside values, boxes (or parts of boxes), or both.	Nothing happens with the comparison circles.	The corresponding records are marked.
		
Activate an outside value.	Nothing happens with the comparison circles.	The corresponding record is activated.
		
Activate a box plot. (The active box plot is labeled with a green dot if the comparison circles are visible.)	The corresponding comparison circle is colored green. Comparison circles of groups that are not significantly different are also green, but with a thin line.	Nothing happens in the visualizations.
		
Highlight an outside value.	Nothing happens with the comparison circles.	The corresponding record is highlighted.

Highlight a box plot.	The corresponding comparison circle is colored red. If a comparison circle has been activated this will be colored blue upon highlighting.	Nothing happens in the visualizations.



-

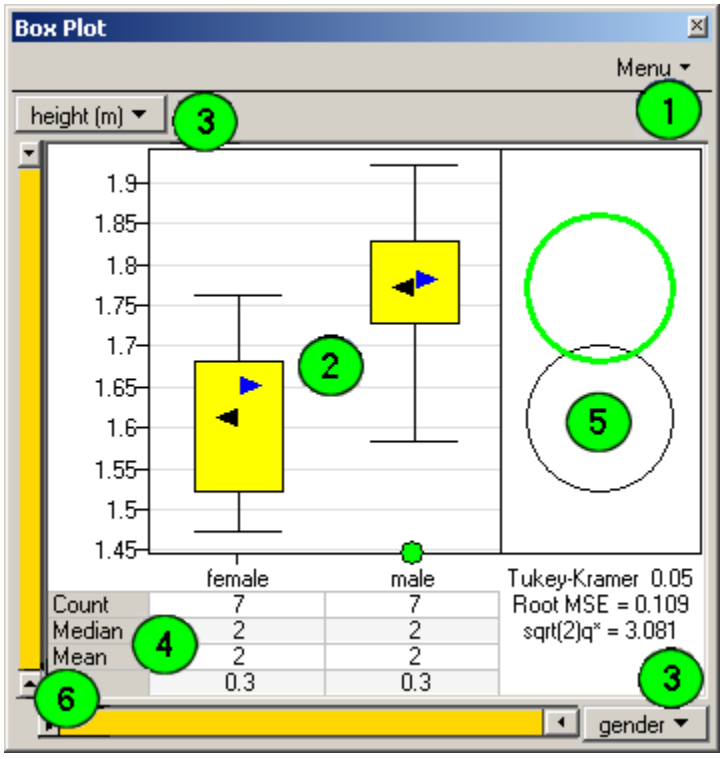


/

If active highlighted / if not active highlighted

10.3 User Interface

10.3.1 Box Plot User Interface Overview



1. Box plot menu

The Box Plot menu contains commands to copy the visualization and to set all properties.

2.Box plot

A box plot displays statistical properties of the value column.

3. Axis selectors

The Y-axis selector controls the column that is currently being analyzed. The X-axis selector controls by which variable the data are split into separate box plots.

4. Box plot table

Optional. Displays the statistical measures of your choice. Which measures should be shown are selected in the Box Plot: Properties dialog.

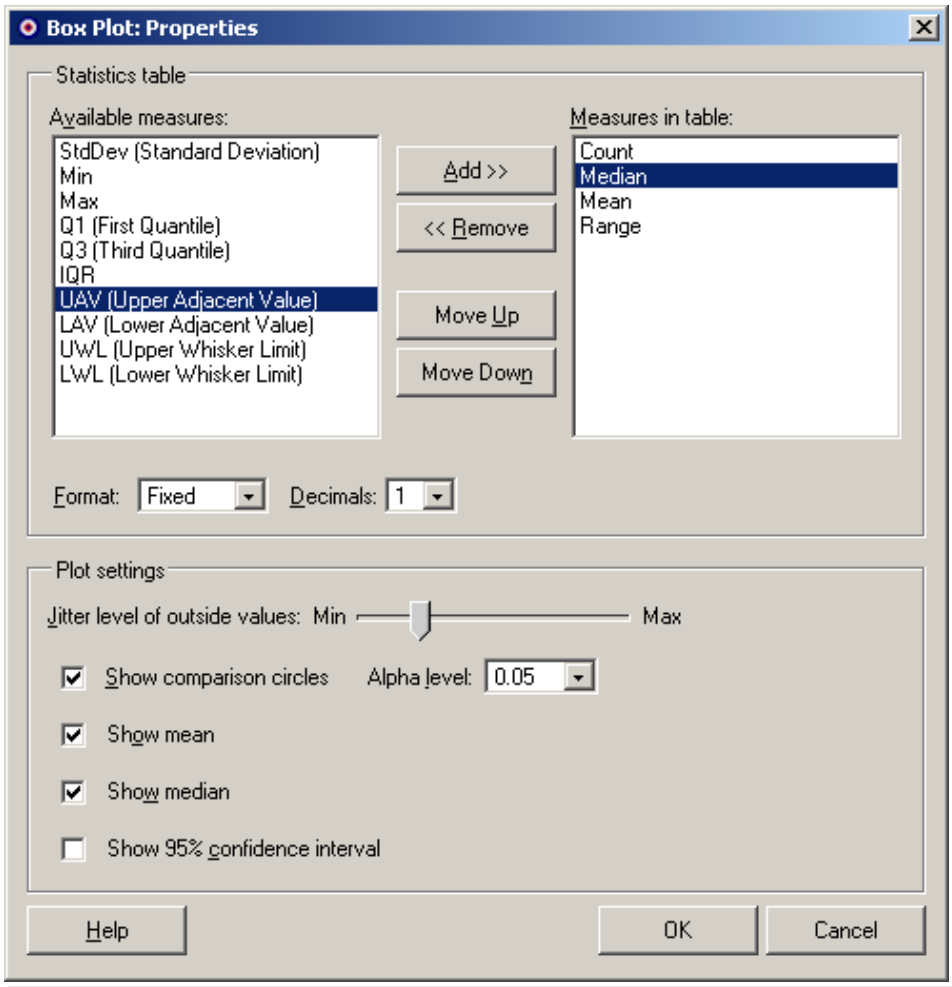
5. Comparison Circles

Optional. Displays comparison circles according to Tukey-Kramer.

6. Zoom bars

Drag the bars to select which box plots to display.

10.3.2 Box Plot Properties Dialog



Option	Description
Available measures	Displays the statistical measures available for display in the box plot table.
Measures in table	Displays the statistical measures currently selected for display in the box plot table.
Add >>	Adds the selected measure to the list of measures to be displayed in the box plot table.
<< Remove	Removes the selected measure from the list of measures to be displayed in the box plot table.
Move Up	Moves the selected measure up one step, thus making it possible to rearrange the order of the measures in the box plot table.
Move Down	Moves the selected measure down one step, thus making it possible to rearrange the order of the measures in the box plot table.
Format	Sets the format of the statistics table to either **General** (displays the values on a decimal format), **Fixed** (displays a fixed number of decimals) or **Scientific** (displays a fixed number of decimals on the form 1.1e-002).

Digits/Decimals	Select the number of significant digits or decimals that should be displayed.
Jitter level of outside values	Displaces outside values to reveal overlapping. Move the slider to change the level of jittering.
Show comparison circles	Select the check box to display comparison circles in the box plot visualization.
Alpha level	The level at which the difference between groups would be significant.
Show mean	Select the check box to display a representation of the mean value in the box plot as a black arrow.
Show median	Select the check box to display a representation of the median value in the box plot as a blue arrow.
Show 95% confidence interval	Select the check box to display the confidence interval in the box plot as a gray area.

► To reach the Box Plot: Properties dialog:

1. Select **Tools** > **Statistics** > **Box Plot**.
2. Select **Properties...** from the Box Plot menu, 

.

10.3.3 Box Plot Menu

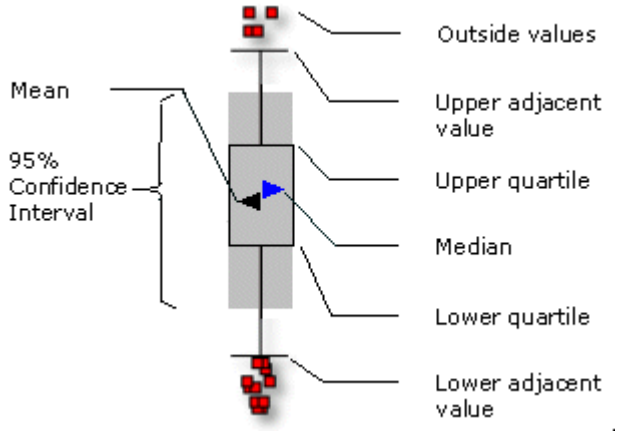
The Box Plot menu is displayed by clicking 

and it contains all commands necessary for working with Box Plot.

Option	Description
Copy Visualization	Copies the current box plot visualization (including the statistics table) to the clipboard as an enhanced metafile. The visualization may then be pasted into any other application (e.g., Microsoft Word or PowerPoint).
Properties	Displays the Box Plot: Properties dialog where you can change the settings of the Box Plot visualization (show comparison circles, mean value, median value and/or confidence intervals) and determine which statistical measures to display in a table.
Help	Launches the online help system.

10.3.4 Box Plot Symbols

The individual box plot is a visual aid to examining key statistical properties of a variable. The diagram below shows how the shape of a box plot encodes these properties. The range of the vertical scale is from the minimum to the maximum value in the selected column.



For details of each measure, see Statistical measures.

10.3.5 Box Plot Axis Selectors

The axis selectors control which column is mapped to which axis. They are located at the end of each axis.

- The Y-axis selector allows only value columns, since this is the column on which the statistical measures are based.
- The X-axis can be set to any column. However, since a separate plot will be drawn for each unique value, the column should not contain too many unique values. To summarize the data in a single plot, select **(None)**.

10.4 Theory and Methods

10.4.1 Comparison Circles Algorithm

The drawing of comparison circles is a way to display whether the group means for all pairs are significantly different from each other or not. Each group (each box plot) gets a circle, where the center of the circle is aligned with the group mean value. The radius of the circle, r_i, is calculated as follows:

$$r_i = |q^*| \sqrt{\frac{MSE}{n_i}}$$

where

$$\mathrm{MSE} = \frac{1}{\mathbf{v}} \sum_{i=1}^{K} \sum_{j=1}^{N} \left(x_{ij} - x_i\right)^2$$

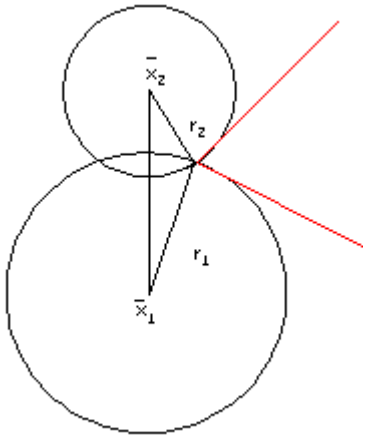
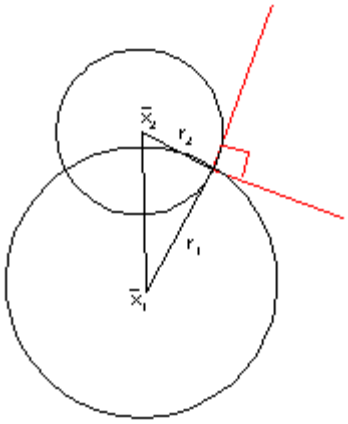
- *MSE* is the pooled sample variance:

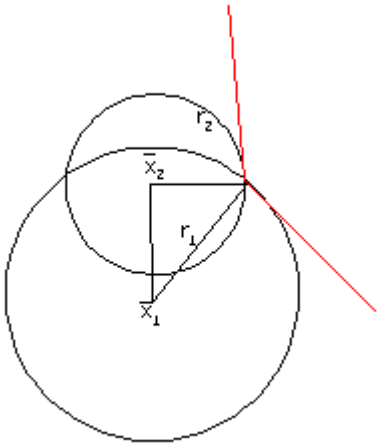
$$\mathbf{v} = \sum_{i=1}^{K} \left(n_i - 1\right)$$

- **v** is the degrees of freedom:
- n_i is the number of records in the group (count)
- *K* is the number of groups
- $|q^*| = \frac{q}{\sqrt{2}}$, where q is the upper alpha quantile of the Studentized range distribution with K groups and **v** degrees of freedom, for details how this is calculated see HSU (1996).

If the circles for different groups do not overlap (or that the external angle of intersection is less than 90 degrees) the means of the two groups are generally significantly different. If the circles have a large overlap, the means are not significantly different.

The explanation to why the overlap defines whether group means are significant or not can be deduced to the Pythagorean Theorem.

Comparison circles	Mathematical expression	Interpretation
	$\lvert\bar{x}_1 - \bar{x}_2\rvert > \sqrt{r_1^2 + r_2^2}$	The groups are significantly different.
	$\lvert\bar{x}_1 - \bar{x}_2\rvert = \sqrt{r_1^2 + r_2^2}$	Borderline significantly different.



$|\bar{x}_1 - \bar{x}_2| < \sqrt{r_1^2 + r_2^2}$

The groups are not significantly different.

10.4.2 Comparison Circles References

Hsu, J.C. (1996), Multiple Comparisons: Theory and Methods, London: Chapman & Hall.

Sall, J. (1992), "Graphical Comparison of Means" Statistical Computing and Statistical Graphics Newsletter, 3, pages 27-32.

11 Summary Table

11.1 Summary Table Overview

The Summary Table is a tool that displays statistical information numerically. The information is based on the data set in Spotfire DecisionSite. You can at any time choose which measures you want to see (such as mean, median, etc.), as well as the columns on which to base these measures. As you change the set of selected records in Spotfire DecisionSite (for example by using the query devices), the Summary Table automatically updates the values displayed to reflect the current selection.

11.2 Using Summary Table

11.2.1 Initializing the Summary Table

► To launch the Summary Table:

1. Select **Tools > Statistics > Summary Table**.
   Response: A new window appears, displaying a selection of statistics for the first ten columns in the data set.
2. If you want to change the columns or measures shown, select **Columns...** or **Measures...** from the **Summary Table** menu,  .
3. If required, organize the table by changing sort order, adjusting column width or reordering measures horizontally.

11.2.2 Selecting Columns for the Summary Table

► To select which columns to display in the Summary Table:

1. If the Summary Table tool is not already open, select **Tools > Statistics > Summary Table**.
   Response: The Summary Table window is displayed.
2. On the Summary Table menu,  , select **Columns...**.
   Response: The Columns dialog is displayed.
3. Select each column for which you want to display statistics and click **Add** >>.
   Comment: For multiple selection, press **Ctrl** and click on the desired columns or click one column and drag to select the following.
4. If you want separate statistics for subsets of data, select the **Group by** check box and choose a categorical column from the drop-down list. This column should not contain a large number of unique values.
5. Click **OK**.
   Response: The Columns dialog is closed and the Summary Table is updated with your new selection of statistical measures.

11.2.3 Selecting Statistical Measures in the Summary Table

► To select measures for display in the Summary Table:

1. If the Summary Table tool is not already open, select **Tools > Statistics > Summary Table**.
   Response: The Summary Table window is displayed.
2. Select **Measures...** from the Summary Table menu,  .
   Response: The Measures dialog is displayed.
3. Select the measures that you want to include and click **Add >>**.
   Comment: For multiple selection, press **Ctrl** and click on the desired measures or click one measure and drag to select the following. For a description of the available measures see Statistical measures.
4. Click **OK**.
   Response: The Measures dialog is closed and the Summary Table updated with your new selection of statistical measures.

11.2.4 Grouping Columns in the Summary Table

Grouping, in this context, refers to the use of a categorical column (one with few unique values) to split the data into subsets. With grouping it is possible to display more detailed statistics.
For example, consider the following data set:

Subject	Gender	Height	Income
1	Male	1.82	3000
2	Male	1.72	2800
3	Female	1.73	2900
4	Female	1.64	3100

In this case, Gender is a suitable column to use for grouping. By doing so, we can display not just the overall mean of Height and Income, but also separate values for the groups Male and Female.

► To use grouping in the Summary Table:

1. If the Summary Table tool is not already open, select **Tools > Statistics > Summary Table**.
2. Select the required measures.
3. Select **Columns...** from the Summary Table menu.
4. Select the columns for which you want to calculate statistics.
5. Select the **Group by** check box and a suitable category column from the list.
   Comment: The category column should contain relatively few unique values. Otherwise the reliability of the statistical measures is reduced, and the information presented in the Summary Table becomes difficult to grasp.
6. Click **OK**.
   Response: The Columns dialog is closed and the Summary Table is updated to show separate statistics for each group.

11.2.5 Controlling Summary Table Layout

The layout of the table can be controlled in three ways: sorting order (vertical), horizontal order (order of columns) and column width.

► To sort by a statistical measure:

- Click on the measure (in the table header) by which you want to sort the table.
  Response: The table sorted in increasing order.
  Comment: Click on the column heading again to toggle between increasing and decreasing order. Note the small arrow beside the column title, showing the sort order.

► To rearrange the horizontal order of the table:

1. Place the mouse pointer on a measure name in the table header.
2. Drag the header to the desired position.

► To adjust column width:

1. Place the mouse pointer on the separator between two column headers.
2. Click-and-drag the separator to the desired position.

Tip: If you double click on the separator, the column width will automatically be adjusted to the longest value in the table.

11.2.6 Exporting Summary Table Results

The measures displayed in the Summary Table can be exported to Excel, as a CSV file, or displayed in HTML format in your browser. This allows you to share your results with colleagues.

► To generate an HTML report from the Summary Table:

1. Launch the Summary Table tool, and select the columns and measures that you want to include.
2. Select **Export To** > **HTML** from the Summary Table menu,  .
   Response: The HTML report is displayed in your default browser.
3. If you want to save the report, select **Save As...** (or equivalent command) from the File menu in your browser.

► To export to Excel from the Summary Table:

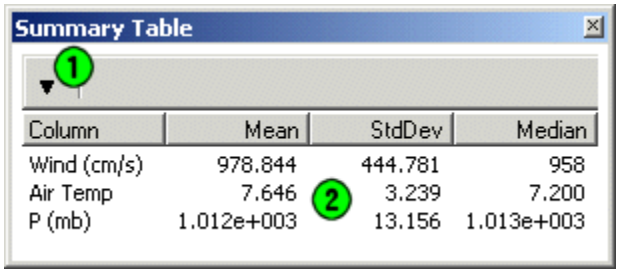
1. Launch the Summary Table tool, and select the columns and measures that you want to include.
2. Select **Export To** > **Excel** from the Summary Table menu,  .
   Response: An Excel spreadsheet is displayed containing the Summary Table results.
3. If you want to save the Excel file, select **Save As...** from the File menu in Excel.

► To export a CSV file from the Summary Table:

1. Launch the Summary Table tool, and select the columns and measures that you want to include.
2. Select **Export To** > **CSV** from the Summary Table menu,  .
   Response: A **Save As** dialog will appear, where you can name and save your file.

11.3 User Interface

11.3.1 Summary Table User Interface



1. Summary Table Menu

 The menu provides all menu commands required to work with Summary Table.

2. Table

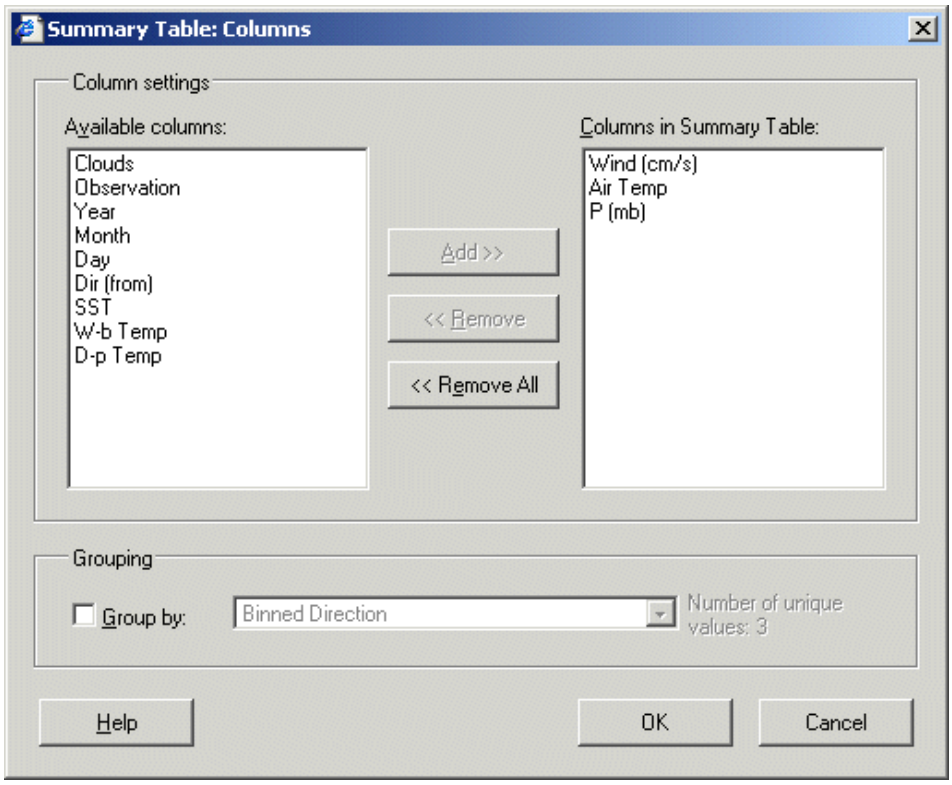
The Summary Table presents statistical information for one or more data columns. On the left is a list of column names (defined in the Summary Table: Columns dialog). For each column name, one or more statistical measures (chosen in the Summary Table: Measures dialog) are displayed. The names of the measures are shown in the table header. You can control the layout of the table.

11.3.2 Summary Table Menu

The menu is displayed by clicking  and it contains all commands necessary for working with the tool.

Option	Description
Columns...	Displays the Summary Table: Columns dialog, for selecting data columns.
Measures...	Displays the Summary Table: Measures dialog, for selecting statistical measures.
Export	Exports the table of statistics as a web page.
Help...	Launches this help system.

11.3.3 Summary Table Columns Dialog

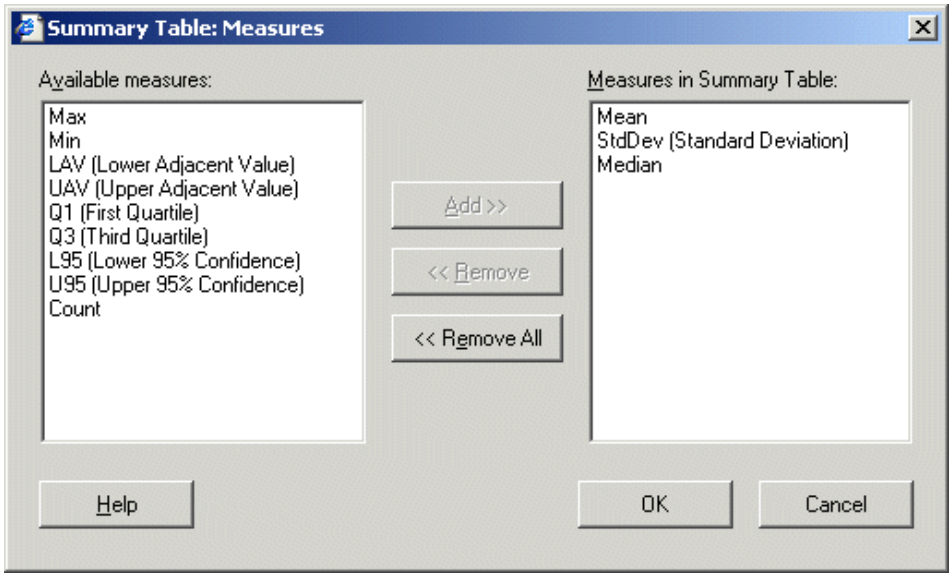


Option	Description
Available columns	The columns available for statistics. This includes all numerical columns, but no string columns. Click on a column name in the list to select it and then click **Add>>** to include it in the Summary Table. To select more than one column, press **Ctrl** and click the columns in the list.
Columns in Summary Table	The columns selected for display in the Summary Table. Click a column name in the list to select it. To select more than one column, press **Ctrl** and click the column names in the list.
Add >>	Adds the selected column to the list of columns to be displayed in the Summary Table.
<< Remove	Removes the selected column from the list of columns to be displayed in the Summary Table.
<< Remove All	Removes all selected columns from the list of columns to be displayed in the Summary Table.
Group by:	Select this check box if you want to use stratification. You must then also select a categorical column (see below).
<drop-down list>	Select a column by which you want to stratify the table of statistics. This means displaying separate statistics for each unique value in the chosen column. This column should preferably contain categorical information, since too many unique values will make the statistical measures less valuable.

► To reach the Summary Table: Columns dialog:

1. Select **Tools** > **Statistics** > **Summary Table**.
2. Select **Columns...** from the **Summary Table** menu.

11.3.4 Summary Table Measures Dialog



Option	Description
Available measures	All measures available for calculating and displaying statistics. Click on a measure name in the list to select it and then click **Add>>** to include it in the Summary Table. To select more than one measure, press **Ctrl** and click the measures in the list. For a mathematical description of the different measures, see Statistical measures.
Measures in Summary Table	Measures selected for display in the Summary Table. Click a column name in the list to select it. To select more than one measure, press **Ctrl** and click the measures in the list.
Add >>	Adds the selected measure to the list of measures chosen for display in the Summary Table.
<< Remove	Removes the selected measure from the list of measures chosen for display in the Summary Table.
<< Remove All	Removes all selected measures from the list of measures chosen for display in the Summary Table.

► To reach the Summary Table: Measures dialog:

1. Select **Tools** > **Statistics** > **Summary Table**.
2. Select **Measures...** from the Summary Table menu.

11.4 Statistical Measures

11.4.1 Statistical Measures Overview

Spotfire DecisionSite contains several tools which calculate various statistical measures. For a description of each measure, see the corresponding section.

11.4.2 Count

The *Count* measure gives the number of values in a column, not counting empty values. In the table below, Column A has a *Count* of 3, while Column B has a *Count* of 4.

Column A	Column B
1	4
	7
8	3
9	6

11.4.3 Unique Values

The *Unique Values* measure gives the number of unique (distinct) values in a column. Empty values are not counted.

11.4.4 Median

The median of a distribution is the value which, when the distribution is sorted, appears in the middle of the list. If the number of values is even, the median is computed by taking the mean of the two middle values.

The median is sometimes called the **location** of the distribution.

11.4.5 Mean

The mean, or average, is calculated as the sum of all values in the distribution divided by the number of values.

The arithmetic mean value, $\bar{x}$, is calculated as:

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

11.4.6 Standard Deviation

The standard deviation (StdDev), *s*, is an indication of how dispersed the probability distribution is about its center. It is computed as follows:

$$s = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

where

- $\bar{x}$ is the mean value of the group
- *n* is the number of values in the group (Count)

11.4.7 Variance

The sample variance, s^2, is an indication of how dispersed the probability distribution is about its center. It is calculated as follows:

$$s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

where

- $\bar{x}$ is the mean value of the group
- *n* is the number of values in the group (Count)

11.4.8 Quartiles

The *first quartile*, Q1, is defined as the value that has an f-value equal to 0.25. The *third quartile*, Q3, has an f-value equal to 0.75. The interquartile range, IQR, is defined as Q3-Q1.

► The quartiles are computed as follows:

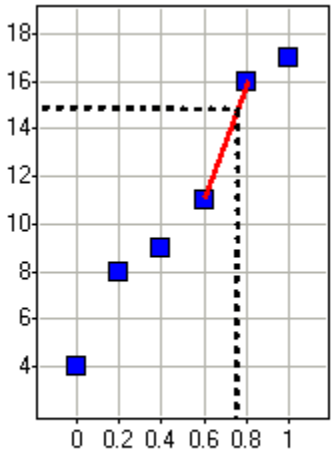
1. The f-value of each value in the data set is computed:

   $$f_i = \frac{i-1}{n-1}$$

   where *i* is the index of the value, and *n* the number of values.
2. The first quartile is computed by interpolating between the f-values immediately below and above 0.25, to arrive at the value corresponding to the f-value 0.25.
3. The third quartile is computed by interpolating between the f-values immediately below and above 0.75, to arrive at the value corresponding to the f-value 0.75.

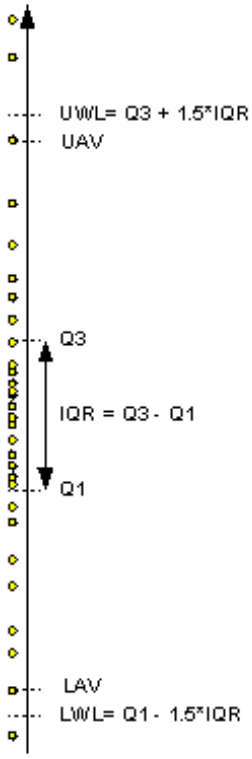
Example:

Value	f-value
4	0
8	0.2
9	0.4
11	0.6
16	0.8
17	1.0



Interpolation at f-value=0.75 yields Q3=14.75.

11.4.9 Adjacent Values and Whisker Limits



Let IQR be the interquartile range.

The upper adjacent value (UAV) is the largest observation that is less than or equal to the upper whisker limit (UWL), which is the third quartile plus 1.5*IQR.

The lower adjacent value (LAV) is the smallest observation that is greater than or equal to the lower whisker limit (LWL), which is the first quartile minus 1.5*IQR.

Note: If, by the above definition, the UAV is such that it is smaller than Q3, then it is set equal to Q3. Similarly, the LAV is never allowed to be greater than Q1.

11.4.10 Confidence Intervals

Confidence intervals are calculated as:

$$\bar{x} \pm \frac{1.959964 \times s}{\sqrt{n}}$$

where

- $\bar{x}$ is the mean value of the group
- *s* is the sample standard deviation
- *n* is the number of values in the group (Count)

11.4.11 Outside Values in Box Plot

Outside values are values beyond the upper and lower adjacent values. In other words, they represent extreme values, or outliers. Not all distributions have outside values.

12 Normal Probability Plot

12.1 Normal Probability Plot Overview

Normal Probability Plots are used to investigate to what extent a data set exhibits normal distribution, also known as "bell curve" or Gaussian distribution.

Knowing if a distribution is normal can be important in many situations. One of the advantages of normally distributed data is that the mean value and the standard deviation can be sufficient to summarize the complete set of data. Also, many statistical tools (such as Anova) assume a normal distribution of the data and may not give satisfying results if the deviation from the normal is too large.

12.2 Using Normal Probability Plots

12.2.1 Using Normal Probability Plot

The Normal Probability Plot tool is used to investigate if your data is normally distributed.

► To generate a Normal Probability Plot:

1. Select **Tools > Statistics > Normal Probability Plot...**.
   Response: The Normal Probability Plot dialog is shown.
2. Select the value column that you want to investigate.
3. Optionally, select a category column.
   Comment: If a category column is used, then a separate line will be plotted for each unique value in the column.
4. Enter a name for the new column that will be generated, or accept the default name.
5. Click **OK**.
   Response: A new scatter plot is created.

12.2.2 Normal Probability Plot Example

Consider the following data set, which lists a few attributes of a group of people:

eye color, gender, height (m), weight (kg), age
blue, female, 1.65, 62.7, 29
blue, female, 1.50, 57.0, 31
blue, female, 1.69, 64.2, 18
blue, male, 1.58, 63.2, 31
green, male, 1.76, 70.4, 44
green, male, 1.82, 72.8, 26
green, male, 1.92, 76.8, 33
green, female, 1.54, 61.6, 39
green, female, 1.76, 70.4, 22
brown, female, 1.67, 66.8, 34
brown, female, 1.47, 58.8, 41
brown, male, 1.69, 71.0, 23
brown, male, 1.78, 74.8, 35
brown, male, 1.83, 76.9, 20

► To determine whether the heights can be approximated by the normal distribution:

1. Select **Tools > Statistics > Normal Probability Plot...**.
   Response: The Normal Probability Plot dialog appears.
2. Select **Height** as value column.
3. Select no category column.
4. Click **OK**.
   Response: A new scatter plot is created.

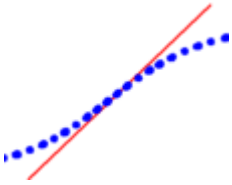
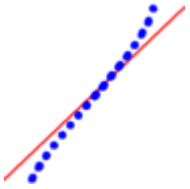
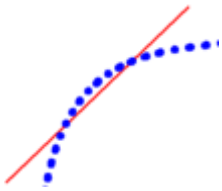
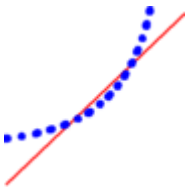
The values are more or less located on a straight line, which means that the distribution can be approximated by the normal.

Note: In a real-life situation the number of records in the investigated data set should be much higher than this example in order to obtain a reasonably accurate result.

12.2.3 Interpreting Normal Plots

The Normal Probability Plot tool calculates the normal quantiles of all values in a column. The values (Y-axis) are then plotted against the normal quantiles (X-axis).

Things to look for:

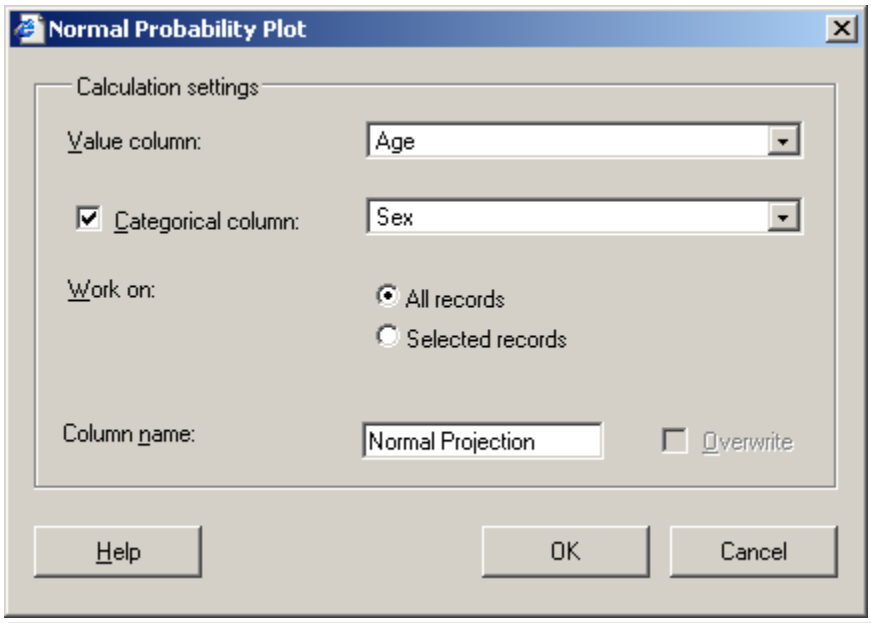
Shape (exaggerated)	Conclusion
	Approximately normal distribution.
	Less variance than expected. While this distribution differs from the normal, it seldom presents any problems in statistical calculations.
	More variance than you would expect in a normal distribution.
	Left skew in the distribution.
	Right skew in the distribution.

Outlier. Outliers can disturb statistical analyses and should always be thoroughly investigated. If the outliers are due to known errors, they should be removed from the data before a more detailed analysis is performed.

Note: Plateaus will occur in the plot if there are only a few discrete values that the variable may take on. However, clustering in the plot may also be due to a second variable that has not been considered in the analysis.

12.3 User Interface

12.3.1 Normal Probability Plot Dialog



Option	Description
Value column	The columns available for analysis. This includes all numerical columns, but no string columns. Select a column name from the drop-down list.
Categorical column	Optional. Column used to categorize the data set. For each unique value in the chosen column, a separate line will be drawn in the generated plot. Select the check box and select a column from the drop-down list.
Work on: All records	All records in the value columns are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Column name	The name of the new column generated by the Normal Probability Plot tool. Use the default name, or enter a new one.

Overwrite	Select this check box to overwrite any existing column with the same name, and to replace the previous Normal Probability Plot with the new one.

► To reach the Normal Probability Plot dialog:

Select **Tools** > **Statistics** > **Normal Probability Plot...**.

12.4 Theory and Methods

12.4.1 The Normal Probability Plot Algorithm

The Normal Probability Plot tool calculates the *normal quantiles* of all values in a column. The values and the normal quantiles are then plotted against each other.

► Normal quantiles are computed as follows:

1. For each value, the f-value is calculated as:

   $$f_i = \frac{i - 0.5}{n}$$

   where i is the index of the value and n is the number of values.
2. The *normal quantile*, *q(f),* for a given f-value is the value for which

   $$P[X <= q] = f$$

   where X is a standard normally distributed variable.

Reference:

Rice, J., A., Mathematical statistics and data analysis / John A. Rice. 2nd ed. Belmont, CA, Duxbury Press, 1995.

12.4.2 Quantiles and F-values

The concept of quantiles is important when you want to visualize distributions.

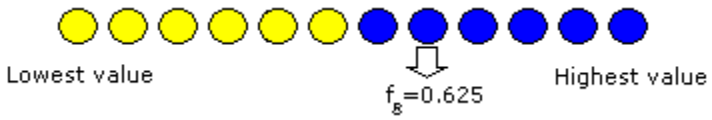
The *f* quantile, *q(f)*, is a value along the measurement scale of the data where *approximately* a fraction *f* of the data are less than or equal to *q(f)*.

If there are *n* values in the record and *i* is an index number for the investigated value, the *f*-value for each record is calculated as:

$$f_i = \frac{i - 0.5}{n}$$

Example:

In the example below, the *f* value for the 8th position in the ordered list of values would be calculated as 7.5/12=0.625, since the total number of values in the list is 12.



13 Profile Anova

13.1 Profile Anova Overview

Anova means **An**alysis **o**f **Va**riance. The Profile Anova tool provides a method for locating records where there is a significant difference between one group of columns and another group, such as in time-series data where experimental parameters change over time.

13.2 Using Profile Anova

13.2.1 Calculating Profile Anova P-values

The Profile Anova is used to determine if there are any differences between the values of different groups in a row. The result is presented as a p-value, where a low p-value represents a large difference.

► To calculate Profile Anova p-values:

1. Select **Tools** > **Statistics** > **Profile Anova...**.

   Response: The Profile Anova dialog is displayed and all available columns are listed in the Value columns field.
2. Move and organize the desired value columns into two or more groups in the **Grouped value columns** field.

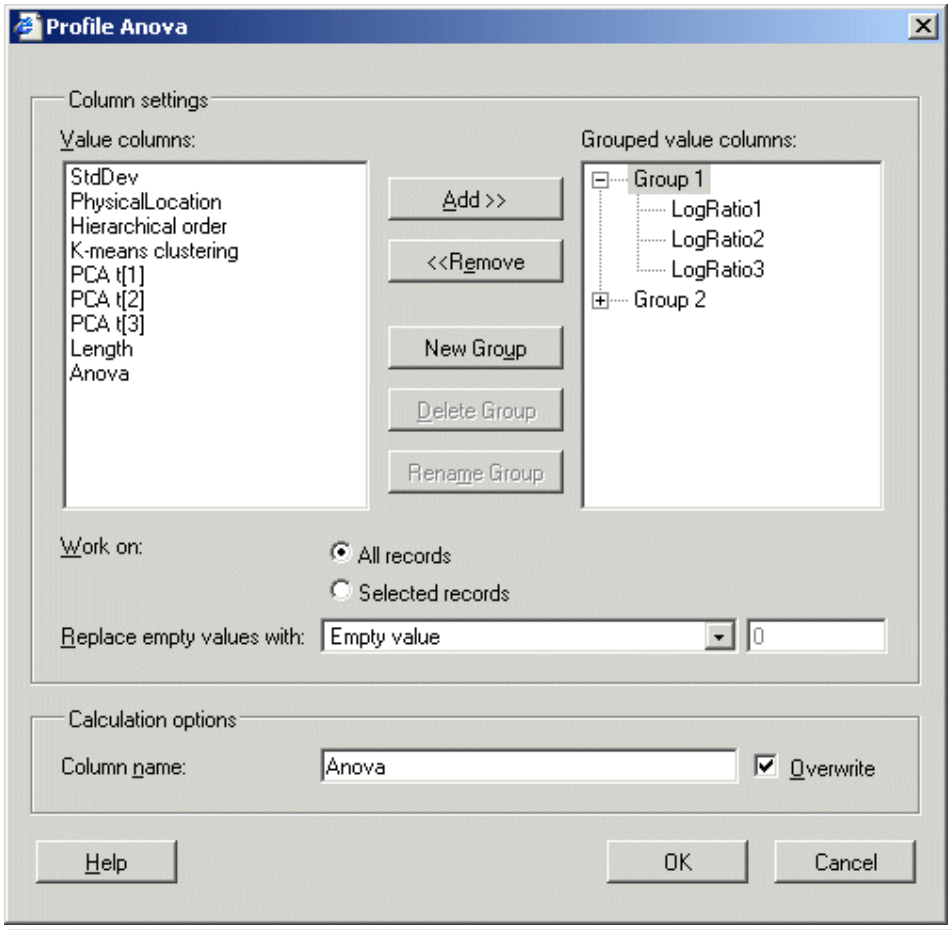
   Comment: Select columns and click on the **Add** >> button. The column will end up in the selected group of the Grouped value columns field. Click **New Group** to add a group, click **Delete Group** to delete a selected group. The tool requires at least two columns in each group to be able to perform the calculations.
3. Click a radio button to select whether to work on **All records** or **Selected records**.
4. Optionally, select a method to **Replace empty values with** from the drop-down list.
5. Optionally, type a new **Column name** in the text box or use the default name.

   Comment: Select the **Overwrite** check box if you want to overwrite a previously added column with the same name. If you do not want to overwrite, make sure Overwrite is cleared or type a unique name in the Column name text box.
6. Click **OK**.

   Response: A new column that contains the p-values is added to the data set. A new profile chart is created, with columns ordered by group. An annotation containing information about which group each variable belongs to may also be added.

13.3 User Interface

13.3.1 Profile Anova Dialog



Option	Description
Value columns	Data columns that you can use in the calculation. Only numerical columns are available. Click a column name in the list to select it. To select more than one column, press **Ctrl** and click the column names in the list.
Grouped value columns	Displays the groups on which the calculation is performed. You can add, delete or rename groups from the field by clicking on the corresponding buttons to the left of the field. You move value columns between the fields using the Add >> and << Remove buttons.
Add >>	Moves selected columns from the Value columns field to a selected group in the Grouped value columns field. Click to select the desired columns and the group that you want to add the columns to, then click on Add >>.
<< Remove	Removes all columns from a selected group and brings them back to the Value Columns field.
New Group	Adds a new group to the Grouped value columns field.
Delete Group	Deletes a selected group from the Grouped value columns field. If the

	group contained any value columns they are moved back to the Value columns field.
Rename Group	Opens the Edit Group Name dialog, where you can change the name of the selected group.
Work on: All records	All records in the value columns are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Replace empty values with	Defines how empty values in the data set should be replaced. **Empty value** simply ignores empty values. **Constant** allows you to replace the empty values by any constant (type a number in the text box). **Row average** replaces the value by the average value of the entire row. **Row interpolation** sets the missing value to the interpolated value between the two neighboring values in the row.
Column name	The name of the new column containing the results from the Profile Anova calculation. The Column name text box is not available when performing Distinction/Multiple distinction calculations, since the names of the result columns are then based on the group names.
Overwrite	Select this check box if you want to replace previously added columns (with the same group names or the same name as the one typed in the **Column name** text box) when you add new columns. Clear the check box if you wish to keep the old columns.

► To reach the Profile Anova dialog:

Select **Tools** > **Statistics** > **Profile Anova...**.

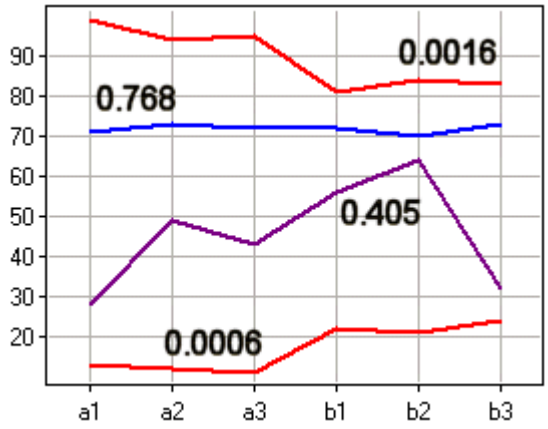
13.4 Theory and Methods

13.4.1 Profile Anova Method Overview

(For a mathematical description of Profile Anova, see The Profile Anova Algorithm.)

The Profile Anova tool requires that we divide the columns in the data set into at least two groups. The tool then produces a new column, giving a *p-value* for each record. The p-value is an indicator of how clearly the groups differ for a particular record.

Consider the following profile chart with four records:



We are comparing two groups of columns, a1-a3 and b1-b3. Where there is minimal difference between the groups (blue profile), the p-value is close to 1. Where there is a clear difference (red profiles) the p-values approach zero.

13.4.2 Profile Anova Algorithm

The Profile Anova tool computes the difference between groups by comparing the mean values of the data in each group. The results are obtained by testing the null hypothesis; the hypothesis that there is no difference between the means of the groups. More formally, the p-value is the probability of the actual *or a more extreme* outcome under the null-hypothesis.

► For each record, a p-value is computed as follows:

1. Values are grouped as selected in the Profile Anova dialog.
2. The total mean value of the record is computed.

$$\bar{x}_{tot} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

3. The mean within each group is computed.
4. The difference between each value and the mean value for the group is calculated and squared.
5. The squared difference values are added. The result is a value that relates to the total deviation of records from the mean of their respective groups. This value is referred to as the *sum of squares within groups*, or **S2Wthn**.
6. For each group, the difference between the total mean and the group mean is squared and multiplied by the number of values in the group. The results are added. The result is referred to as the *sum of squares between groups*, or **S2Btwn.**

$$S2Btwn = N_1(\bar{x}_1 - \bar{x}_{tot})^2 + N_2(\bar{x}_2 - \bar{x}_{tot})^2 + \ldots + N_N(\bar{x}_N - \bar{x}_{tot})^2$$

7. The two sums of squares are used to obtain a statistic for testing the null hypothesis, the so called F-statistic. The F-statistic is calculated as:

$$F = \frac{S2Btwn/dfB}{S2Wthn/dfW}$$

where, *dfB* (degree of freedom between groups) equals the number of groups minus 1, and *dfW* (degree of freedom within groups) equals the total number of values minus the number of groups.

8. The F-value is distributed according to the F-distribution (commonly presented in mathematical tables/handbooks). The F-value, in combination with the degrees of freedom and an F-distribution table, yields the p-value.

The p-value is the probability of the actual *or a more extreme* distribution under the null-hypothesis. If the p-value is below a certain level (usually 0.05) it is assumed that there is a significant difference between the group means.

13.4.3 Requirements on Input Data for Profile Anova

Experimental design

In this tool, a one-way layout of Anovas has been employed. This means that the experimental design should be of the type where the outcome of a single continuous variable is compared between different groups. The tool cannot be used to analyze experiments where two or more variables vary together.

Distribution of data

The Anova comparison assumes the following:

- The data is approximately normally distributed.
- The variances of the separate groups are approximately equal.

If the data do not fulfill these conditions, the Anova comparison may produce unreliable results.

14 Column Relationships

14.1 Column Relationships Overview

The Column Relationships tool is used for investigating the relationships between different column pairs. The Linear regression option allows you to compare numerical columns, the Anova option will help you determine how well a category column categorizes values in a (numerical) value column, the Kruskal-Wallis option is used to compare sortable columns to categorical columns, and the Chi-square option helps you to compare categorical columns.

For each combination of columns, the tool calculates a *p-value*, representing the degree to which the first column predicts values in the second column. A low p-value indicates a probable strong connection between two columns. The resulting table is sorted by p-value for the Anova, Kruskal-Wallis and Chi-square calculations, and by p-value and RSq (squared correlation value) for the Linear regression calculation.

14.2 Using Column Relationships

14.2.1 Calculating Column Relationships

The Column Relationships tool is used for investigating the relationships between numerical and/or categorical columns using different statistical tests. For each combination of columns, the tool calculates a p-value, representing the degree to which the first column predicts values in the second column.

► To calculate Column Relationships:

1. Select **Tools** > **Statistics** > **Column Relationships...**.

   Response: The Column Relationships dialog is displayed and all available columns are listed in the Available columns field.
2. Select the comparison method you wish to use, depending on the type of columns that you want to compare.

   Comment: Choose from **Linear regression (numerical vs numerical), Anova (numerical vs categorical)**, **Kruskal-Wallis (sortable vs categorical)** and **Chi-square (categorical vs categorical)**.
3. Move the desired columns into either of the two fields *Y columns* (*categorical/sortable/numerical*) and *X columns* (*categorical/numerical*).

   Comment: Select columns from *Available columns* and click on one of the **Add >>** buttons. You must select at least one column for the Y-columns field and one for the X-columns field. Click **<< Remove** to move a column back to the list of available columns.
4. Select whether to base the p-values on **All records** or **Selected records** only.
5. Click **OK**.

   Response: The Column Relationships window is launched.
6. Click on the column pair you are interested in.

   Response: A new visualization is created. If an Anova or Linear regression has been calculated the result is a scatter plot. You may want to jitter the plot to reveal overlapping markers. Use the Properties dialog in DecisionSite to do this. If two categorical columns have been compared (Chi-square), the result is a pie chart

Tip: If you have a data set with many columns you can right-click on the header of the columns in the Available columns list box (e.g., Name) and select **Show Search Field** from the pop-up menu. This will display a search field where you can type a search string and limit the number of items in the list. It is possible to use the wildcard characters * and ? in the search.

14.2.2 Controlling Column Relationships Table Layout

The layout of the table can be controlled in three ways: sorting order (vertical), horizontal order (order of columns) and column width. It is also possible to show or hide calculation details such as degree of freedom or certain statistics in the table. See Pop-up menu for more information.

► To sort by Y or X column, or by p-value:

- Click on the column header by which you want to sort the table.

  Response: The table is sorted in increasing order.

  Comment: Click on the column heading again to sort in decreasing order. Note the small arrow beside the column title, showing the sort order. Click a third time to return to the default sort order.

► To rearrange the horizontal order of the table:

1. Place the mouse pointer on a table header.
2. Drag the header to the desired position.

► To adjust column width:

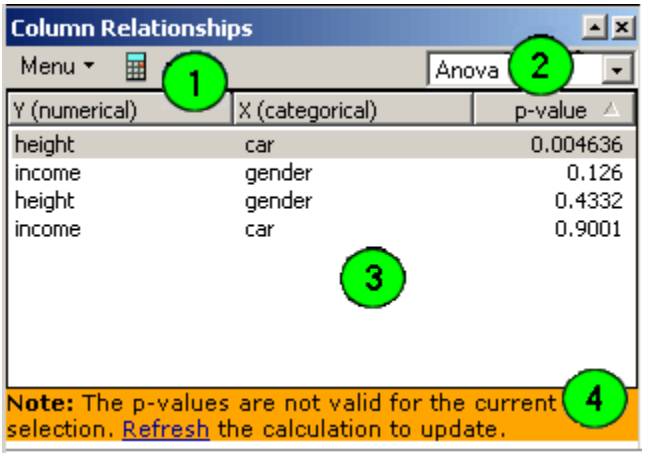
1. Place the mouse pointer on the separator between two column headers.
2. Click-and-drag the separator to the desired position.

   Comment: If you double click on the separator, the column width will automatically be adjusted to the longest value in the table.

14.3 User Interface

14.3.1 Column Relationships User Interface Overview

This is the Column Relationships main window:



1. Column Relationships menu and toolbar

The Column Relationships menu contains commands to perform a new calculation, copy the table or get help.

The toolbar includes the menu and a button that launches the Column Relationships dialog so that you can perform a new calculation.

2. Drop-down list

The latest list of each comparison type during a DecisionSite session will be temporarily stored here. Hence, it is possible to have one Anova, one Linear regression and one Chi-square

comparison active at the same time and change between the different comparisons without having to recalculate the results.

3. Column Relationships table

This table displays a p-value for each combination of Y and X columns. A low p-value indicates a probable strong connection between two columns.

Clicking on a column heading will sort the rows according to that column. By default, the table is sorted according to increasing p-values for Anova and Chi-square calculations, and by p-value and RSq for Linear regression calculations. Clicking on a row in the table will produce a new scatter plot, or, in the case of Chi-square calculations, a pie chart.

It is possible to add more information to the table by right-clicking on any of the table headers and selecting either of the available statistics. See Pop-up menu for more information.

4. Calculation information

This field will inform you of whether the current p-values are based on the currently selected records in DecisionSite or not. If you filter your data using the query devices or zooming after performing a column relationships calculation on selected records, the p-values in the table will no longer reflect the current selection in your visualizations. To update the p-values, click on the **Refresh** link in the orange field.

► To reach the Column Relationships window:

1. Select **Tools > Statistics > Column Relationships...**.
2. Perform the calculation by making your selections and clicking **OK** in the Column Relationships dialog. See also Calculating column relationships.

14.3.2 Column Relationships Menu

The Column Relationships menu is displayed by clicking 

in the Column Relationships window and contains the following commands:

Option	Description
New Calculation	Launches the Column Relationships dialog where you can specify settings for new column comparisons.
Copy	Copies the currently selected contents of the table to the clipboard as a tab separated list, which can then be pasted elsewhere.
Help	Opens this help file to the Column Relationships overview topic.

14.3.3 Column Relationships Pop-up Menu

It is possible to display more information in the Column Relationships table than the default columns Y (numerical/categorical), X (numerical/categorical), and p-value. Which items are displayed is selected on the pop-up menu. To bring up the pop-up menu, right-click on any of the table headers (e.g., Y (numerical)) in the Column Relationships window.

All calculations

Option	Description
Show Search Field	This will display or hide a search field where you can type a search string and limit the number of items in the list. It is possible to use the wildcard characters * and ? in the search.

Y (numerical/categorical)	The name of the Y column concerned.
X (numerical/categorical)	The name of the X column concerned.
p-value	The calculated p-value, representing the degree to which the first column predicts values in the second column. A low p-value indicates a probable strong connection between two columns.

Linear regression

Option	Description
F-stat	The F-statistic calculated according to [Ref. Arnold].
RSq	The squared correlation value.
df	The degrees of freedom = the number of non-empty records in the column - 2.

Anova

Option	Description
F-stat	The F-statistic. See Anova algorithm for more information.
S2Btwn	The sum of squares between groups.
S2Wthn	The sum of squares within groups.
dfBtwn	The degree of freedom between groups.
dfWthn	The degree of freedom within groups.

Kruskal-Wallis

Option	Description
H-stat	The H-statistic. See Kruskal-Wallis algorithm for more information.
df	The degrees of freedom = k-1, where k is the number of categories.

Chi-square

Option	Description
Chi2-stat	The Chi2-statistic, which is a direct relationship between the observed and the expected values. A high Chi2-value indicates that the observed values diverges from the expected values.
df	The degrees of freedom = (I-1)(J-1) where I is the number of unique values in the first column and J is the number of unique values in the second column.

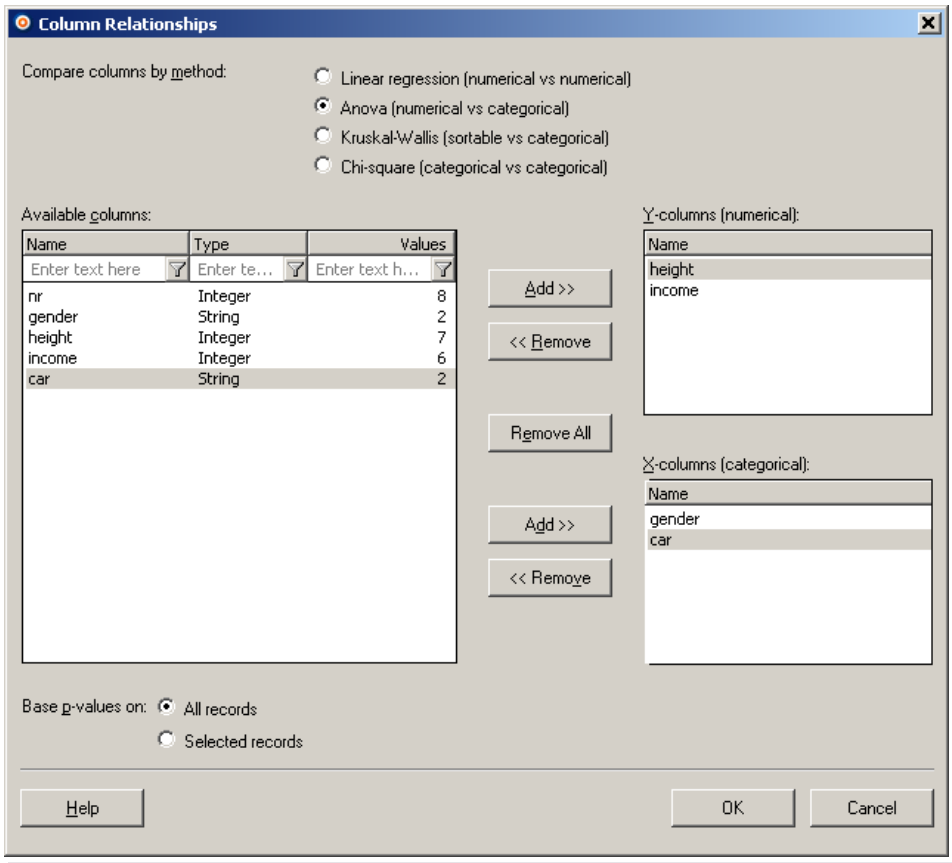
14.3.4 Column Relationships Toolbar

The Column Relationships toolbar includes the following buttons. Click the button on the toolbar to activate the corresponding function.

	Displays the Column Relationships menu.

Launches the Column Relationships dialog where you can perform a new calculation and compare columns.

14.3.5 Column Relationships Dialog



Option	Description
Linear regression (numerical vs numerical)	Use this option to compare numerical columns with one another.
Anova (numerical vs categorical)	Use this option to compare numerical columns with categorical columns.
Kruskal-Wallis (sortable vs categorical)	Use this option to compare ordered columns with categorical columns.
Chi-square (categorical vs categorical)	Use this option to compare categorical columns with one another.
Available columns	The columns available for use in the calculation. Click a column name in the list to select it. To select more than one column, press **Ctrl** and click the column names in the list. Use one of the Add >> buttons to send the selected column to either the Y-columns or X-columns field, see below.
Enter text here 	If you have a data set with many columns, you can right-click on the header of the columns in the Available columns list box and select **Show Search Field** from the pop-up menu.

	This will display a search field where you can type a search string and limit the number of items in the list. It is possible to use the wildcard characters * and ? in the search.
Y-columns (categorical/numerical)	The selected dependent columns that you wish to compare against the independent columns below.
X-columns (categorical/numerical)	The selected independent columns. Categorical columns should typically not contain too many unique values.
Add >>	Moves selected columns from the Available columns field to the field next to the button.
<< Remove	Removes a column and brings it back to the Available columns field.
Remove All	Removes all columns from the selected columns fields.
Base p-values on:	Choose whether to base calculations on the entire data set or only the subset selected using the query devices and zooming.

► To reach the Column Relationships dialog:

Select **Tools** > **Statistics** > **Column Relationships...**.

14.4 Theory and Methods

14.4.1 Overview of Column Relationships Theory

The Column Relationships tool calculates a probability value (p-value) for any combination of columns. This p-value can be used to determine whether or not the association between the columns is statistically significant.

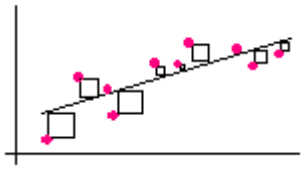
- Linear regression
- Anova
- Kruskal-Wallis
- Chi-square

Linear regression

(For a mathematical description of linear regression, see Column Relationships Linear regression algorithm.)

The linear regression option is used to calculate an F-test investigating whether the independent variable X predicts a significant proportion of the variance of the dependent variable Y.

Linear regression, or the "least squares" method, works by minimizing the sum of the square of the vertical distances of the points from the regression line.

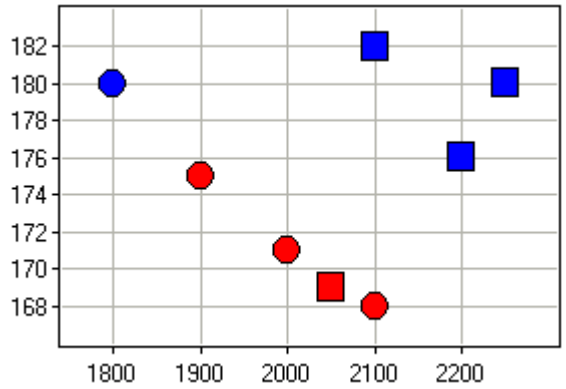


Anova

(For a mathematical description of Anova, see Column Relationships Anova algorithm.)

Anova means **An**alysis **o**f **Va**riance. The Anova option is used for investigating how well a category column categorizes a value column. For each combination of category column and value column, the tool calculates a p-value, representing the degree to which the category column predicts values in the value column. A low p-value indicates a probable strong connection between two columns.

Consider the following scatter plot representing data about eight subjects: gender (male/female), owns car (yes/no), income ($), and height (cm). Income is plotted on the horizontal axis, and height on the vertical.



Blue markers represent car owners, red markers represent non-car owners. Squares represent male subjects, circles female subjects. If we perform an Anova calculation with gender and car as category columns, and income and height as value columns, the result will be four p-values as follows.

Value column	Category column	p-value
Height	Car	0.00464
Income	Gender	0.047
Height	Gender	0.433
Income	Car	0.519

A low p-value indicates a higher probability that there is a connection between category and value column. In this case, Height and Car seem closely related, while Income and Car are not. We can verify this by examining the scatter plot.

See Requirements on input data for column relationships for more information about what data to use with this tool.

Kruskal-Wallis

(For a mathematical description of the Kruskal-Wallis test, see Column Relationships Kruskal-Wallis algorithm.)

The Kruskal-Wallis option is used to compare independent groups of sampled data. It is the nonparametric version of one-way Anova and is a generalization of the Wilcoxon test for two independent samples. The test uses the ranks of the data rather than their actual values to calculate the test statistic. This test can be used as an alternative to the Anova, when the assumption of normality or equality of variance is not met.

Chi-square

(For a mathematical description of the chi-square calculation, see Column Relationships Chi-square independence test algorithm.)

The chi-square option is used to compare observed data with the data that would be expected according to a specific hypothesis (e.g., the null-hypothesis which states that there is no significant difference between the expected and the observed result). The chi-square is the sum

of the squared difference between observed and expected data, divided by the expected data in all possible categories. A high chi-square statistic indicates that there is a large difference between the observed counts and the expected counts.

From the chi-square statistic it is possible to calculate a p-value. This value is low if the chi-square statistic is high. Generally, a probability of 0.05 or less is considered to be a significant difference.

14.4.2 Column Relationships Linear Regression Algorithm

The Linear Regression option calculates the p-value under the assumption that there are no empty values in the data set.

Note: If there are empty values in the data set, the data set will first be reduced to the rows containing values for both the first and the second column.

Let n be the total number of values and denote by (x_i, y_i), $i = 1, ..., n$ the set of data points to fit a straight line

$$y = \beta_0 + \beta_1 x$$

The least square estimates of β_0 and β_1 are:

$$\beta_0 = \frac{\left(\sum_{i=1}^{n} x_i^2\right)\left(\sum_{i=1}^{n} y_i\right) - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} x_i y_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$\beta_1 = \frac{n\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

The p-value is then calculated from the F-distribution where the F-statistic is calculated with the sum of squares between the estimated line and the total mean of the y_i's having one degree of freedom as numerator and the residual sum of squares divided by the number of degrees of freedom (n-2) as denominator.

References

Arnold, Steven F., The Theory of Linear Models and Multivariate Analysis.

Rice, John A., Mathematical Statistics and Data Analysis, 2nd ed. pp 509.

14.4.3 Column Relationships Anova Algorithm

The Anova option computes the difference between groups by comparing the mean values of the data in each group. The results are obtained by testing the null hypothesis; the hypothesis that there is no difference between the means of the groups. More formally, the p-value is the probability of the actual *or a more extreme* outcome under the null-hypothesis.

Note: If there are empty values in the data set, the data set will first be reduced to the rows containing values for both the first and the second column.

► For each combination of category and value column, a p-value is computed as follows:

1. Records are grouped according to their value in the category column.

2. The total mean value of the value column is computed.

$$\bar{x}_{tot} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

3. The mean within each group is computed.
4. The difference between each value and the mean value for the group is calculated and squared.
5. The squared difference values are added. The result is a value that relates to the total deviation of records from the mean of their respective groups. This value is referred to as the *sum of squares within groups*, or **S2Wthn**.
6. For each group, the difference between the total mean and the group mean is squared and multiplied by the number of values in the group. The results are added. The result is referred to as the *sum of squares between groups*, or **S2Btwn.**

$$S2Btwn = N_1(\bar{x}_1 - \bar{x}_{tot})^2 + N_2(\bar{x}_2 - \bar{x}_{tot})^2 + \ldots + N_N(\bar{x}_N - \bar{x}_{tot})^2$$

7. The two sums of squares are used to obtain a statistic for testing the null hypothesis, the so called F-statistic. The F-statistic is calculated as:

$$F = \frac{S2Btwn/dfB}{S2Wthn/dfW}$$

   where, *dfB* (degree of freedom between groups) equals the number of groups minus 1, and *dfW* (degree of freedom within groups) equals the total number of values minus the number of groups.
8. The F-value is distributed according to the F-distribution (commonly presented in mathematical tables/handbooks). The F-value, in combination with the degrees of freedom and an F-distribution table, yields the p-value.

The p-value is the probability of the actual *or a more extreme* outcome under the null-hypothesis. If the p-value is below a certain level (usually 0.05) it is assumed that there is a significant difference between the group means. The lower the p-value, the larger the difference.

Note: A very small p-value may also arise if an effect is tiny but the sample sizes are large. Similarly, a higher p-value can arise if the effect is large but the sample size is small.

14.4.4 Column Relationships Kruskal-Wallis Algorithm

The Kruskal-Wallis option calculates the p-value under the assumption that there are no empty values in the data set.

Note: If there are empty values in the data set, the data set will first be reduced to the rows containing values for both the first and the second column.

The Kruskal-Wallis test can be seen as the nonparametric version of a one-way Anova. The test uses the ranks of the data rather than their actual values to calculate the test statistic. This test can be used as an alternative to the Anova, when the assumption of normality or equality of variance is not met.

For k groups of observations, all N observations are combined into one large sample, the result is sorted from smallest to largest values and ranks are assigned, assigning ties (when values occur more than once) the same rank.

Now, after regrouping the observations, the sum of the ranks are calculated in each group. The test statistic, H, is then:

$$H = \frac{\frac{12}{N(N+1)} \sum_{i=1}^{k} N_i \left(\bar{R}_i - \frac{(N+1)}{2} \right)^2}{1 - \frac{\sum_{j=1}^{m} \left(T_j^3 - T_j \right)}{\left(N^3 - N \right)}}$$

k = number of categories
N = number of cases in the sample
N_i = number of cases in the i^{th} category
$\bar{R}_i$ = average of the ranks in the i^{th} category
T_j = ties for the j^{th} unique rank
m = number of unique ranks
A p-value can be calculated from the test statistic by referring the value of H to a table with the chi-square distribution with k-1 degrees of freedom. This can be used to test the hypothesis that all k population distributions are identical.

Example:

For the following data set, the different parameters used in the test are as follows:

Data set		Parameters	
Category	**Value**	**Rank**	**Ties**
A	1	1	1
A	3	2.5	2
A	3	2.5	
B	5	5.5	2
B	5	5.5	
B	4	4	1

k = 2
N = 6
N_A= 3
N_B= 3
$\bar{R}_A$ = 2
$\bar{R}_B$ = 5
T_1= 1
T_2= 2
T_3= 2
T_4= 1
m = 4
H = 4.091

14.4.5 Column Relationships Chi-square Independence Test Algorithm

The Chi-square option calculates the p-value under the assumption that there are no empty values in the data set.

Note: If there are empty values in the data set, the data set will first be reduced to the rows containing values for both the first and the second column.

Let n be the total number of values and denote by I the number of unique values in the first column and by J the number of unique values in the second column. Also for $i = 1, ..., I$ let n_i be the number of occurrences of the i^{th} unique value and for $j = 1, ..., J$, let n_j be the number of occurrences of the j^{th} unique value. If we now let n_{ij} denote the number of rows containing the i^{th} unique value in the first column and the j^{th} unique value in the second column, the Pearson's chi-square statistic is:

$$T = \sum_{i=1}^{I} \sum_{j=1}^{J} \frac{(n_{ij} - n_i n_j / n)^2}{n_i n_j / n}$$

with *(I-1)(J-1)* degrees of freedom.

The p-value is then calculated from the chi-square distribution with *(I-1)(J-1)* degrees of freedom.

Reference

Rice, John A., Mathematical Statistics and Data Analysis, 2nd ed. pp 489-491.

14.4.6 Requirements on Input Data for Column Relationships

Experimental design

In this tool, a one-way layout of Anovas has been employed. This means that the experimental design should be of the type where the outcome of a single continuous variable is compared between different groups. The tool cannot be used to analyze experiments where two or more variables vary together.

Tip: You can create a new column using the Concatenate function (or '&') of the New Column from Expression tool (**Edit > New Column > From Expression...**) if you want to analyze two or more variables together.

Distribution of data

The Anova and Linear regression comparisons assume the following:

- The data is approximately normally distributed.
- The variances of the separate groups, or the variances of the errors in the case of linear regression, are approximately equal.

If the data do not fulfill these conditions, the comparisons may produce unreliable results.

Note: If more than one test is performed at the same time, then it is more likely that there will be at least one p-value less than 0.05 than in the case where only one test is performed. A guideline of when to reject the hypothesis is then "Reject the hypothesis if the p-value is less than 0.05 divided by the number of tests". This is called the Bonferroni method for multiple tests.

15 Index

D

Q

R

S