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ADE-4: a multivariate analysis and graphical display software

Jean Thioulouse (1), **Daniel Chessel** (2), **Sylvain Dolédec** (2) & **Jean-Michel Olivier** (2)

(1) Laboratoire de Biométrie, Université Lyon 1, 43 boulevard du 11 novembre 1918, F-69622 Villeurbanne Cedex, France.
(2) Laboratoire d'Ecologie des Eaux Douces, Université Lyon 1, 43 boulevard du 11 novembre 1918, F-69622 Villeurbanne Cedex, France.

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Abstract

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Abstract:

We present ADE-4, a multivariate analysis and graphical display software. Multivariate analysis methods available in ADE-4 include most classic tools of the multivariate analysis, as principal component analysis, correspondence analysis, discriminant analysis, canonical correlation analysis, principal coordinate analysis, canonical variate analysis, canonical correspondence analysis, linear regression analysis, partial least squares regression, multivariate regression analysis, and Fourier analysis. Graphical display and data exploration are powerful tools for the multivariate analysis of ecological data. Most of the ADE-4 multivariate analysis methods are available for one, two, or three tables. Ordinations can be displayed and interpreted simultaneously with other variables, statistics and tests, using various graphical displays and interactive techniques. The ADE-4 software is simple and homogeneous among all the programs. This contributes to make the use of ADE-4 very easy for non specialists in statistics, data analysis or computer science.

Keywords:

Multivariate analysis, principal component analysis, correspondence analysis, instrumental variables, canonical correspondence analysis, partial least squares regression, canonical analysis, graphics, multivariate graphics, ecological graphics, interactive graphics, Macintosh, HyperCard, Windows 95.

Corresponding author:

Jean Thioulouse
Laboratoire de Biométrie - Université Lyon 1
43 boulevard du 11 novembre 1918
F-69622 Villeurbanne Cedex - France

1. Introduction

Data exploration analysis and graphical display software for Apple Macintosh and Windows 95 microcomputers. It is made of several stand alone applications, called modules, that feature a wide range of multivariate analysis methods, from simple one-table analysis to three-way table analysis and two-table analysis methods. It also provides many possibilities for exploratory data analysis, data editing and data management, and for the production of publication quality graphics. The ADE-4 software is made of 30 modules, 25 for Macintosh and 28 for Windows, including 4 multivariate analysis modules, as the Kyte and Doolittle plot, and 3 utilities as the Internet archiver. The user interface is simple and homogeneous among all the programs. This contributes to make the use of ADE-4 very easy for non specialists in statistics, data analysis or computer science.

ADE-4 is made of a series of small independent modules that can be used independently from each other or launched through a HyperCard interface. There are two categories of modules: multivariate analysis modules and other modules, as data editors, or utilities.

1.1 Multivariate analysis modules

Computational modules present an "Options" menu that enables the user to choose between the possibilities available in the example. For example, in the PCA (principal component analysis) module, it is possible to choose between PCA on correlation or on covariance (see Figure 1).

Fig. 1. Elements of the user interface of principal modules. In the Options menu screen is shown the dotted method. By the mean dotting window allows the user to type in the parameters of the dotted method (here, the number of dots and the seed for the random number generator). The "Help/Hide" button allows to display or hide the help text. The "Go" button launches the analysis. The "Help" button launches the help window. The "Quit" button allows to quit the application and saves the current options. The "Help" button launches the help window. The "Quit" button allows to quit the application and saves the current options.

According to the option selected by the user, a dotting window is displayed, showing the parameters required for the execution of the analysis (Figure 1B). The user can click on the buttons at the bottom of the screen to see the other dotted parameters (number of dots, random seed, and dotting method). The "Help" button allows to display the help text, and the "Go" button launches the analysis. A project window shows the computation steps while the analysis is being performed (Figure 1D), and a text report that contains a description of input and output files and of analysis parameters is created.

1.2 Graphical modules

Graphical modules also present an "Options" menu to choose the type of graphic. They have an additional "Windows" menu (Figure 2A). This menu can be used to close one of the graphical windows (where data are displayed) or to tile all the opened graphical windows. The user can then freely modify the values of all the parameters and the resulting graphic is displayed in the "Graphics" window (Figure 2B).

Fig. 2. Elements of the user interface of graphical modules. In the Options menu screen is shown the type graphic, and the Windows menu can be used to choose one of the three parameter windows (B, C, D and E). The main dotting window (B) works in the same way as in computation modules. The "Bar/Bars" window (C) allows to set the values of parameters concerning the barplots (number of bars, and of bars per page, and the "Go" button allows to launch the barplot drawing. The "Boxplot" window (D) allows to set the values of parameters concerning the boxplots (notch and height, number of bars, and the "Go" button allows to launch the boxplot drawing. The "Histogram" window (E) allows to set the values of parameters concerning the histogram (number of bars, and the "Go" button allows to launch the histogram drawing.

2. The new interface of ADE-4

The new interface of ADE-4 is based on the use of HyperCard stacks. It allows to access to the data sheets, to the data editors, to the computation modules, and to the graphical modules. The main window (Figure 3) shows the different stacks available in the current directory. The user can then easily navigate from one stack to the other. The Windows version uses the Linkwitz HyperCard emulator.

2.1 Data sheets and data editors

These basic multivariate analysis methods can be applied to one table data sets (Dolédec and Chessel, 1991). The corresponding modules are the PCA (principal components analysis) module, the CoA (correspondence analysis) module, the DCA (detrended correspondence analysis) module, the MCA (multiple correspondence analysis) module, the PCoA (principal coordinate analysis) module, the DA (discriminant analysis) module, the MDA (multiple discriminant analysis) module, the CCA (canonical correlation analysis) module, the PLS (partial least squares regression analysis) module, the MRA (multivariate regression analysis) module, the CVA (canonical variate analysis) module, the CCorA (canonical correlation analysis) module, the CWA (within-class canonical variate analysis) module, the CBA (between-class canonical variate analysis) module, the CCA (canonical correspondence analysis) module, the PCoiv (principal coordinate analysis with instrumental variables) module, the CWiv (within-class canonical variate analysis with instrumental variables) module, the CBiv (between-class canonical variate analysis with instrumental variables) module, the CCAiv (canonical correspondence analysis with instrumental variables) module, the Fourier module, the Kyte and Doolittle plot module, the Internet archiver module, and the Internet archiver module (Thioulouse and Chessel, 1994) for the different analysis methods available in the current version of ADE-4 (see http://biomsun.univ-lyon1.fr/ade4/).

2.2 Graphical modules

A HyperCard (Macintosh) version or WinPlus (Windows 95 version) stack (ADE*Draw) can be used to launch the modules. This stack also displays the files that are in the current data directory, and allows to launch the appropriate module for the data file to be analyzed.

ADE*Draw is a library of c, C++ compiler data sets of varying size that can be used for trial runs of data analysis methods. Most of these data sets come from environmental studies. Documentation about the use of the graphical modules is provided in the documentation of the statistical methods and data sets available in ADE-4.

2.3 Data editors

These basic multivariate analysis methods can be applied to one table data sets (Dolédec and Chessel, 1991). The corresponding modules are the PCA (principal components analysis) module, the CoA (correspondence analysis) module, the DCA (detrended correspondence analysis) module, the MCA (multiple correspondence analysis) module, the PCoA (principal coordinate analysis) module, the DA (discriminant analysis) module, the MDA (multiple discriminant analysis) module, the CCA (canonical correlation analysis) module, the PLS (partial least squares regression analysis) module, the MRA (multivariate regression analysis) module, the CVA (canonical variate analysis) module, the CCorA (canonical correlation analysis) module, the CWA (within-class canonical variate analysis) module, the CBA (between-class canonical variate analysis) module, the CCA (canonical correspondence analysis) module, the PCoiv (principal coordinate analysis with instrumental variables) module, the CWiv (within-class canonical variate analysis with instrumental variables) module, the CBiv (between-class canonical variate analysis with instrumental variables) module, the CCAiv (canonical correspondence analysis with instrumental variables) module, the Fourier module, the Kyte and Doolittle plot module, the Internet archiver module, and the Internet archiver module (Thioulouse and Chessel, 1994).

2.4 Factorial and Discriminant Analyses

A HyperCard (Macintosh) version or WinPlus (Windows 95 version) stack (ADE*Draw) can be used to launch the modules. This stack also displays the files that are in the current data directory, and allows to launch the appropriate module for the data file to be analyzed.

ADE*Data is a library of c, C++ compiler data sets of varying size that can be used for trial runs of data analysis methods. Most of these data sets come from environmental studies. Documentation about the use of the graphical modules is provided in the documentation of the statistical methods and data sets available in ADE-4.

3. Data analysis methods

The data analysis methods available in ADE-4 will not be presented here, due to lack of space. They are based on the duality diagram (Cailliez and Pagès, 1976; Escoufier 1987). In many cases, the duality diagram has been (Good 1969), (Jaggi 1973) are available to study the significance of observed structures.

3.1 Data sheets and data editors

These basic multivariate analysis methods can be applied to one table data sets (Dolédec and Chessel, 1991). The corresponding modules are the PCA (principal components analysis) module, the CoA (correspondence analysis) module, the DCA (detrended correspondence analysis) module, the MCA (multiple correspondence analysis) module, the PCoA (principal coordinate analysis) module, the DA (discriminant analysis) module, the MDA (multiple discriminant analysis) module, the CCA (canonical correlation analysis) module, the PLS (partial least squares regression analysis) module, the MRA (multivariate regression analysis) module, the CVA (canonical variate analysis) module, the CCorA (canonical correlation analysis) module, the CWA (within-class canonical variate analysis) module, the CBA (between-class canonical variate analysis) module, the CCA (canonical correspondence analysis) module, the PCoiv (principal coordinate analysis with instrumental variables) module, the CWiv (within-class canonical variate analysis with instrumental variables) module, the CBiv (between-class canonical variate analysis with instrumental variables) module, the CCAiv (canonical correspondence analysis with instrumental variables) module, the Fourier module, the Kyte and Doolittle plot module, the Internet archiver module, and the Internet archiver module (Thioulouse and Chessel, 1994).

3.2 Data sheets with spatial structure

These basic multivariate analysis methods can be applied to one table data sets (Dolédec and Chessel, 1991). The corresponding modules are the PCA (principal components analysis) module, the CoA (correspondence analysis) module, the DCA (detrended correspondence analysis) module, the MCA (multiple correspondence analysis) module, the PCoA (principal coordinate analysis) module, the DA (discriminant analysis) module, the MDA (multiple discriminant analysis) module, the CCA (canonical correlation analysis) module, the PLS (partial least squares regression analysis) module, the MRA (multivariate regression analysis) module, the CVA (canonical variate analysis) module, the CCorA (canonical correlation analysis) module, the CWA (within-class canonical variate analysis) module, the CBA (between-class canonical variate analysis) module, the CCA (canonical correspondence analysis) module, the PCoiv (principal coordinate analysis with instrumental variables) module, the CWiv (within-class canonical variate analysis with instrumental variables) module, the CBiv (between-class canonical variate analysis with instrumental variables) module, the CCAiv (canonical correspondence analysis with instrumental variables) module, the Fourier module, the Kyte and Doolittle plot module, the Internet archiver module, and the Internet archiver module (Thioulouse and Chessel, 1994).

3.3 Factorial Analyses (1-table analyses)

The ADE-4 Analyses 1D graphical modules, that belong to four categories: one dimensional graphics, curves, scalars, and geographical maps. Most modules have the possibility to draw several graphics in the same window, and to link them together. For example, the Lorenz curve, the histogram, and the boxplot can be drawn in the same window, and the points that belong to a given group will be selected in all the three graphics when one of them is selected. The Lorenz curve, the histogram, and the boxplot are powerful tools for the exploratory data analysis, when one always deals with many variables and/or groups of samples. Some other modules have two versions, according to the way they read the collections (binary groups can be either single pop table by table, or superimposed). Superimposed graphics can be drawn in the same window, or in different windows.

The GraphESR module is intended for one dimensional data exploration, such as the Lorenz curve. It has two options: histogram and boxplot. The histogram option computes and draws the histogram of the given data set. It also computes and draws the corresponding density function, which optionally the adjusted Gaussian curve (superimposed over it. The Lebesgue spline density function (Lebesgue spline) is also available. The boxplot option computes and draws the boxplot (Figure 4A). This boxplot is particularly useful when one deals with many variables and/or groups of samples. The successive exploratory graphics corresponds to several partitions of the set of cases, or several quantitative variables. All these parameters are interactively set by the user.

Fig. 4. Example of graphics drawn with the GraphESR module. The eleven dimensional graphics (numbered 1 to 11) corresponds to eleven qualitative variables. In each elementary graphics, the boxplot (in the upper part of the figure) shows the distribution of the quantitative variable, and the successive histograms (in the lower part of the figure) correspond to the successive partitions of the qualitative variable. The eleven curves represent the mean and the variance of the samples belonging to each of these partitions. The Lebesgue spline density function (in the upper part of the figure) is also drawn. The successive histograms can be drawn in the same window, or in different windows. The successive boxplots can be superimposed, or drawn in different windows. The successive curves can be superimposed, or drawn in different windows.

3.4 Curves

The GraphCurve module draws curves, i.e. series of values (ordinates) that are plotted along an axis (abscissa). It features four options: Lines, Bars, Steps and Boxes. Here also, colours and groups of sets can correspond to the elementary graphics of a collection. Boxes are simply the classical "box and whiskers" display, showing the median, quartiles, minimum and maximum.

The GroupCurve module is the twin module to the GroupHist module. It allows to compare several curves, that are the means of the samples belonging to each of these partitions. The Kolmogorov-Smirnov statistics is also computed and displayed (which can be chosen by the user) relatively to heterogeneity among an axis, these labels are connected by lines to the corresponding coordinates on the axis. The columns and rows of the data table can be permuted, and the resulting new table can be saved in a new data file.

The GroupCOUNT module allows to count the number of occurrences in the successive classes, for each of the successive partitions. This module is useful for non-stationnary point processes, which must be superimposed instead of pooled out by rule. Because superimposed histograms and tables are not convenient, this is used only for Gamma curves (Figure 5). Gamma curves are a family of curves that are the means of the successive partitions of the set of points, according to their nearest neighbour, the second nearest neighbour, etc. The successive elementary graphics corresponds to several partitions of the set of points, or several quantitative variables. All these parameters are interactively set by the user.

Fig. 5. Example of graphics drawn with the GroupCOUNT module. The eleven elementary graphics (numbered 1 to 11) correspond to eleven qualitative variables. In each elementary graphics, the curve (in the upper part of the figure) shows the distribution of the quantitative variable, and the successive histograms (in the lower part of the figure) correspond to the successive partitions of the qualitative variable. The eleven curves represent the means and the variance of the samples belonging to each of these partitions. The Lebesgue spline density function (in the upper part of the figure) is also drawn. The successive histograms can be drawn in the same window, or in different windows. The successive boxplots can be superimposed, or drawn in different windows. The successive curves can be superimposed, or drawn in different windows.

3.5 Scalars

The Lebesgue spline computes the density function of a given set of points (or weights). The Lebesgue spline is a kind of kernel method, which has some perfect several actions that help interpreting the factors underlying the distribution of the set of points, interactively set by the user.

3.6 Cartography modules

The GeoEsther module is linked to the GeoDist module, and allows to compute and display the variogram cloud (Figure 6). This module also computes the Geary's Test statistics, and Moran's Test statistics, and displays the corresponding values.

Fig. 6. Example of graphics drawn with the GeoEsther module. Left: the variogram cloud. Right: the variogram cloud, in which the user can perform several actions that help interpreting the factors underlying the distribution of the set of points, interactively set by the user.

3.7 Kyte and Doolittle plot module

The Kyte and Doolittle plot module (Figure 7) is a simple plot module, which allows to plot the values of a variable (or two variables) on a map, according to their coordinates. It includes an option to display the values on the map, and to save the map in a new data file.

Fig. 7. Example of graphics drawn with the Kyte and Doolittle plot module. The Lynx mondes (left) shows contour curves with grey level patterns that indicate the curve value. The Meuse module (B) shows grey level patterns on a geographical map. For both modules, collections correspond to the columns of the table containing the values displayed on the map (grey levels, or contour curves). Contour curves maps and the values of grey levels can be saved in new data files.

The Lynx mondes draws contour curves on the map (Figure 8A). It can be used with sampling points having any distribution in the map: an interpolated regular grid is computed before drawing the contour curves. The Lynx mondes module also computes and displays the variogram cloud (Figure 8B) for the two variables. Thioulouse et al. 1995 for description and example of use of the Lynx mondes module.

The Meuse module draws maps with grey level polygons (Figure 8B), starting from a file containing the coordinates of the vertices of each of the areas making the map, and a second file containing the values of the variables.

3.8 Conclusion

The current version of ADE-4 contains 30 modules, 25 for the Macintosh version, and 28 for the Windows version. The modules are written in two different languages, Pascal for Macintosh version, and C++ for Windows version. The Macintosh version runs on Macintosh computers with at least 4 Mo of RAM, and requires the System 7 and HyperCard 2.2 or later versions. The Windows version runs under Windows 95 or Windows NT, and requires at least 8 Mo of RAM. The Macintosh version runs faster than the Windows version, because the Macintosh version is a native application, while the Windows version runs under an emulator. The ADE-4 software is simple and homogeneous among all the programs. This contributes to make the use of ADE-4 very easy for non specialists in statistics, data analysis or computer science.

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