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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 proximities (distances or similarities) 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 positive and negative distances and similarities.
- 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

1. Input data

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

	a	b	c	d
a	0	2	4	7
b	2	0	2	5
с	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
- 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.
- The diagonal elements are used in the non-uniform origin option.
- Blank lines and lines starting with the comment symbol ('#') are discarded.

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 0.0 2.0 5.0	4.0	7.0
b	2.0	0.0	2.0	5.0
С	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

a	0.5	2.0	4.0	7.0
b	2.0	1.0	2.0	5.0
С	4.0	2.0 1.0 2.0 5.0	0.0	3.0
d	7.0	5.0	3.0	3.0

Matrix-like with node labels in the first column, data separated by spaces, and non-zero diagonal values

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

Triangular-like file format

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

- 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.
- The diagonal elements are used in the non-uniform origin option.
- Blank lines and lines starting with the comment symbol ('#') are discarded.

Some different representations for the previous data could be:

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

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

Triangular-like file without node labels

Triangular-like file without node labels, and non-zero diagonal values

List-like file format

Each line in the text file contains three elements, which represent the labels of two nodes and the distance (or similarity) 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.
- *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.
- Diagonal elements, i.e. values from an element to itself (e.g. "a a 1.5"), if present, are used in the non-uniform origin option.
- If there are missing pairs (other than diagonal elements), the default value in the md.ini
 configuration file is assigned.
- Blank lines and lines starting with the comment symbol ('#') are discarded.

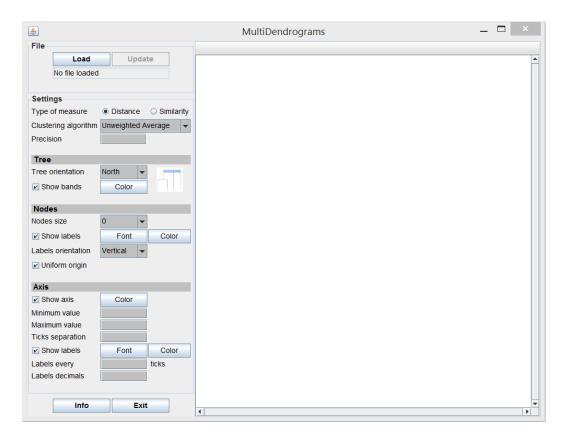
For example, three list-like files for the previous data could be:

		a a O
		a b 2
		a c 4
		a d 7
	ab2	ba2
	a c 4	b b 0
	ad7	b c 2
	ba2	b d 5
	b c 2	ca4 ab2
	b d 5	cb2 ac4
a b 2	c a 4	cc0 ad7
a c 4	c b 2	cd3 bc2
ad7	c d 3	da7 bd5
b c 2	da7	db5 cd3
b d 5	d b 5	dc3 bb1
c d 3	d c 3	dd0 dd3
Simple list	Complete list	Lists with diagonal elements

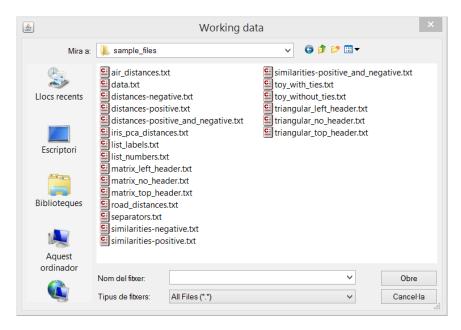
2. Loading data

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

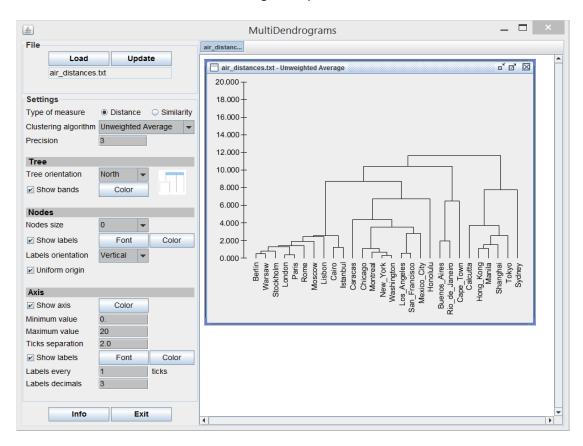
- 1. Choose the desired settings, mainly the Type of measure and the Clustering algorithm. These settings will be explained in detail in the next sections.
- 2. Click on the 'Load' button:



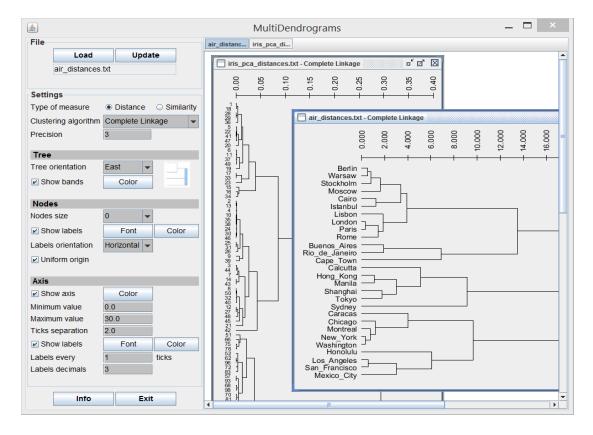
3. Select the file to open and then click on the 'Open' button:



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



5. Take advantage of the right and bottom scrollbars to handle large dendrograms:

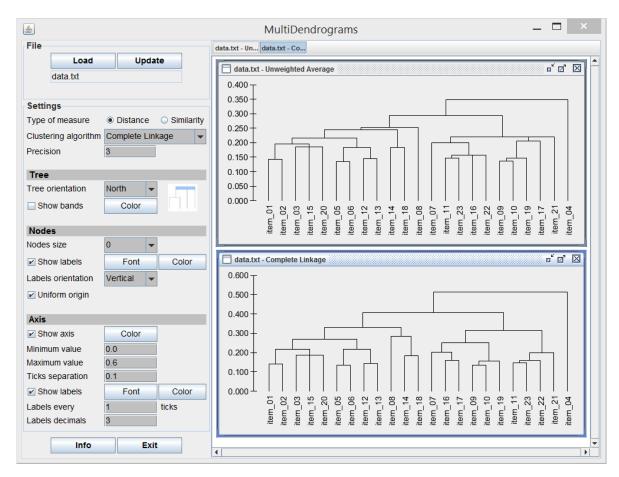


3. Actions

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.

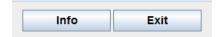


It is possible to load the same data file several times, in order to compare the dendrogram appearance for different parameters settings.



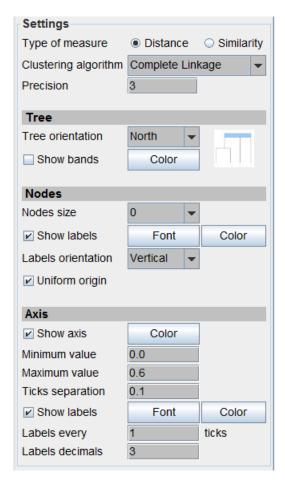
The parameters shown always correspond to the active (selected) dendrogram window.

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



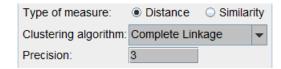
4. Settings

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:



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.

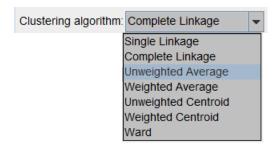
Main data representation settings



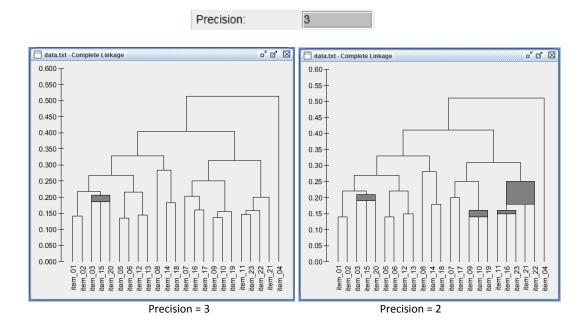
- Type of measure: It allows choosing between two kinds of measures, distance and similarity. Choose between them according to the meaning of the loaded data. With distances, the closer the elements the lower their distance. On the contrary, with similarity, the closer the elements the larger their weight.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



 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.



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.

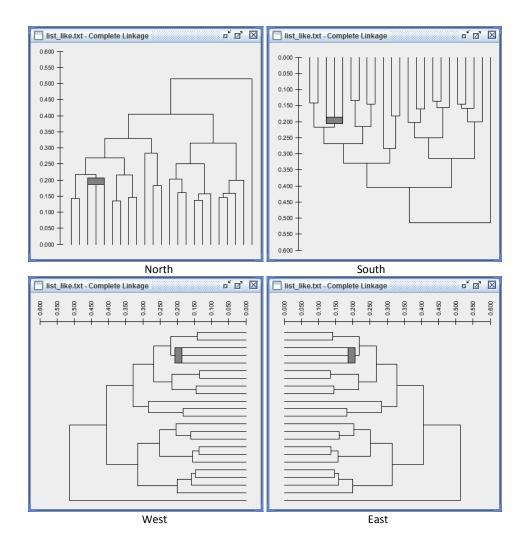


Tree settings

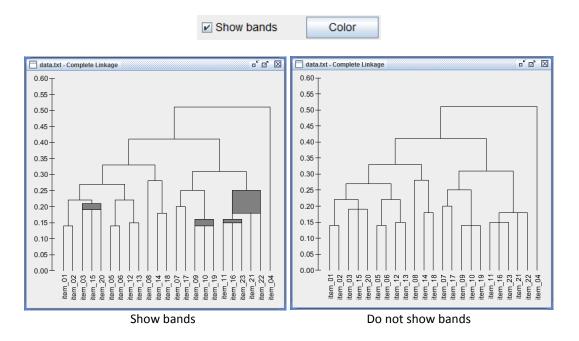


- **Tree orientation**: Four orientations are available, *north*, *south*, *east* and *west*, which refer to the relative position of the root of the tree. By default, *north* is selected.



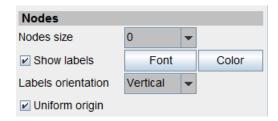


Show bands: It allows showing a band or not in case of tied minimum distances between three or more elements, and selecting the color of the band. If selected, the bands show the heterogeneity of all the distances between the clustered elements. Otherwise, the elements are grouped at their minimum distance.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

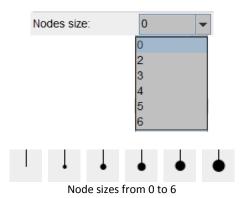


Let us explain the meaning of the bands. In *MultiDendrograms*, if several pairs of elements share the same minimal distance, they are clustered together in one step. For instance, suppose that the minimal distance is 0.4, and that they correspond to the tied pairs (A,B) and (B,C). *MultiDendrograms* 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.

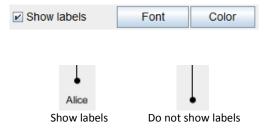
Nodes settings



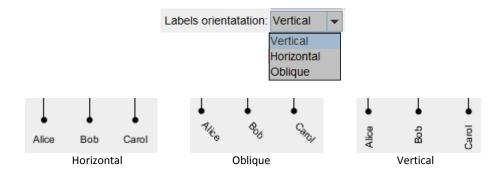
- **Nodes size**: Six different node sizes are available. By default, 0 is selected (i.e. nodes not shown):



- **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**:

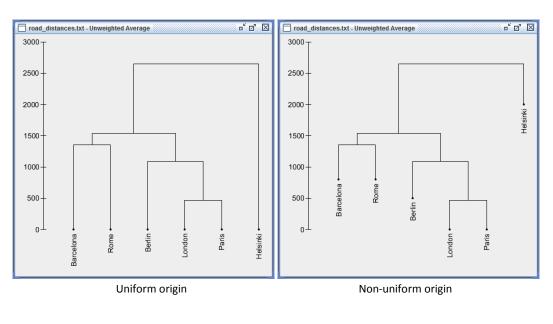


- **Labels orientation**: Three orientations are available: *vertical, horizontal* and *oblique*. By default, *vertical* is selected:



- **Uniform origin**: It allows choosing between uniform and non-uniform origins of the nodes. By default, *uniform origin* is selected. In the non-uniform mode, the height at which the nodes are drawn is taken from the data file, in the form of values (distances or similarities) between an element and itself (e.g. "a a 3.5" in list form, or diagonal values in matrix and triangular forms). For missing diagonal values, height infinity is chosen (minus infinity in the case of distances, plus infinity in the case of similarities):

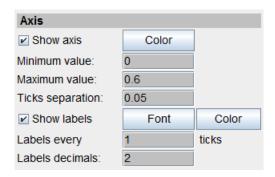
✓ Uniform origin



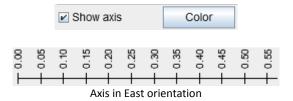
Barcelona	800	1864	3448	1494	1036	1355
Berlin	1864	500	1620	1099	1068	1505
Helsinki	3448	1620	2000	2680	2636	2864
London	1494	1099	2680	0	462	1875
Paris	1036	1068	2636	462	0	1424
Rome	1355	1505	2864	1875	1424	800

Note the values in the diagonal of the matrix

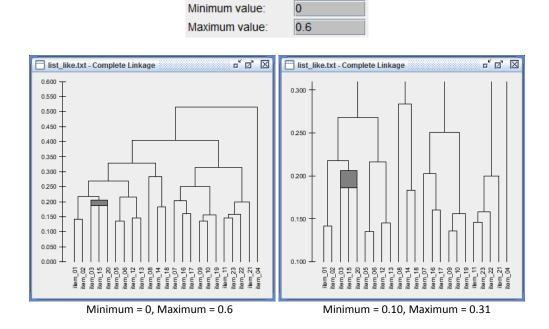
Axis settings



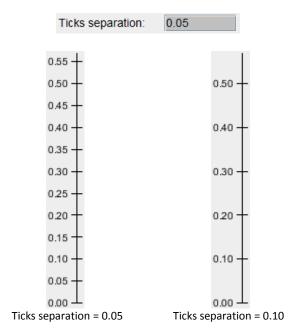
- **Show axis**: It allows showing or not the axis, and selecting its color. By default, **show axis** is selected and the selected color is **black**.



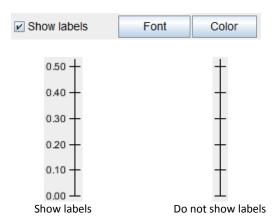
- **Minimum value / Maximum value**: They allow choosing the minimum and maximum value of the axis, respectively. They also affect the view of the dendrogram. The default values are calculated from the data.



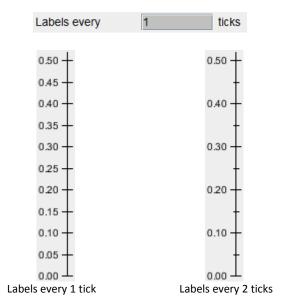
- **Ticks separation**: It allows choosing the separation between consecutive ticks of the axis. The default value is calculated from the data:



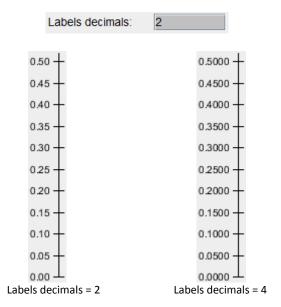
- **Show labels**: It allows showing or not the labels of the axis, and selecting their color and font. By default, **show labels** is selected, the font is **Arial** and the color is **black**.



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

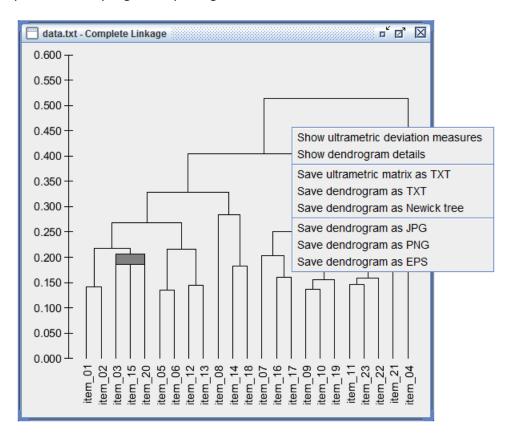


- **Labels decimals**: Number of decimal digits of the tick labels. By default it is set equal to the **precision** parameter.

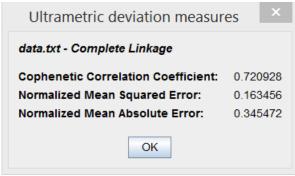


5. Analyzing and exporting results

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

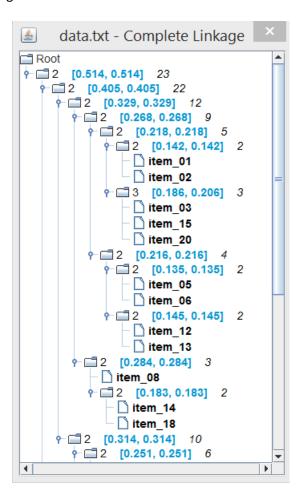


- Show ultrametric deviation measures: Calculates the ultrametric matrix corresponding to the active dendrogram and obtains three differents deviation measures between the original and the ultrametric matrices: the cophenetic correlation coefficient, the normalized mean squared error and the normalized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



Deviation measures

- **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.
- Minimum and maximum 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 (leafs 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.

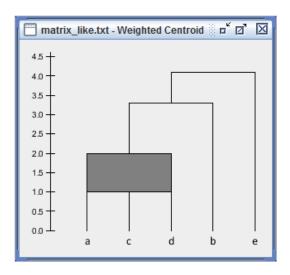
- Save ultrametric matrix as TXT: Calculates the ultrametric matrix corresponding to the loaded data and saves it to a text file in matrix form, with the nodes labels in the first row. This text file can then be easily loaded into any text editor or spreadsheet application (e.g. Microsoft Excel).

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

Original distances matrix

a	С	d	b 3.3 3.3 3.3 0.0 4.1	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 distances or maximum similarities are 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 similarities.
- 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 type of origin: uniform or non-uniform. In uniform type the diagonal values of the data are discarded and all elements are assigned the same height, otherwise the diagonal values define the heights of the elements.

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 PARAMETERS

where the PARAMETERS are:

FILE NAME PROX TYPE METHOD [PRECISION] [ORIGIN]

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
```

```
-direct FILE_NAME PROX_TYPE METHOD [ PRECISION ] [ ORIGIN ]

Direct calculation of the multidendrogram without graphic interface

FILE_NAME: name of the data file

PROX_TYPE: proximity type, one of
```

D, DIST, DISTANCE, DISTANCES S, SIM, SIMILARITY, SIMILARITIES

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

ORIGIN: origin type, one of

UO, UNIFORM_ORIGIN
NUO, NON_UNIFORM_ORIGIN
default value: UNIFORM_ORIGIN

There are sample script files to show some direct calculations:

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

Examples:

```
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
java -jar multidendrograms.jar -direct data.txt D CL UO
java -jar multidendrograms.jar -direct data.txt D CL 3 NUO
```

APPENDIX B. Customization of the graphical user interface

In the ini folder, under the installation directory, there is a configuration file, md.ini, which is used to define many of the characteristics of the graphical user interface (GUI) of *MultiDendrograms*. It is a text file that you may edit at your convenience. After any modification, the changes will take effect the next time you start *MultiDendrograms*. The most important uses are the selection of the language and changing the font sizes, styles and colors of the text in the application.

Language

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
- German

There is a language file (e.g. lang_english.l) in the ini folder for each of the languages available. The selection of the language is made in the first lines of the configuration file md.ini. To change the selected language, just open md.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 file selection
language = ini/lang_english.l
#language = ini/lang_catalan.l
#language = ini/lang_spanish.l
#language = ini/lang_deutsch.l
```

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

Size

MultiDendrograms was initially configured to be used in screens with resolutions starting from 1024x768 pixels. In the last years, with the advent of high resolution screens, the text in MultiDendrograms may appear very small, being difficult to be read. To alleviate this problem, we have prepared configuration files for three different font sizes: 10, 12 and 14 pt:

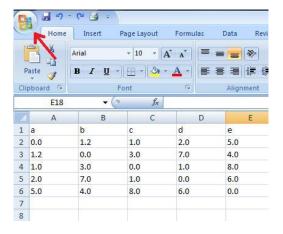
```
md_size10.inimd_size12.inimd_size14.ini
```

To select one of them, e.g. that of size 14pt, simply rename md.ini to md_old.ini and copy the file md_size14.ini into md.ini. Of course, you may edit it as you desire to adapt any parameter you want.

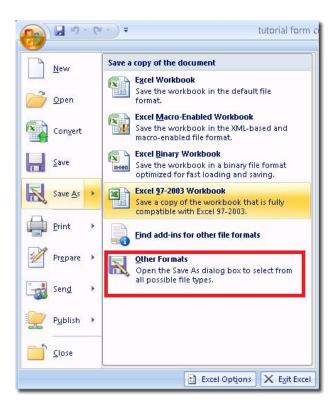
APPENDIX C. Preparing input data with Microsoft Excel

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 you have Microsoft Excel 2007, but similar procedures apply to other versions and similar programs.

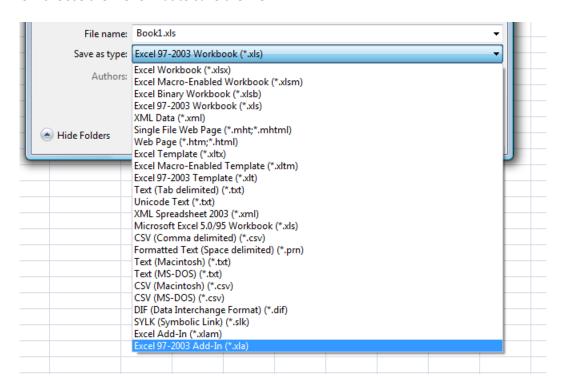
1. Click on the button with the Microsoft Office logo:



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

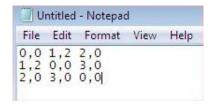


3. Now choose the file format to save the file:



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):



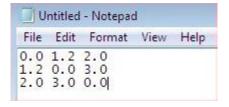
- Go to the 'Edit' menu and select 'Replace':



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



- Save the modified file:



APPENDIX D. History of changes

MultiDendrograms 4.0

- Graphical user interface at different sizes
- Positive and negative distances and similarities
- Uniform and non-uniform origin of nodes
- Improved configuration file
- Translation to German
- Improved performance

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. Request, comments, bugs and acknowledgements

If you have any comment about *MultiDendrograms*, e.g. to request some functionality in future versions, or if you find a bug, please send us an email to any of the following addresses:

- Sergio Gómez: sergio.gomez@urv.cat
- Alberto Fernández: alberto.fernandez@urv.cat

In the case of bugs, please send us all the information needed to reproduce it: a detailed description, a sample data file, the version of the program, the operating system, the Java version, the parameters, the series of actions which result in the bug, the expected result, snapshots, etc. Don't worry if you cannot supply all this information from the beginning, let's just start a conversation and try to find the solution.

Finally, we want to acknowledge all the people who have contributed to the development of this application: Justo Montiel and David Torres, who developed the first versions of *MultiDendrograms* as part of their studies in Computer Science at Universitat Rovira i Virgili (Tarragona) under our supervision; Luce Prignano, for being one of the first users and providing useful comments; Roger Gómez and Mireia Gómez for the translation to German; Franco Lancia for his interest in *MultiDendrograms*, which has resulted in an incorporation of our algorithms in his <u>T-Lab</u> software for text analysis. We also want to thank all the people who have trusted in *MultiDendrograms* for their research, even citing in their publications the program and our paper appeared in *Journal of Classification*.

APPENDIX F. License

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