



MultiDendrograms 3.2

Manual

Departament d'Enginyeria



Informàtica i
Matemàtiques



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<http://deim.urv.cat/~sgomez/multidendrograms.php>



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Introduction

MultiDendrograms is a simple yet powerful program to make the Hierarchical Clustering of real data, distributed under an Open Source license. Starting from a distances (or weights) matrix, *MultiDendrograms* calculates its dendrogram using the most common Agglomerative Hierarchical Clustering algorithms (e.g. Single Linkage, Complete Linkage, Unweighted Average and Ward), allows the tuning of many of the graphical representation parameters, and the results may be easily exported to file.

MultiDendrograms implements the variable-group algorithms in [1] to solve the non-uniqueness problem found in the standard pair-group algorithms and implementations. This problem arises when two or more minimum distances between different clusters are equal during the amalgamation process. The standard approach consists in choosing a pair, breaking the ties between distances, and proceeds in the same way until the final hierarchical classification is obtained. However, different clusterings are possible depending on the criterion used to break the ties (usually a pair is just chosen at random!), and the user is unaware of this problem.

The variable-group algorithms group more than two clusters at the same time when ties occur, given rise to a graphical representation called *multidendrogram*. Their main properties are:

- When there are no ties, the variable-group algorithms give the same results as the standard pair-group ones.
- They always give a uniquely determined solution.
- In the multidendrogram representation for the results one can explicitly observe the occurrence of ties during the agglomerative process. Furthermore, the height of any fusion interval (the *bands* in the program) indicates the degree of heterogeneity inside the corresponding cluster.

In this manual we show how to prepare the data file, load it into *MultiDendrograms*, the meaning of the parameters of the program, and how to export the results to file.

The main characteristics of *MultiDendrograms* are:

- Multiplatform, runs in Windows, Linux and MacOS.
- Graphical user interface.
- Also command-line direct calculation without graphical user interface.
- Implementation of variable-group algorithms for Agglomerative Hierarchical Clustering.
- Works with distance and weight matrices.
- Many parameters for the customization of the dendrogram layout.
- Navigation through the dendrogram information in a folder-like window.
- Calculation of corresponding ultrametric matrix.
- Calculation of deviation measures such as the cophenetic correlation coefficient.
- Save dendrogram details in text and Newick tree format.
- Save dendrogram image as JPG, PNG and EPS.

MultiDendrograms web page: <http://deim.urv.cat/~sgomez/multidendrograms.php>

Please cite [1] if you use *MultiDendrograms* in your publications.

[1] Alberto Fernández and Sergio Gómez, *Solving Non-Uniqueness in Agglomerative Hierarchical Clustering Using Multidendrograms*, Journal of Classification **25** (2008) 43-65

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1. Input data

The data file must represent a distances (or weights) matrix, like the one in the following table:

	a	b	c	d
a	0	2	4	7
b	2	0	2	5
c	4	2	0	3
d	7	5	3	0

There are three different arrangements these data can be stored in a text file such that *MultiDendrograms* may accept them: matrix, triangular and list formats.

Matrix-like file format

Each line in the text file contains a data matrix row. The characteristics of these files are:

- The matrix must be symmetric, and the diagonal elements should be zeros (any value different from zero is ignored).
- Within each row, the elements are separated by: spaces (' '), tab character, semicolon (';'), comma (',') or vertical bar ('|').
- It is possible to include the names in an additional first row or column, but not in both.
- If present, the labels of the nodes can not contain any of the previous separators.

Some different representations for the previous data could be:

Node_a	Node_b	Node_c	Node_d
0.0	2.0	4.0	7.0
2.0	0.0	2.0	5.0
4.0	2.0	0.0	3.0
7.0	5.0	3.0	0.0

Matrix-like with node labels in first row, data separated by tabs

a	0.0	2.0	4.0	7.0
b	2.0	0.0	2.0	5.0
c	4.0	2.0	0.0	3.0
d	7.0	5.0	3.0	0.0

Matrix-like with node labels in the first column, data separated by spaces

0.0,2.0,4.0,7.0
2.0 0.0 2.0 5.0
4.0 2.0 0.0 3.0
7.0 5.0;3.0 0.0

Matrix-like file without node labels, data separated by all kind of separators

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Triangular-like file format

The text file contains the lower triangular data of the distances or weights matrix. The characteristics of these files are:

- The diagonal elements must be included and should be zeros (any value different from zero is ignored).
- Within each row, the elements are separated by: spaces (' '), tab character, semicolon (';'), comma (',') or vertical bar ('|').
- It is possible to include the names in an additional first row or column, but not in both.
- If present, the labels of the nodes can not contain any of the previous separators.

Some different representations for the previous data could be:

```
Alice Bob Carol Dave
0
2 0
4 2 0
7 5 3 0
```

Triangular-like with node labels in first row, data separated by tabs

```
a 0
b 2 0
c 4 2 0
d 7 5 3 0
```

Triangular-like with node labels in the first column, data separated by spaces

```
0
2 0
4 2 0
7 5 3 0
```

Triangular-like file without node labels

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List-like file format

Each line in the text file contains three elements, which represent the labels of two nodes and the distance (or weight) between them. The characteristics of these files are:

- The separators between the three elements may be: spaces (' '), tab character, semicolon (';'), comma (',') or vertical bar ('|').
- The labels of the nodes can not contain any of the previous separators.
- Distances from an element to itself (e.g. "a a 0.0") are ignored.
- *MultiDendrograms* accepts either the presence or absence of the symmetric data elements, i.e. if the distance between nodes a and b is 2.0, it is possible to include in the list the line "a b 2.0", or both "a b 2.0" and "b a 2.0". If both are present, the program checks if the values are equal.

For example, three list-like files for the previous data could be:

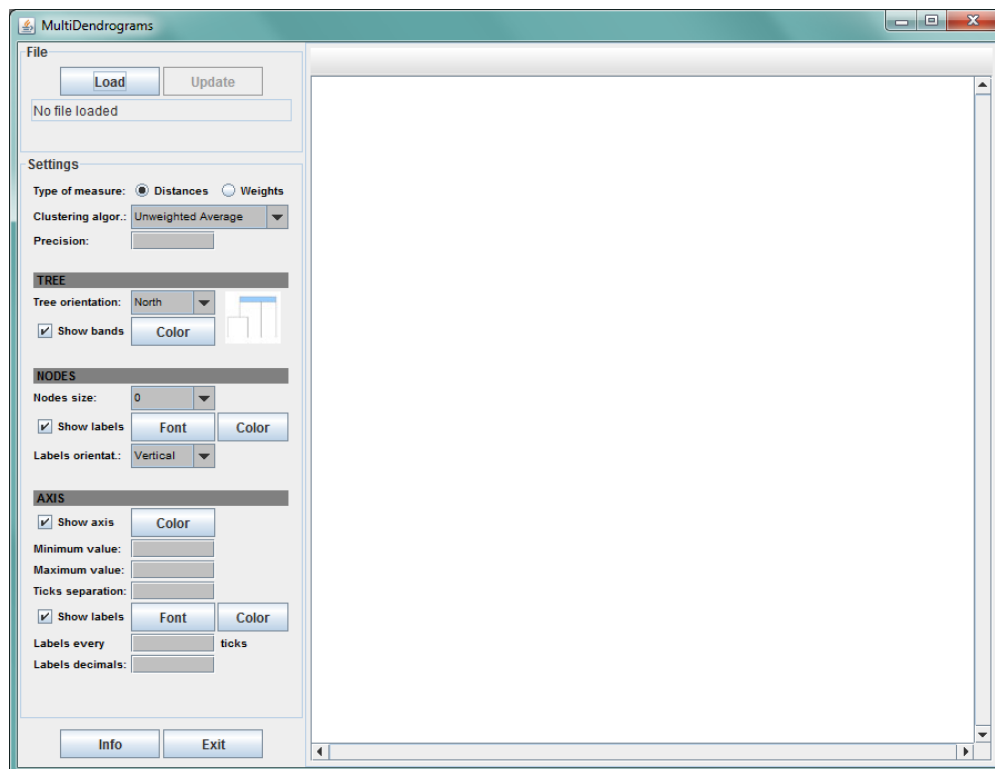
<div>a b 2 a c 4 a d 7 b c 2 b d 5 c d 3</div>	<div>a b 2 a c 4 a d 7 b a 2 b c 2 b d 5 c a 4 c b 2 c d 3 d a 7 d b 5 d c 3</div>	<div>a a 0 a b 2 a c 4 a d 7 b a 2 b b 0 b c 2 b d 5 c a 4 c b 2 c c 0 c d 3 d a 7 d b 5 d c 3 d d 0</div>
Simple list	Complete list	Complete list

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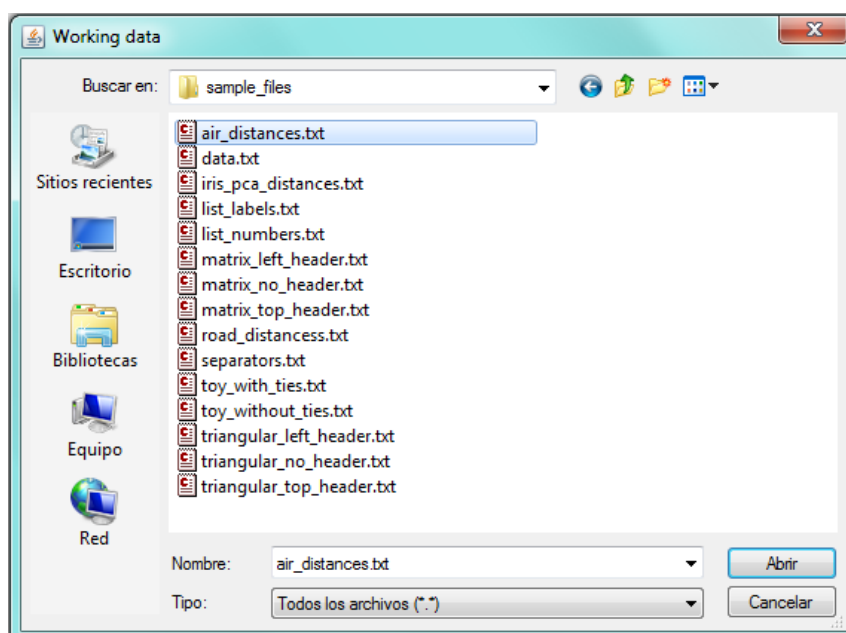
2. Loading data

Once we have our data in a compatible format, we can load them into *MultiDendrograms*.

1. Choose the desired settings, mainly the Type of measure and the Clustering algorithm. These settings will be explained in detail in the next sections.
2. Click on the 'Load' button:

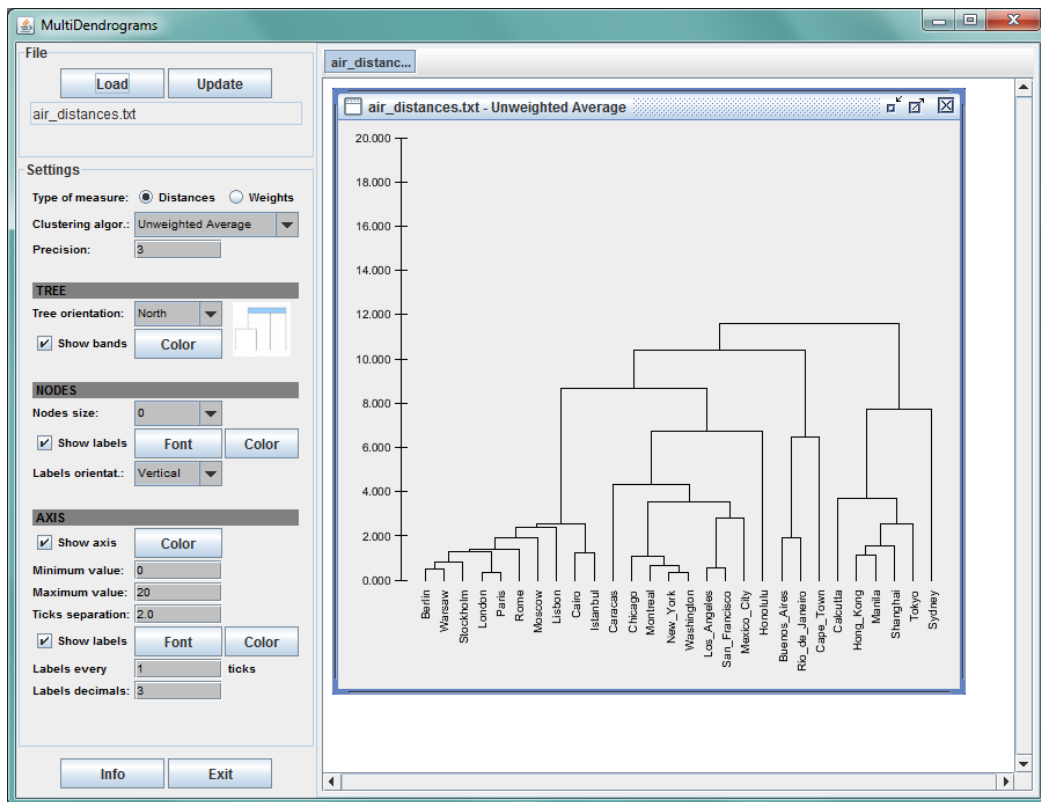


3. Select the file to open and then click on the 'Open' button:



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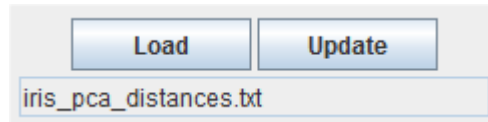
4. Now the data is loaded and its dendrogram representation is shown:



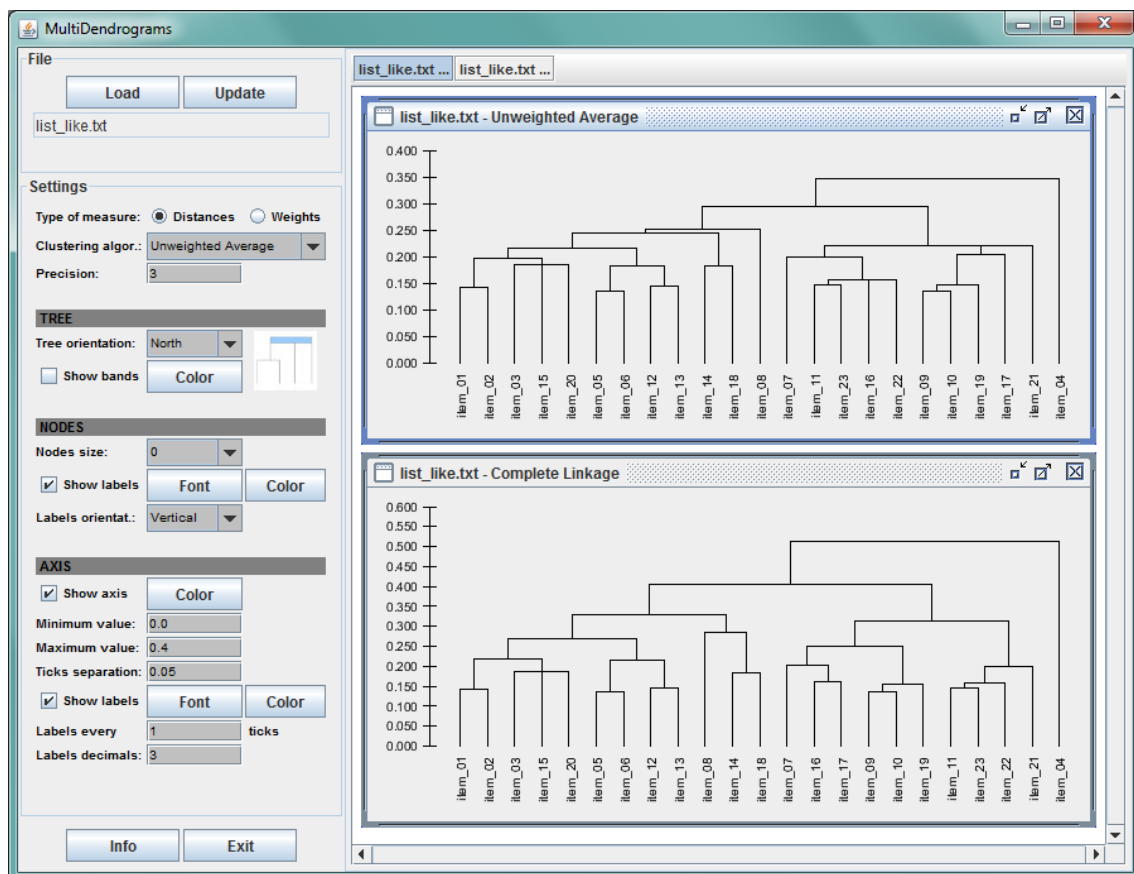
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3. Actions

MultiDendrograms only has two action buttons, **Load** and **Update**. **Load** is used to read data from a file and create a new window for the dendrogram, using the current values of the parameters, while **Update** is needed for the actualization of the active dendrogram when one or more parameters are changed. Below these buttons it is shown the name of the data file of the active dendrogram.



It is possible to load the same data file several times, in order to compare the dendrogram appearance for different parameters settings.



The parameters shown always correspond to the active (selected) dendrogram window.

Finally, there are two additional buttons, **Info** to show the information of the program, and **Exit** to quit the application.



4. Settings

The program automatically applies default values to the parameters depending on the data loaded, which should be adjusted as desired. The following figure shows the settings tab, with four different areas corresponding to the main data representation, tree, nodes and axis settings respectively:

The screenshot shows a 'Settings' dialog box with four main sections: 'Type of measure', 'Clustering algor.', 'Precision', 'TREE', 'NODES', and 'AXIS'. The 'Type of measure' section has radio buttons for 'Distances' (selected) and 'Weights'. The 'Clustering algor.' section has a dropdown menu set to 'Unweighted Average'. The 'Precision' section has a text input field set to '3'. The 'TREE' section has a 'Tree orientation' dropdown set to 'North', a 'Show bands' checkbox (unchecked), and a 'Color' button. The 'NODES' section has a 'Nodes size' dropdown set to '0', a 'Show labels' checkbox (checked), 'Font' and 'Color' buttons, and a 'Labels orientat.' dropdown set to 'Vertical'. The 'AXIS' section has a 'Show axis' checkbox (checked), a 'Color' button, 'Minimum value' (0.0), 'Maximum value' (0.4), 'Ticks separation' (0.05), a 'Show labels' checkbox (checked), 'Font' and 'Color' buttons, 'Labels every' (1 ticks), and 'Labels decimals' (3).

Section	Parameter	Value
General	Type of measure	Distances
	Clustering algor.	Unweighted Average
	Precision	3
TREE	Tree orientation	North
	Show bands	False
	Color	Default
NODES	Nodes size	0
	Show labels	True
	Font	Default
	Color	Default
AXIS	Labels orientat.	Vertical
	Show axis	True
	Color	Default
	Minimum value	0.0
	Maximum value	0.4
	Ticks separation	0.05
	Show labels	True
	Font	Default
Color	Default	
Labels every	1 ticks	
Labels decimals	3	

Changes in the main data representation parameters affect the structure of the dendrogram tree, thus it needs to be fully recalculated, operation which may take several seconds, even minutes (depending of the data size and the computer speed). On the other hand, changes in the tree, nodes and axis settings only modify the visual representation of the dendrogram, which are much faster to update.

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Main data representation settings

Type of measure: ☒ Distances ☐ Weights
Clustering algor.: Complete Linkage
Precision: 3

- **Type of measure:** It allows choosing between two kinds of measures, **distances** and **weights**. Choose between them according to the meaning of the loaded data. With **distances**, the closer the elements the lower their distance. On the contrary, with **weights**, the closer the elements the larger their weight. By default, **distances** is selected.

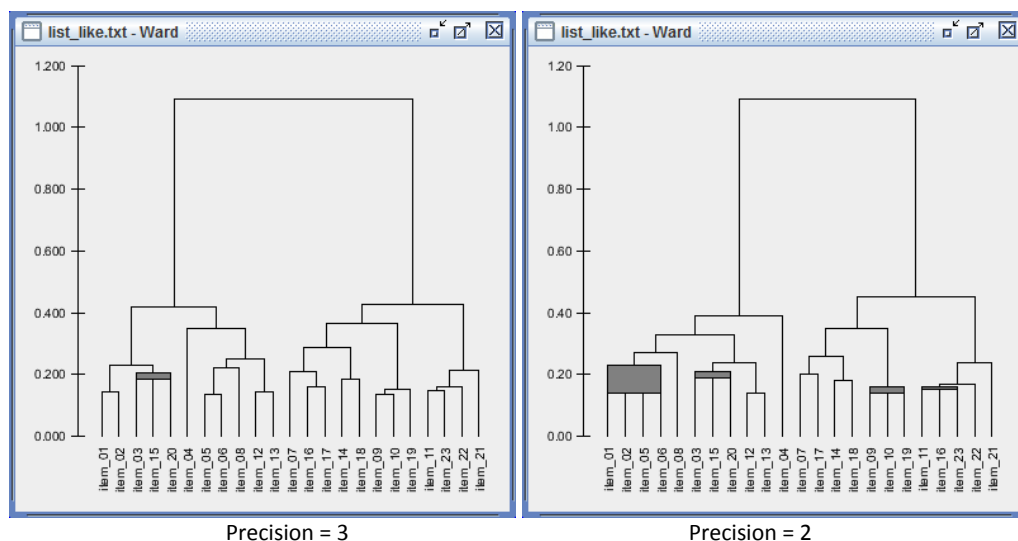
Type of measure: ☒ Distances ☐ Weights

- **Clustering algorithm:** Seven clustering algorithms are available, **single linkage**, **complete linkage**, **unweighted average**, **weighted average**, **unweighted centroid**, **weighted centroid** and **ward**. By default, **unweighted average** is selected.

Clustering algor.: Complete Linkage
Single Linkage
Complete Linkage
Unweighted Average
Weighted Average
Unweighted Centroid
Weighted Centroid
Ward

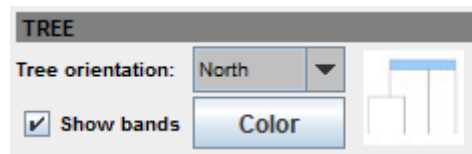
- **Precision:** Number of decimal significant digits of the data and for the calculations. This is a very important parameter, since equal distances at a certain precision may become different by increasing its value. Thus, it may be responsible of the existence of tied distances. The rule should be not to use a precision larger than the resolution given by the experimental setup which has generated the data. By default, the precision is set to that of the data value with the largest number of decimal significant digits.

Precision: 3

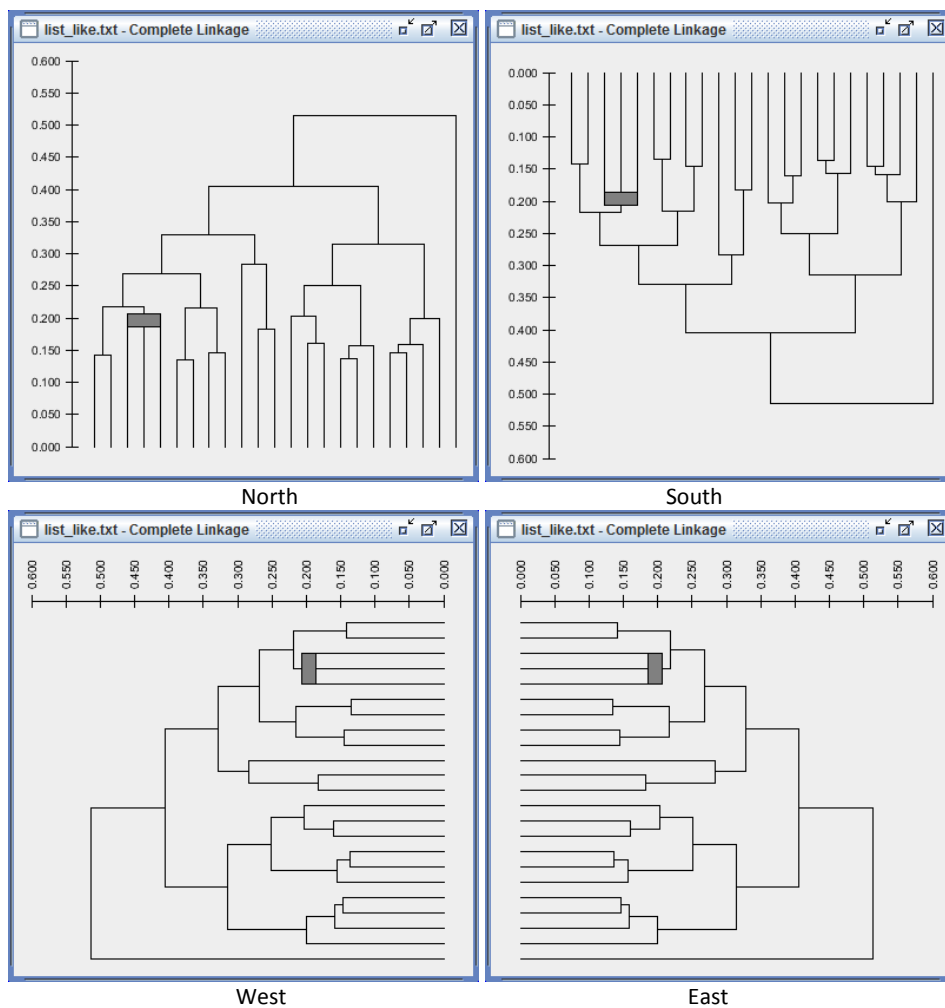
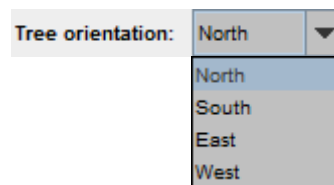


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Tree settings

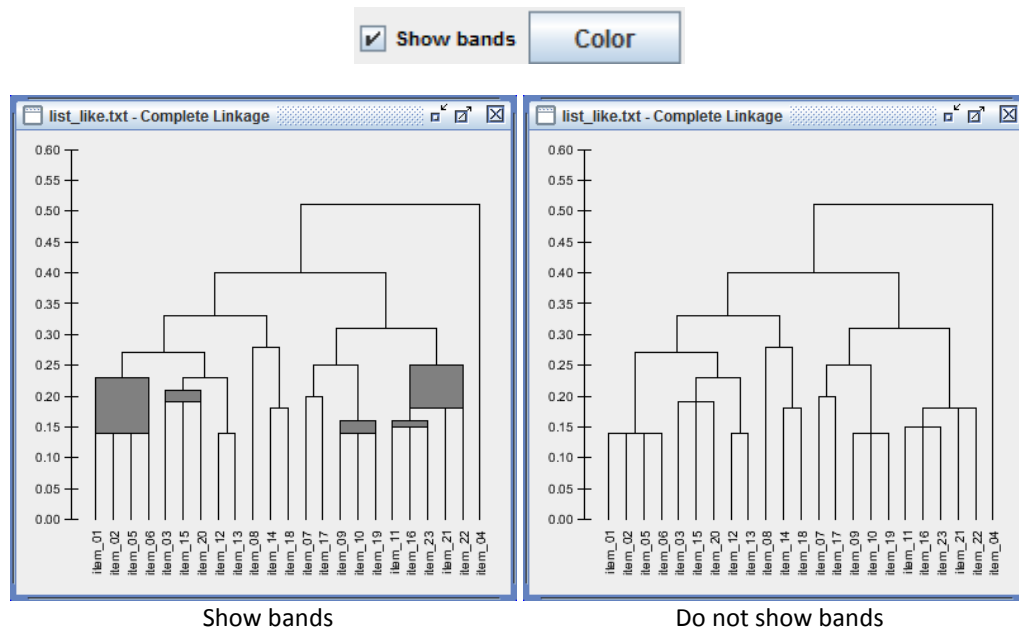


- **Tree orientation:** Four orientations are available, *north*, *south*, *east* and *west*, which refer to the relative position of the root of the tree. By default, *north* is selected.



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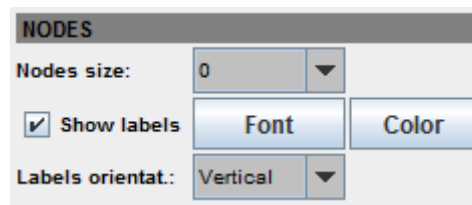
- **Show bands:** It allows showing a band or not in case of tied minimum distances between three or more elements, and selecting the color of the band. If selected, the bands show the heterogeneity of all the distances between the clustered elements. Otherwise, the elements are grouped at their minimum distance. By default, **show bands** is selected, and its default color is **light gray**.



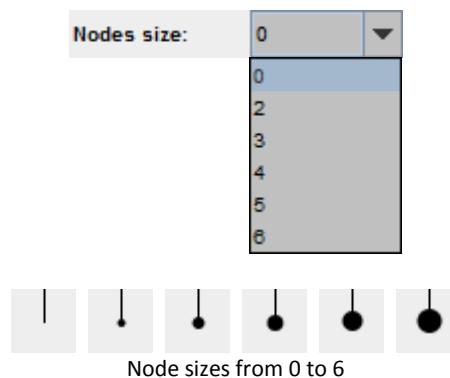
Let us explain the meaning of the bands. In *MultiDendrograms*, if several pairs of elements share the same minimal distance, they are clustered together in one step. For instance, suppose that the minimal distance is 0.4, and that they correspond to the tied pairs (A,B) and (B,C). *MultiDendrograms* puts them together in the same cluster (A,B,C) at height 0.4. However, if the distance (A,C) is 0.5, it is possible to represent the cluster (A,B,C) as a rectangle which spans between heights 0.4 and 0.5, thus showing the heterogeneity of the clustered elements.

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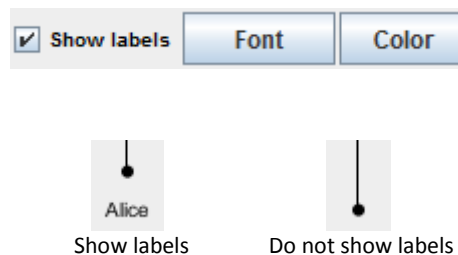
Nodes settings



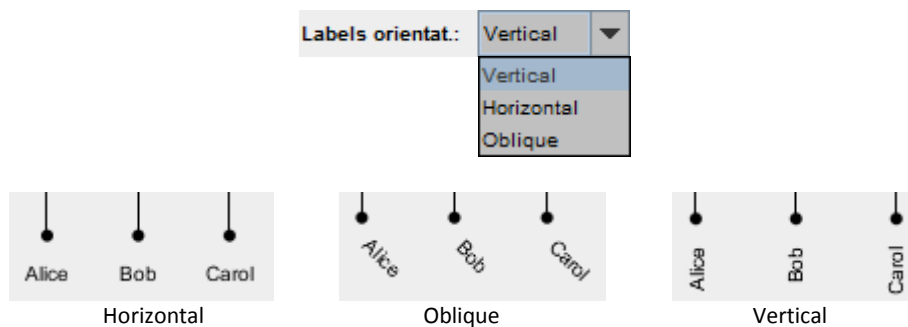
- **Nodes size:** Six different node sizes are available. By default, 0 is selected (i.e. nodes not shown):



- **Show labels:** It allows showing or not the labels of the nodes, and selecting their color and font. By default, **show labels** is selected, the font is **Arial** and the color is **black**:



- **Labels orientation:** Three orientations are available: **vertical**, **horizontal** and **oblique**. By default, **vertical** is selected:

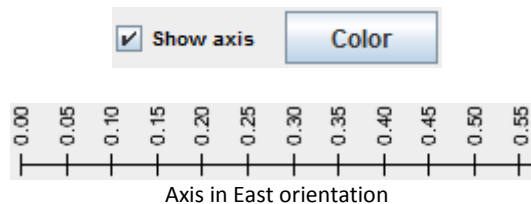


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Axis settings

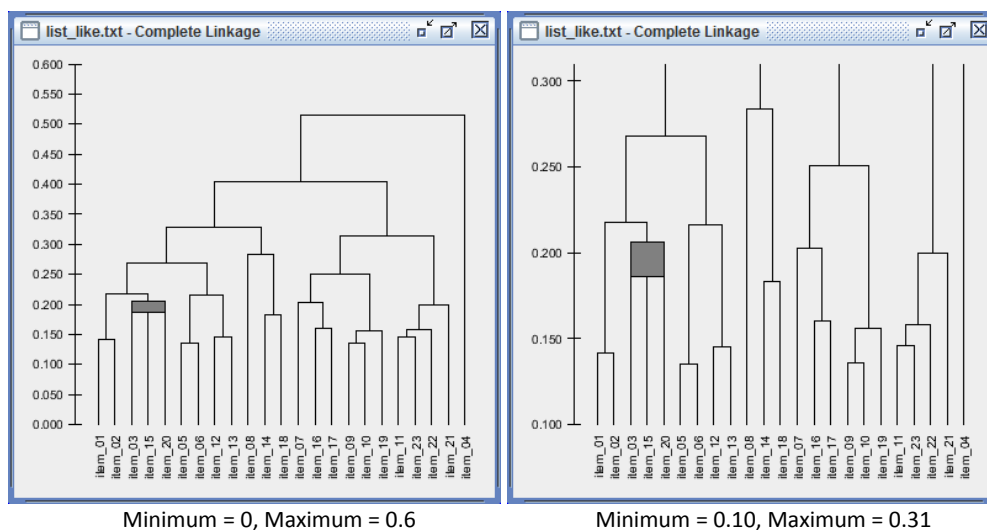
AXIS		
<input checked="" type="checkbox"/> Show axis	Color	
Minimum value:	0	
Maximum value:	0.570	
Ticks separation:	0.050	
<input checked="" type="checkbox"/> Show labels	Font	Color
Labels every	1	ticks
Labels decimals:	3	

- **Show axis:** It allows showing or not the axis, and selecting its color. By default, **show axis** is selected and the selected color is **black**.



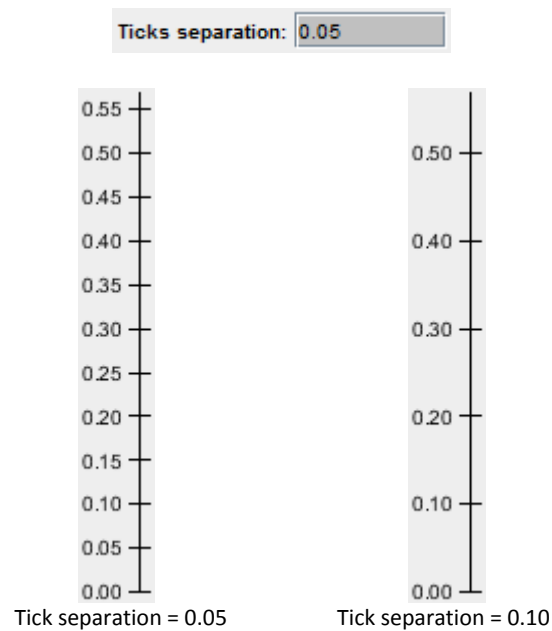
- **Minimum value / Maximum value:** They allow choosing the minimum and maximum value of the axis, respectively. They also affect the view of the dendrogram. The default values are calculated from the data.

Minimum value:	0.10
Maximum value:	0.31

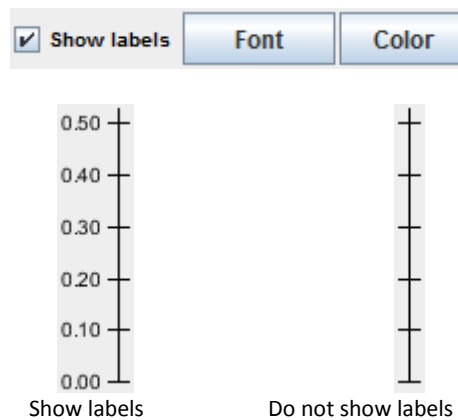


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- **Tick separation:** It allows choosing the separation between consecutive ticks of the axis. The default value is calculated from the data:

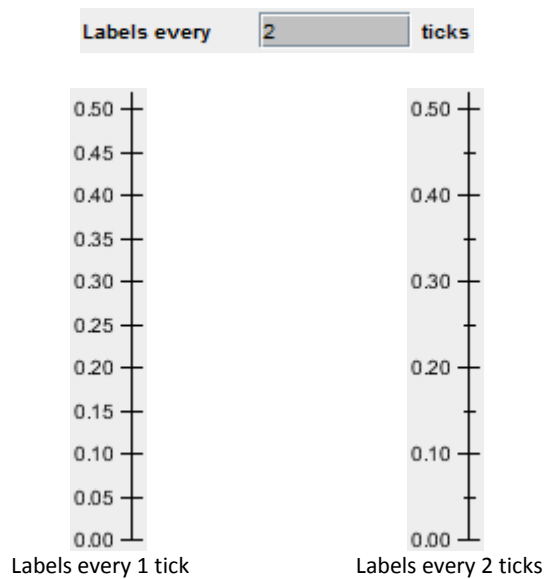


- **Show labels:** It allows showing or not the labels of the axis, and selecting their color and font. By default, **show labels** is selected, the font is **Arial** and the color is **black**.

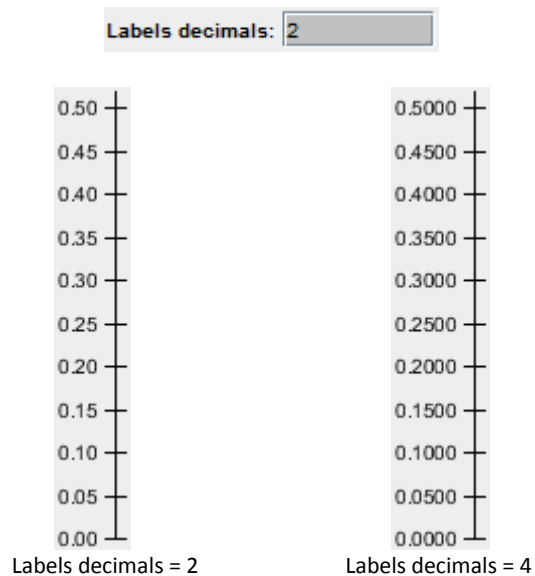


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- **Labels every ... ticks:** Number of consecutive ticks to find the next labeled tick. By default is set to 1.

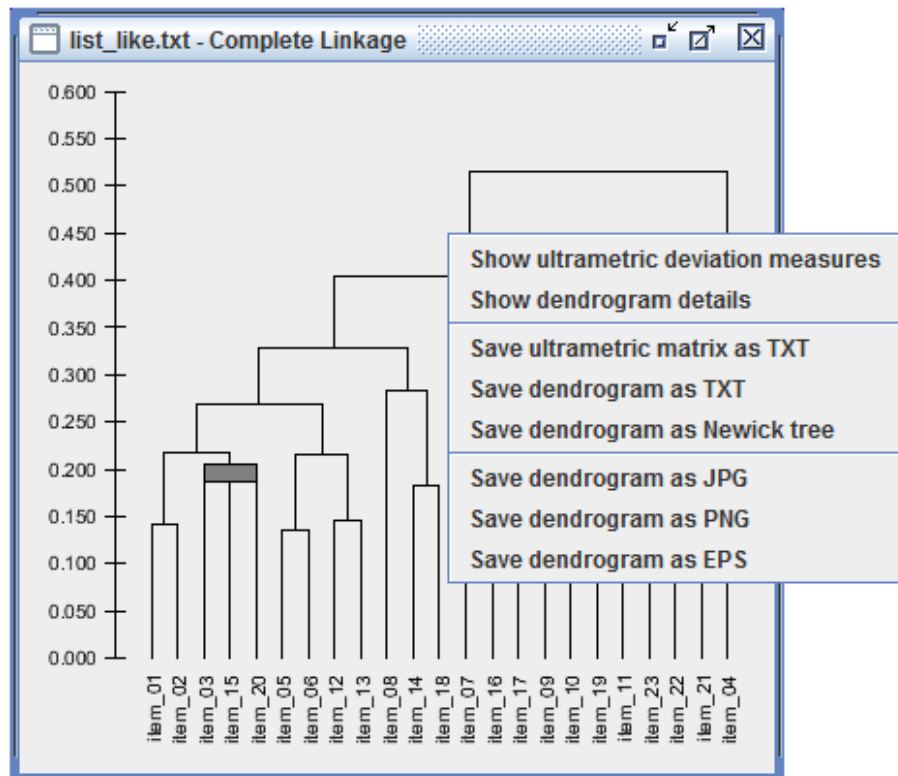


- **Labels decimals:** Number of decimal digits of the tick labels. By default it is set equal to the **precision** parameter.

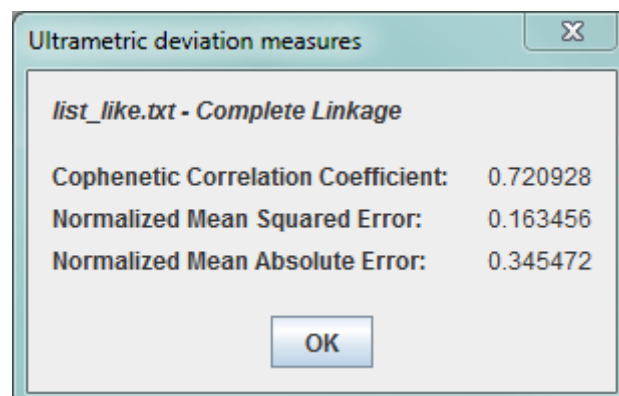


5. Analyzing and exporting results

The contextual menu, available by right-clicking the dendrogram windows, gives access to several options for analyzing and exporting the results to file.



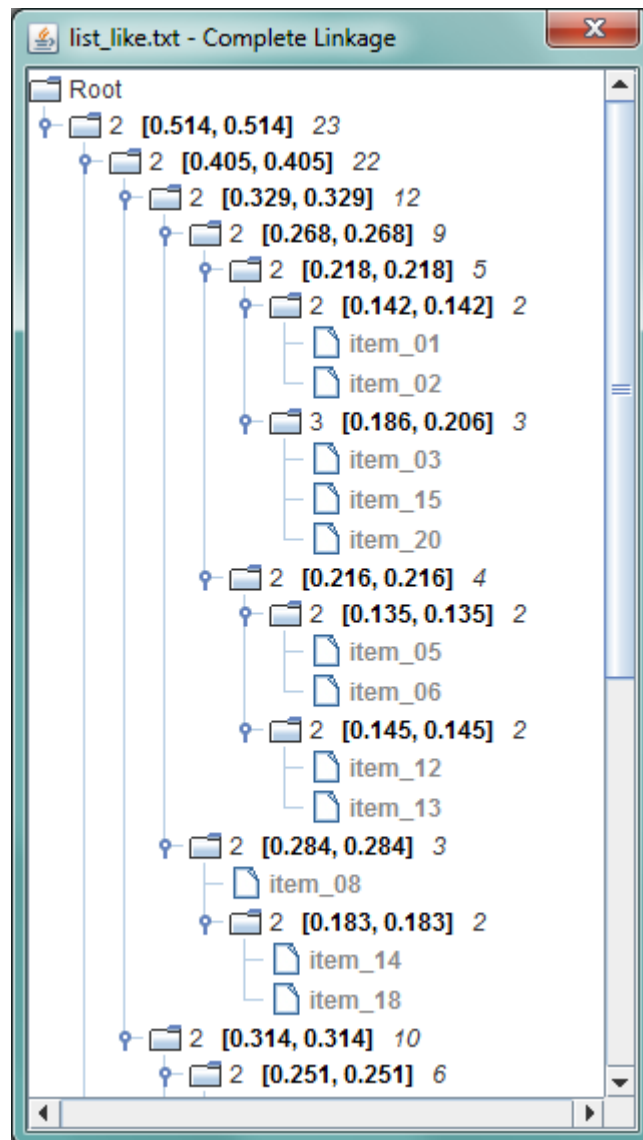
- **Show ultrametric deviation measures:** Calculates the ultrametric matrix corresponding to the active dendrogram and obtains three different deviation measures between the original and the ultrametric matrices: the **cophenetic correlation coefficient**, the **normalized mean squared error** and the **normalized mean absolute error**.



Deviation measures

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- **Show dendrogram details:** Opens a window which contains all the information of the dendrogram in a navigable folder-like structure:



The available information in the details window is:

- Number of children of each interior node of the dendrogram. The interior nodes in the dendrogram representation correspond to the clusters found during the agglomeration process, and the children may be other interior nodes or data items.
- Maximum and minimum distances at which the children of an interior node are joined to form a new cluster. These values may only be different in case of tied distances, which become a band in the multidendrogram representation.
- Number of data items (leaves of the tree) under each interior node of the dendrogram.
- List of children of each interior node, which may be either interior nodes or data items.

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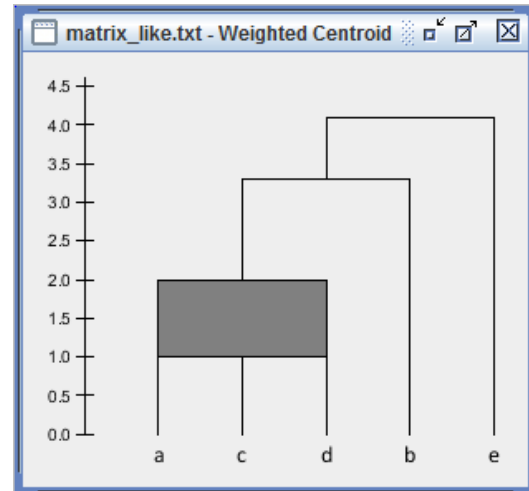
- **Save ultrametric matrix as TXT:** Calculates the ultrametric matrix corresponding to the loaded data and saves it to a text file in matrix form, with the nodes labels in the first row. This text file can then be easily loaded into any text editor or spreadsheet application (e.g. Microsoft Excel).

a	b	c	d	e
0.0	1.2	1.0	2.0	5.0
1.2	0.0	3.0	7.0	4.0
1.0	3.0	0.0	1.0	8.0
2.0	7.0	1.0	0.0	6.0
5.0	4.0	8.0	6.0	0.0

Original distances matrix

a	c	d	b	e
0.0	1.0	1.0	3.3	4.1
1.0	0.0	1.0	3.3	4.1
1.0	1.0	0.0	3.3	4.1
3.3	3.3	3.3	0.0	4.1
4.1	4.1	4.1	4.1	0.0

Ultrametric matrix



- **Save dendrogram as TXT:** Saves the dendrogram details to a text file.

```
+ 2 [4.1, 4.1] 5
+ 2 [3.3, 3.3] 4
+ 3 [1.0, 2.0] 3
* a
* c
* d
* b
* e
```

Dendrogram in text format

- **Save dendrogram as Newick tree:** Saves the dendrogram details in Newick tree format (see http://en.wikipedia.org/wiki/Newick_format).

```
((a:1.0,c:1.0,d:1.0):2.3,b:3.3):0.8,e:4.1);
```

Dendrogram in Newick format

In this format the information given by the bands is lost, only the minimum distance is used. However, it has the advantage that is a standard format used in many other applications, thus allowing their use to generate other graphical representations.

- **Save dendrogram as JPG, PNG, EPS:** It is also possible to save the image of the dendrogram in three different formats (JPG, PNG and EPS) using their corresponding **Save dendrogram as ...** context menu items.

6. Command-line direct calculation

It is possible to use *MultiDendrograms* in command-line mode to calculate the dendrogram without the graphical interface. This is useful in several situations:

- To automate the generation of many dendrograms using scripts.
- When there is no need of a plot of the dendrogram.
- When the plot of the dendrogram is to be performed with a different program.
- When the number of elements is too large to allow a graphical representation.
- To be able to call *MultiDendrograms* from a different application.

The input parameters of a command-line call are:

- The name of the input data file, in matrix, triangular or list format.
- The type of measure: distances or weights.
- The clustering algorithm: single linkage, complete linkage, unweighted average, weighted average, unweighted centroid, weighted centroid or ward.
- The precision, i.e. the number of decimal significant digits of the data and for the calculations. This parameter is optional, if not given it is calculated from the data. However, the rule should be not to use a precision larger than the resolution given by the experimental setup which has generated the data.

The output results are:

- A file with the dendrogram tree in text format.
- A file with the dendrogram in Newick format.
- A file with the ultrametric matrix.
- The ultrametric deviation measures: the cophenetic correlation coefficient, the normalized mean squared error and the normalized mean absolute error.

The syntax of a command-line direct calculation is:

java -jar multidendrograms.jar -direct FILE_NAME SIM_TYPE METHOD [PRECISION]

The details are given in Appendix A.

APPENDIX A. Requirements, installation and execution

Requirements

To run *MultiDendrograms* it is necessary to have installed a recent version of the Java Runtime Environment (JRE):

- Java: <http://java.com>

You can check if Java is already in your computer following these steps:

1. Open a shell or command prompt (In Windows: Start -> Run -> type "cmd" -> Enter):
2. Type: `java -version`

If JRE is installed, you will get its version.

Installation

MultiDendrograms does not require installation. Just unpack the main ZIP file into a folder using any unzip program, e.g. 7-zip, iZarc, WinRAR or WinZip.

Basic execution

- Windows: double-click **multidendrograms.bat** or **multidendrograms.jar**
- Linux: run **multidendrograms.sh** or **multidendrograms.jar**
- MacOS: double-click **multidendrograms.jar** or run **multidendrograms.sh**

Advanced execution

In the command-line:

`java -jar multidendrograms.jar [options]`

The program accepts these options:

```
-h | -help
    Syntax help

-loglevel LEVEL
    Sets the verbosity level of the logger
    LEVEL: verbosity level, one of
        OFF
        SEVERE
        WARNING
        INFO
        CONFIG
        FINE
        FINER
        FINEST
        ALL
    Default value of LEVEL: WARNING
```

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-direct FILE_NAME SIM_TYPE METHOD [PRECISION]

Direct calculation of the multidendrogram without graphic interface

FILE_NAME: name of the data file name

SIM_TYPE: similarity type, one of

D, DISTANCES

W, WEIGHTS

METHOD: agglomeration type, one of

SL, SINGLE_LINKAGE

CL, COMPLETE_LINKAGE

UA, UNWEIGHTED_AVERAGE

WA, WEIGHTED_AVERAGE

UC, UNWEIGHTED_CENTROID

WC, WEIGHTED_CENTROID

WD, WARD

PRECISION : number of decimal significant digits, auto if missing value

There is a sample script file to show some direct calculations:

- Windows: **multidendrograms-cmd.bat**
- Linux and MacOS: **multidendrograms-cmd.sh**

Examples:

java -jar multidendrograms.jar

java -jar multidendrograms.jar -loglevel off

java -jar multidendrograms.jar -direct data.txt DISTANCES Complete_Linkage 3

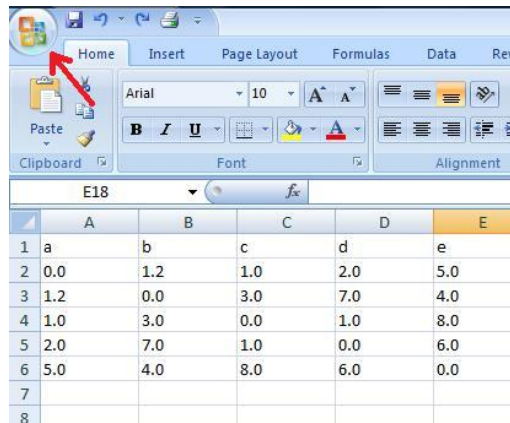
java -jar multidendrograms.jar -direct data.txt D CL

java -jar multidendrograms.jar -direct data.txt D CL 3

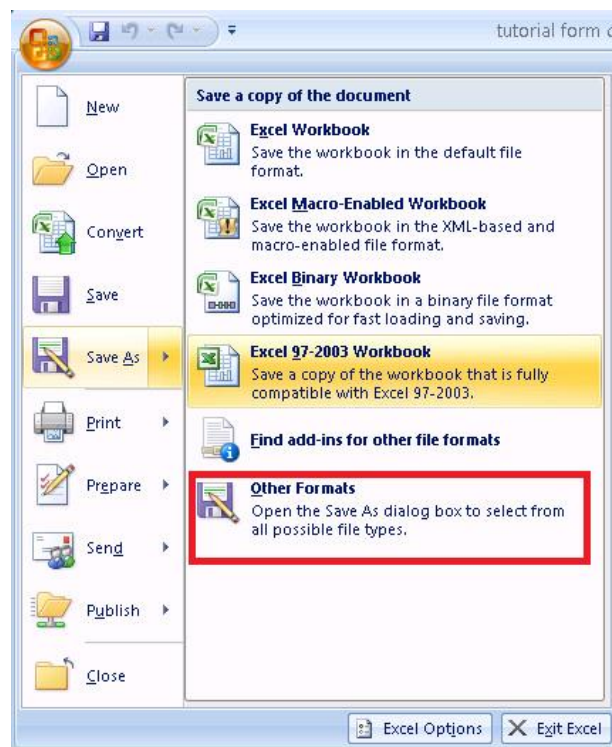
APPENDIX B. Preparing input data with Microsoft Excel

MultiDendrograms cannot load data directly from a Microsoft Excel (or similar) file, we first need to save our data in a compatible format. We will assume Microsoft Excel 2007, but similar procedures apply to other versions and similar programs.

1. Click on the button with the Microsoft Office logo:

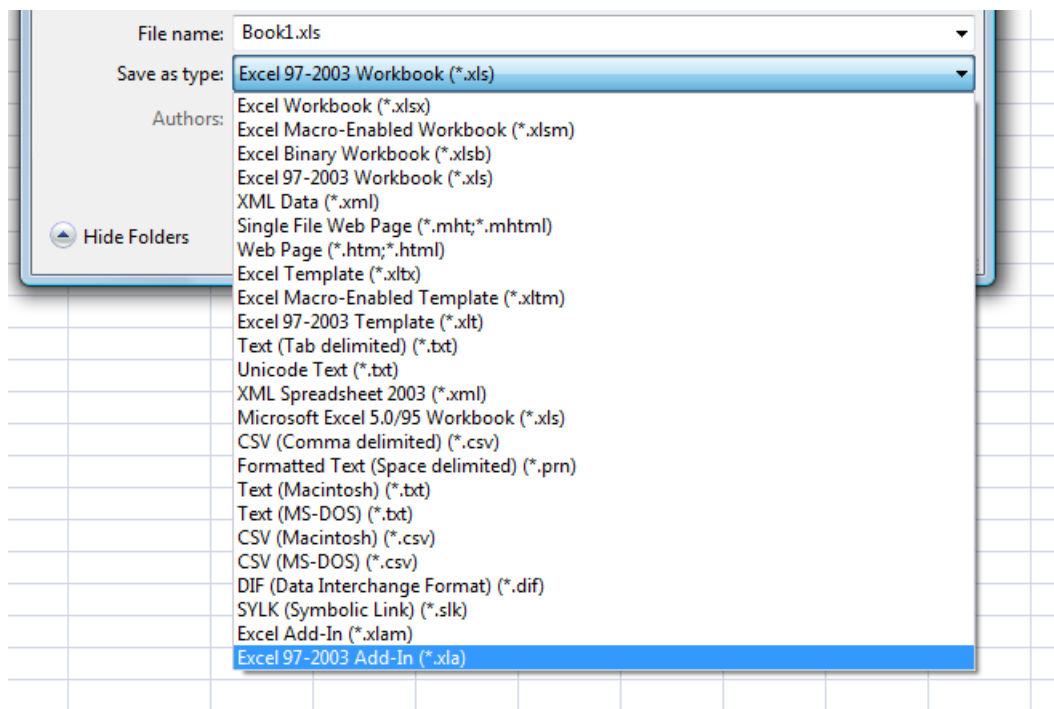


2. Select the option 'Save As' and then 'Other Formats':



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3. Now choose the file format to save the file:

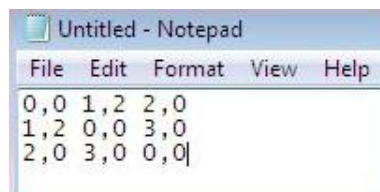


The compatible formats are the following:

- Text (Tab delimited)
- Unicode Text
- CSV (Comma delimited)
- Formatted text (Space delimited)
- Text (Macintosh)
- Text (MS-DOS)
- CSV (Macintosh)
- CSV (MS-DOS)

4. *MultiDendrograms* needs that decimal numbers use the character ‘.’ as the decimal symbol, e.g. “3.1416”. Unfortunately, some regional system configurations use different decimal symbols, e.g. in Spanish it is ‘,’ as in “3,1416”. In these cases, the previously exported file has to be edited to change the decimal symbol to ‘.’:

- Open the file with Notepad (or any other file editor):



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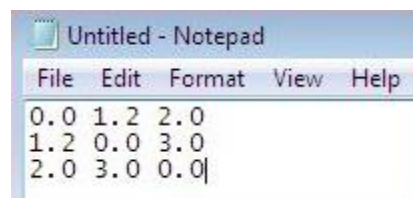
- Go to the 'Edit' menu and select 'Replace':



- Replace all appearances of ',' with ' .':



- Save the modified file:



APPENDIX C. Languages

By default, the graphical user interface of *MultiDendrograms* is shown in English. Currently, it is possible to choose between the following languages:

- English
- Catalan
- Spanish

In the `ini` folder there is a language file (e.g. `english.l`) for each of the languages available. The selection of the language is made in the first lines of the configuration file `dendo.ini` found in the `ini` folder. To change the selected language, just open `dendo.ini` in an editor, uncomment the desired language and comment the rest (comments start with a '#' character). For example, to choose English the contents should be:

```
# Language
language = ini/english.l
#language = ini/catalan.l
#language = ini/spanish.l
```

To translate *MultiDendrograms* to other languages, just create a new language file `newlanguage.l`, containing the translation of all the lines in any other language file, and add the corresponding line to the configuration file `dendo.ini`. If you send us your new language file, we can include it in future versions of *MultiDendrograms*.

APPENDIX D. History of changes

MultiDendrograms 3.2

- New format for dendrogram navigation and save as text file

MultiDendrograms 3.1

- Data in triangular form

MultiDendrograms 3.0

- Scrollbars in dendrograms panel
- Command-line direct calculation of multidendrogram
- Ward hierarchical clustering
- Check if new version is available
- Confirmation before closing
- Improved performance
- Major source code refactoring

MultiDendrograms 2.1

- Export dendrograms to Newick format
- Show calculation progress
- Improved GUI
- Improved performance

MultiDendrograms 2.0

- Completely new multiplatform (Windows, Linux, MacOS, etc.) application
- Added Graphical User Interface (GUI)
- Control of the dendrogram appearance
- Navigation through the dendrogram details
- Accepts distance and similarity matrices
- Export dendrograms to JPG, PNG and EPS
- Calculation of ultrametric deviation measures

MultiDendrograms 1.0

- Windows command-line application to compute multidendrograms
- Windows command-line application to compute ultrametric matrices
- Windows command-line application to generate EPS plots

APPENDIX E. License

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