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BiplotGUI

Interactive Biplots in R

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DRAFT

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PREFACE

This manual documents the features of version 0.0-4.1 of the BiplotGUI package. The package makes it easy for users to construct and interact with biplots in R.

[Chapter 1](#) gives an overview of the package and its techniques. All the features of the graphical user interface (GUI) are documented in full in [Chapter 2](#). Changes made to the package are listed in [Appendix A](#).

While the statistical output provided by the BiplotGUI has been checked for accuracy, the GUI itself occasionally gives console warnings or even crashes. It's quick to simply restart the GUI. If the behaviour is replicable, please contact me at the address below with the details. Otherwise, visit <http://biplotgui.r-forge.r-project.org/> for more information, for help, or to report bugs. Some known issues are listed in [Appendix B](#).

The BiplotGUI package was written as part of my Masters degree at Stellenbosch University in South Africa. I would like to thank my two supervisors, Prof Niël le Roux and Dr Sugnet Gardner-Lubbe, for their continued support. I would also like to thank Prof Patrick Groenen, whose suggestions inadvertently gave rise to the project.

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ABBREVIATIONS

| | |
|-----|--------------------------------|
| AOD | analysis of distance |
| CLI | command line interface |
| CV | canonical variate |
| CVA | canonical variate analysis |
| GDP | gross domestic product |
| GUI | graphical user interface |
| IM | iterative majorisation |
| MDS | multidimensional scaling |
| PC | principal component |
| PCA | principal component analysis |
| PCO | principal coordinates analysis |
| PPP | purchasing price parity |
| RAE | relative absolute error |

KEYBOARD SHORTCUTS

| | |
|--------|---|
| A | Shows points determined by PCO . |
| B | Shows points determined by MDS (identity transformation). |
| C | Shows points determined by MDS (monotone regression transformation). |
| D | Shows points determined by MDS (monotone spline transformation). |
| R | Shows points determined by MDS (currently selected transformation). |
| 0 | Shows no biplot axes. |
| 1 | Constructs a PCA biplot. |
| 2 | Constructs a covariance/correlation biplot. |
| 3 | Constructs a CVA biplot. |
| 4 | Shows regression biplot axes. |
| 5 | Shows Procrustes biplot axes. |
| 6 | Shows circular non-linear biplot axes. |
| Ctrl+N | Interpolates a new sample. |
| Ctrl+L | Clears all additional descriptors from the biplot. |
| F11 | Shows the currently displayed biplot region in an external window. |
| F12 | Shows the currently displayed biplot in 3D in an external window. |
| Ctrl++ | Shows the next set of legend entries. |
| Ctrl+- | Shows the previous set of legend entries. |
| Ctrl+G | Allows many graphical parameters to be set for the different groups of points. |
| Ctrl+A | Allows many graphical parameters to be set for the different biplot axes. |
| Ctrl+R | Reverts all the graphical parameters to their default values. |
| Ctrl+S | Saves the currently displayed biplot region in the currently selected file format. |
| Ctrl+C | Copies the currently displayed biplot region to the clipboard. |
| Ctrl+P | Prints the currently displayed biplot region. |
| F1 | Enables pop-up help messages for the components of the main GUI window. |

CHAPTER 1

OVERVIEW

1.1 INTRODUCTION

In this section we give a brief overview of biplots, existing biplot software, and the statistical programming language and environment R. In [Section 1.2](#) we set out the main aims of the **BiplotGUI** package, while its most important features are showcased in [Sections 1.3](#) and [1.4](#) through the exploration of three data sets. Further features are illustrated in [Section 1.5](#). In [Section 1.6](#) we list some ideas for future releases. The present version of the package is 0.0-4. The article is intentionally non-mathematical.¹ This allows the focus to lie firmly with the package and its features. However, detailed references are provided for those who wish to gain a fuller understanding of the underlying theory. In addition, the main computations performed by the package are set out in [Section 1.A](#).

1.1.1 Biplots

Introduced by [Gabriel \(1971\)](#), the biplot is described by [Gower and Hand \(1996\)](#) in their authoritative monograph as the multivariate analogue of the ordinary scatter plot. As such, biplots are representations of multivariate data in which information on both the samples (observations) and the variables of a data matrix is given simultaneously in two or three dimensions: the samples are represented as points, while the variables are represented as labelled, calibrated axes. The axes are either linear and oblique, or non-linear. This new approach to biplots differs from the more traditional approach in which samples and variables are represented as points and/or uncalibrated vectors.

Some dimension-reduction technique is typically used to represent the samples as points, often principal component analysis (PCA) ([Pearson, 1901](#); [Hotelling, 1933](#)) or canonical variate analysis (CVA) ([Hotelling, 1935, 1936](#)). More generally, scaling techniques such as principal coordinates analysis (PCO) ([Torgerson, 1952](#); [Gower, 1966](#)) or metric or non-metric multidimensional scaling (MDS) ([Kruskal, 1964a,b](#); [Sammon, 1969](#)) are used. [Jolliffe \(2002\)](#) dedicates a monograph to PCA, while [Krzanowski \(2000\)](#) covers general multivariate topics. [Cox and Cox \(2001\)](#) and [Borg and Groenen \(2005\)](#) are standard references for scaling techniques.

The placement of the axes depends partly on the mechanism used in the placement of the points. The PCA biplot provides linear axes for points placed by PCA ([Gower and Hand, 1996](#), Chapter 2); similarly the CVA biplot provides linear axes for points placed by CVA ([Gabriel, 1972](#); [Gower and Hand, 1996](#), Chapter 5). The regression biplot ([Gower and Hand, 1996](#), Chapter 3) gives approximate linear axes for any ordination of points. So too does the Procrustes biplot ([Gower and Hand, 1996](#), Chapter 3). The regression and Procrustes biplots correspond to the PCA biplot for points determined by PCO based on Pythagorean dissimilarities. The covariance biplot ([Greenacre, 1984](#); [Underhill, 1990](#)) adjusts the points and axes of the PCA biplot so that the cosines of the angles between the axes approximate the correlations between the corresponding variables. The correlation biplot is similar, except that the variables are first scaled to have unit variances.

The placement of the axes may also depend on how they are to be used. *Predictive* axes are

¹This chapter was submitted for publication by La Grange, Le Roux and Gardner-Lubbe.

positioned and calibrated so that the orthogonal projection of a point onto an axis ‘predicts’ as best as is graphically possible the value of the corresponding sample on the corresponding variable. *Interpolative* axes, on the other hand, are positioned and calibrated so that a new sample may be added to an existing configuration of points at the most appropriate position graphically possible. Interpolation can be either by the centroid or vector sum of the positions on the axes corresponding to the respective variable values of the new sample.

For additive inter-sample dissimilarities (Gower and Hand, 1996, p. 105), biplots with non-linear axes (or trajectories) may be constructed for points determined by PCO. The PCO solution itself requires the inter-sample dissimilarities to be Euclidean-embeddable (Gower, 1982); dissimilarity measures for which this is the case are discussed by Gower and Legendre (1986). Non-linear predictive axes may make use of circular projection (Gower and Hand, 1996, Chapter 6), while non-linear interpolative axes (Gower and Harding, 1988; Gower and Hand, 1996, Chapter 6) are used in the same way as the linear variety. Non-linear biplots are often most useful to gauge what is otherwise approximated by linear biplots.

While very many examples of biplots of the traditional approach may be found in the literature, there are fewer examples of biplots of the new approach. An important reason has been the lack of software, as is discussed in Sections 1.1.2 and 1.1.3. The value of biplots of the new approach, however, has often been demonstrated. In an easy to read introduction, for example, Le Roux and Gardner (2005) cite and showcase many examples of the uses of linear biplots, from such diverse fields as archaeology, agriculture, antiques, education, financial management, mineralogy and process control. Other recent fields of application include cephalometry (Naidoo, Harris, Swanevelder and Lombard, 2006), chemistry (Alves, Cunha, Amaral, Pereira and Oliveira, 2005) and mineralogy (Jemwa and Aldrich, 2006). Examples of non-linear biplots may be found in Gower and Harding (1988), Gower and Hand (1996), Cox and Cox (2001) and Gower and Ngouenet (2005).

Given the ubiquity of multivariate data and the usefulness of biplots in describing such data, there is still much scope for the further popularisation of the technique.

1.1.2 Existing biplot software

Many statistical packages can be used to produce at least the simplest of biplots of the traditional approach. These include the major statistical packages Minitab (Minitab Inc, 2007), SPSS (SPSS Inc, 2008), STATA (StataCorp LP, 2007) and various products from SAS (2009). However, functionality is often limited, and the results hard to obtain. Greater functionality is provided by the three dedicated biplot programs XLS-Biplot (Udina, 2005a,b), GGEbiplot (Yan and Kang, 2006) and BiPlot (Lipkovich and Smith, 2002a,b). XLS-Biplot is based on XLisp-Stat (Tierney, 1990) and has many useful features including a related web-server that can be used to construct biplots online. GGEbiplot is aimed mainly at agronomists, crop scientists and geneticists. It supplements the book by Yan and Kang (2003). BiPlot is an add-on for Excel, and although therefore potentially widely useful, it unfortunately has some minor but serious shortcomings (see Udina, 2005b).

The Genstat package (VSN International Ltd, 2008) can be used to calculate the coordinates of the elements of a biplot. These can then be drawn using a procedure from an add-on library. Other packages, offering some traditional biplot functionality, include Manet (Hofmann, 2000), for Macintosh only, and ViSta (Young, 2001). Some packages are aimed at ecologists—brodgar (Highland Statistics Ltd, 2008) with R, Canoco (Plant Research International, 2002) with CanoDraw (Smilauer, 2003), MVSP (Kovach Computing Services, 2008) and PC-ORD (MjM Software Design, 2007)—while the Excel add-on BrandMap (WRC Research Systems Inc, 2007) is aimed at marketers.

STATISTICA (StatSoft Inc, 2007) is currently the only mainstream statistical package capable of producing calibrated new-approach biplots, albeit the PCA biplot only. All the software mentioned are for purchase, except XLS-Biplot, BiPlot, Manet and ViSta which are available free of charge. So too is R.

1.1.3 R

R (R Development Core Team, 2008) is a free statistical programming language and environment capable of producing high-quality graphics. Initiated by Ihaka and Gentleman (1996), it has become ‘the *de facto* standard for statistical computing’ (Greenacre, 2007, p. 213). It is an open-source implementation of the S programming language, available for download for all the major platforms from the R Project homepage at <http://www.r-project.org>. The R core is updated regularly with minor version revisions released roughly every six months. The current version (as of December 2008) is R 2.8.1. Updates are relatively painless. R is easily extensible: a large number of user-written packages is available for download from repositories such as CRAN and BioConductor. These repositories can be accessed via the R Project homepage. As R has increased in popularity, so too has the number of books devoted to it. Recent general-topic books on R include Braun and Murdoch (2007), Chambers (2007) and Spector (2008). The book by Murrel (2005) deals specifically with graphics in R. Many more resources are freely available from the R Project homepage.

As far as biplots are concerned, the `biplot` method in R can be used to produce two variations of Gabriel’s (1971) classical biplot. The classical biplot is most similar to the covariance/correlation biplot described earlier. Packages with support for traditional biplots include `ade4` (Dray and Dufour, 2007, 2008), `ade4TkGUI` (Thioulouse and Dray, 2008, 2007), `bpca` (Faria and Demetrio, 2008) and `vegan` (Oksanen *et al.*, 2008). In addition, the `calibrate` package (Graffelman, 2007) can be used to calibrate both scatter plot and biplot axes as described by Graffelman and van Eeuwijk (2005). In general, however, these calibrations do not correspond to those of Gower and Hand (1996).

As opposed to the many solutions for biplots of the traditional approach listed in this section and in the previous one, software for biplots of the new approach has not been readily available. To produce biplots of the new approach, users have had to do their own programming in a suitable environment (for example, Gardner, 2001). To many potential users, such a task represents a major obstacle.

1.2 A NEW PACKAGE

The primary aim with the `BiplotGUI` package is to make it easy to construct biplots of the kind advocated by Gower and Hand (1996) – biplots in which samples are represented as points and variables are represented as calibrated axes. The package goes beyond this, however, allowing users to interact with the data through the biplots which are produced. Naturally, the graphical output should be of a high quality and easily customisable. Its characteristics make R the ideal environment for the development of such a package.

In the next two sections, the most important features of the `BiplotGUI` package are illustrated. This is done through the exploration of three data sets. Further features are highlighted in Section 1.5. A systematic account of all features is given in Chapter 2. The package does not currently support biplots of categorical variables. Further resources and tools are available via the package home page at <http://biplotgui.r-forge.r-project.org>.

Table 1.1. The country data. Eight variables measured on the countries with the 15 largest economies (PPP GDP) in 2007; countries listed in alphabetical order.

| Country | GDP | HIV.Aids | Life exp. | Mil. | Oil cons. | Pop. | Tel. | Unempl. |
|-----------|--------|----------|-----------|------|-----------|------|-------|---------|
| Brazil | 8710 | 0.7 | 72.2 | 2.6 | 4.0 | 190 | 204.2 | 9.6 |
| Canada | 35 370 | 0.3 | 80.3 | 1.1 | 25.1 | 33 | 622.3 | 6.4 |
| China | 7724 | 0.1 | 72.9 | 4.3 | 1.8 | 1322 | 278.4 | 4.2 |
| France | 29 852 | 0.4 | 80.6 | 2.6 | 11.3 | 64 | 543.5 | 8.7 |
| Germany | 31 941 | 0.1 | 79.0 | 1.5 | 11.7 | 82 | 657.8 | 7.1 |
| India | 3685 | 0.9 | 68.6 | 2.5 | 0.8 | 1130 | 44.0 | 7.8 |
| Indonesia | 4041 | 0.1 | 70.2 | 3.0 | 1.8 | 235 | 63.2 | 12.5 |
| Italy | 30 199 | 0.5 | 79.9 | 1.8 | 11.8 | 58 | 430.8 | 7.0 |
| Japan | 33 100 | 0.1 | 82.0 | 0.8 | 16.0 | 127 | 432.8 | 4.1 |
| Mexico | 10 570 | 0.3 | 75.6 | 0.5 | 6.6 | 109 | 182.7 | 3.2 |
| Russia | 12 350 | 1.1 | 65.9 | 2.7 | 6.5 | 141 | 283.6 | 6.6 |
| S Korea | 24 386 | 0.1 | 77.2 | 2.7 | 16.0 | 49 | 547.8 | 3.3 |
| Spain | 27 418 | 0.7 | 79.8 | 1.2 | 14.2 | 40 | 454.5 | 8.1 |
| UK | 31 723 | 0.2 | 78.7 | 2.4 | 11.0 | 61 | 552.9 | 2.9 |
| USA | 43 369 | 0.6 | 78.0 | 4.1 | 25.1 | 301 | 571.2 | 4.8 |

1.3 A FIRST EXAMPLE

In this section we introduce a country-comparative data set. It is used to show how the graphical user interface (GUI) may be initialised, how its features are laid out, and how it may be used to explore multivariate data using, amongst other things, PCA and regression biplots.

1.3.1 The country data

Table 1.1 gives measurements of eight variables for the countries with the 15 largest economies (by purchasing price parity (PPP) gross domestic product (GDP)) in 2007. These data have been derived largely from the 2007 CIA World Factbook (Agency, 2007) and are for illustrative purposes only. The variables are: PPP GDP per capita in US dollars (GDP); HIV/Aids prevalence as a percentage of the population (HIV.Aids); life expectancy in years (Life exp.); military spending as a percentage of GDP (Mil.); oil consumption in barrels per annum per capita (Oil cons.); population in millions (Pop.); number of fixed line telephones per 1000 people (Tel.); and percentage unemployed (Unempl.). The aim is to represent these data in two or three dimensions so that a single, multivariate visual impression may be obtained, with the calibrated biplot axes incorporating information on the original variables.

1.3.2 Getting started

After R has been downloaded and installed, it is also necessary to install the BiplotGUI package and its dependencies (details are provided in Section 1.B). This process needs to be performed only once. To then load the BiplotGUI package into R, the following command is entered at the R prompt, followed as usual by the enter key:

```
library(BiplotGUI)
```

If the user is acquainted with R, data may be entered at the keyboard or be imported into R and saved as a matrix or a data frame. The country data have already been included in the package as a data frame, and may be viewed from within R by typing the commands

```
data(Countries)
Countries
```

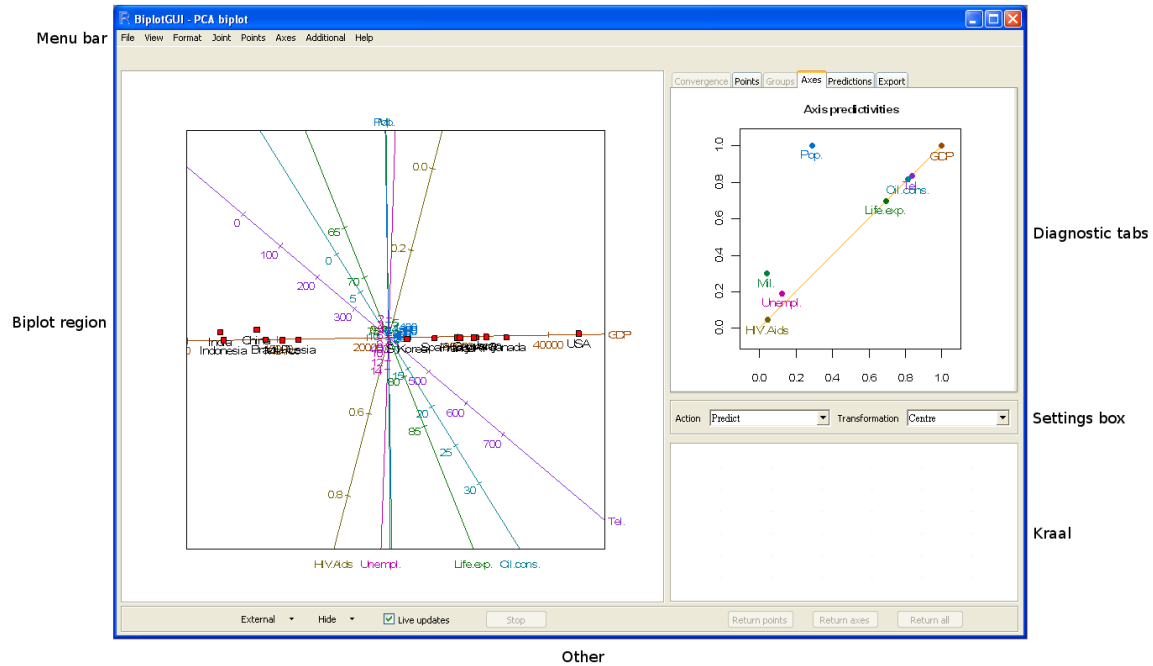


Figure 1.1. A screenshot of the BiplotGUI window as it initially appears. A predictive PCA biplot of the country data is shown towards the left. The axis predictivities are shown top right.

at the R prompt. To initialise the GUI with the country data, the command

```
Biplots(Data = Countries)
```

is entered. No further R commands are necessary.

1.3.3 The layout

Figure 1.1 shows the layout of the GUI after it has launched. Six regions are indicated:

- **The menu bar**, in addition to the settings box, contains the most important options. The three most important drop-down menus are **Joint**, **Points** and **Axes**. The biplots listed under Joint have both their points and axes determined according to a single, joint mechanism. The other biplots have their points determined from the Points menu and their axes determined from the Axes menu.
- **The biplot region** is where the biplot and optional title and legend are displayed. This space is responsive to mouse clicks and motion.
- **The settings box** may be used to set the action of the biplot axes, either predictive, centroid interpolative or vector sum interpolative. Various data transformations may be effected.
- **The diagnostics tabs** show output related to the currently displayed biplot. The convergence tab shows a graph of convergence; the points, groups and axes tabs show context-specific graphs of goodness-of-fit for points, groups and axes, respectively; the predictions tab shows dynamically predicted variable values; while the export tab allows various objects to be exported to R.

- **The [kraal](#)** is where points and axes may be kept, temporarily removing them from consideration.
- **Other.** The options in this section can be used to show the currently displayed [biplot](#) in an external window (in [two](#) or [three](#) dimensions), to control the [biplot region](#) or to control the [kraal](#). While the [GUI](#) is busy, a [progress bar](#) is shown towards the left of this area.

The [Show pop-up help](#) option in the [Help](#) menu activates pop-up help messages which appear when the mouse cursor is hovered over the components of the main [GUI](#) window.

1.3.4 Exploring

The [PCA](#) biplot with predictive axes is shown by default. For the country data, this is the biplot shown towards the left of the screenshot in [Figure 1.1](#). As should be the case for all biplots, a unit aspect ratio is used to ensure that distances within the biplot are properly represented. In this biplot, the points representing the countries lie ordered along a virtually straight line. In fact, the imagined line corresponds very closely to the biplot axis for [GDP](#), and importantly, the line is almost horizontal. The reason for this becomes clear by looking at the [GDP](#) column of the country data set. The values of [GDP](#) are orders larger than those of the other variables. Therefore, that linear combination of the variables that has the largest possible variation (the first principal component) is heavily weighted towards [GDP](#). In effect, [GDP](#) drowns out the other variables. To avoid this, we choose the [Centre, scale](#) transformation from the available [transformations](#) in the [settings box](#). This transformation independently transforms each variable to unit variance and automatically updates the biplot to the one shown in the top left panel of [Figure 1.2](#) (see [Section 1.A.2](#) for details on the calculations involved). Irrespective of the chosen transformation, however, the axes are always calibrated in terms of the original variable values. The first principal component in this new figure still ranks the countries from least to most wealthy, in some more complicated sense. The developed countries of the West, together with Japan and newly-industrialised South Korea, cluster in the south-east quadrant. Brazil, Russia and Indonesia lie more towards the west, with Mexico straddling the divide. India, and especially China, lie further away.

While the relative positions of the points are interesting, biplots come into their own when the points are related to their original variable values through the axes. By right clicking inside the predictive linear biplot and selecting [Predict cursor positions](#) from the pop-up menu, an array of orthogonally projecting lines emanates from, and follows, the cursor as it moves over the biplot. If [Predict points closest to cursor positions](#) is selected instead, the lines project from the point closest to the cursor as it moves, rather than from the cursor itself. So for example, the image in the top right panel of [Figure 1.2](#) was created by hovering the cursor closer to the point for China than to any other point. These orthogonally projecting lines intersect the axes at the positions at which the optimal approximations to the original variables values are to be read off. It can be seen from the image that China scores relatively low on all the variables except population and military spending. As the cursor moves, these predictions are also given numerically, in real time, in the [predictions tab](#). Dynamic prediction is disabled by right clicking inside the biplot and selecting [Don't predict](#) from the pop-up menu. (Some numerical predictions are given below.) Notice that although the predictions are optimal, they remain approximations. An unfortunate consequence is that values close to zero on variables measured on the ratio scale can have negative predicted values. For example, in [Figure 1.2](#) the population of Spain is predicted to be less than zero.

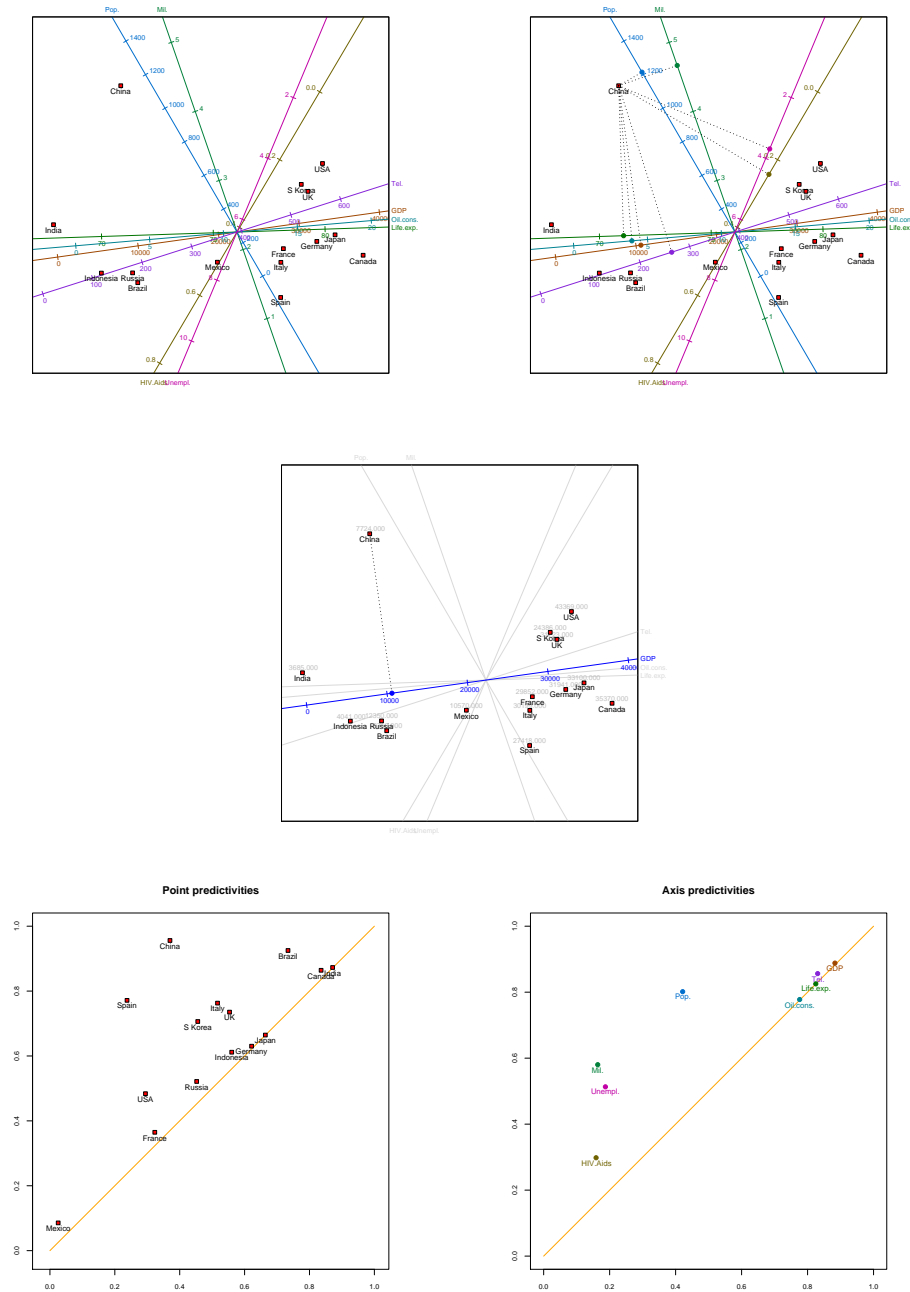


Figure 1.2. Top left panel: a predictive PCA biplot of the centred, scaled country data. Top right panel: a predictive PCA biplot of the centred, scaled country data with China projected onto all the biplot axes. Centre panel: a predictive PCA biplot of the centred, scaled country data with GDP highlighted and China projected. Bottom left panel: PCA point predictivities of the centred, scaled country data. Bottom right panel: PCA axis predictivities of the centred, scaled country data.

With many variables, a biplot may become crowded. A particular axis can be highlighted by right clicking it and then selecting [Highlight](#) from the pop-up menu. Doing so greys the other axes, and displays the true variable values of the highlighted axis above the corresponding points. The displays in the [diagnostic tabs](#) are shaded accordingly and orthogonal projections are drawn to the highlighted axis only. An example is shown in the centre panel of [Figure 1.2](#), where [GDP](#) is highlighted and China is predicted.

The question of course, is how good the biplot approximation is. This depends on both the points and the axes. As for the points, the ‘quality’ of the [PCA](#) approximation is found by clicking to the [export tab](#), selecting ‘quality’, and then clicking [Display in console](#) to display the result in the R console, or otherwise clicking [Save to workspace](#) to save the result as an object in the R workspace. In the case of the country data, the quality, 0.693, implies that 69.3% of the variation in the samples is accounted for by the first two principal components. Point and axis predictivities may also be calculated ([Gardner-Lubbe, Le Roux and Gower, 2008](#)). Predictivities indicate how well *individual* points or axes are represented in various dimensions of the biplot. Diagrams of point and axis predictivities are available in the [points](#) and [axes](#) tabs, respectively. Those for the country data are shown in the bottom panels of [Figure 1.2](#). The points and axes in these figures always appear above the diagonal in the unit square. The further to the right a point or axis appears, the better represented it is in the first (or horizontal) biplot dimension. The closer to the top of the diagram, the better the point or axis is represented overall in the biplot, taking into account the contribution of both the first and the second (vertical) biplot dimension. The marginal contribution of the second biplot dimension is indicated by the vertical distance between the diagonal line and the point or axis. This interpretation suggests that India, Canada and Brazil are relatively well represented in the first biplot dimension. Japan, Germany and Indonesia are represented reasonably in the first dimension, but poorly in the second. France, the United States and Russia are poorly represented overall, and Mexico extremely poorly. China is the best represented country overall. The axes may be similarly interpreted. The two diagrams were saved by right clicking them in the [GUI](#), then making use of the [Save as](#) options in the pop-up menus. Predictivities are also available numerically from the [export tab](#). The formulae for quality, point predictivities and axis predictivities for [PCA](#) biplots are given in [Section 1.A.3](#).

Another measure of the goodness of the approximation is the relative absolute error, which may be calculated for any sample on any variable. The relative absolute error is defined to be the absolute difference between the predicted and actual values, expressed as a percentage of the range (max – min) of the actual values of the particular variable. For [GDP](#), for example, the following output is obtained for the country data by selecting ‘Pred’ from the [export tab](#):

| GDP | Prediction | Actual | RelAbsErr% |
|-----------|------------|--------|------------|
| Brazil | 9330.3 | 8710 | 1.6 |
| Canada | 37282.7 | 35370 | 4.8 |
| China | 10606.7 | 7724 | 7.3 |
| France | 27669.1 | 29852 | 5.5 |
| Germany | 31869.4 | 31941 | 0.2 |
| India | 40.2 | 3685 | 9.2 |
| Indonesia | 5054.5 | 4041 | 2.6 |
| Italy | 27130.3 | 30199 | 7.7 |
| Japan | 34209.8 | 33100 | 2.8 |
| Mexico | 19392.0 | 10570 | 22.2 |
| Russia | 8865.5 | 12350 | 8.8 |
| S Korea | 30946.1 | 24386 | 16.5 |

| | | | |
|-------|---------|-------|------|
| Spain | 26507.7 | 27418 | 2.3 |
| UK | 31644.7 | 31723 | 0.2 |
| USA | 33889.0 | 43369 | 23.9 |

Although the United States, Mexico and South Korea predict poorly on the [GDP](#) axis, the overall configuration is optimal. By taking means over the samples, mean relative absolute errors may be obtained for the different variables. From the export tab's 'MeanRelAbsErr' entry these are:

| | | | | | | | |
|-----|----------|-----------|------|-----------|------|------|---------|
| GDP | HIV.Aids | Life.exp. | Mil. | Oil.cons. | Pop. | Tel. | Unempl. |
| 7.7 | 20.1 | 9.8 | 14.4 | 11.2 | 11.3 | 8.8 | 15.1 |

These error rates reinforce what is conveyed by the axis predictivities: that HIV/Aids prevalence, unemployment and military spending are relatively poorly represented, the other variables better. Mean relative absolute errors are useful as a measure of the loss of information in biplots since they can be calculated for any type of biplot. Predictivities are defined only when certain orthogonal decompositions exist ([Gardner-Lubbe *et al.*, 2008](#)), as they do in the case of [PCA](#), [CVA](#) and analysis of distance ([AOD](#)) ([Krzanowski, 2004](#); [Gardner, Le Roux, Rypstra and Swart, 2005](#)) biplots.

For a biplot to be usable in printed form, it must necessarily be two-dimensional. However, assisted by a computer, a user may easily interact with a biplot in three dimensions. Three-dimensional, non-MDS biplots may be obtained in the [BiplotGUI](#) package by clicking the [External](#) menu button at the bottom left of the [GUI](#) and then selecting the [In 3D](#) option. Alternatively, the user may simply press the F12 shortcut key shown alongside the option. Doing so renders the three-dimensional version of the currently displayed two-dimensional [biplot](#) in an external window. This feature makes use of the [rgl](#) package ([Adler and Murdoch, 2009](#)) and allows the biplot to be rotated and enlarged dynamically. [Figure 1.3](#) shows the three-dimensional predictive [PCA](#) biplot of the country data that corresponds to the two-dimensional version at the top left of [Figure 1.2](#). A further 12.9% of the total variation in the samples is accounted for in the additional dimension – the third value from 'eigen' in the export tab divided by the sum of the eigenvalues. An initial 360 degree 'fly-by' of three-dimensional biplots can be enabled via the [File → Options](#) dialogue box.

A [PCA](#) approximation results from the projection of samples onto the plane of best fit. In a covariance biplot ([Joint → Covariance/Correlation](#)), these 'scores' are adjusted so that the cosines of the angles between the biplot axes approximate the correlations between the corresponding variables. The correlation biplot is the same as the covariance biplot, but with the variables first scaled to have unit variances (via the settings box, in the usual manner). The correlation biplot of the country data is shown in the top left panel of [Figure 1.4](#). Three groups of variables are seen to be highly positively correlated (the angles between them are small):

- the number of telephone lines, [GDP](#), oil consumption, life expectancy;
- HIV/Aids prevalence, unemployment;
- population, military spending.

The computations underlying these biplots are set out in [Section 1.A.4](#). Notice that the labels of the axes are attached to those ends of the axes that have the higher calibrations. This is the default option for all linear biplots. Alternatively, the axis labels may be given in a [legend underneath the biplot](#), or [no axis labels](#) may be given whatsoever. These and other

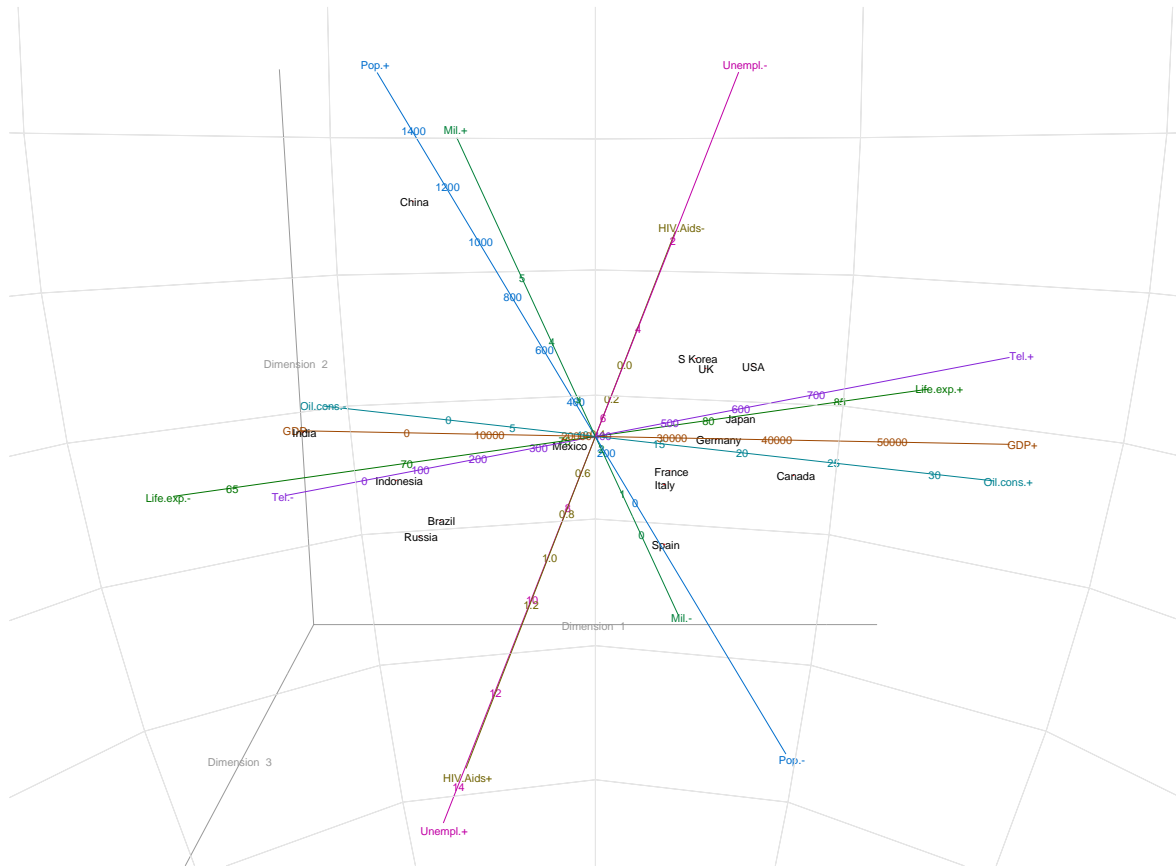


Figure 1.3. The predictive PCA biplot of the centred, scaled country data, in three dimensions. This figure corresponds to the two-dimensional biplot at the top left of Figure 1.2.

similar options may be set via the **View** menu. Notice also that the option **Joint → CVA** is disabled since the samples of the country data have not been grouped in any way, for example by continent. We return to **CVA** biplots in Section 1.4.1, where the samples of the antique furniture data set are grouped, and where group differences are investigated.

As opposed to dimension reduction by projection, in **MDS** the points are chosen so that *stress*, the sum of the squared differences between the inter-sample *disparities* and the inter-point *distances*, is explicitly minimised (details in Section 1.A.8). The **Points → MD'** menu gives various options. These include taking the inter-sample disparities to be the inter-sample *dissimilarities* themselves (the **identity transformation**); retaining merely the order of the inter-sample dissimilarities by optimally transforming them into disparities (**monotone regression**, Kruskal, 1964b); or monotonically smoothing the inter-sample dissimilarities into disparities (the **monotone spline transformation**, Ramsey, 1982, 1988). Therefore metric, non-metric and semi-metric **MDS** representations are available. The inter-sample dissimilarities are calculated according to the chosen dissimilarity metric (Section 1.A.6). Four metrics are currently available from the **Points → Dissimilarity metric** menu: **Pythagoras**, **Square-root-of-Manhattan**, **Clark** and **Mahalanobis**. Inter-point distances are always Pythagorean. An iterative majorisation (**IM**) algorithm (De Leeuw, 1977; De Leeuw and Heiser, 1980) is used to find the **MDS** solutions. The **IM** algorithm converges uniformly, and usually leads to a local minimum, although in theory a saddle-point cannot be ruled out. Practical convergence criteria need to be specified.

The top right panel of Figure 1.4 shows a metric **MDS** of the country data, expressed in terms of its principal axes, with approximate regression biplot axes superimposed (from **Points →**

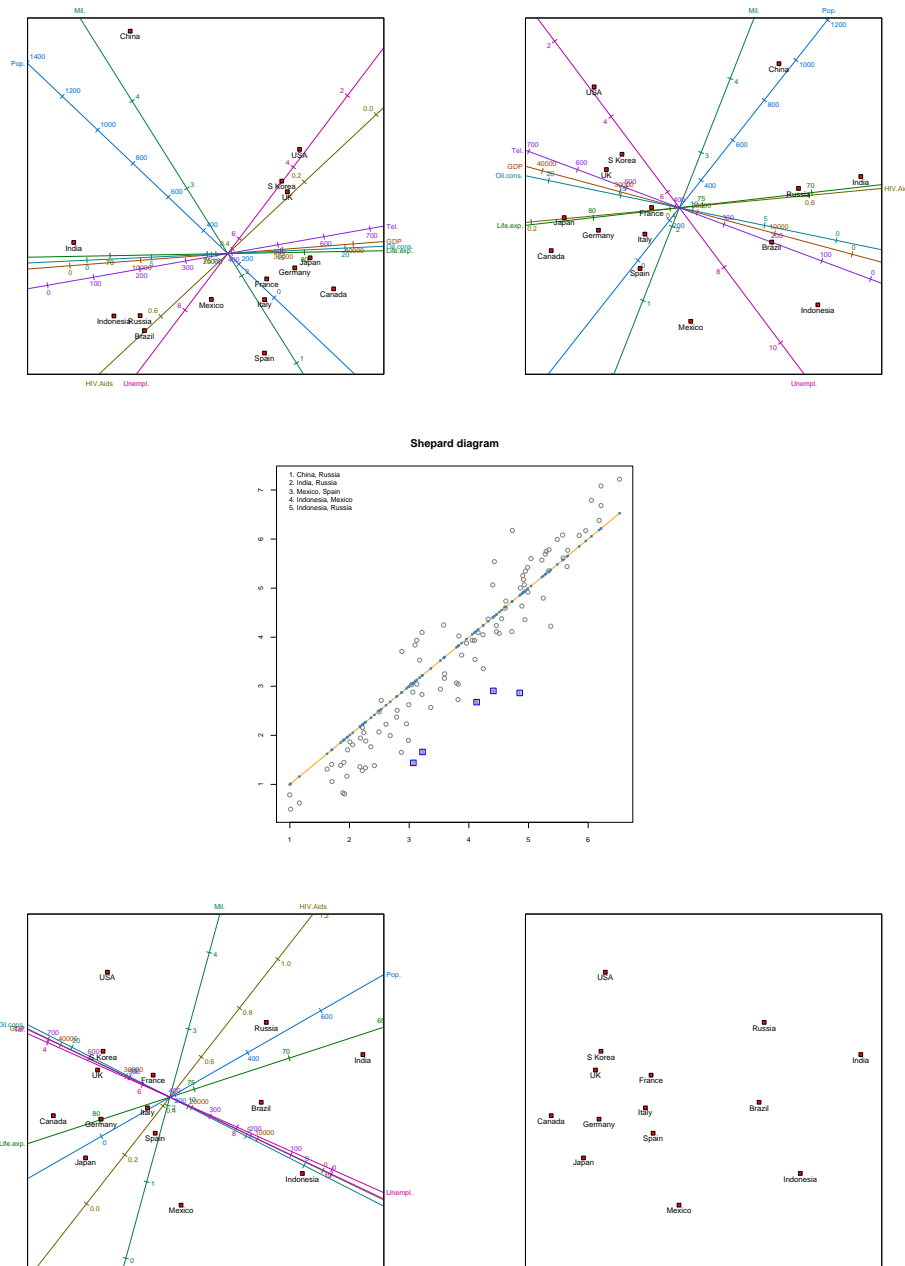


Figure 1.4. Top left panel: a predictive correlation biplot of the centred, scaled country data. Top right panel: a predictive regression biplot for the metric MDS representation of the centred, scaled country data. The MDS representation is in terms of its principal axes. Centre panel: the Shepard diagram corresponding to the regression biplot of the top right panel. Bottom left panel: a predictive regression biplot for the metric MDS representation of the centred, scaled country data, but with China removed. Bottom right panel: the metric MDS of the centred, scaled data with China removed.

MDS → In terms of principal axes, thereafter Points → MDS → Identity transformation). The default dissimilarity metric, Pythagoras, is retained. In this representation, the relative distances between the points are directly related to the corresponding dissimilarities between the countries. The United Kingdom and South Korea, therefore, are more similar to one another than they are to the other countries with respect to the eight variables. As the algorithm converges, updates of the configuration are shown in the [biplot region](#), together with updates of the graphs in the [diagnostic tabs](#). The [Live updates](#) option, however, may be disabled to increase the speed at which the algorithm runs (the checkbox in question is amongst the buttons at the bottom of the [GUI](#)). A graph of the stress values over iterations is given in the [convergence tab](#); in this instance, from the [export tab](#), convergence is reached after 96 iterations, with a final stress value of 45.8. By default, the [IM](#) algorithm is taken to have converged as soon as the relative decrease in stress is lower than 10^{-6} . The algorithm is also stopped once more than 5000 iterations have been performed. These options can be adjusted via the [File → Options](#) dialogue box. A Shepard diagram ([Borg and Groenen, 2005](#), Section 3.3; [Shepard, 1962](#)) can be found in the [points tab](#) and is shown at the centre of [Figure 1.4](#). Each circle in the Shepard diagram represents a pair of samples. The horizontal axis indicates the inter-sample dissimilarity; the vertical axis indicates the corresponding inter-point distance. The blue dots on the yellow line (which generalises to a step function or a curve) indicate the disparities. Thus the closer the circles are to the line (or step function or curve), the better the overall fit. The five worst-fitting point pairs are identified in the top left corner of the diagram. The dissimilarity between China and Russia, therefore, is most poorly approximated by the points. The [Points → MDS → Random initial configuration](#) option forces the algorithm to start from a random configuration at each run; a new run is initiated by clicking [Points → MDS → Run](#) or by re-clicking [Points → MDS → Identity transformation](#). Otherwise, the last [PCO](#) or [MDS](#) solution is taken to be the new initial configuration, as is the case for [Figure 1.4](#).

To conclude with the country data, suppose that we feel that China is in many ways atypical, and that we would like to see what the effect would be of removing it from consideration. To do so we need simply ‘drag’ the point representing China from the [biplot](#) into the [kraal](#). We may also right click the point representing China and select [Send to kraal](#) from the pop-up menu. The [biplot region](#) is then automatically updated as if China were never part of the data set. The updated biplot is given in the bottom left panel of [Figure 1.4](#). Russia’s position relative to the other countries seems to have been most greatly affected. There has also been a re-alignment amongst the axes, most notably the axes for HIV/Aids, population and unemployment. Axes may also be removed to the [kraal](#). Points and axes which have been removed to the [kraal](#) may be dragged back onto the biplot, or the [kraal](#) may be emptied of its [points only](#), its [axes only](#), or of both its [points and axes](#) simultaneously by making use of the buttons below it, or by right clicking inside it and selecting the desired option from the [pop-up menu](#). At any stage, the points and/or axes of any representation may be hidden by clicking on the options in the [hide](#) menu button at the bottom of the window. The figure at the bottom right of [Figure 1.4](#) is the same as the one in the bottom left panel, but with the biplot axes hidden as described.

1.4 TWO MORE EXAMPLES

In this section we consider two more examples. In [Section 1.4.1](#) we focus our attention on grouped data by investigating antique furniture, while non-linear prediction is illustrated in [Section 1.4.2](#) at the hand of fighter aircraft data.

1.4.1 Antique furniture

It is often of great interest to collectors, auctioneers and cultural historians to be able to correctly identify the type of wood used to make antique furniture. In the period between 1652 and 1900, wood from both the indigenous *Ocotea bullata* ('Stinkwood') and the imported *Ocotea porosa* ('Imbuia') were used to make Old-Cape furniture in South Africa. Being from the same genus and family (*Lauraceae*), it is often difficult to distinguish between the two types of wood based solely on a traditional analysis of colour, smell, and other observable characteristics. [Burden, Gardner, Le Roux and Swart \(2001\)](#) and [Le Roux and Gardner \(2005\)](#) make use of **CVA** biplots of anatomical measurements to distinguish between the species. A third species, *Ocotea kenyensis*, is also included in the analyses. The microscopically measured variables are: tangential vessel diameter in μm (VesD); vessel element length in μm (VesL); fibre length in μm (FibL); ray height in μm (RayH); ray width in μm (RayW); and the number of vessels per mm^2 (NumVes). The 37 observations are the mean values over fifty repeat-measurements made on 20 samples of *Ocotea bullata*, 10 of *Ocotea porosa*, and 7 of *Ocotea kenyensis*. The data are included in the **BiplotGUI** package as the data frame **AntiqueFurniture**, of which the first column contains the group specifications. The data may be viewed from within R by entering the following instructions at the prompt of the R console:

```
data(AntiqueFurniture)
AntiqueFurniture
```

To initialise the **GUI** with the antique furniture data, the following command may be entered at the R prompt:

```
Biplots(Data = AntiqueFurniture[, -1], groups = AntiqueFurniture[, 1])
```

In other words, the data consist of all the columns of **AntiqueFurniture** except the first, while the group specifications are precisely the contents of the first column.

As was mentioned earlier, upon initialisation of the **GUI**, the predictive **PCA** biplot is shown by default. To show the **CVA** biplot instead, the user simply needs to click the option **Joint → CVA**. This option is now available since, in the call to the **Biplots** function, groups were specified. The predictive **CVA** biplot of the antique furniture data is shown in the top left panel of [Figure 1.5](#). The positions of the points are determined by the first two canonical variates – those linear combinations of the original variables that maximally separate the group means, subject to certain restrictions ([Krzanowski, 2000](#), Section 11.1). The group means themselves are shown as larger but corresponding symbols (activated by clicking **Additional → Interpolate → Sample group means**, retaining the default options). Since there is more than one group, an optional **legend** is included below the **biplot** by default. The mechanism for the prediction of the variable values is the same as before and is illustrated in the figure in the case of sample 29.

The top right panel of [Figure 1.5](#) shows the same biplot, now overlain onto a two-dimensional density estimate of the points. The density estimate is obtained by clicking **Additional → Point densities** and accepting the default options (amongst other things, for the point densities to be estimated for all points, as opposed to certain groups of points only). The point densities are calculated using the default arguments to the **bkde2D** function of the **KernSmooth** package ([Wand, 2008](#)). Similar biplots can be found in [Blasius, Eilers and Gower \(2008\)](#).

Sometimes it is helpful to zoom into or out of portions of a biplot. This is done by right clicking on a focal point inside the **biplot**, and selecting the **Zoom in** or **Zoom out** option from the pop-up menu which then appears. The bottom panel of [Figure 1.5](#) shows the **CVA** biplot of antique furniture, enlarged around the mean of the species *Ocotea bullata*. The original view can be restored by choosing the **Reset zoom** option from the pop-up menu.

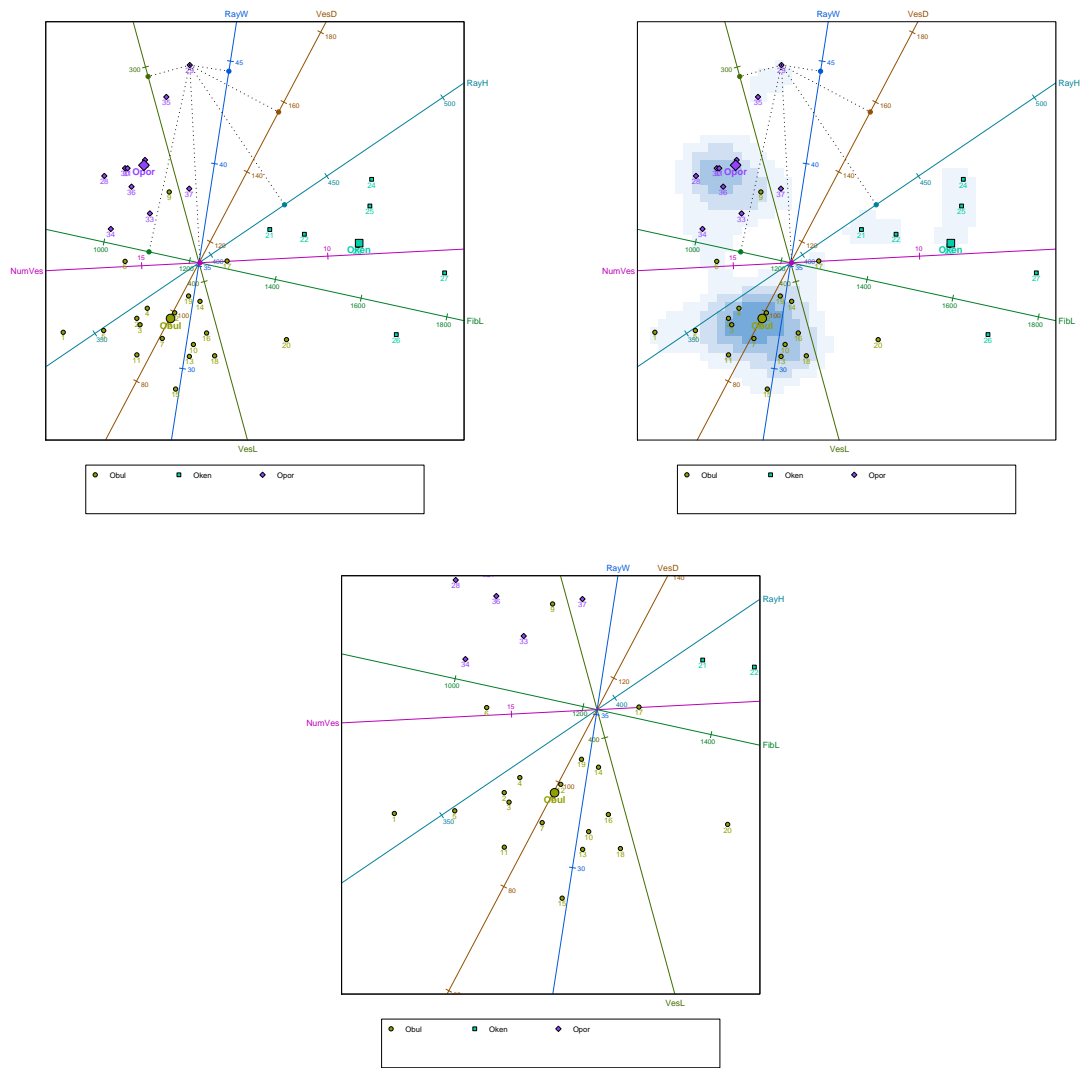


Figure 1.5. Top left panel: a predictive CVA biplot of the antique furniture data with sample 29 projected onto all the biplot axes. The group means are also shown. Top right panel: as in the top left panel, but with the biplot overlain onto the two-dimensional density estimate of the points. Bottom panel: the same biplot as the other two, but zoomed in around the mean of the species *Ocotilla bullata*.

A screenshot of the GUI is shown in Figure 1.6. To the left, a CVA biplot of the antique furniture data appears. From the settings box, it can be seen that the axes are not predictive; in fact they are `Action.InterpolateVectorSum` vector sum interpolative. Also, the data have not been transformed, except for the obligatory centring of the columns to have zero means. In any case, CVA biplots are unaffected by the scaling of the variables to have unit variance. Sample 18 has been dragged from the biplot into the kraal. It has therefore not been taken into account in the construction of the biplot. However, using its original variable values—104, 387, 1290, 381, 22 and 12, respectively—it has subsequently been interpolated onto the biplot towards the bottom of the image (using the `Additional → Interpolate → A New Sample` option). This is the most appropriate position for the sample in the existing biplot. It is reassuring that the positions assigned to sample 18 in Figures 1.5 and 1.6 correspond so closely. This need not have been the case. Also notice that, notwithstanding the removal of sample 18, the calibrations and directions of the predictive and interpolative biplot axes differ. This is in general the case for CVA biplots. More details are given in Section 1.A.5.

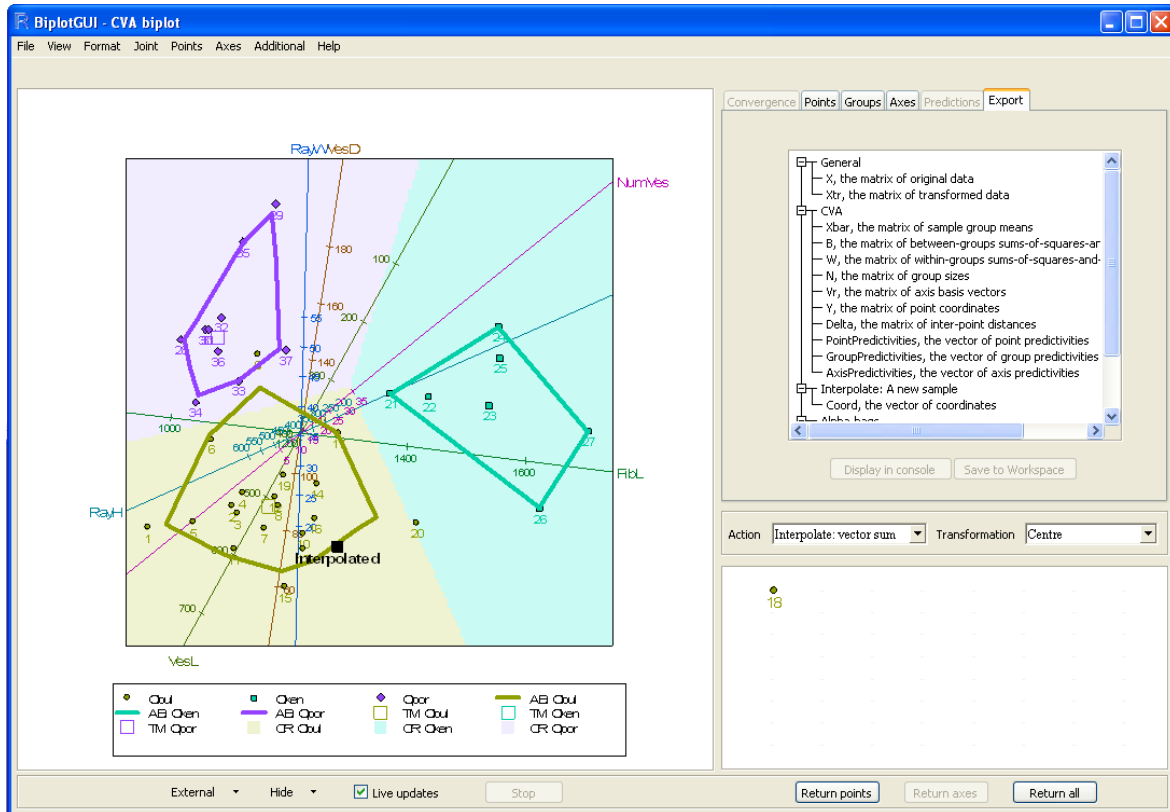


Figure 1.6. A screenshot of the GUI. A vector sum interpolative CVA biplot of the antique furniture data is shown towards the left, with sample 18 removed to the kraal. Sample 18 has then been interpolated to give its implied position. Classification regions are shown, as well as 90% alpha-bags for the species *Ocotea bullata* and *Ocotea porosa*. A convex hull surrounds the points of the species *Ocotea kenyensis*. The export tab is shown top right.

The biplot in Figure 1.6 also sports colour-coded classification regions. These are the regions in the display space plane closest to the respective group means in a specified number of canonical dimensions, here the default number, two. The classification regions are included by selecting [Classification regions](#) from the [Additional](#) menu. They may be used for the classification of interpolated samples. For more on the links between biplots and discrimination, see [Gardner and Le Roux \(2005\)](#). Furthermore, by clicking [Additional](#) → [Alpha-bags](#), alpha-bags ([Gardner, 2001](#); [Aldrich, Gardner and Le Roux, 2004](#)) and Tukey medians have been superimposed for the species *Ocotea bullata* and *Ocotea porosa* (there are too few samples for an alpha-bag for *Ocotea kenyensis* to be constructed; with an appropriate warning, a convex-hull is displayed instead). Alpha-bags are closely related to the bagplots of [Rousseeuw, Ruts and Tukey \(1999\)](#) and enclose regions that contain approximately the inner 100 α % of samples, here 90% of the samples for the two species separately. The alpha-bags and convex hull do not overlap. This emphasises the high degree of separation between the species. For CVA biplots, group predictivities may also be calculated, in addition to the point and axis predictivities discussed earlier ([Gardner-Lubbe et al., 2008](#)). A diagram of these is available in the [groups](#) tab. Finally, Figure 1.6 also shows the [export](#) tab. As has been explained, various objects are available for export from this tab, and may be either [displayed in the R console](#), or [saved to the current R workspace](#). The list of available objects depends on what is shown in the [biplot](#).

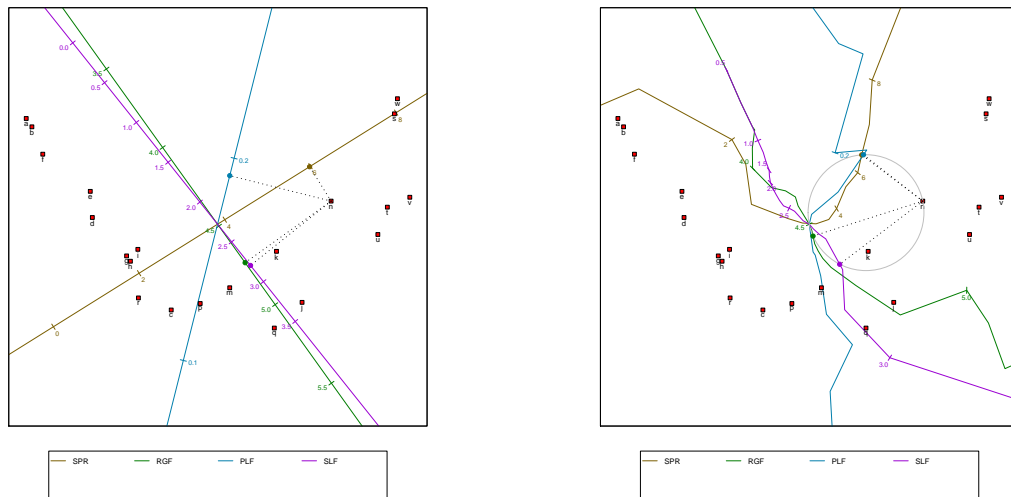


Figure 1.7. Left panel: a predictive regression biplot of the fighter aircraft data, with points determined by [PCO](#) based on the Square-root-of-Manhattan dissimilarity metric. The orthogonal prediction of the variables values of aircraft ‘n’ is shown. Right panel: a predictive circular non-linear biplot of the fighter aircraft data, with points determined by [PCO](#) based on the Square-root-of-Manhattan dissimilarity metric. The circular prediction of the variable values of aircraft ‘n’ is shown.

1.4.2 Fighter aircraft

Measurements of four variables on 22 types of fighter aircraft were extracted by [Cook and Weisberg \(1982\)](#) from a report by [Stanley and Miller \(1979\)](#). Following [Gower and Hand \(1996\)](#), we consider only the first 21 of these aircraft in the biplots below. The four variables are: specific power, proportional to power per unit weight (SPR); flight range factor (RGF); payload as a fraction of gross weight (PLF); and sustained load factor (SLF). These data can be found in the `FighterAircraft` data frame included in the `BiplotGUI` package. The `GUI` is initialised in the same way as it was for the country data in [Section 1.3.2](#).

The left panel of [Figure 1.7](#) shows a regression biplot of the fighter aircraft data with the points determined by [PCO](#) and the inter-sample dissimilarities calculated according to the Square-root-of-Manhattan dissimilarity metric. The figure is obtained by clicking [Points](#) → [Dissimilarity metric](#) → [Square-root-of-Manhattan](#) and then [Axes](#) → [Regression](#). Making use of orthogonal projection, the variable values for aircraft ‘n’ are predicted to be 5.980, 4.73, 0.191 and 2.80, respectively. These can be compared to the actual values, 5.855, 4.53, 0.172 and 2.50. The right panel of [Figure 1.7](#) shows the corresponding circular non-linear biplot (obtained by clicking [Axes](#) → [Circular non-linear](#)). Here prediction is performed by completing the circle which has, as diagonal, the line stretching from the origin of the biplot to the point to be predicted. The predicted values are read off at the points at which the circle intersects the axes ([Gower and Hand, 1996](#), Section 6.3.2). If a particular axis is intersected at more than one position, the position closest to the point being predicted is used. If an axis isn’t intersected at all, no prediction for the corresponding variable can be made. For aircraft ‘n’, the valid points of intersection are shown in the figure as small, filled circles on the circumference of the larger circle. From the [predictions](#) or [export tabs](#), the circular non-linear predictions for aircraft ‘n’ are 6.090, 4.54, 0.174 and 2.90, respectively (these values depend on how finely the non-linear axes are constructed; by default 20 positions are taken into account from each calibrated marker to the next). Except for the fourth variable, the non-linear predictions are very close to the actual values.

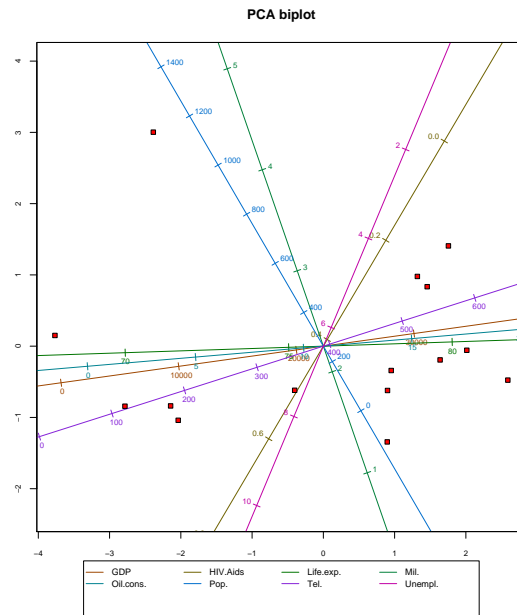


Figure 1.8. A modified version of the biplot given in the top left panel of [Figure 1.2](#): a predictive PCA biplot of the country data with a title, hidden point labels, axis labels in a legend, and the axes of the display space calibrated.

[Section 1.A.7](#) provides the steps required to perform a PCO; the formulae underlying the regression and circular non-linear biplots are provided in [Sections 1.A.9](#) and [1.A.11](#), respectively.

1.5 FURTHER FEATURES

This section touches upon the customisation and export of biplots and other graphs produced using the **BiplotGUI** package.

There are two main ways in which graphs can be customised. Basic customisation can be performed using the options of the **View** menu, while the **Format** menu options can be used to alter a large number of graphical parameters.

[Figure 1.8](#) shows the same predictive PCA biplot of the country data as was shown in the top left panel of [Figure 1.2](#). However, the biplot in [Figure 1.8](#) has been modified by changing the default selections in the **View** menu. The **Show title** option places a title above the biplot; by default the title reflects the type of biplot, but it may be changed via the **Format** → **Title** option. Furthermore, the point labels have been hidden by deselecting **Show point labels**. Instead of showing the axis labels around the edges of the biplot as in [Figure 1.2](#), the labels in [Figure 1.8](#) are shown in a legend (**Show axis labels in legend**). The **View** → **Calibrate display space axes** option calibrates the two dimensions of the biplot, but this is generally undesirable in biplots of the new approach ([Gower and Hand, 1996](#), Section 2.6).

The **Format** menu allows virtually any of the graphical parameters used internally by the package to be altered. The biplot in [Figure 1.9](#) serves as an example. This biplot is the same as the biplot that appears in the left panel of [Figure 1.5](#), but with some of the default graphical parameters changed. The **By group** option allows the graphical parameters which relate to points, sample group means, convex hulls / alpha-bags and classification regions to be set for all groups simultaneously, or for a single group at a time. [Figure 1.10](#) shows the ‘By group’ dialogue box as it appears for the points of the species *Ocotea bullata*. The parameter

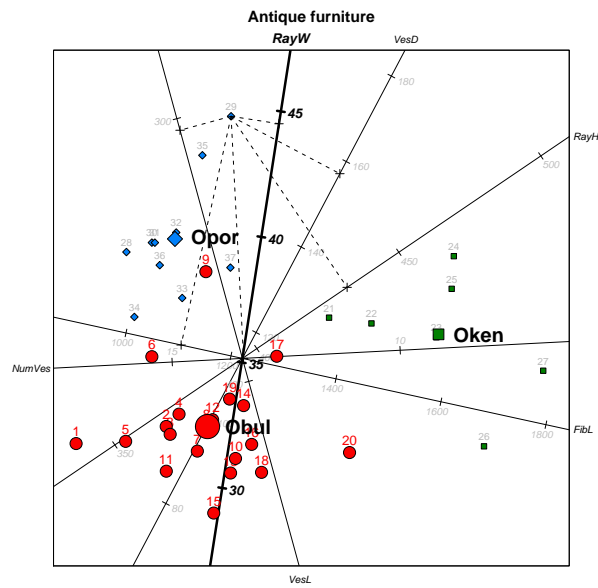


Figure 1.9. A modified version of the biplot given in the left panel of [Figure 1.5](#): a predictive CVA biplot of the antique furniture data.

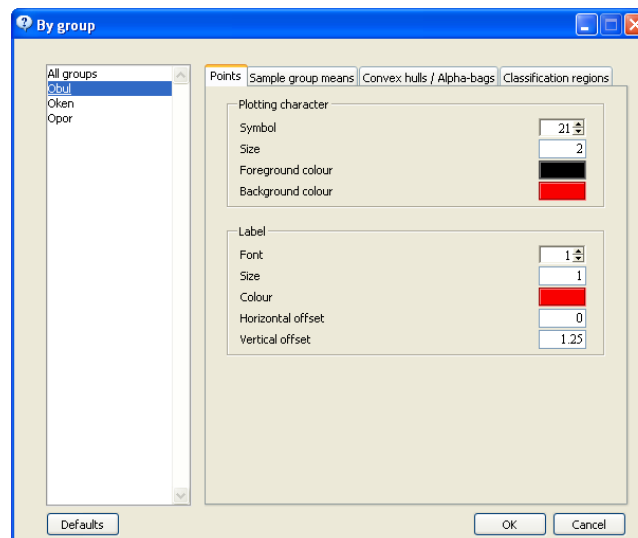


Figure 1.10. The 'Format → By group' dialog box as it appears for the biplot in [Figure 1.9](#).

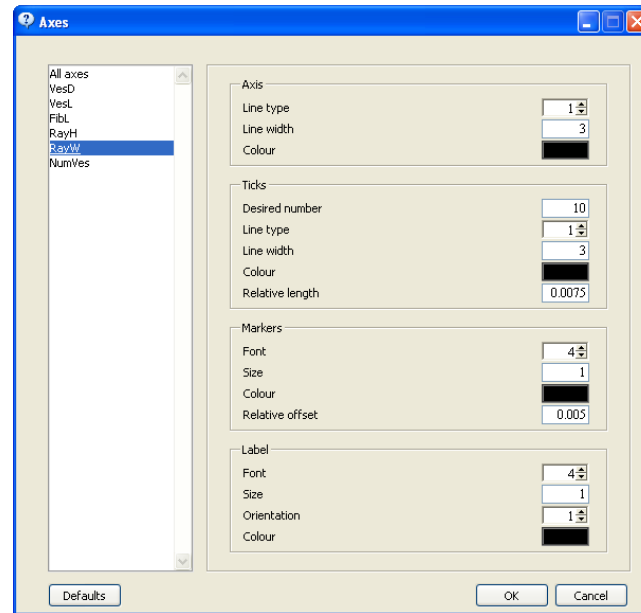


Figure 1.11. The ‘Format → Axes’ dialogue box as it appears for the biplot in Figure 1.9.

values shown are as they have been set for Figure 1.9. The [Axes](#) option similarly allows the graphical parameters for axes to be set. Figure 1.11 shows the ‘Axes’ dialogue box in the case of the graphical parameters for the axis ‘RayW’, again with the parameters as they have been adjusted for Figure 1.9. The graphical parameters used in dynamic variable value prediction and in the highlighting of axes can also be modified by clicking [Format → Interaction](#), while [diagnostic tab](#) customisation may be performed via the [Diagnostic tabs](#) option. The [Reset all](#) option reverts all the graphical parameters back to their default values. In all, more than 80 different graphical parameters may be set, often-times differently for different groups or axes. All these parameters are documented in detail in the package manual.

[Biplots](#) and [diagnostic tab](#) graphs can be saved in various file formats: [PDF](#), [Postscript](#), [Metafile](#), [Bmp](#), [Png](#), [Jpeg](#) (50%, 75%, 100% quality) and [PicTeX](#). Any graph can be saved by right clicking it and navigating the Save as menu. The biplot region may also be saved via the [File → Save as](#) menu. While the images shown onscreen are by necessity Metafile images, the images that appear in this article—besides the screenshots—were saved in PDF format. Together with Postscript, such images are of the highest quality. [Copy](#) and [Print](#) options are also available.

1.6 FUTURE WORK

Being in its first release, there is much that may be improved and expanded upon. Amongst the techniques which might sensibly be incorporated into the package are:

- Special options for [CVA](#) biplots in the case of two groups only ([Le Roux and Gardner-Lubbe, 2008](#));
- Orthogonal predictive non-linear biplots ([Gower and Ngouenet, 2005](#));
- [AOD](#) biplots ([Krzanowski, 2004](#); [Gardner et al., 2005](#));
- The adjustments to the regression and Procrustes biplots suggested by [Gower, Meulman and Arnold \(1999\)](#) to better suit non-metric [MDS](#) representations;

- Sensitivity analysis for PCO-based biplots (Krzanowski, 2006);
- Support for categorical variables in the form of generalised biplots (Gower, 1992);
- A better approach to the calculation of classification regions (Gower, 1993).

Other improvements may also be made. These include:

- Allowing any pair of principal components, canonical variates or principal coordinates to be shown, as opposed to only the first two;
- Supporting a greater number of dissimilarity metrics;
- Allowing interactive orthogonal parallel translation so that axes can be moved towards the edges of biplots (Blasius *et al.*, 2008);
- Incorporating a graded legend for point density estimates;
- Improving the three-dimensional biplots (providing support for additional descriptors, allowing dynamic variable value prediction);
- Otherwise improving the GUI and general performance.

As for any such package, suggestions and bug-reports by users are important and greatly encouraged.

1.7 SUMMARY

In this paper, the BiplotGUI package for R was introduced. Its features were illustrated using three data sets; ideas for future releases were briefly explored; and computational details were provided in an appendix.

The package makes it possible to easily construct many types of biplots and to interact with them in various ways. The package is free and its source code shared. Amongst linear biplots, the PCA, covariance/correlation, CVA, regression and Procrustes biplots are supported. Circular non-linear biplots can be created. In addition, PCO and MDS representations can be displayed on their own, without added biplot axes. Additional descriptors can be superimposed, and three-dimensional biplots can be explored using the `rgl` package. Various goodness-of-fit measures are easily accessible.

1.A COMPUTATIONS

This section outlines the main formulae used to produce the biplots of the BiplotGUI package. Fuller explanations and derivations may be found in the cited works.

1.A.1 General

Let $\mathbf{X} : n \times p$ represent a data matrix. The n samples of \mathbf{X} are to be represented as points in a biplot; the p (numerical) variables are to be represented as calibrated biplot axes. Biplots are displayed in r dimensions. Typically r is taken to be 2 or 3. Biplots with higher values of r are abstractions that cannot be drawn.

1.A.2 Data transformations

The data matrix \mathbf{X} is first transformed into a matrix $\tilde{\mathbf{X}} : n \times p$ on which further calculations are performed. By convention, however, biplot axes are always calibrated in terms of the original variable values, those of \mathbf{X} . Six transformations are supported: ‘centre’, ‘centre, scale’, ‘unitise, centre’, ‘log, centre’, ‘log, centre, scale’ and ‘log, unitise, centre’. The transformations are compound functions. The base functions (log, centre, scale, unitise) are performed in the order in which they appear in the option names. When a matrix $\mathbf{A} : n \times p$ is transformed into a matrix $\mathbf{B} : n \times p$ by taking *logarithms*, $[\mathbf{B}]_{ij} = \log_e([\mathbf{A}]_{ij})$. This requires that all $[\mathbf{A}]_{ij} > 0$. When a matrix \mathbf{A} is transformed into a matrix \mathbf{B} by *centring*, $[\mathbf{B}]_{ij} = [\mathbf{A}]_{ij} - \text{mean}(\mathbf{A}_{(j)})$, where $\mathbf{A}_{(j)}$ is the j th column of \mathbf{A} and $\text{mean}(\mathbf{a})$ returns the mean of the elements of \mathbf{a} . When a matrix \mathbf{A} is transformed into a matrix \mathbf{B} by *scaling*, $[\mathbf{B}]_{ij} = [\mathbf{A}]_{ij}/\text{sd}(\mathbf{A}_{(j)})$, where $\text{sd}(\mathbf{a})$ returns the sample standard deviation of the elements of \mathbf{a} . When a matrix \mathbf{A} is transformed into a matrix \mathbf{B} by *unitising*, $[\mathbf{B}]_{ij} = ([\mathbf{A}]_{ij} - \min(\mathbf{A}_{(j)}))/(\max(\mathbf{A}_{(j)}) - \min(\mathbf{A}_{(j)}))$, where $\max(\mathbf{a})$ and $\min(\mathbf{a})$ return the maximum and minimum, respectively, of the elements of \mathbf{a} .

1.A.3 The PCA biplot

Points: The normalised eigenvectors corresponding to the r largest eigenvalues of $\tilde{\mathbf{X}}'\tilde{\mathbf{X}}$ form the columns of a *basis matrix* $\mathbf{V}_r : p \times r$. The samples of \mathbf{X} are represented as points in the display space at coordinates $\mathbf{Y} : n \times r = \tilde{\mathbf{X}}\mathbf{V}_r$. These are simply the ‘scores’ of the first r principal components.

Axes: All biplot axes pass through the origin. Predictive and interpolative biplot axes coincide in direction. The j th *predictive* biplot axis is calibrated μ at coordinates $(\tilde{\mu}\mathbf{e}_j'\mathbf{V}_r)/(\mathbf{e}_j'\mathbf{V}_r\mathbf{V}_r'\mathbf{e}_j)$, with $\tilde{\mu}$ the consistently transformed μ , and with \mathbf{e}_j the j th column of the identity matrix \mathbf{I}_p . Convenient markers, representative of the j th column of \mathbf{X} , are variously substituted into μ to calibrate the entire axis. The j th *vector sum interpolative* biplot axis is similarly calibrated μ at coordinates $\tilde{\mu}\mathbf{e}_j'\mathbf{V}_r$, while the j th *centroid interpolative* biplot axis is calibrated μ at coordinates $\tilde{\mu}p\mathbf{e}_j'\mathbf{V}_r$.

Goodness-of-fit: With λ_j the j th largest eigenvalue of $\tilde{\mathbf{X}}'\tilde{\mathbf{X}}$, the *quality* of the representation is given by $(\sum_{j=1}^r \lambda_j)/(\sum_{j=1}^p \lambda_j)$. The *adequacy* of the j th biplot axis is $\mathbf{e}_j'\mathbf{V}_r\mathbf{V}_r'\mathbf{e}_j$. The r -dimensional *point predictivities* are given by the diagonal elements of

$$\text{diag}(\hat{\tilde{\mathbf{X}}}\hat{\tilde{\mathbf{X}}}')\text{diag}(\tilde{\mathbf{X}}\tilde{\mathbf{X}}')^{-1},$$

with $\hat{\tilde{\mathbf{X}}}$ the reconstructed matrix $\hat{\tilde{\mathbf{X}}} = \tilde{\mathbf{X}}\mathbf{V}_r\mathbf{V}_r'$. The r -dimensional *axis predictivities* are given by the diagonal elements of

$$\text{diag}(\hat{\tilde{\mathbf{X}}}\hat{\tilde{\mathbf{X}}}')\text{diag}(\tilde{\mathbf{X}}'\tilde{\mathbf{X}})^{-1}.$$

Quality, adequacies and predictivities always lie in the interval $[0, 1]$, with higher values better.

More: Full details may be found in [Gower and Hand \(1996, Chapter 2\)](#), and, for point and axis predictivities, in [Gardner-Lubbe et al. \(2008\)](#).

1.A.4 The covariance/correlation biplot

When \mathbf{X} is transformed into $\tilde{\mathbf{X}}$ by centring only, the biplot is known as a *covariance* biplot. If in addition \mathbf{X} is transformed by scaling, the biplot is known as a *correlation* biplot.

Points: The *basis matrix for interpolation* is given by

$$\mathbf{V}_{r,\text{int}} = (n-1)^{1/2}\mathbf{V}_{r,\text{pca}}\text{diag}(\lambda_1, \dots, \lambda_r)^{-1/2},$$

where $\lambda_1, \dots, \lambda_r$ are the r largest eigenvalues of $\tilde{\mathbf{X}}'\tilde{\mathbf{X}}$ and where the columns of $\mathbf{V}_{r,\text{pca}}$ contain the corresponding normalised eigenvectors. In the case of both interpolative and predictive biplots, the samples are represented as points in the display space at coordinates $\mathbf{Y} = \tilde{\mathbf{X}}\mathbf{V}_{r,\text{int}}$.

Axes: All biplot axes pass through the origin. Predictive and interpolative biplot axes do *not* in general coincide in direction. The *basis matrix for prediction* is

$$\mathbf{V}_{r,\text{pr}} = n^{-1/2}\mathbf{V}_{r,\text{pca}}\text{diag}(\lambda_1, \dots, \lambda_r)^{1/2}.$$

The j th *predictive* biplot axis is calibrated μ at coordinates $(\tilde{\mu}\mathbf{e}_j'\mathbf{V}_{r,\text{pr}})/(\mathbf{e}_j'\mathbf{V}_{r,\text{pr}}\mathbf{V}_{r,\text{pr}}'\mathbf{e}_j)$. The j th *vector sum interpolative* biplot axis is calibrated μ at coordinates $\tilde{\mu}\mathbf{e}_j'\mathbf{V}_{r,\text{int}}$, while the j th *centroid interpolative* biplot axis is calibrated μ at coordinates $\tilde{\mu}\mathbf{p}\mathbf{e}_j'\mathbf{V}_{r,\text{int}}$.

Goodness-of-fit: The *quality* of the representation is given by $(\sum_{j=1}^r \lambda_j)/(\sum_{j=1}^p \lambda_j)$.

More: Full details may be found in [Gardner \(2001, Section 2.3.2\)](#). See also [Greenacre \(1984\)](#), [Underhill \(1990\)](#) and [Gower and Hand \(1996, Section 11.5.1\)](#).

1.A.5 The CVA biplot

Points: In CVA biplots, the n samples are grouped. Suppose that there are g groups of size n_1, \dots, n_g , respectively, and that the matrix of *group sizes* is given by $\mathbf{N} = \text{diag}(n_1, \dots, n_g)$. Suppose further that $\tilde{\mathbf{X}} : g \times p$ is the matrix of *sample group means* based on the transformed data matrix $\tilde{\mathbf{X}}$. The *between groups sums-of-squares-and-crossproducts* matrix is given by

$$\mathbf{B} = \tilde{\mathbf{X}}'\tilde{\mathbf{N}}\tilde{\mathbf{X}},$$

while the *within groups sums-of-squares-and-crossproducts* matrix is given by

$$\mathbf{W} = \tilde{\mathbf{X}}'\tilde{\mathbf{X}} - \tilde{\mathbf{X}}'\tilde{\mathbf{N}}\tilde{\mathbf{X}}.$$

The normalised eigenvectors corresponding to the non-increasing eigenvalues of the matrix $\mathbf{W}^{-1/2}\mathbf{B}\mathbf{W}^{-1/2}$ are placed into the columns of a matrix \mathbf{V}_{temp} . Then with $\mathbf{V} = \mathbf{W}^{-1/2}\mathbf{V}_{\text{temp}}$, the *basis matrix for interpolation*, $\mathbf{V}_{r,\text{int}}$, consists of the first r columns of \mathbf{V} . In the case of both interpolative and predictive biplots, the samples are represented as points in the display space at coordinates $\mathbf{Y} = \tilde{\mathbf{X}}\mathbf{V}_{r,\text{int}}$. These are simply the ‘scores’ of the first r canonical variates.

Axes: All biplot axes pass through the origin. Predictive and interpolative biplot axes do *not* in general coincide in direction. The *basis matrix for prediction*, $\mathbf{V}_{r,\text{pr}}$, consists of the first r columns of $(\mathbf{V}^{-1})'$. The j th *predictive* biplot axis is calibrated μ at coordinates $(\tilde{\mu}\mathbf{e}_j'\mathbf{V}_{r,\text{pr}})/(\mathbf{e}_j'\mathbf{V}_{r,\text{pr}}\mathbf{V}_{r,\text{pr}}'\mathbf{e}_j)$. The j th *vector sum interpolative* biplot axis is calibrated μ at coordinates $\tilde{\mu}\mathbf{e}_j'\mathbf{V}_{r,\text{int}}$, while the j th *centroid interpolative* biplot axis is calibrated μ at coordinates $\tilde{\mu}\mathbf{p}\mathbf{e}_j'\mathbf{V}_{r,\text{int}}$.

Goodness-of-fit: The r -dimensional *point predictivities* are given by the diagonal elements of

$$\text{diag}(\hat{\mathbf{Y}}_g'\hat{\mathbf{Y}}_g)\{\text{diag}(\mathbf{Y}_g'\mathbf{Y}_g)\}^{-1},$$

where $\mathbf{Y}_g = (\mathbf{I} - \mathbf{G}(\mathbf{G}'\mathbf{G})^{-1}\mathbf{G}')\tilde{\mathbf{X}}$ and \mathbf{G} is the sample-group indicator matrix which has i th row \mathbf{e}_k if sample i belongs to group k , $i = 1, \dots, n$, $k = 1, \dots, g$. The matrix $\hat{\mathbf{Y}}_g$ is given by $\hat{\mathbf{Y}}_g = \mathbf{Y}_g\mathbf{V}_{r,\text{int}}(\mathbf{V}_{r,\text{pr}})'$. The r -dimensional *group predictivities* are given by the diagonal elements of

$$\text{diag}(\hat{\mathbf{X}}'\hat{\mathbf{W}}^{-1}\hat{\mathbf{X}})\{\text{diag}(\tilde{\mathbf{X}}'\mathbf{W}^{-1}\tilde{\mathbf{X}})\}^{-1},$$

with $\hat{\tilde{\mathbf{X}}}$ the reconstructed matrix $\hat{\tilde{\mathbf{X}}} = \tilde{\mathbf{X}}\mathbf{V}_{r,\text{int}}(\mathbf{V}_{r,\text{pr}})'$. The r -dimensional *axis predictivities* are given by the diagonal elements of

$$\text{diag}(\hat{\tilde{\mathbf{X}}} \mathbf{N} \hat{\tilde{\mathbf{X}}}) \{ \text{diag}(\tilde{\mathbf{X}}' \mathbf{N} \tilde{\mathbf{X}}) \}^{-1}.$$

More: Full details may be found in [Gower and Hand \(1996, Chapter 5\)](#), and, in the case of point, group and axis predictivities, in [Gardner-Lubbe *et al.* \(2008\)](#).

1.A.6 Dissimilarity metrics

One of four dissimilarity metrics can be used to calculate an inter-sample dissimilarity matrix $\mathbf{D} : n \times n$ from the transformed data matrix $\tilde{\mathbf{X}}$. Under the *Pythagoras* dissimilarity metric, $[\mathbf{D}]_{ii'}^2 = d_{ii'}^2 = (\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_{i'})'(\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_{i'})$, with $\tilde{\mathbf{x}}_i$ the i th row of $\tilde{\mathbf{X}}$. Under the *Square-root-of-Manhattan* dissimilarity metric, $d_{ii'}^2 = \sum_{j=1}^p |\tilde{x}_{ij} - \tilde{x}_{i'j}|$. According to [Clark's \(1952\)](#) dissimilarity metric, $d_{ii'}^2 = \sum_{j=1}^p ((\tilde{x}_{ij} - \tilde{x}_{i'j})/(\tilde{x}_{ij} + \tilde{x}_{i'j}))^2$. Finally, under the [Mahalanobis \(1936\)](#) dissimilarity metric, $d_{ii'}^2 = (\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_{i'})' \mathbf{S}_{\tilde{\mathbf{X}}}^{-1} (\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_{i'})$, with $\mathbf{S}_{\tilde{\mathbf{X}}}$ the sample covariance matrix of $\tilde{\mathbf{X}}$. Note that the term ‘Pythagoras’ is used instead of ‘Euclidean’ in order to avoid confusion with the term ‘Euclidean-embeddable’ of the next section.

More: See also [Cox and Cox \(2001, Section 1.3\)](#) and [Borg and Groenen \(2005, Section 6.3\)](#).

1.A.7 PCO

Points: An inter-sample dissimilarity matrix \mathbf{D} is calculated from $\tilde{\mathbf{X}}$ according to one of the four dissimilarity metrics of [Section 1.A.6](#). All four dissimilarity metrics are Euclidean-embeddable ([Gower, 1982](#)), as required by PCO. The *sums-of-squares-and-crossproducts* matrix is given by

$$\mathbf{B} = (\mathbf{I} - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n') \mathbf{D} (\mathbf{I} - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n').$$

The r largest eigenvalues of \mathbf{B} , $\lambda_1, \dots, \lambda_r$, are taken to form the diagonal elements of matrix $\mathbf{\Lambda} : r \times r$. The corresponding normalised eigenvectors are placed into the columns of matrix $\mathbf{V}_r : n \times r$. The samples are then represented as points in the display space at principal coordinates $\mathbf{Y} = \mathbf{V}_r \mathbf{\Lambda}^{1/2}$. PCO is also known as ‘classical scaling’.

Goodness-of-fit: The *quality* of the representation is given by $(\sum_{j=1}^r \lambda_j) / (\sum_{j=1}^p \lambda_j)$. A Shepard diagram may also be drawn.

More: Full details may be found in [Gower and Hand \(1996, Section A.5.2\)](#) and [Cox and Cox \(2001, Section 2.2\)](#). The Shepard diagram is described in [Borg and Groenen \(2005, Section 3.3\)](#).

1.A.8 MDS

Points: An inter-sample dissimilarity matrix \mathbf{D} is calculated from $\tilde{\mathbf{X}}$ according to one of the four dissimilarity metrics of [Section 1.A.6](#). The samples are represented in the display space at coordinates $\mathbf{Y} : n \times r$, with \mathbf{Y} found algorithmically to minimise the *stress* criterion

$$S(\hat{\mathbf{d}}, \mathbf{Y}) = \sum_{i < i'} (\hat{d}_{ii'} - \delta_{ii'}(\mathbf{Y}))^2.$$

In this expression, $\hat{d}_{ii'}$ represents the inter-sample *disparity* between sample i and i' . Inter-sample disparities are derived from the inter-sample dissimilarities \mathbf{D} by one of three transformations: the identity transformation, monotone regression, or a monotone spline transformation.

The quantity $\delta_{ii'}(\mathbf{Y})$, in turn, represents the Pythagoras distance between rows i and i' of \mathbf{Y} , called the inter-point *distance*. An **IM** algorithm is used to find the minimising matrix \mathbf{Y} . The algorithm converges uniformly to a local minimum, although in theory a saddle-point cannot be ruled out. In practice, the algorithm is taken to have converged as soon as the relative decrease in stress becomes smaller than some pre-set value. The algorithm is also stopped as soon as a certain maximum number of iterations has been performed.

Goodness-of-fit: A Shepard diagram may be drawn.

More: For more details and a full description of the implementation of the **IM** algorithm, see [Borg and Groenen \(2005, Chapters 8, 9\)](#). The Shepard diagram is described in [Borg and Groenen \(2005, Section 3.3\)](#).

1.A.9 The regression biplot

Points: The samples are represented as points with coordinates $\mathbf{Y} : n \times r$. The coordinates are typically determined by **PCO** or **MDS**, but any scaling method can be used.

Axes: The *basis matrix* is given by $\mathbf{V}_r = (\mathbf{Y}'\mathbf{Y})^{-1}\mathbf{Y}'\tilde{\mathbf{X}}$. All other details are the same as for the axes of the **PCA** biplot.

More: Full details may be found in [Gower and Hand \(1996, Sections 3.3.2, 3.4.3\)](#).

1.A.10 The Procrustes biplot

Points: The samples are represented as points with coordinates $\mathbf{Y} : n \times r$. The coordinates are typically determined by **PCO** or **MDS**, but any scaling method can be used. When the points are determined by **PCO** based on Pythagorean dissimilarities, the **PCA**, regression and Procrustes biplots coincide.

Axes: All biplot axes pass through the origin. Predictive and interpolative biplot axes do *not* in general coincide in direction. By orthogonal Procrustes analysis, the *basis matrix for prediction*, $\mathbf{V}_{r,\text{pr}}$, is given by the first r columns of $\mathbf{B}\mathbf{A}'$ where $\tilde{\mathbf{X}}'\mathbf{Y} = \mathbf{A}\mathbf{\Sigma}\mathbf{B}'$ is the singular value decomposition of $\tilde{\mathbf{X}}'\mathbf{Y}$. The j th *predictive* biplot axis is calibrated μ at coordinates $(\tilde{\mu}\mathbf{e}_j'\mathbf{V}_{r,\text{pr}})/(\mathbf{e}_j'\mathbf{V}_{r,\text{pr}}\mathbf{V}_{r,\text{pr}}'\mathbf{e}_j)$. The *basis matrix for interpolation*, $\mathbf{V}_{r,\text{int}}$, minimises $\|\mathbf{Y} - \tilde{\mathbf{X}}\mathbf{V}\|$ out of all projection matrices \mathbf{V} with orthonormal columns. The solution is found by minimal error projection Procrustes. The j th *vector sum interpolative* biplot axis is calibrated μ at coordinates $\tilde{\mu}\mathbf{e}_j'\mathbf{V}_{r,\text{int}}$, while the j th *centroid interpolative* biplot axis is calibrated μ at coordinates $\tilde{\mu}\mathbf{p}\mathbf{e}_j'\mathbf{V}_{r,\text{int}}$.

More: Full details may be found in [Gower and Hand \(1996, Sections 3.3.1, 3.4.2\)](#). For more on orthogonal Procrustes analysis, see [Gower and Hand \(1996, Appendix A.10.1\)](#). The algorithm for minimal error projection Procrustes is described in [Gower and Dijksterhuis \(2004, p. 57\)](#).

1.A.11 The circular non-linear biplot

Points: The samples are represented as points with coordinates $\mathbf{Y} : n \times r$ determined by **PCO**. The dissimilarity metric is assumed to be additive ([Gower and Hand, 1996, p. 105](#)), as all the dissimilarity metrics of [Section 1.A.6](#) are besides Mahalanobis. Matrices \mathbf{B} and \mathbf{A} are carried forward from **PCO**. Define $[\mathbf{E}]_{ii'} = -\frac{1}{2}[\mathbf{D}]_{ii'}^2$, with \mathbf{D} the dissimilarity matrix.

Axes: The biplot axes can be chosen to pass through a common point. Predictive and interpolative biplot axes do *not* in general coincide. To find the position of marker μ on the j th *vector sum interpolative* biplot axis, the vector $\mathbf{d}_{n+1} : n \times 1$ is taken to contain the

dissimilarities, divided by -2 , between $\tilde{\mu}\mathbf{e}_j$ and the n samples of $\tilde{\mathbf{X}}$. The axis is calibrated μ at the first r coordinates of $\mathbf{y} = \mathbf{\Lambda}^{-1}\mathbf{Y}'(\mathbf{d}_{n+1} - \frac{1}{n}\mathbf{E}\mathbf{1})$. The j th *centroid interpolative* biplot axis is calibrated μ at the first r coordinates of $\mathbf{y} = p\mathbf{\Lambda}^{-1}\mathbf{Y}'(\mathbf{d}_{n+1} - \frac{1}{n}\mathbf{E}\mathbf{1})$. The construction of predictive non-linear biplot axes is more complicated and is described in Gower and Hand (1996, Section 6.3.2).

More: Full details may be found in Gower and Hand (1996, Chapter 6). See also Gower and Harding (1988) and Gower and Ngouenet (2005).

1.B SETUP

R can be downloaded from CRAN via the R Project homepage at <http://www.r-project.org> for any of the three major platforms: Linux, MacOS X and Windows. At the time of writing, the latest version of R is 2.8.1. At present, BiplotGUI is intended to be run under Windows. Future releases will be more general.

The BiplotGUI package and its dependencies can most easily be downloaded and installed into R by issuing the following command in the R console:

```
install.packages("BiplotGUI")
```

BiplotGUI depends on the following R packages: *colorspace* (Ihaka, Murrel, Hornik and Zeileis, 2008), *deldir* (Turner, 2007), *KernSmooth* (Wand, 2008), *MASS* (Venables and Ripley, 2002), *rgl* (Adler and Murdoch, 2009), *tcltk* (R Development Core Team, 2008), *tcltk2* (Grosjean, 2009) and *tkrplot* (Tierney, 2008).

BiplotGUI runs slightly better when the R console is in SDI mode, rather than MDI mode.

1.C GUIs IN R

R is a functional programming language with a command line interface (CLI). However, it is possible to incorporate GUIs. Thioulouse and Dray (2007), amongst others, discuss the advantages and the disadvantages of doing so within a statistical context.

The principal GUI toolkit available to R users is Tcl/Tk. R bindings to this toolkit are provided through the *tcltk* package (R Development Core Team, 2008), with enhancements available through the *tcltk2* (Grosjean, 2009) and *tkrplot* (Tierney, 2008) packages. The *tcltk* package comes as part of the basic R distribution.

The GTK+ toolkit, with its roots in the GNOME desktop manager for Linux, can also be used. Bindings for this toolkit are available through the *RGtk2* (Lawrence and Temple Lang, 2009) and related packages. The *gWidgets* package (Verzani, 2008) provides R users with a toolkit-independent interface to the widgets of Tcl/Tk, GTK+ and Java. The *rJava* package (Urbanek, 2009) gives access to the Java virtual machine.

The BiplotGUI package is based on the Tcl/Tk toolkit. Although the GTK+ toolkit is more comprehensive, and the *gWidgets* package perhaps more convenient, R has basic built-in support for Tcl/Tk so that no additional software is required to write, and more importantly, run such GUIs. This is not an insignificant point when made to a novice or hesitant user. However, GTK+ offers many advantages which may outweigh those of Tcl/Tk as time progresses.

DETAIL

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2.2 FEATURES

After an introductory sentence, each feature is discussed under standard headings. These headings are listed below, together with a short description of each. Headings appear only when applicable.

| | |
|----------------|---|
| DETAIL | More detailed information on the feature |
| DEFAULT VALUE | For graphical parameters, the default value |
| SHORTCUT | A keyboard shortcut to the feature |
| ALTERNATIVE TO | Mutually exclusive features |
| SREENSHOT | For dialogue boxes, a reference to a screenshot |
| REFERENCES | References to external material |

Features are indented as in [Section 2.1](#). The symbols used, from the outer-most to inner-most levels of indentation, are ►, •, ▷, ◦ and ◇, respectively. Information on the options in dialogue boxes is given in framed sections.

► **Menu bar**

The primary interface of the [GUI](#).

DETAIL · The menu bar is located at the top of the [GUI](#). It consists of a number of drop-down menus, each with a number of entries. Entries may have sub-entries. The entries of menus are arranged around common themes of action. The [Joint](#) menu is for biplots with a joint mechanism for determining the positions of both points and axes. For other biplots, the [Points](#) menu determines the positions of the points while the [Axes](#) menu determines the positions of the axes. Many entries contained in the menu bar can also be accessed from the pop-up menus which appear when various parts of graphs are right clicked.

SHORTCUTS · Often-used entries have dedicated keyboard shortcuts displayed to their right. These keyboard shortcuts are listed on page [vii](#). Menu bar entries may also be accessed via the keyboard by pressing the Alt key together with the underlined letter in the name of the corresponding drop-down menu, followed by the sequence of underlined letters in the path to the entry.

SCREENSHOT · [Figure 1.1](#)

• **File**

Contains export and other options.

DETAIL · The File menu lets the user [save](#), [copy](#) or [print](#) the currently displayed [biplot region](#). In addition, general [options](#) may be set, or the user may [exit](#) the [GUI](#).

▷ **Save as**

Lets the user save the currently displayed [biplot region](#) in a number of widely-used file formats.

DETAIL · Depending on how the [GUI](#) has been resized onscreen, the proportions within a saved biplot region may differ from what is shown onscreen. To ensure consistency, saved biplot regions always have both their width and height set to 20.32 centimeters (8 inches). The [PDF](#) and [Postscript](#) file formats offer the highest quality, better even than that shown onscreen.

SHORTCUT · Ctrl+S. Saves the currently displayed biplot region in the currently selected file format.

○ **PDF...**

Saves the currently displayed [biplot region](#) as a PDF file.

DETAIL · Together with [Postscript](#), the PDF file format offers the highest quality.

ALTERNATIVE TO · [Postscript](#), [Metafile](#), [Bmp](#), [Png](#), [Jpeg 50% quality](#), [Jpeg 75% quality](#), [Jpeg 100% quality](#), [PicTeX](#)

A standard dialogue box appears which lets the user specify the name and location of the PDF file.

○ **Postscript...**

Saves the currently displayed [biplot region](#) as a Postscript file (.ps).

DETAIL · Together with [PDF](#), the Postscript file format offers the highest quality.

ALTERNATIVE TO · [PDF](#), [Metafile](#), [Bmp](#), [Png](#), [Jpeg 50% quality](#), [Jpeg 75% quality](#), [Jpeg 100% quality](#), [PicTeX](#)

A standard dialogue box appears which lets the user specify the name and location of the Postscript file.

○ **Metafile...**

Saves the currently displayed [biplot region](#) as a Windows Metafile (.wmf).

ALTERNATIVE TO · [PDF](#), [Postscript](#), [Bmp](#), [Png](#), [Jpeg 50% quality](#), [Jpeg 75% quality](#), [Jpeg 100% quality](#), [PicTeX](#)

A standard dialogue box appears which lets the user specify the name and location of the Windows Metafile.

○ **Bmp...**

Saves the currently displayed [biplot region](#) as a bitmap (.bmp).

ALTERNATIVE TO · [PDF](#), [Postscript](#), [Metafile](#), [Png](#), [Jpeg 50% quality](#), [Jpeg 75% quality](#), [Jpeg 100% quality](#), [PicTeX](#)

A standard dialogue box appears which lets the user specify the name and location of the bitmap file.

- **Png...**

Saves the currently displayed [biplot region](#) as a png file.

ALTERNATIVE TO · [PDF](#), [Postscript](#), [Metafile](#), [Bmp](#), [Jpeg 50% quality](#), [Jpeg 75% quality](#), [Jpeg 100% quality](#), [PicTeX](#)

A standard dialogue box appears which lets the user specify the name and location of the png file.

- **Jpeg**

Lets the user save the currently displayed [biplot region](#) as a Jpeg file (.jpg, .jpeg).

- ◇ **50% quality...**

Saves the currently displayed [biplot region](#) as a Jpeg file at 50% quality.

ALTERNATIVE TO · [PDF](#), [Postscript](#), [Metafile](#), [Bmp](#), [Png](#), [Jpeg 75% quality](#), [Jpeg 100% quality](#), [PicTeX](#)

A standard dialogue box appears which lets the user specify the name and location of the 50% quality Jpeg file.

- ◇ **75% quality...**

Saves the currently displayed [biplot region](#) as a Jpeg file at 75% quality.

ALTERNATIVE TO · [PDF](#), [Postscript](#), [Metafile](#), [Bmp](#), [Png](#), [Jpeg 50% quality](#), [Jpeg 100% quality](#), [PicTeX](#)

A standard dialogue box appears which lets the user specify the name and location of the 75% quality Jpeg file.

- ◇ **100% quality...**

Saves the currently displayed [biplot region](#) as a Jpeg file at 100% quality.

ALTERNATIVE TO · [PDF](#), [Postscript](#), [Metafile](#), [Bmp](#), [Png](#), [Jpeg 50% quality](#), [Jpeg 75% quality](#), [PicTeX](#)

A standard dialogue box appears which lets the user specify the name and location of the 100% quality Jpeg file.

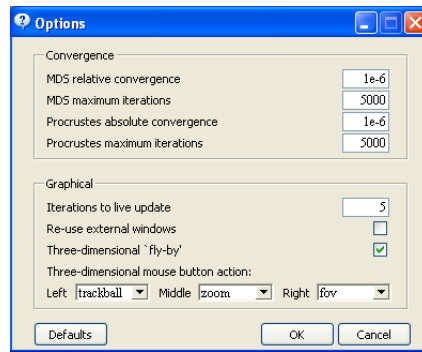
- **PicTeX...**

Saves the currently displayed [biplot region](#) in the PicTeX format (.tex).

ALTERNATIVE TO · [PDF](#), [Postscript](#), [Metafile](#), [Bmp](#), [Png](#), [Jpeg 50% quality](#), [Jpeg 75% quality](#), [Jpeg 100% quality](#)

REFERENCES · See the R help file of the `pictex` function for the limitations of the conversion to this format.

A standard dialogue box appears which lets the user specify the name and location of the PicTeX file.

Screenshot 2.1: The *File* → *Options* dialogue box.▷ **Copy**

Copies the currently displayed [biplot region](#) to the clipboard as a Windows Metafile.

DETAIL · Depending on how the [GUI](#) has been resized onscreen, the proportions within a copied biplot region may differ from what is shown onscreen. To ensure consistency, copied biplot regions always have both their width and height set to 20.32 centimeters (8 inches). Biplots saved as [PDF](#) or [Postscript](#) files are of a higher quality than those copied to the clipboard.

SHORTCUT · Ctrl+C

▷ **Print...**

Prints the currently displayed [biplot region](#).

DETAIL · Depending on how the [GUI](#) has been resized onscreen, the proportions within a printed biplot region may differ from what is shown onscreen. To ensure consistency, printed biplot regions always have both their width and height set to 20.32 centimeters (8 inches).

SHORTCUT · Ctrl+P

A standard dialogue box appears which lets the user set various options before printing.

▷ **Options...**

Lets the user set various general options.

SCREENSHOT · [2.1](#)

Convergence

Lets the user set various convergence criteria.

MDS relative convergence

If still running, the [IM](#) algorithm for [MDS](#) stops when the *proportional* decrease in stress becomes smaller than this value.

DEFAULT VALUE · 10^{-6}

REFERENCES · [Borg and Groenen \(2005, pp. 191–192, 204–205\)](#)

MDS maximum iterations

If still running, the **IM** algorithm for **MDS** stops when the number of iterations reaches this value.

DEFAULT VALUE · 5000

REFERENCES · [Borg and Groenen \(2005, pp. 191–192, 204–205\)](#)

Procrustes absolute convergence

If still running, the Procrustes algorithm for interpolative biplots stops when the absolute decrease in stress first becomes smaller than this value.

DEFAULT VALUE · 10^{-6}

REFERENCES · [Gower and Hand \(1996, Section A.10.2\)](#), [Gower and Dijksterhuis \(2004, p. 57\)](#)

Procrustes maximum iterations

If still running, the Procrustes algorithm for interpolative biplots stops when the number of iterations reaches this value.

DEFAULT VALUE · 5000

REFERENCES · [Gower and Hand \(1996, Section A.10.2\)](#), [Gower and Dijksterhuis \(2004, p. 57\)](#)

Graphical

Lets the user set general graphical options.

Iterations to live update

The **biplot region** and relevant graphs in the **diagnostic tabs** are updated after this number of **MDS** iterations, and multiples of it.

DETAIL · The smaller the value of this option, the smoother the transitions in the graphs; the larger the value of this option, the smaller the time to convergence. Irrespective of the value of this option, the biplot region and the relevant graphs in the diagnostic tabs are only updated during **MDS** convergence if **Live updates** is checked below the biplot region.

DEFAULT VALUE · 5

Re-use external windows

Toggles between re-using windows for external graphics, or creating new windows.

DETAIL · If checked, the same window is used to display any two-dimensional external graphs that are produced. Such graphs can be created by clicking **External → As is** below the **biplot region**, or by right clicking the graphs of the **diagnostic tabs** and selecting **External** from the pop-up menu. If clear, new windows are used to show any additional two-dimensional graphs, retaining previous external graphs, if any. Similar comments hold for three-dimensional external biplots created by clicking **External → In 3D** below the biplot region. The windows of the two- and three-dimensional graphs operate independently.

DEFAULT VALUE · clear

Three-dimensional ‘fly-by’

Toggles between including an initial ‘fly-by’ in three-dimensional biplots, or not.

DEFAULT VALUE · clear

Three-dimensional mouse button action: left

The action of the left mouse button in three-dimensional biplots.

DEFAULT VALUE · trackball

REFERENCES · See the R help file of the `par3d` function of the `rgl` package ([Adler and Murdoch, 2009](#)) for details on the choices.

Three-dimensional mouse button action: middle

The action of the middle mouse button in three-dimensional biplots.

DEFAULT VALUE · zoom

REFERENCES · See the R help file of the `par3d` function of the `rgl` package ([Adler and Murdoch, 2009](#)) for details on the choices.

Three-dimensional mouse button action: right

The action of the right mouse button in three-dimensional biplots.

DEFAULT VALUE · fov

REFERENCES · See the R help file of the `par3d` function of the `rgl` package ([Adler and Murdoch, 2009](#)) for details on the choices.

Defaults

Reverts the options to their default values.

OK

Saves the options and returns to the [GUI](#).

Cancel

Cancels the changes made since the dialogue box was opened, and returns to the [GUI](#).

▷ **Exit**

Lets the user exit the [GUI](#).

DETAIL · Upon exiting, all [GUI](#) settings changed during the session are lost. The user is returned to the R prompt of the R console.

A standard dialogue box appears which asks the user to confirm whether or not to exit the [GUI](#).

• **View**

Lets the user customise the [biplot region](#).

▷ **Show title**

Shows a [title](#) above the [biplot](#).

DETAIL · The biplot retains the same size and relative position, irrespective of whether or not a title is shown.

▷ **Clip around points**

Sets the [biplot](#) borders around the points, ignoring the axes.

DETAIL · If selected, the biplot borders are set just large enough to show all the points and their labels in their entirety. [Non-linear axes](#) may not be visible in their entirety.

ALTERNATIVE TO · [Clip around points and axes](#)

▷ **Clip around points and axes**

Sets the [biplot](#) borders around the points and axes.

DETAIL · If selected, the biplot borders are set large enough to show all the points, their labels, and the axes in their entirety. Available only for [non-linear axes](#) and when the axes are not [hidden](#).

ALTERNATIVE TO · [Clip around points](#)

▷ **Show point labels**

Shows the point labels in the [biplot](#).

DETAIL · If selected, the biplot borders are enlarged so that all the point labels are visible in their entirety. Not available when the points are [hidden](#).

▷ **Show point values**

Shows the variable values of a [highlighted axis](#) alongside the corresponding points in the [biplot](#).

DETAIL · Only available when an axis has been highlighted.

▷ **Show group labels in legend**

Shows the group labels in the [legend](#).

DETAIL · Not available when there is only one group of samples, or when the points are [hidden](#).

▷ **Don't show axis labels**

Suppresses the axis labels.

DETAIL · Not available if there are [no axes](#), or when the axes are [hidden](#).

ALTERNATIVE TO · [Show clinging axis labels](#), [Show axis labels in legend](#)

▷ **Show clinging axis labels**

Shows the axis labels at those edges of the axes with the higher calibrations.

DETAIL · Available only for linear axes that are not [hidden](#).

ALTERNATIVE TO · [Don't show axis labels](#), [Show axis labels in legend](#)

▷ **Show axis labels in legend**

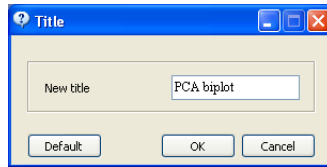
Shows the axis labels in the [legend](#).

DETAIL · Not available if there are [no axes](#), or when the axes are [hidden](#).

ALTERNATIVE TO · [Don't show axis labels](#), [Show clinging axis labels](#)

▷ **Show Additional labels in legend**

Shows the labels of descriptors from the [Additional](#) menu in the [legend](#).



Screenshot 2.2: The *Format* → *Title* dialogue box.

▷ **Show next legend entries**

Shows the succeeding set of 16 legend entries, if any, in the [legend](#).

DETAIL · The legend can contain up to a maximum of 16 entries at once. This option updates the legend to show the succeeding set of at most 16 entries. The option does not show the first set of entries after the last set. Not available when there are no succeeding entries, or when no legend is shown.

SHORTCUT · Ctrl++

▷ **Show previous legend entries**

Shows the preceding set of 16 legend entries, if any, in the [legend](#).

DETAIL · The legend can contain up to a maximum of 16 entries at once. This option updates the legend to show the preceding set of 16 entries. The option does not show the last set of entries before the first set. Not available when there are no preceding entries, or when no legend is shown.

SHORTCUT · Ctrl+-

▷ **Calibrate display space axes**

Calibrates the two [biplot](#) dimensions.

DETAIL · This runs counter to the spirit of biplots of the new approach. [Gower and Hand \(1996\)](#) call such biplots ‘bad’.

REFERENCES · [Gower and Hand \(1996, Section 2.6\)](#)

• **Format**

Lets the user customise the internally used graphical parameters.

▷ **Title...**

Lets the user change the [title](#).

DETAIL · The title is shown only if [View](#) → [Show title](#) is selected.

SCREENSHOT · [2.2](#)

New title

The new [title](#).

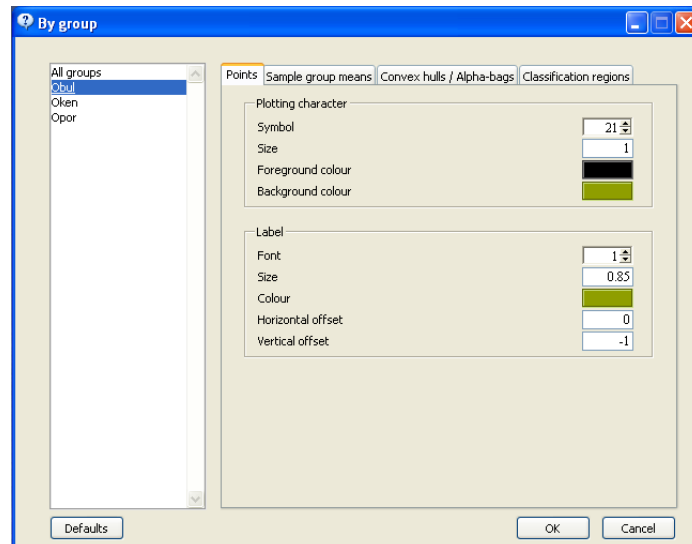
DEFAULT VALUE · Depends on the currently displayed biplot; can be seen from the title bar of the [GUI](#).

Default

Reverts the option to its default value.

OK

Saves the [title](#), returns to the [GUI](#), and redraws the [biplot region](#).



Screenshot 2.3: The *Points* tab of the *Format* → *By group* dialogue box.

Cancel

Cancels the changes made since the dialogue box was opened, and returns to the [GUI](#).

▷ By group...

Lets the user set graphical parameters for [points](#), [sample group means](#), [convex hulls](#) / [alpha-bags](#) and [classification regions](#) for a particular group, or for all groups simultaneously.

DETAIL · When *All groups* is selected from the list to the left of the dialogue box, changes made to the parameter values to the right of the dialogue box affect all groups. Changes to particular groups can be made by clicking the group names in the list to the left of the dialogue box. Parameter values which differ amongst groups are left blank when *All groups* is selected.

SHORTCUT · Ctrl+G

SCREENSHOT · [2.3](#)

Only the Points tab is discussed here. The other tabs are discussed together with the options of the [Additional](#) menu.

Plotting character

Lets the user change the graphical parameters of the points that represent the samples, by group.

Symbol

Sets the symbol used to represent the points, by group.

DETAIL · Corresponds to R's `pch` argument. Possible values: NA, 0, ..., 25.

DEFAULT VALUE · If there is only one group, 22. Otherwise the values are recycled by group with the values 21 to 25.

Size

Sets the size of the points, by group.

DETAIL · Corresponds to R's `cex` argument. Larger values result in larger points. Possible values: positive real numbers.

DEFAULT VALUE · 1

Foreground colour

Sets the exterior colour of the points, by group.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · "black"

Background colour

Sets the interior colour of the points, by group.

DETAIL · Corresponds to R's `bg` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · If there is only one group, "red". Otherwise equally spaced colours from the `hcl` spectrum.

Label

Lets the user change the graphical parameters of the point labels, by group.

Font

Sets the font of the point labels, by group.

DETAIL · Corresponds to R's `font` argument. Possible values: 1: regular; 2: bold; 3: italic; 4: bold italic.

DEFAULT VALUE · 1

Size

Sets the size of the point labels, by group.

DETAIL · Corresponds to R's `cex` argument. Larger values result in larger text. Possible values: positive real numbers.

DEFAULT VALUE · 0.85

Colour

Sets the colour of the point labels, by group.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · If there is only one group, "black". Otherwise equally spaced colours from the `hcl` spectrum.

Horizontal offset

Sets the horizontal offset of the point labels from the corresponding points, by group.

DETAIL · The point labels are shifted horizontally from the corresponding points with this multiple of the width of the letter 'x' (in the selected font size).

Positive values shift the labels to the right; negative values shift the labels to the left.

DEFAULT VALUE · 0

Vertical offset

Sets the vertical offset of the point labels from the corresponding points, by group.

DETAIL · The point labels are shifted vertically from the corresponding points with this multiple of the height of the letter ‘x’ (in the selected font size). Positive values shift the labels towards the top; negative values shift the labels towards the bottom.

DEFAULT VALUE · -1

Defaults

Reverts the options of all the tabs of the dialogue box to their default values.

OK

Saves the options of all the tabs of the dialogue box, returns to the [GUI](#), redraws the currently displayed [biplot region](#) and other graphs if necessary.

Cancel

Cancels the changes made since the dialogue box was opened, and returns to the [GUI](#).

▷ **Axes...**

Lets the user set graphical parameters for a particular axis, or for all axes simultaneously.

DETAIL · When *All axes* is selected from the list to the left of the dialogue box, changes made to the parameter values to the right of the dialogue box affect all axes. Changes to particular axes can be made by clicking the variable names from the list to the left of the dialogue box. Parameter values which differ amongst axes are left blank when *All axes* is selected.

SHORTCUT · Ctrl+A

SCREENSHOT · [2.4](#)

Axis

Lets the user change the graphical parameters associated with the axis that represents the variable.

Line type

Sets the type of line used to draw the axis.

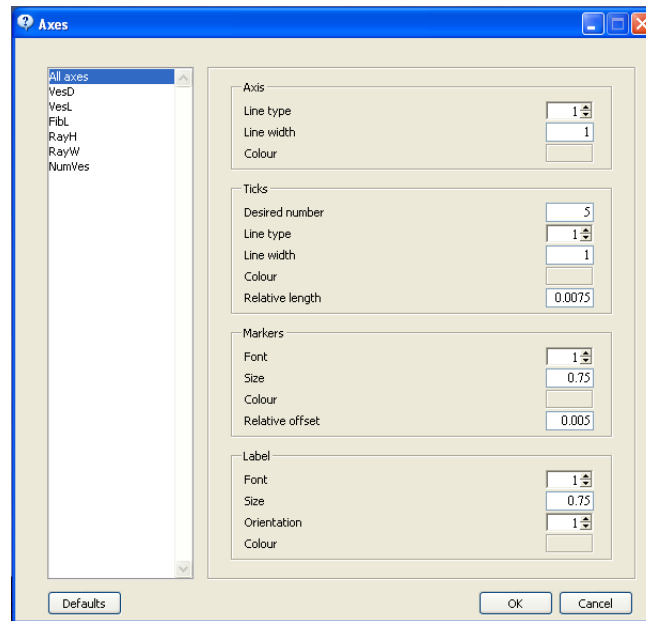
DETAIL · Corresponds to R’s `lty` argument. Possible values: 0, ..., 6.

DEFAULT VALUE · 1

Line width

Sets the width of the axis.

DETAIL · Corresponds to R’s `lwd` argument. Larger values result in wider axes.

Screenshot 2.4: The *Format* → *Axes* dialogue box.

Possible values: positive real numbers.

DEFAULT VALUE · 1

Colour

Sets the colour of the axis.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · Equally spaced colours from the `hcl` spectrum.

Ticks

Lets the user change graphical parameters associated with the ticks of the axis.

DETAIL · The ticks, together with the markers, calibrate the axis. The ticks are the short lines orthogonal to the axis, alongside which the markers (the numbers) are given. For [non-linear axes](#), the slopes of the ticks are approximated numerically.

Desired number

Sets the desired number of ticks on the axis.

DETAIL · Corresponds to the argument `n` of R's `pretty` function. This number is not strictly adhered to; it is only approximate.

DEFAULT VALUE · 5

REFERENCES · See the R help file of the `pretty` function.

Line type

Sets the type of line used to draw the ticks on the axis.

DETAIL · Corresponds to R's `lty` argument. Possible values: 0, ..., 6.

DEFAULT VALUE · 1

Line width

Sets the width of the ticks of the axis.

DETAIL · Corresponds to R's `lwd` argument. Larger values result in wider ticks. Possible values: positive real numbers.

DEFAULT VALUE · 1

Colour

Sets the colour of the ticks of the axis.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · The same as the default colour of the axis.

Relative length

Sets the relative length of the ticks of the axis.

DETAIL · The length of the ticks is twice this fraction of the width of the [biplot](#).

DEFAULT VALUE · 0.0075

Markers

Lets the user change graphical parameters associated with the markers of the axis.

DETAIL · The markers, together with the ticks, calibrate the axis. The markers are the numbers, in terms of the original variable values, given alongside the ticks (the short lines orthogonal to the axis). The markers are positioned on that side of the axis that would place them below the axis if the axis were to be rotated to be horizontal (so that the marker values increase from left to right).

Font

Sets the font of the markers of the axis.

DETAIL · Corresponds to R's `font` argument. Possible values: 1: regular; 2: bold; 3: italic; 4: bold italic.

DEFAULT VALUE · 1

Size

Sets the size of the markers of the axis.

DETAIL · Corresponds to R's `cex` argument. Larger values result in larger text. Possible values: positive real numbers.

DEFAULT VALUE · 0.75

Colour

Sets the colour of the markers of the axis.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · The same as the default colour of the axis.

Relative offset

Sets the relative offset of the markers from the corresponding ticks of the axis.

DETAIL · The markers are shifted this fraction of the width of the [biplot](#) from the edge of the corresponding ticks.

DEFAULT VALUE · 0.005.

Label

Lets the user change the graphical parameters of the axis label.

Font

Sets the font of the axis label.

DETAIL · Corresponds to R's `font` argument. Possible values: 1: regular; 2: bold; 3: italic; 4: bold italic.

DEFAULT VALUE · 1

Size

Sets the size of the axis label.

DETAIL · Corresponds to R's `cex` argument. Larger values result in larger text. Possible values: positive real numbers.

DEFAULT VALUE · 0.75

Orientation

Sets the orientation of clinging axis labels.

DETAIL · Corresponds to R's `las` argument. Possible values: 0: always parallel to the [biplot](#) edge; 1: always horizontal; 2: always perpendicular to the biplot edge; 3: always vertical.

DEFAULT VALUE · 1

Colour

Sets the colour of the axis label.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

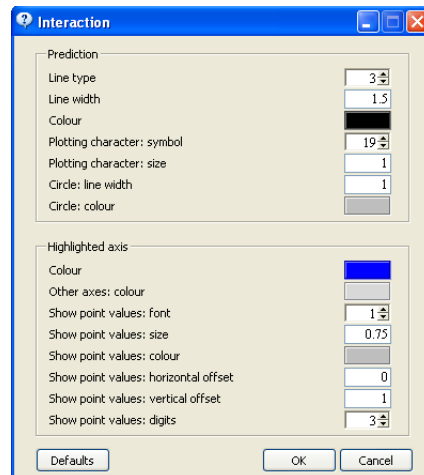
DEFAULT VALUE · The same as the default colour of the axis.

Defaults

Reverts the options to their default values.

OK

Saves the options, returns to the [GUI](#), redraws the currently displayed [biplot region](#) and other graphs if necessary.



Screenshot 2.5: The *Format* → *Interaction* dialogue box.

Cancel

Cancels the changes made since the dialogue box was opened, and returns to the [GUI](#).

▷ Interaction...

Lets the user set graphical parameters for variable value prediction and [highlighted axes](#).

SCREENSHOT · [2.5](#)

Prediction

Lets the user change the graphical parameters associated with variable value prediction.

Line type

Sets the line type used for projection.

DETAIL · Corresponds to R's `lty` argument. Possible values: 0, ..., 6.

DEFAULT VALUE · 3

Line width

Sets the width of the projection lines.

DETAIL · Corresponds to R's `lwd` argument. Larger values result in wider ticks. Possible values: positive real numbers.

DEFAULT VALUE · 1.5

Colour

Sets the colour of the projection lines.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · "black"

Plotting character: symbol

Sets the symbol used to represent the projected points on the axes.

DETAIL · Corresponds to R's `pch` argument. Possible values: NA, 0, ..., 25.

DEFAULT VALUE · 19

Plotting character: size

Sets the size of the projected points on the axes.

DETAIL · Corresponds to R's `cex` argument. Larger values result in larger points. Possible values: positive real numbers.

DEFAULT VALUE · 1

Circle: line width

Sets the width of the circle used in circular projection in the circular non-linear biplot.

DETAIL · Corresponds to R's `lwd` argument. Larger values result in wider ticks. Possible values: positive real numbers.

DEFAULT VALUE · 1

Circle: colour

Sets the colour of the circle used in circular projection in the circular non-linear biplot.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · "gray75"

Highlighted axis

Lets the user change the graphical parameters associated with [highlighted axes](#).

DETAIL · The graphical parameters prefixed with 'Show point values' are for the customisation of the variable values which are shown when an axis is highlighted and [View → Show point values](#) is selected.

Colour

Sets the colour of the highlighted axis.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · "blue"

Other axes: colour

Sets the colour of the non-highlighted axes.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · "gray85"

Show point values: font

Sets the font of the point values.

DETAIL · Corresponds to R's `font` argument. Possible values: 1: regular; 2: bold; 3: italic; 4: bold italic.

DEFAULT VALUE · 1

Show point values: size

Sets the size of the point values.

DETAIL · Corresponds to R's `cex` argument. Larger values result in larger text. Possible values: positive real numbers.

DEFAULT VALUE · 0.75

Show point values: colour

Sets the colour of the point values.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · "gray75"

Show point values: horizontal offset

Sets the horizontal offset of the point values from the corresponding points.

DETAIL · The point values are shifted horizontally from the corresponding points with this multiple of the width of the letter 'x' (in the selected font size). Positive values shift the values to the right; negative values shift the values to the left.

DEFAULT VALUE · 0

Show point values: vertical offset

Sets the vertical offset of the point values from the corresponding points.

DETAIL · The point values are shifted vertically from the corresponding points with this multiple of the height of the letter 'x' (in the selected font size). Positive values shift the values towards the top; negative values shift the values towards the bottom.

DEFAULT VALUE · 1

Show point values: digits

Sets the number of decimal places to show in the point values.

DETAIL · Possible values: 0, ..., 8.

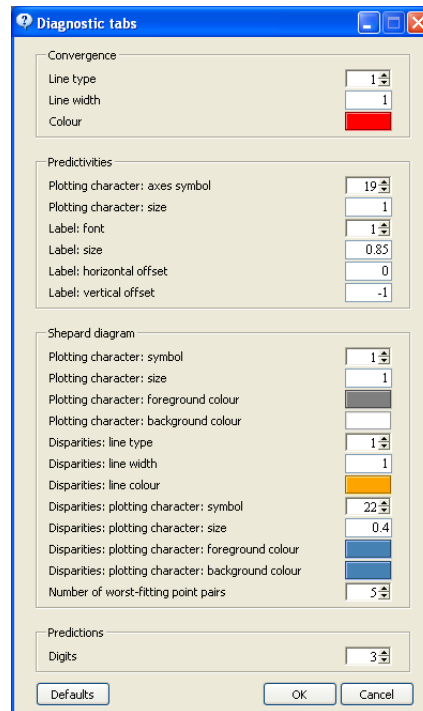
DEFAULT VALUE · 3

Defaults

Reverts the options to their default values.

OK

Saves the options, returns to the [GUI](#), and redraws the currently displayed [biplot region](#).



Screenshot 2.6: The *Format* → *Diagnostics* dialogue box.

Cancel

Cancels the changes made since the dialogue box was opened, and returns to the [GUI](#).

▷ Diagnostic tabs...

Lets the user set graphical parameters for the graphs of the [diagnostic tabs](#).

SCREENSHOT · [2.6](#)

Convergence

Lets the user change the graphical parameters of the graph of the [convergence tab](#).

Line type

Sets the line type.

DETAIL · Corresponds to R's `lty` argument. Possible values: 0, ..., 6.

DEFAULT VALUE · 1

Line width

Sets the line width.

DETAIL · Corresponds to R's `lwd` argument. Possible values: positive real numbers.

DEFAULT VALUE · 1

Colour

Sets the line colour.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · “red”

Predictivities

Lets the user change the graphical parameters of the points, groups and axes predictivities graphs of the [points](#), [group](#) and [axes](#) tabs, respectively.

Plotting character: axes symbol

Sets the symbol used to represent axes in the [axes tab](#).

DETAIL · Corresponds to R's `pch` argument. Possible values: NA, 0, ..., 25.

DEFAULT VALUE · 19

Plotting character: size

Sets the size of the plotting characters.

DETAIL · Corresponds to R's `cex` argument. Larger values result in larger plotting characters. Possible values: positive real numbers.

DEFAULT VALUE · 1

Label: font

Sets the font of the labels.

DETAIL · Corresponds to R's `font` argument. Possible values: 1: regular; 2: bold; 3: italic; 4: bold italic.

DEFAULT VALUE · 1

Label: size

Sets the size of the labels.

DETAIL · Corresponds to R's `cex` argument. Larger values result in larger text. Possible values: positive real numbers.

DEFAULT VALUE · 0.85

Label: horizontal offset

Sets the horizontal offset of the labels from the corresponding plotting characters.

DETAIL · The labels are shifted horizontally from the corresponding plotting characters with this multiple of the width of the letter ‘x’ (in the selected font size). Positive values shift the labels to the right; negative values shift the labels to the left.

DEFAULT VALUE · 0

Label: vertical offset

Sets the vertical offset of the labels from the corresponding plotting characters.

DETAIL · The labels are shifted vertically from the corresponding plotting characters with this multiple of the height of the letter ‘x’ (in the selected font

size). Positive values shift the labels towards the top; negative values shift the labels towards the bottom.

DEFAULT VALUE · -1

Shepard diagram

Lets the user change the graphical parameters of the Shepard diagram of the [points tab](#).

Plotting character: symbol

Sets the symbol used to represent the inter-point distances.

DETAIL · Corresponds to R's `pch` argument. Possible values: NA, 0, ..., 25.

DEFAULT VALUE · 1

Plotting character: size

Sets the size of the plotting character used for inter-point distances.

DETAIL · Corresponds to R's `cex` argument. Larger values result in larger plotting characters. Possible values: positive real numbers.

DEFAULT VALUE · 1

Plotting character: foreground colour

Sets the exterior colour of the plotting character used for inter-point distances.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · "gray50"

Plotting character: background colour

Sets the interior colour of the plotting character used for inter-point distances.

DETAIL · Corresponds to R's `bg` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · "white"

Disparities: line type

Sets the line type used for inter-sample disparities.

DETAIL · Corresponds to R's `lty` argument. Possible values: 0, ..., 6.

DEFAULT VALUE · 1

Disparities: line width

Sets the width of the line used for inter-sample disparities.

DETAIL · Corresponds to R's `lwd` argument. Larger values result in a wider line. Possible values: positive real numbers.

DEFAULT VALUE · 1

Disparities: line colour

Sets the colour of the line used for inter-sample disparities.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the

colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · “orange”

Disparities: plotting character: symbol

Sets the symbol used to represent the inter-sample disparities.

DETAIL · Corresponds to R’s `pch` argument. Possible values: NA, 0, ..., 25.

DEFAULT VALUE · 22

Disparities: plotting character: size

Sets the size of the plotting character used for inter-samples disparities.

DETAIL · Corresponds to R’s `cex` argument. Larger values result in larger plotting characters. Possible values: positive real numbers.

DEFAULT VALUE · 0.4

Disparities: plotting character: foreground colour

Sets the exterior colour of the plotting character used for inter-samples disparities.

DETAIL · Corresponds to R’s `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · “steelblue”

Disparities: plotting character: background colour

Sets the interior colour of the plotting character used for inter-samples disparities.

DETAIL · Corresponds to R’s `bg` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · “steelblue”

Number of worst-fitting point pairs

Sets the number of worst-fitting point pairs to show at the top left of the Shepard diagram.

DETAIL · The degree of misfit between a pair of points is quantified as the difference between the inter-point distance and the corresponding inter-sample disparity. Therefore as the vertical distance from the plotting character that represents the inter-point distance to the line representing the inter-sample disparities.

DEFAULT VALUE · 5

Predictions

Lets the user change the settings associated with the [predictions tab](#).

Digits

Sets the number of decimal places to show in the variable value predictions of the [predictions tab](#).

DETAIL · Possible values: 0, ..., 8.

DEFAULT VALUE · 3

Defaults

Reverts the options to their default values.

OK

Saves the options, returns to the [GUI](#), and redraws the the graphs of the [diagnostic tabs](#).

Cancel

Cancels the changes made since the dialogue box was opened, and returns to the [GUI](#).

▷ **Reset all...**

Lets the user revert all the parameters of the [Format](#) menu to their default values.

SHORTCUT · Ctrl+R

A standard dialogue box appears asking the user to confirm whether or not to reset the graphical parameters of the [Format](#) menu.

DETAIL · Upon confirmation, the graphical parameters are reset and the [bipot region](#) and the graphs of the [diagnostic tabs](#) are redrawn.

• **Joint**

For the construction of joint-mechanism biplots.

DETAIL · The biplots of this menu have both their points and axes determined according to a single, joint mechanism. Other biplots have their points determined from the [Points](#) menu and their axes determined from the [Axes](#) menu.

▷ **PCA**

Constructs a [PCA](#) biplot.

DETAIL · The points correspond to the scores of the first two [PCs](#).

SHORTCUT · 1

ALTERNATIVE TO · [Covariance/Correlation](#), [CVA](#), [None](#), [Regression](#), [Procrustes](#), [Circular non-linear](#)

REFERENCES · [Gower and Hand \(1996, Chapter 2\)](#)

▷ **Covariance/Correlation**

Constructs a covariance/correlation biplot.

DETAIL · If the data are only [centred](#), a covariance biplot is produced. If the data are [centred and scaled](#), a correlation biplot is produced.

SHORTCUT · 2

ALTERNATIVE TO · [PCA](#), [CVA](#), [None](#), [Regression](#), [Procrustes](#), [Circular non-linear](#)

REFERENCES · [Gabriel \(1971\)](#), [Greenacre \(1984\)](#), [Gardner \(2001, Section 2.3.2\)](#), [Gower and Hand \(1996, Section 11.5.1\)](#)

▷ **CVA**

Constructs a [CVA](#) biplot.

DETAIL · The points correspond to the first two [CVs](#). The group means can be

included by clicking [Additional](#) → [Interpolate](#) → [Sample group means](#). CVA biplots are invariant to the [scaling of data to have unit variances](#). Only available when there is more than one group.

SHORTCUT · 3

ALTERNATIVE TO · [PCA](#), [Covariance/Correlation](#), [None](#), [Regression](#), [Procrustes](#), [Circular non-linear](#)

REFERENCES · [Gower and Hand \(1996, Chapter 5 except Section 5.5\)](#)

• Points

Determines the positions of the points of those biplots which have their axes determined from the [Axes](#) menu.

DETAIL · As opposed to the biplots of the [Joint](#) menu, the Points and Axes menus are used together. The options of the Points menu determine the points, while the options of the Axes menu determine the axes.

▷ Dissimilarity metric

Lets the user set the dissimilarity metric to be used in [PCO](#) and [MDS](#).

DETAIL · All the dissimilarity metrics that are available are Euclidean-embeddable. Therefore points exist in Euclidean space which have the same distances between them in Pythagorean distance as the samples have between them in the Euclidean-embeddable dissimilarity metric. If the axes previously selected in the [Axes](#) menu are no longer available because of the change in dissimilarity metric, the most appropriate replacement is automatically chosen.

REFERENCES · [Gower and Legendre \(1986\)](#), [Gower and Hand \(1996, Section A.5.1\)](#)

◦ Pythagoras

The [dissimilarity metric](#) is set to Pythagoras.

DETAIL · ‘Pythagoras’ and ‘Euclidean’ are synomomous. However, to avoid confusion with the term ‘Euclidean-embeddable’, the term ‘Pythagoras’ is used rather than ‘Euclidean’. Under this dissimilarity metric, the dissimilarity between a vector $\mathbf{x} : p \times 1$ and a vector $\mathbf{y} : p \times 1$ is given by $((\mathbf{x} - \mathbf{y})'(\mathbf{x} - \mathbf{y}))^{1/2}$.

ALTERNATIVE TO · [Square-root-of-Manhattan](#), [Clark](#), [Mahalanobis](#)

REFERENCES · [Loomis \(1968\)](#), [Cox and Cox \(2001, p. 11\)](#), [Borg and Groenen \(2005, p. 122\)](#)

◦ Square-root-of-Manhattan

The [dissimilarity metric](#) is set to Square-root-of-Manhattan.

DETAIL · Dissimilarities under this metric are the square root of those under the Manhattan or City Block dissimilarity metric. Therefore the dissimilarity between a vector $\mathbf{x} : p \times 1$ and a vector $\mathbf{y} : p \times 1$ is given by $(\sum_{i=1}^p |x_i - y_i|)^{1/2}$.

ALTERNATIVE TO · [Pythagoras](#), [Clark](#), [Mahalanobis](#)

REFERENCES · [Gower and Harding \(1988\)](#), [Gower and Hand \(1996, p. 103\)](#), [Cox and Cox \(2001, p. 11\)](#), [Borg and Groenen \(2005, p. 122\)](#)

◦ Clark

The [dissimilarity metric](#) is set to Clark.

DETAIL · Under this dissimilarity metric, the dissimilarity between a vector

$\mathbf{x} : p \times 1$ and a vector $\mathbf{y} : p \times 1$ is given by $\sum_{i=1}^p \left(\frac{x_i - y_i}{x_i + y_i} \right)^2$.

ALTERNATIVE TO · [Pythagoras](#), [Square-root-of-Manhattan](#), [Mahalanobis](#)

REFERENCES · [Clark \(1952\)](#), [Gower and Ngouenet \(2005\)](#)

◦ Mahalanobis

The [dissimilarity metric](#) is set to Mahalanobis.

DETAIL · Under this dissimilarity metric, the dissimilarity between a vector $\mathbf{x} : p \times 1$ and a vector $\mathbf{y} : p \times 1$ is given by $((\mathbf{x} - \mathbf{y})' \mathbf{S}^{-1} (\mathbf{x} - \mathbf{y}))^{1/2}$ where \mathbf{S} is the covariance matrix of the matrix with all the observations as rows.

ALTERNATIVE TO · [Pythagoras](#), [Square-root-of-Manhattan](#), [Clark](#)

REFERENCES · [Mahalanobis \(1936\)](#), [Cox and Cox \(2001, p. 11\)](#)

▷ PCO

The points are determined by [PCO](#), with inter-sample dissimilarities calculated according to the chosen [dissimilarity metric](#).

DETAIL · The coordinates of the points are taken to be the first two principal coordinates. [PCO](#) is also known as ‘classical scaling’.

SHORTCUT · A

ALTERNATIVE TO · [MDS Identity transformation](#), [MDS Monotone regression](#), [MDS Monotone spline transformation](#).

REFERENCES · [Gower \(1966\)](#), [Gower and Hand \(1996, Section A.5.2\)](#), [Cox and Cox \(2001, Section 2.2\)](#), [Borg and Groenen \(2005, Chapter 12\)](#)

▷ MDS

The points are determined by [MDS](#), with inter-sample dissimilarities calculated according to the chosen [distance metric](#).

REFERENCES · [Cox and Cox \(2001\)](#), [Borg and Groenen \(2005\)](#)

◦ Run

Performs an [MDS](#) with the currently selected transformation.

DETAIL · The inter-sample disparities are taken to be the transformed inter-sample dissimilarities, calculated according to the chosen [dissimilarity metric](#). Using an [IM](#) algorithm, the points are chosen so that stress, the sum of squared differences between the inter-point distances and the inter-sample disparities, is minimised.

SHORTCUT · R

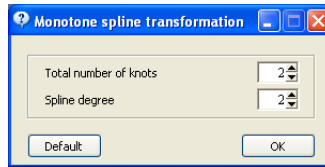
ALTERNATIVE TO · [PCO](#)

REFERENCES · [Borg and Groenen \(2005, Chapters 8, 9\)](#)

◦ Identity transformation

Performs an [MDS](#) with the identity transformation.

DETAIL · The inter-sample disparities are taken to be the inter-sample dissimilarities, calculated according to the chosen [dissimilarity metric](#). Using an [IM](#) algorithm, the points are chosen so that stress, the sum of squared



Screenshot 2.7: The *Points* \rightarrow *MDS* \rightarrow *Monotone spline transformation* dialogue box.

differences between the inter-point distances and the inter-sample disparities, is minimised.

SHORTCUT · B

ALTERNATIVE TO · [PCO](#), [Monotone regression](#), [Monotone spline transformation](#)

REFERENCES · [Borg and Groenen \(2005, Section 8.6\)](#)

◦ **Monotone regression**

Performs a non-metric [MDS](#).

DETAIL · The inter-sample disparities are calculated by the up-and-down-blocks algorithm from the inter-sample dissimilarities, based on the chosen [dissimilarity metric](#). In essence, merely the order of the inter-sample dissimilarities is preserved. Using an [IM](#) algorithm, the points are chosen so that stress, the sum of squared differences between the inter-point distances and the inter-sample disparities, is minimised. The [Primary approach to ties](#) or the [Secondary approach to ties](#) can be used.

SHORTCUT · C

ALTERNATIVE TO · [PCO](#), [Identity transformation](#), [Monotone spline transformation](#),

REFERENCES · [Borg and Groenen \(2005, Sections 9.1, 9.2\)](#)

◦ **Monotone spline transformation...**

Performs an [MDS](#) with a monotone spline transformation

DETAIL · The inter-sample dissimilarities are smoothed using monotone splines to obtain the inter-sample disparities, based on the chosen [dissimilarity metric](#). Using an [IM](#) algorithm, the points are chosen so that stress, the sum of squared differences between the inter-point distances and the inter-sample disparities, is minimised.

SHORTCUT · D

SCREENSHOT · [2.7](#)

ALTERNATIVE TO · [PCO](#), [Identity transformation](#), [Monotone regression](#)

REFERENCES · [Borg and Groenen \(2005, Sections 9.1, 9.6\)](#)

Lets the user select the spline transformation.

Total number of knots

The total number of spline knots, including the two exterior knots.

DETAIL · Between each successive pair of knots, a polynomial of degree

Spline degree is fit.

DEFAULT VALUE · 2

REFERENCES · [Borg and Groenen \(2005, Section 9.6\)](#)

Spline degree

The degree of the polynomial of the spline transformation.

DETAIL · Between each successive pair of knots, a polynomial of degree *Spline degree* is fit.

DEFAULT VALUE · 2

REFERENCES · [Borg and Groenen \(2005, Section 9.6\)](#)

Default

Reverts the options to their default values.

OK

Saves the options, returns to the [GUI](#), and starts the [MDS](#) iteration process.

Cancel

Cancels the changes made since the dialogue box was opened, and returns to the [GUI](#).

○ **Primary approach to ties**

If selected, equality in dissimilarities need not translate to equality in disparities in monotone regression.

DETAIL · Only available when [Monotone regression](#) is selected.

ALTERNATIVE TO · [Secondary approach to ties](#)

REFERENCES · [Borg and Groenen \(2005, Section 9.4\)](#)

○ **Secondary approach to ties**

If selected, equality in dissimilarities implies equality in disparities in monotone regression.

DETAIL · Only available when [Monotone regression](#) is selected.

ALTERNATIVE TO · [Primary approach to ties](#)

REFERENCES · [Borg and Groenen \(2005, Section 9.4\)](#)

○ **Random initial configuration**

The next [MDS](#) algorithm will start from a random initial configuration.

DETAIL · If selected, the initial [MDS](#) configuration is taken to have points uniformly distributed over $[-1, 1]$ in both dimensions. If not selected, the initial configuration is taken to be the previous configuration of points. Useful to avoid local minima.

○ **In terms of principal axes**

If selected, newly converged [MDS](#) configurations are rotated to be in terms of their principal axes.

DETAIL · Since scaling techniques are invariant to rotation (amongst other

things), expressing [MDS](#) solutions in terms of their principal axes can make different configurations more comparable.

REFERENCES · [Borg and Groenen \(2005, Section 24.1\)](#)

- **Axes**

Determines the axes to be shown along with the points determined from the [Points](#) menu.

DETAIL · As opposed to the biplots of the [Joint](#) menu, the [Points](#) and [Axes](#) menus are used together. The options of the [Points](#) menu determine the points, while the options of the [Axes](#) menu determine the axes. The available axes depend on the choice of [dissimilarity metric](#) and the scaling technique from the [Points](#) menu.

- ▷ **None**

No biplot axes are shown, only points.

SHORTCUT · 0

ALTERNATIVE TO · [PCA](#), [Covariance/Correlation](#), [CVA](#), [Regression](#), [Procrustes](#), [Circular non-linear](#)

- ▷ **Regression**

Shows regression biplot axes.

DETAIL · Not available when the [dissimilarity metric](#) is [Mahalanobis](#) and the scaling technique is [PCO](#).

SHORTCUT · 4

ALTERNATIVE TO · [PCA](#), [Covariance/Correlation](#), [CVA](#), [None](#), [Procrustes](#), [Circular non-linear](#)

REFERENCES · [Gower and Hand \(1996, Sections 3.3.2, 3.4.3\)](#), [Cox and Cox \(2001, Section 3.7\)](#)

- ▷ **Procrustes**

Shows Procrustes biplot axes.

DETAIL · Not available when the [dissimilarity metric](#) is [Mahalanobis](#) and the scaling technique is [PCO](#).

SHORTCUT · 5

ALTERNATIVE TO · [PCA](#), [Covariance/Correlation](#), [CVA](#), [None](#), [Regression](#), [Circular non-linear](#)

REFERENCES · [Gower and Hand \(1996, Sections 3.3.1, 3.4.2, A.10.2\)](#), [Gower and Dijksterhuis \(2004, p. 57\)](#)

- ▷ **Circular non-linear**

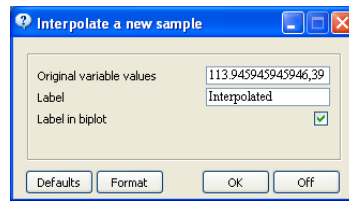
Shows circular non-linear biplot axes.

DETAIL · Only available when the points are determined by [PCO](#), except when the [dissimilarity metric](#) is [Mahalanobis](#).

SHORTCUT · 6

ALTERNATIVE TO · [PCA](#), [Covariance/Correlation](#), [CVA](#), [None](#), [Regression](#), [Procrustes](#)

REFERENCES · [Gower and Harding \(1988\)](#), [Gower and Hand \(1996, Chapter 6\)](#),



Screenshot 2.8: The *Additional* → *Interpolate* → *A new sample* dialogue box.

Gower and Ngouenet (2005)

▷ Default

Selects the default biplot type from the [Axes](#) menu.

DETAIL · The default biplot type depends on the choice of [dissimilarity metric](#) and scaling technique from the [Points](#) menu.

• Additional

Contains additional descriptors which can be included in the [biplot](#).

DETAIL · When the entries of the Additional menu appear in the [legend](#), the group names are preceded by short prefixes. The prefixes are as follows: SGM for ‘Sample Group Mean’; CH for ‘Convex Hull’; AB for ‘Alpha-Bag’; TM for ‘Tukey Median’; and CR for ‘Classification Region’.

▷ Interpolate

Lets the user interpolate additional points onto the [biplot](#).

DETAIL · Only a single new point can be interpolated at one time.

◦ A new sample...

Lets the user interpolate a new sample as a point in the [biplot](#).

DETAIL · Not available if there are [no axes](#), as opposed to the axes being [hidden](#).

SHORTCUT · Ctrl+N

SCREENSHOT · [2.8](#)

REFERENCES · [Gower and Hand \(1996, Sections 2.3, 6.3.1\)](#)

Original variable values

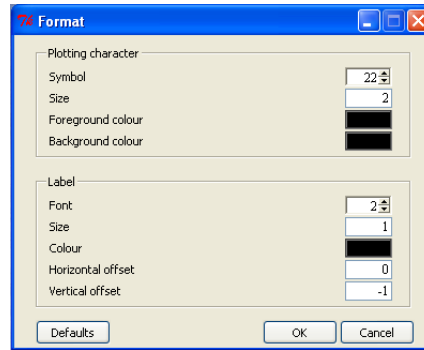
The variable values of the sample which is to be interpolated.

DETAIL · The variable values are given in terms of the units of the original variables, and in the order of the original variables. The variable values are separated by commas, without spaces. The variable values of variables that have been dragged from the [biplot](#) into the [kraal](#) are not entered. If axes are dragged back onto the biplot from the kraal, the option is disabled.

DEFAULT VALUE · The mean values of the non-kraal variables.

Label

The label to be used to annotate the interpolated point in the [biplot](#) or in



Screenshot 2.9: The *Additional* → *Interpolate* → *A new sample* → *Format* dialogue box.

the [legend](#).

DEFAULT VALUE · Interpolated

Label in biplot

If checked, shows the interpolated point's label in the [biplot](#) itself. Otherwise the label is shown in the [legend](#).

DEFAULT VALUE · checked

Defaults

Reverts the options to their default values.

Format

See the next framed section.

OK

Saves the options, returns to the [GUI](#), and redraws the [biplot region](#) with the interpolated point.

Off

Disables the option, and returns to the [GUI](#), not showing the interpolated point.

Format

Lets the user set graphical parameters for interpolated samples.

SCREENSHOT · [2.9](#)

Plotting character

Lets the user change the graphical parameters of the of the interpolated point.

Symbol

Sets the symbol used to represent the interpolated point.

DETAIL · Corresponds to R's `pch` argument. Possible values: NA, 0, ..., 25.

DEFAULT VALUE · 22

Size

Sets the size of the interpolated point.

DETAIL · Corresponds to R's `cex` argument. A larger value results in a larger point. Possible values: positive real numbers.

DEFAULT VALUE · 2

Foreground colour

Sets the exterior colour of the interpolated point.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · "black"

Background colour

Sets the interior colour of the interpolated point.

DETAIL · Corresponds to R's `bg` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · "black"

Label

Lets the user change the graphical parameters of the interpolated point label.

Font

Sets the font of the interpolated point label.

DETAIL · Corresponds to R's `font` argument. Possible values: 1: regular; 2: bold; 3: italic; 4: bold italic.

DEFAULT VALUE · 2

Size

Sets the size of the interpolated point label.

DETAIL · Corresponds to R's `cex` argument. Larger values result in larger text. Possible values: positive real numbers.

DEFAULT VALUE · 1

Colour

Sets the colour of the interpolated point label.

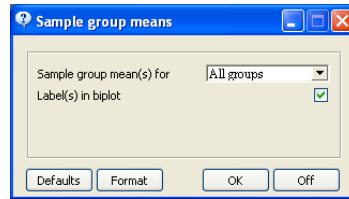
DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · "black"

Horizontal offset

Sets the horizontal offset of the interpolated point label from the interpolated point.

DETAIL · The interpolated point label is shifted horizontally from the interpolated point with this multiple of the width of the letter 'x' (in the



Screenshot 2.10: The *Additional* → *Interpolate* → *Sample group means* dialogue box.

selected font size). Positive values shift the label to the right; negative values shift the label to the left.

DEFAULT VALUE · 0

Vertical offset

Sets the vertical offset of the interpolated point label from the interpolated point.

DETAIL · The interpolated point label is shifted vertically from the interpolated point with this multiple of the height of the letter ‘x’ (in the selected font size). Positive values shift the label towards the top; negative values shift the label towards the bottom.

DEFAULT VALUE · −1

Defaults

Reverts the options to their default values.

OK

Saves the options and returns to the [Additional](#) → [Interpolate](#) → [A new sample](#) dialogue box.

Cancel

Cancels the changes made since the dialogue box was opened, and returns to the [Additional](#) → [Interpolate](#) → [A new sample](#) dialogue box.

○ **Sample group means...**

Lets the user interpolate the sample group means as points in the [biplot](#).

DETAIL · This option is especially important in the case of [CVA](#) biplots, where the optimality criterion is in terms of separation of the group means. If the sample group mean labels are shown in the [legend](#), the group names are preceded by the prefix SGM for ‘Sample Group Mean’. Not available if there are [no axes](#), as opposed to the axes being [hidden](#).

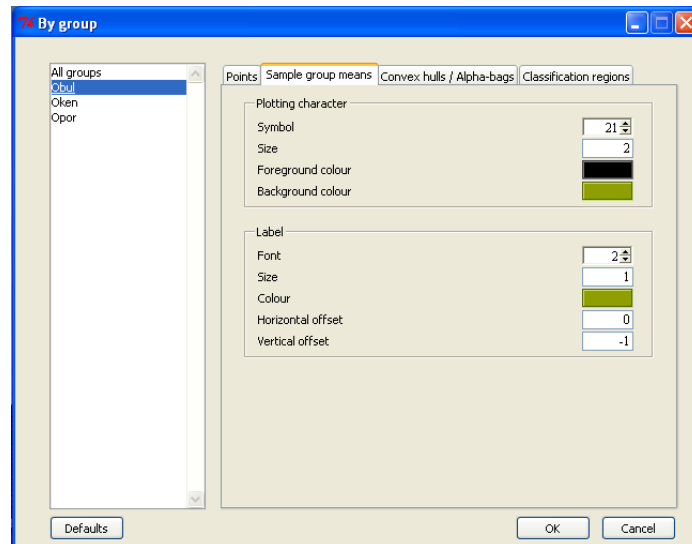
SCREENSHOT · [2.10](#)

REFERENCES · [Gower and Hand \(1996, Sections 2.3, 6.3.1\)](#)

Sample group mean(s) for

Sets the group(s) of samples for which sample group means must be interpolated.

DETAIL · Possible options: All samples (the overall mean is interpolated),



Screenshot 2.11: The *Additional* → *Interpolate* → *Sample group means* → *Format* dialogue box. This is also the *Sample group means* tab of the *Format* → *By group* dialogue box

all groups (the mean of each group is interpolated), or a specific group.

DEFAULT VALUE · All groups

Label(s) in biplot

If checked, shows the sample group mean labels in the [biplot](#) itself. Otherwise the labels are shown in the [legend](#).

DEFAULT VALUE · checked

Defaults

Reverts the options to their default values.

Format

See the next framed region.

OK

Saves the options, returns to the [GUI](#), and redraws the currently displayed [biplot region](#) with the interpolated sample group mean(s).

Off

Disables the option, and returns to the [GUI](#), not showing sample group mean(s).

Format

Lets the user set graphical parameters for interpolated sample group means, for a particular group, or for all groups simultaneously.

SCREENSHOT · [2.11](#)

This is also the Sample group means tab of the [Format](#) → [By group](#) dialogue box.

Plotting character

Lets the user change the graphical parameters of the point that represents the sample group mean, by group.

Symbol

Sets the symbol used to represent the sample group mean, by group.

DETAIL · Corresponds to R's `pch` argument. Possible values: NA, 0, ..., 25.

DEFAULT VALUE · If there is only one group, 22. Otherwise the values are recycled by group with the values 21 to 25.

Size

Sets the size of the point that represents the sample group mean, by group.

DETAIL · Corresponds to R's `cex` argument. A larger value results in a larger point. Possible values: positive real numbers.

DEFAULT VALUE · 2

Foreground colour

Sets the exterior colour of the point that represents the sample group mean, by group.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · "black"

Background colour

Sets the interior colour of the sample group mean, by group.

DETAIL · Corresponds to R's `bg` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · If there is only one group, "red". Otherwise equally spaced colours from the `hcl` spectrum.

Label

Lets the user change the graphical parameters of the sample group mean label, by group.

Font

Sets the font of the sample group mean label, by group.

DETAIL · Corresponds to R's `font` argument. Possible values: 1: regular; 2: bold; 3: italic; 4: bold italic.

DEFAULT VALUE · 2

Size

Sets the size of the sample group mean label, by group.

DETAIL · Corresponds to R's `cex` argument. Larger values result in larger text. Possible values: positive real numbers.

DEFAULT VALUE · 1

Colour

Sets the colour of the sample group mean label, by group.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · If there is only one group, "black". Otherwise equally spaced colours from the `hcl` spectrum.

Horizontal offset

Sets the horizontal offset of the sample group mean label from the corresponding sample group mean, by group.

DETAIL · The sample group mean label is shifted horizontally from the sample group mean with this multiple of the width of the letter 'x' (in the selected font size). Positive values shift the labels to the right; negative values shift the labels to the left.

DEFAULT VALUE · 0

Vertical offset

Sets the vertical offset of the sample group mean label from the corresponding sample group mean, by group.

DETAIL · The sample group mean label is shifted vertically from the sample group mean with this multiple of the height of the letter 'x' (in the selected font size). Positive values shift the label towards the top; negative values shift the label towards the bottom.

DEFAULT VALUE · -1

Defaults

Reverts the options of all the tabs of the dialogue box to their default values.

OK

Saves the options of all the tabs of the dialogue box, and returns to the [Additional → Interpolate → Sample group means](#) dialogue box.

Cancel

Cancels the changes made since the dialogue box was opened, and returns to the [Additional → Interpolate → Sample group means](#) dialogue box.

▷ **Convex hulls...**

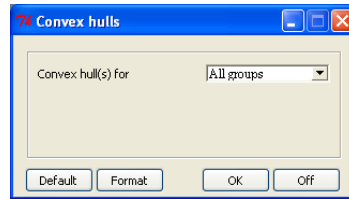
Lets the user superimpose convex hulls around one or more of the groups of points.

DETAIL · Convex hulls may be drawn around all the points, around each group of points, or around a specific group of points. If the convex hull labels are shown in the [legend](#), the group names are preceded by the prefix CH for 'Convex Hull'.

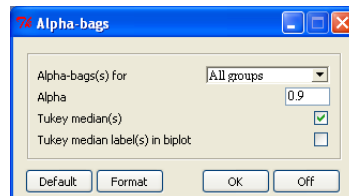
SCREENSHOT · [2.12](#)

ALTERNATIVE TO · [Alpha-bags](#)

REFERENCES · See the R help file of the `chull` function.



Screenshot 2.12: The *Additional* \rightarrow *Convex hulls* dialogue box.



Screenshot 2.13: The *Additional* \rightarrow *Alpha-bags* dialogue box.

Convex hull(s) for

The group(s) of points for which convex hull(s) must be drawn.

DETAIL · Possible options: All points (a single convex hull is drawn around all points), All groups (a convex hull is drawn around each group), or a specific group.

DEFAULT VALUE · All groups

Defaults

Reverts the options to their default values.

Format

Discussed under [Alpha-bags](#).

OK

Saves the option, returns to the [GUI](#), and redraws the [biplot region](#) with the convex hull(s).

Off

Disables the option, and returns to the [GUI](#), not showing convex hulls.

▷ **Alpha-bags...**

Lets the user superimpose alpha-bags around one or more of the groups of points.

DETAIL · Alpha-bags may be drawn around all the points, around each group of points, or around a specific group of points. Alpha-bags are closely related to bagplots which can be considered to be two-dimensional boxplots. Alpha-bags enclose approximately the inner $100\alpha\%$ of the points of a group. If the alpha-bag labels are shown in the [legend](#), the group names are preceded by the prefix AB for ‘Alpha-Bag’. If the Tukey median labels are shown in the legend, the group names are preceded by the prefix TM for ‘Tukey Median’.

SCREENSHOT · [2.13](#)

ALTERNATIVE TO · [Convex hulls](#)

REFERENCES · [Rousseeuw *et al.* \(1999\)](#), [Gardner \(2001\)](#), [Wurz, Le Roux, Gardner and Deacon \(2003\)](#)

Alpha-bag(s) for

The group(s) of points for which alpha-bag(s) must be drawn.

DETAIL · Possible options: All points (a single alpha-bag is drawn for all points), All groups (an alpha-bag is drawn for each group), or a specific group.

DEFAULT VALUE · All groups

Alpha

The value of alpha for the alpha-bag(s) to be shown.

DETAIL · Approximately the inner $100\alpha\%$ of the points of the group are enclosed in an alpha-bag.

DEFAULT VALUE · 0.9

Tukey median(s)

If checked, the tukey median(s) of the groups are also shown.

DEFAULT VALUE · checked

REFERENCES · [Rousseeuw *et al.* \(1999\)](#), [Gardner \(2001\)](#)

Tukey median label(s) in biplot

If checked and Tukey median(s) are shown, the Tukey median labels are shown in the [biplot](#), rather than in the [legend](#).

DETAIL · Approximately the inner $100\alpha\%$ of the points of the group are enclosed in an alpha-bag.

DEFAULT VALUE · clear

Defaults

Reverts the options to their default values.

Format

See the next framed section.

OK

Saves the options, returns to the [GUI](#) and redraws the [biplot region](#) with the alpha-bag(s) as selected.

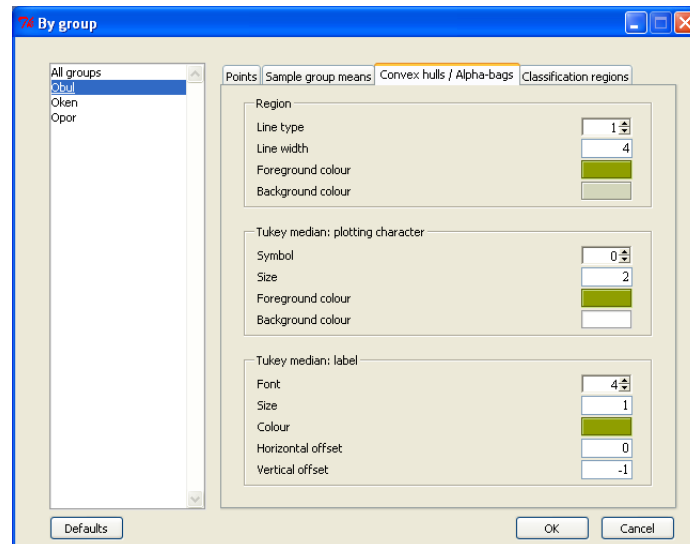
Off

Disables the option, and returns to the [GUI](#), not showing alpha-bags.

Format

Lets the user set graphical parameters for convex hulls and alpha-bags, for a particular group, or for all groups simultaneously.

SCREENSHOT · [2.14](#)



Screenshot 2.14: The *Additional* → *Convex hulls / Alpha-bags* → *Format* dialogue box. This is also the *Convex hulls / Alpha-bags* tab of the *Format* → *By group* dialogue box.

This is also the Convex hulls / Alpha-bags tab of the [Format](#) → [By group](#) dialogue box.

Region

Lets the user change graphical parameters associated with convex hulls or alpha-bags.

Line type

Sets the type of line used to draw the convex hull or alpha-bag, by group.

DETAIL · Corresponds to R's `lty` argument. Possible values: 0, ..., 6.

DEFAULT VALUE · 1

Line width

Sets the width of the convex hull or alpha-bag, by group.

DETAIL · Corresponds to R's `lwd` argument. Larger values result in wider border for convex hulls and alpha-bags. Possible values: positive real numbers.

DEFAULT VALUE · 4

Foreground colour

Sets the exterior colour of the convex hull or alpha-bag, by group.

DETAIL · Corresponds to R's `col` argument.

DEFAULT VALUE · If there is only one group, `#919191`. Otherwise equally spaced colours from the `hcl` spectrum.

Background colour

Sets the interior colour of the convex hull or alpha-bag, by group.

DETAIL · Corresponds to R's `bg` argument.

DEFAULT VALUE · If there is only one group, `#D4D4D4`. Otherwise equally

spaced colours from the `hcl` spectrum.

Tukey median: Plotting character

Lets the user change the graphical parameters of the Tukey median, by group.

Symbol

Sets the symbol used to represent the Tukey median, by group.

DETAIL · Corresponds to R's `pch` argument. Possible values: `NA`, 0, ..., 25.

DEFAULT VALUE · 0

Size

Sets the size of the Tukey medians, by group.

DETAIL · Corresponds to R's `cex` argument. A larger value results in a larger point. Possible values: positive real numbers.

DEFAULT VALUE · 2

Foreground colour

Sets the exterior colour of the Tukey median, by group.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · If there is only one group, "red". Otherwise equally spaced colours from the `hcl` spectrum.

Background colour

Sets the interior colour of the Tukey median, by group.

DETAIL · Corresponds to R's `bg` argument. Can be changed by clicking the colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · `NA`

Tukey median: label

Lets the user change the graphical parameters of the Tukey median label, by group.

Font

Sets the font of the Tukey median label, by group.

DETAIL · Corresponds to R's `font` argument. Possible values: 1: regular; 2: bold; 3: italic; 4: bold italic.

DEFAULT VALUE · 4

Size

Sets the size of the Tukey median label, by group.

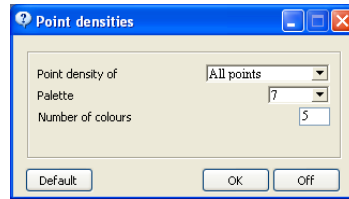
DETAIL · Corresponds to R's `cex` argument. Larger values result in larger text. Possible values: positive real numbers.

DEFAULT VALUE · 1

Colour

Sets the colour of the Tukey median label, by group.

DETAIL · Corresponds to R's `col` argument. Can be changed by clicking the



Screenshot 2.15: The *Additional* → *Point densities* dialogue box.

colour, producing a standard colour selection dialogue box.

DEFAULT VALUE · If there is only one group, “black”. Otherwise equally spaced colours from the `hcl` spectrum.

Horizontal offset

Sets the horizontal offset of the Tukey median label from the corresponding Tukey median, by group.

DETAIL · The Tukey median label is shifted horizontally from the Tukey median with this multiple of the width of the letter ‘x’ (in the selected font size). Positive values shift the labels to the right; negative values shift the labels to the left.

DEFAULT VALUE · 0

Vertical offset

Sets the vertical offset of the Tukey median label from the corresponding Tukey median.

DETAIL · The Tukey median label is shifted vertically from the Tukey median with this multiple of the height of the letter ‘x’ (in the selected font size). Positive values shift the label towards the top; negative values shift the label towards the bottom.

DEFAULT VALUE · -1

Defaults

Reverts the options of all the tabs of the dialogue box to their default values.

OK

Saves the options of all the tabs of the dialogue box, and returns to the [Additional](#) → [Convex hulls](#) or [Additional](#) → [Alpha-bags](#) dialogue box.

Cancel

Cancels the changes made since the dialogue box was opened, and returns to the [Additional](#) → [Convex hulls](#) or [Additional](#) → [Alpha-bags](#) dialogue box.

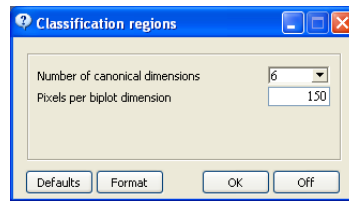
▷ **Point densities...**

Lets the user superimpose the biplot onto a background of point density estimates.

SCREENSHOT · [2.15](#)

ALTERNATIVE TO · [Classification regions](#)

REFERENCES · [Wand \(2008\)](#), [Blasius et al. \(2008\)](#)



Screenshot 2.16: The *Additional* → *Classification regions* dialogue box.

Point density of

Sets the group of points on which the point densities are to be based.

DETAIL · Possible options: All points, or a specific group of points.

DEFAULT VALUE · All points

Palette

The colour palette in which the point densities are represented.

DETAIL · Possible options: Terrain, Heat, 1, . . . , 8

DEFAULT VALUE · 7

Number of colours

The number of distinct colours to include in the palette.

DETAIL · The higher the number, the smoother the image. The lower the number, the easier to distinguish between different levels.

DEFAULT VALUE · 5

Defaults

Reverts the options to their default values.

OK

Saves the options, returns to the [GUI](#) and redraws the [biplot region](#) with the point density estimates as chosen.

Off

Disables the option, and returns to the [GUI](#), not showing point density estimates.

▷ **Classification regions. . .**

Lets the user superimpose a [CVA](#) biplot onto a background of coloured classification regions.

DETAIL · Pixels are coloured in according to the closest group mean in a specified number of canonical dimensions, except when the specified number of canonical dimensions is two, in which case a Voronoi diagram gives the classification regions. If the classification region labels are shown in the [legend](#), the group names are preceded by the prefix CR for ‘Classification Region’. Only available for [CVA](#) biplots.

SCREENSHOT · [2.16](#)

ALTERNATIVE TO · [Point densities](#)

REFERENCES · [Gower and Hand \(1996, Section 7.3.2\)](#), [Gardner and Le Roux \(2005\)](#)

Number of canonical dimensions

The number of canonical dimensions in which classification are to be made.

DETAIL · From 1, ..., min(the number of variables, one less than the number of groups).

DEFAULT VALUE · 2

Pixels per biplot dimension

This number of pixels, squared, are classified into one of the groups and colour-coded accordingly.

DETAIL · The larger the number, the finer the image, but the more time and memory required to produce it. The smaller the number, the grainier the image.

DEFAULT VALUE · 150

Default

Reverts the option to its default value.

Format

See the next framed region.

OK

Saves the options, returns to the [GUI](#) and redraws the [biplot region](#) with the classification regions shown.

Off

Disables the option, and returns to the [GUI](#), without classification regions.

Format

Lets the user set graphical parameters for classification regions, for a particular group, or for all groups simultaneously.

SCREENSHOT · [2.17](#)

This is also the Classification regions tab in the [Format → By group](#) dialogue box.

Region***Background colour***

The background colour of classification region, by group.

DETAIL · Equally spaced colours from the [hcl](#) spectrum.

Defaults

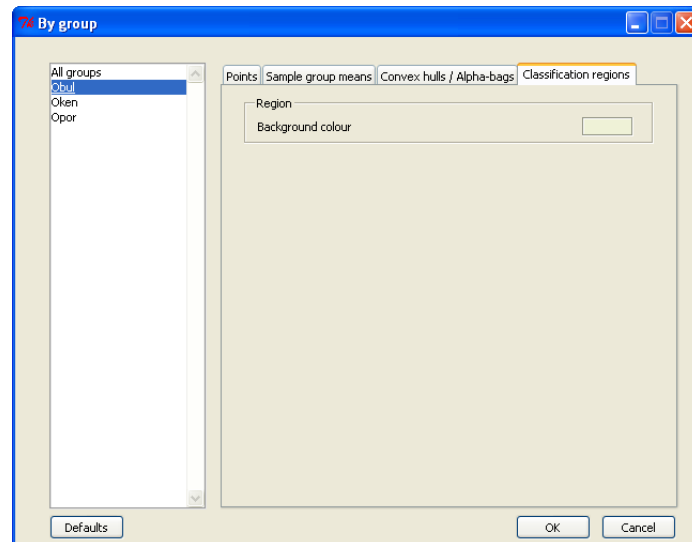
Reverts the options to their default values.

OK

Saves the options, returns to the [GUI](#) and redraws the [biplot region](#) with classification regions.

Off

Disables the option, and returns to the [GUI](#), not showing classification regions.



Screenshot 2.17: The *Additional* → *Classification regions* → *Format* dialogue box. This is also the *Classification regions* tab in the *Format* → *By group* dialogue box.

▷ **Clear all**

Disables all additional descriptors.

SHORTCUT · Ctrl+L

• **Help**

Some help options.

▷ **Manual (in PDF)**

Opens this manual.

SHORTCUT · F1

▷ **Homepage**

Opens the package homepage at <http://biplotgui.r-forge.r-project.org/> if an Internet connection is available.

▷ **Show pop-up help**

If selected, pop-up help is shown as the mouse cursor is hovered over the major elements of the main view of the GUI.

▷ **About...**

Shows information about the author, version and license.

► **Biplot region**

Contains the [biplot](#), optional [title](#), and optional [legend](#).

DETAIL · The biplot region is located towards the left of the GUI. The biplot itself is positioned at the centre of the biplot region. An optional title is shown above the biplot when [View](#) → [Show title](#) is selected. An optional legend may be shown below the biplot.

The biplot region is responsive to mouse clicks and motion. Different pop-up menus appear when right clicking [inside the biplot](#), [on a point](#), [on an axis](#), or [outside the biplot](#).

Depending on how the GUI has been resized onscreen, the proportions within the biplot region onscreen may differ from the proportions in biplot regions that have been [saved](#), [copied](#), [printed](#) or shown in [external](#) windows. To ensure consistency, saved and copied biplot regions always have both their width and height set to 20.32 centimeters (8 inches). Two-dimensional external-window biplot regions always have both their width and height set to 17.78 centimeters (7 inches). This is the default size of R graphs.

SCREENSHOT · [Figure 1.1](#)

- **Title**

Provides a [title](#) to the [biplot](#).

DETAIL · The title is only shown if [View → Show title](#) is selected. The default title depends on the currently displayed biplot. The biplot retains the same size and relative position, irrespective of whether or not a title is shown.

- **Biplot**

A graph that displays samples as points, and variables as calibrated axes.

DETAIL · This is the graph of main interest. Right clicking on a [point](#), on an [axis](#), or [elsewhere](#) within the biplot produces pop-up menus. Points and axes may be dragged from the biplot into the [kraal](#), and be dragged back onto the biplot from the kraal.

REFERENCES · [Gabriel \(1971\)](#), [Gower and Hand \(1996\)](#)

- **Legend**

A legend to the elements which appear in the [biplot](#).

DETAIL · If necessary, a legend is provided below the biplot. The legend can identify groups, axes, an interpolated point, sample group means, convex hulls, alpha-bags, Tukey medians and classification regions, in that order. All these elements can separately be included or excluded from the legend.

The legend can contain a maximum of 16 entries at any one time. If there are more than 16 entries, only the first 16 are shown initially. The succeeding set of entries can be shown by right clicking outside the biplot but inside the [biplot region](#), and selecting [Show next legend entries](#) from the [popup-menu](#). The keyboard shortcut is Ctrl++. Similar options are available with which to show the preceding entries. All legend entries are restricted to be 14 characters long.

When the entries of the [Additional](#) menu appear in the legend, the group names are preceded by short prefixes. The prefixes are as follows: SGM for Sample Group Mean; CH for Convex Hull; AB for Alpha-Bag; TM for Tukey Median; CR for Classification Region.

- **Inner pop-up menu**

Provides access to biplot options.

DETAIL · This pop-up menu appears when the user right clicks inside the [biplot](#) (as opposed to the [biplot region](#)), but not on a point or on an axis.

- ▷ **Zoom in**

Zooms in around the right clicked position.

DETAIL · The [biplot](#) is enlarged and the focus is shifted so that that position which was right clicked to produce the pop-up menu appears at the centre of the biplot.

▷ **Zoom out**

Zooms out from the right clicked position.

DETAIL · The [biplot](#) is reduced in size and the focus is shifted so that that position which was right clicked to produce the pop-up menu appears at the centre of the [biplot](#).

▷ **Reset zoom**

Resets the [biplot](#) to its original zoom factor.

▷ **Don't predict**

Dynamic variable prediction is disabled.

DETAIL · Not shown if there are [no axes](#), as opposed to the axes being [hidden](#).

ALTERNATIVE TO · [Predict cursor positions](#), [Predict points closest to cursor positions](#)

▷ **Predict cursor positions**

The variable values of the point under the cursor position are dynamically predicted.

DETAIL · For linear biplots, the orthogonal projections onto the biplot axes are shown. For non-linear biplots, circular projections are shown. The predicted variable values themselves are shown in the [predictions tab](#). Not available when the axes are [hidden](#), or if the biplot is interpolative rather than predictive. Not shown when there are [no axes](#).

ALTERNATIVE TO · [Don't predict](#), [Predict points closest to cursor positions](#)

REFERENCES · ([Gower and Hand, 1996](#), Sections 2.3, 6.3.2)

▷ **Predict points closest to cursor positions**

The variable values of the point closest to the cursor position are dynamically predicted.

DETAIL · For linear biplots, orthogonal projections onto the biplot axes are shown. For non-linear biplots, circular projections are shown. The predicted variable values themselves are shown in the [Predictions tab](#). Not available when the [points are hidden](#), the [axes are hidden](#), or if the biplot is interpolative rather than predictive. Not shown when there are [no axes](#).

ALTERNATIVE TO · [Don't predict](#), [Predict cursor positions](#)

REFERENCES · ([Gower and Hand, 1996](#), Sections 2.3, 6.3.2)

▷ **Remove axis highlight**

If an axis has been highlighted, this option removes the highlight.

DETAIL · Only available if an axis has been highlighted. Axes are highlighted by right clicking them and selecting [Highlight](#) from the pop-up menu. Not shown when there are [no axes](#), as opposed to the axes being [hidden](#).

▷ **Format by group...**

The same as [Format](#) → [By group](#).

▷ **Format axes...**

The same as [Format](#) → [Axes](#).

DETAIL · Not shown when there are [no axes](#), as opposed to the axes being [hidden](#).

▷ **Save as**

The same as [File → Save as](#).

▷ **Copy**

The same as [File → Copy](#).

▷ **Print...**

The same as [File → Print](#).

• **Point pop-up menu**

Provides access to options associated with points.

DETAIL · This pop-up menu appears when the user right clicks a point inside the [biplot](#). A point or axis is under the mouse if the mouse cursor changes from an arrow to a hand.

▷ **Send to kraal**

Sends the point which was right clicked to the [kraal](#).

DETAIL · Sending a point to the kraal temporarily removes it from consideration. The [biplot region](#) and [diagnostic tabs](#) are automatically updated. Points and axes may also be dragged from the [biplot](#) to the kraal.

▷ **Format...**

Opens the *Points* tab of the [Format → By group](#) dialogue box at the group of the point that was right clicked.

• **Axis pop-up menu**

Provides access to options associated with axes.

DETAIL · This pop-up menu appears when the user right clicks an axis inside the [biplot](#). A point or axis is under the mouse if the mouse cursor changes from an arrow to a hand.

▷ **Highlight**

Highlights the axis which was right clicked.

DETAIL · This option highlights the axis which was right clicked by greying the other axes in the [biplot region](#) and [diagnostic tabs](#). By default, the variable values of the highlighted axis are also then shown in the [biplot](#). An axis highlight may be removed by right clicking inside the biplot and selecting [Remove axis highlight](#) from the pop-up menu. The highlight is automatically removed if the highlighted axis is moved to the [kraal](#).

▷ **Send to kraal**

Sends the axis which was right clicked to the [kraal](#).

DETAIL · Sending an axis to the [kraal](#) temporarily removes it from consideration. The [biplot region](#) and [diagnostic tabs](#) are automatically updated. At least three axes must be left in the [biplot](#).

▷ **Format...**

Opens the [Format → Axes](#) dialogue box at the axis that was right clicked.

• **Outer pop-up menu**

Provides access to biplot options.

▷ **Show title**

The same as [View → Show title](#).

▷ **Format title...**

The same as [Format → Title](#).

▷ **Show group labels in legend**

The same as [View → Show group labels in legend](#).

▷ **Don't show axis labels**

The same as [View → Don't show axis labels](#).

DETAIL · Not shown when there are [no axes](#), as opposed to the axes being [hidden](#).

▷ **Show clinging axis labels**

The same as [View → Show clinging axis labels](#).

DETAIL · Not shown when there are [no axes](#), as opposed to the axes being [hidden](#).

▷ **Show axis labels in legend**

The same as [View → Show axis labels in legend](#).

DETAIL · Not shown when there are [no axes](#), as opposed to the axes being [hidden](#).

▷ **Show Additional labels in legend**

The same as [View → Show Additional labels in legend](#).

▷ **Show next legend entries**

The same as [View → Show next legend entries](#).

▷ **Show previous legend entries**

The same as [View → Show previous legend entries](#).

▷ **Save as**

The same as [File → Save as](#).

▷ **Copy**

The same as [File → Copy](#).

▷ **Print...**

The same as [File → Print](#).

► **Settings box**

Lets the user choose the action of the biplot axes, and effect data transformations.

DETAIL · The settings box is located towards the centre right of the [GUI](#).

SCREENSHOT · [Figure 1.1](#)

• **Action**

Lets the user choose the action of the biplot axes.

DETAIL · Disabled when there are no axes, or the axes are hidden.

▷ **Predict**

A predictive biplot is shown.

DETAIL · Predictive biplot axes are positioned and calibrated to optimally predict

variable values from the positions of points in a biplot.

ALTERNATIVE TO · [Interpolate: centroid](#), [Interpolate: vector sum](#)

REFERENCES · ([Gower and Hand, 1996](#), Sections 2.3, 6.3.2)

▷ **Interpolate: centroid**

A centroid interpolative biplot is shown.

DETAIL · Centroid interpolative biplot axes are positioned and calibrated to allow for interpolation of new samples onto an existing biplot by finding a centroid.

ALTERNATIVE TO · [Predict](#), [Interpolate: vector sum](#)

REFERENCES · [Gower and Hand \(1996, Section 5.3\)](#)

▷ **Interpolate: vector sum**

A vector sum interpolative biplot is shown.

DETAIL · Vector sum interpolative biplot axes are positioned and calibrated to allow for interpolation of new samples onto an existing biplot by finding a vector sum.

ALTERNATIVE TO · [Predict](#), [Interpolate: centroid](#)

REFERENCES · ([Gower and Hand, 1996](#), Sections 2.3, 6.3.1)

• **Transformation**

Lets the user effect data transformations.

DETAIL · These transformations are performed on **Data** argument of the **Biplots** function. Data are always centred to have zero column means. Log-transformations are only available if all the non-[kraal](#) variable values of the non-[kraal](#) points are strictly positive. Irrespective of the transformation, the biplot axes are always calibrated in terms of the original variable values. In order to have a biplot calibrated in terms of transformed variable values, the transformation has to be performed outside of the [GUI](#) and passed to the [GUI](#) via the **Data** argument.

▷ **Centre**

Transforms the data to have zero column means.

DETAIL · The mean of each column is subtracted from the elements of that column. The data are always centred to have zero column means.

ALTERNATIVE TO · [Centre, scale](#); [Unitise, centre](#); [Log, centre](#); [Log, centre, scale](#); [Log, unitise, centre](#)

▷ **Centre, scale**

Transforms the data to have zero column means, and then scales the data so that each column has unit variance.

DETAIL · The mean of each column is first subtracted from the elements of that column. Each column is then divided by its standard deviation.

ALTERNATIVE TO · [Centre](#); [Unitise, centre](#); [Log, centre](#); [Log, centre, scale](#); [Log, unitise, centre](#)

▷ **Unitise, centre**

Shifts and scales each column to have minimum value 0 and maximum value 1; thereafter centres to have zero column means.

DETAIL · The minimum of each column is subtracted from the elements of that column, the answers divided by the range of the (original) column.

ALTERNATIVE TO · [Centre](#); [Centre, scale](#); [Log, centre](#); [Log, centre, scale](#); [Log, unitise, centre](#)

▷ **Log, centre**

Takes natural logarithms, then transforms the data to have zero column means.

DETAIL · Natural logarithms are taken of all elements. Thereafter the mean of each column is subtracted from the elements of that column. Only available if all the non-[kraal](#) variable values of the non-kraal points are strictly positive.

ALTERNATIVE TO · [Centre](#); [Centre, scale](#); [Unitise, centre](#); [Log, centre, scale](#); [Log, unitise, centre](#)

▷ **Log, centre, scale**

Takes natural logarithms, transforms to have zero column means, then scales so that each column has unit variance.

DETAIL · Natural logarithms are taken of all elements. Thereafter the mean of each column is first subtracted from the elements of that column. Each column is then divided by its standard deviation. Only available if all the non-[kraal](#) variable values of the non-kraal points are strictly positive.

ALTERNATIVE TO · [Centre](#); [Centre, scale](#); [Unitise, centre](#); [Log, centre](#); [Log, unitise, centre](#)

▷ **Log, unitise, centre**

Takes natural logarithms, shifts and scales each column to have minimum value 0 and maximum value 1; thereafter centres to have zero column means.

DETAIL · Natural logarithms are taken of all elements. Thereafter the minimum of each column is subtracted from the elements of that column, the answers divided by the range of the (post-log) column. Only available if all the non-[kraal](#) variable values of the non-kraal points are strictly positive.

ALTERNATIVE TO · [Centre](#); [Centre, scale](#); [Unitise, centre](#); [Log, centre](#); [Log, centre, scale](#);

► **Diagnostic tabs**

Consists of tabs for diagnostic graphs, dynamic variable value predictions, and quantities for export back to R.

DETAIL · The diagnostic tabs are located towards the top right of the [GUI](#).

*Note: A [known issue](#) affects the diagnostic tabs of version 0.0-4.1 of the *BiplotGUI* package.*

SCREENSHOT · [Figure 1.1](#)

- **Convergence**

If the points are determined by [MDS](#), a graph of stress values over iterations is shown.

DETAIL · If [Live updates](#) is checked, the graph is updated live. Only available when the points are determined by [MDS](#).

- ▷ **Pop-up menu**

Makes various options available with respect to the graph of the convergence tab.

DETAIL · The convergence pop-up menu is obtained by right clicking the graph in the convergence tab.

- **Show title**

The same as [View → Show title](#). However, it applies to the graph in the tab rather than to the [biplot region](#).

- **Format...**

The same as [Format → Diagnostic tabs](#).

- **Save as**

The same as [File → Save as](#). However, it applies to the graph in the tab rather than to the [biplot region](#).

DETAIL · Diagnostic graphs are saved with the same proportions that would be used if the currently displayed biplot region were to be saved. This ensures that the graphs can be used alongside one another. Specifically, if the biplot region has a [legend](#), in the saved version of diagnostic graphs, an equivalent open space will be left at the bottom of the graph. To remove the space, temporarily remove the legend from the biplot and save the diagnostic graph once more.

- **Copy**

The same as [File → Copy](#). However, it applies to the graph in the tab rather than to the [biplot region](#).

DETAIL · Diagnostic graphs are copied with the same proportions that would be used if the currently displayed biplot region were to be copied. This ensures that the graphs can be used alongside one another. Specifically, if the biplot region has a [legend](#), in the copied version of diagnostic graphs, an equivalent open space will be left at the bottom of the graph. To remove the space, temporarily remove the legend from the biplot and copy the diagnostic graph once more.

- **Print...**

The same as [File → Print](#). However, it applies to the graph in the tab rather than to the [biplot region](#).

DETAIL · Diagnostic graphs are printed with the same proportions that would be used if the currently displayed biplot region were to be printed. This ensures that the graphs can be used alongside one another. Specifically, if the biplot region has a [legend](#), in the printed version of diagnostic graphs, an equivalent open space will be left at the bottom of the graph. To remove the space, temporarily remove the legend from the biplot and print the diagnostic graph once more.

- **External**

The same as [External](#) → [As is](#) below the [biplot region](#). However, it applies to the graph in the tab rather than to the biplot region.

DETAIL · External diagnostic graphs have the same proportions that would be used if the currently displayed [biplot](#) were to be placed in an external window. This ensures that the graphs can be used alongside one another. Specifically, if the biplot has a [legend](#), in the diagnostic graph will have an equivalent open space. To remove the space at the bottom of the graph, temporarily remove the legend and choose the External option for the diagnostic graph once more.

- **Points**

Shows graphs of goodness of fit of the points.

DETAIL · For [PCA](#) and [CVA](#) biplots, graphs of point predictivities are shown. The first axis shows the point predictivities in the first [biplot](#) dimension. Therefore, the closer a point is to the right of the graph, the better it is represented in the first dimension of the biplot. The distance above the diagonal line represents the contribution of the second biplot dimension. Therefore, the second axis of the point predictivities graph shows the point predictivities of the first two biplot dimensions jointly. The closer a point is to the top of the graph, the better represented it is in the two dimensions of the biplot.

When the points in a biplot are based either on [PCO](#) or [MDS](#), a Shepard diagram is shown in this tab. In a Shepard diagram, inter-sample dissimilarities are shown on the x-axis. On the y-axis, inter-point disparities are shown on the line, while inter-point distances are shown as points. The closer the inter-point distances are to the inter-point disparities, the better the fit. By default, the five worst-fitting point pairs are identified. A Shepard diagram is only shown if there are fewer than 250 non-kraal samples.

Not available for covariance/correlation biplots.

REFERENCES · [Borg and Groenen \(2005, Section 3.3\)](#), [Gardner-Lubbe et al. \(2008\)](#)

- ▷ **Pop-up menu**

The same as the [convergence pop-up menu](#). However, it acts on the graphs of the [points tab](#).

- **Groups**

Shows graphs of goodness of fit of the groups.

DETAIL · For [CVA](#) biplots, graphs of group predictivities are shown. The first axis shows the group predictivities in the first [biplot](#) dimension. Therefore, the closer a point is to the right of the graph, the better represented the corresponding group is in the first dimension of the biplot. The distance above the diagonal line represents the contribution of the second biplot dimension. Therefore, the second axis of the group predictivities graph shows the group predictivities of the first two biplot dimensions jointly. The closer a point is to the top of the graph, the better represented the corresponding group is in the two dimensions of the biplot.

Only available for [CVA](#) biplots.

REFERENCES · [Gardner-Lubbe et al. \(2008\)](#)

- ▷ **Pop-up menu**

The same as the [convergence pop-up menu](#). However, it acts on the graph of the [groups tab](#).

- **Axes**

Shows graphs of goodness of fit of the axes.

DETAIL · For [PCA](#) and [CVA](#) biplots, graphs of axis predictivities are shown. The first axis shows the axis predictivities in the first [biplot](#) dimension. Therefore, the closer a point is to the right of the graph, the better represented the corresponding axis is in the first dimension of the biplot. The distance above the diagonal line represents the contribution of the second biplot dimension. Therefore, the second axis of the axis predictivities graph shows the axis predictivities of the first two biplot dimensions jointly. The closer a point is to the top of the graph, the better represented the corresponding axis is in the two dimensions of the biplot.

Only available for [PCA](#) and [CVA](#) biplots.

REFERENCES · [Gardner-Lubbe et al. \(2008\)](#)

- ▷ **Pop-up menu**

The same as the [convergence pop-up menu](#). However, it acts on the graph of the [axes tab](#).

- **Predictions**

The tab in which live variable value predictions are shown.

DETAIL · Dynamic variable value prediction is enabled by right clicking inside the [biplot](#) and choosing either [Predict cursor positions](#) or [Predict points closest to cursor positions](#) from the pop-up menu. If [Predict cursor positions](#) is chosen, the second column of the table in the predictions tab contains the variable value predictions corresponding to the position of the mouse cursor as it moves over the biplot. If [Predict points closest to cursor positions](#) is chosen, the variable values of the point closest to the mouse cursor as it moves over the biplot, are predicted. In this case, the third column contains the actual variable values of the points. The fourth column contains the [RAE](#), which is calculated as $(\text{prediction} - \text{actual}) / (\text{maximum actual for variable} - \text{minimum actual for variable}) \times 100$. Biplots are not exact but optimal.

Not available when there are [no axes](#), the axes are [hidden](#), or the biplot is interpolative rather than predictive.

REFERENCES · [Gower and Hand \(1996, Sections 2.3, 6.3.2\)](#)

- **Export**

Allows various quantities to be exported back to R to view or manipulate.

DETAIL · Depending on the representation in the [biplot region](#), various quantities are available for export back to R. A quantity can be displayed in the R console by selecting it and clicking [Display in console](#). Alternatively, a quantity can be saved to the current R workspace by selecting it and clicking [Save to workspace](#).

REFERENCES · [Gower and Hand \(1996\)](#), [Borg and Groenen \(2005\)](#)

- ▷ **Display in console**

Displays the quantity selected in the [export tab](#) in the R console.

DETAIL · Only available if a quantity has been selected in the export tab.

- ▷ **Save to workspace**

Saves the quantity selected in the [export tab](#) in the current R workspace under the

name given in the list of quantities.

DETAIL · Only available if a quantity has been selected in the export tab.

► Kraal

Points and axes may be dragged to the kraal, temporarily removing them from consideration.

DETAIL · The kraal is located towards the bottom right of the [GUI](#). A point or axis can be removed to the kraal by first hovering the mouse cursor over it so that the cursor changes from an arrow to a hand, and then dragging the point or axis beyond the [biplot](#) borders. Alternatively, the point or axis can be right clicked, and Send to kraal selected from the pop-up menu. The [biplot region](#) and [diagnostic tabs](#) are then automatically updated as if the corresponding sample or variable were never part of the data set; the point or axis itself appears in the kraal. Many points and axes can simultaneously be kept in the kraal, but at least three axes must remain in the biplot.

The kraal itself is responsive to mouse clicks and motion. Different pop-up menus appear when right clicking [inside the kraal](#), [on a point](#), or [on an axis](#). Points and axes may be dragged around in the kraal over a grid of possible positions, or back onto the biplot. Alternatively, the buttons below the kraal may be used to send back the [points only](#), the [axes only](#), or both the [points and axes](#).

SCREENSHOT · [Figure 1.1](#)

• Kraal pop-up menu

Shows options associated with the [kraal](#).

DETAIL · The kraal pop-up menu is obtained by right clicking inside the kraal but not on points or axes in the kraal.

▷ Return points

Returns all the points in the [kraal](#) to the [biplot](#) and updates the biplot and the [diagnostic tabs](#).

DETAIL · Not available when there are no points in the [kraal](#).

▷ Return axes

Returns all the axes in the [kraal](#) to the [biplot](#) and updates the biplot and the [diagnostic tabs](#).

DETAIL · Not available when there are no axes in the [kraal](#).

▷ Return all

Returns all the points and axes in the [kraal](#) to the [biplot](#) and updates the biplot and [diagnostic tabs](#).

DETAIL · Not available when there are no points or axes in the [kraal](#).

▷ Format by group...

The same as [Format](#) → [By group](#).

▷ Format axes...

The same as [Format](#) → [Axes](#).

• Kraal point pop-up menu

Shows options associated with a point in the [kraal](#).

DETAIL · The [kraal](#) point pop-up menu is obtained by right clicking a point in the [kraal](#).

When the mouse cursor is above a point or axis, the cursor changes from an arrow to a hand.

▷ **Return to biplot**

Returns the right clicked point to the [biplot](#) and updates the biplot and [diagnostic tabs](#).

▷ **Format...**

Opens the points tab of the [Format → By group](#) dialogue box at that group of the point that was right clicked.

• **Kraal axis pop-up menu**

Shows options associated with an axis in the [kraal](#).

DETAIL · The kraal axis pop-up menu is obtained by right clicking an axis in the kraal. When the mouse cursor is above a point or axis, the cursor changes from an arrow to a hand.

▷ **Return to biplot**

Returns the right clicked axis to the [biplot](#) and updates the biplot and [diagnostic tabs](#).

▷ **Format...**

Opens the [Format → Axes](#) dialogue box at that axis that was right clicked.

► **Other**

Contains miscellaneous features.

DETAIL · These features are located in the strip at the bottom of the [GUI](#).

SCREENSHOT · [Figure 1.1](#)

• **Progress bar**

Shows the progress while performing an action.

DETAIL · The progress bar appears at the bottom left of the screen while an action is being performed. While the [GUI](#) is busy, no new actions should be initiated. Changing tabs is not considered to constitute action.

• **External**

Options to display the currently displayed [biplot region](#) in an external window.

DETAIL · Whether external windows are re-used or not can be set by clicking [File → Options](#).

▷ **As is**

Shows the currently displayed [biplot region](#) in an external R graph.

DETAIL · Depending on how the [GUI](#) has been resized onscreen, the proportions within an external [biplot region](#) may differ from what is shown onscreen. To ensure consistency, external biplot regions always have both their width and height set to 17.78 centimeters (7 inches). This is the default size of R graphs.

SHORTCUT · F11

▷ **In 3D**

Creates a three-dimensional version of the currently displayed [biplot](#) which can be dynamically navigated.

DETAIL · This option is only available for non-[MDS](#) representations so that the first two dimensions of the three-dimensional biplot corresponds to the two-dimensional biplot shown in the [GUI](#). Various options can be set by clicking [File → Options](#). By default the left mouse button acts as a trackball for navigation, the middle mouse button allows zooming in and out, and the right mouse button sets the field of view. Not all options from the [View](#) menu or graphical parameters from the [Format](#) menu transfer to the three-dimensional biplots.

SHORTCUT · F12

REFERENCES · See the R help file of the `par3d` function of the `rgl` package ([Adler and Murdoch, 2009](#)) for details on the choices.

- **Hide**

Hides the points and/or the axes of a biplot.

▷ **Points**

Hides the points of the [biplot](#).

▷ **Axes**

Hides the axes of the [biplot](#).

DETAIL · Not available when there are [no axes](#).

- **Live updates**

Toggles between showing live updates of [MDS](#) convergence (both in the [biplot](#) and [diagnostic tabs](#)), and merely showing the graphs for the final, converged configuration.

DETAIL · It can be informative to see the [MDS](#) configuration converges. However, if checked, the [biplot region](#) and Shepard diagram is redrawn after a number of iterations, taking more time. To speed up convergence, the checkbox can be cleared. The number of iterations to the next update can be changed by clicking [File → Options](#).

- **Stop**

Stops the [IM](#) algorithm for [MDS](#).

DETAIL · Stops the iterations and proceeds with the current configuration, fitting biplot axes and all the rest. Such representations do not meet optimality criteria and may therefore be misleading. Available only while an [MDS](#) configuration is being found.

- **Return points**

Returns all the points in the [kraal](#) to the [biplot](#) and updates the biplot and the [diagnostic tabs](#).

DETAIL · Not available when there are no points in the [kraal](#).

- **Return axes**

Returns all the axes in the [kraal](#) to the [biplot](#) and updates the biplot and the [diagnostic tabs](#).

DETAIL · Not available when there are no axes in the [kraal](#).

- **Return all**

Returns all the points and axes in the [kraal](#) to the [biplot](#) and updates the biplot and [diagnostic tabs](#).

DETAIL · Not available when there are no points or axes in the [kraal](#).

CHAPTER A

HISTORY

VERSION 0.0-1

29 JULY 2008. The first release. Contains support for

- Biplots: [PCA](#), covariance/correlation, [CVA](#), regression, Procrustes, circular non-linear
- Interpolation and prediction
- Scaling techniques: [PCO](#), metric [MDS](#) (identity transformation), non-metric [MDS](#) (monotone regression), semi-metric [MDS](#) (monotone spline transformation)
- Data transformations: centre; centre, scale; unitise, centre; log, centre; log, centre, scale; log, unitise, centre
- Distance metrics: Pythagoras, Square-root-of-Manhattan, Clark, Mahalanobis
- Additional descriptors: convex hulls, alpha-bags, point densities, classification regions
- Export of intermediate quantities back to R
- Diagnostic graphs: convergence; point, group and axis predictivities; Shepard diagrams
- Interactivity: variable value prediction, zooming, point and axis drag-and-drop; 3D biplots
- Customisation of graphs
- Import of data from Excel 1997–2003 files

VERSION 0.0-2

12 AUGUST 2008. The first CRAN release.

- The [Help](#) → [Homepage](#) option is added
- The names of two graphical parameters in the [Format](#) → [Interaction](#) dialogue box are corrected
- The `CountryData` data set is renamed the `Countries` data set
- Changes are made to the package help files, including correcting the units of the GDP variable of the countries data. The variable measures ‘[PPP GDP](#) per capita in US dollars’ rather than ‘[PPP GDP](#) in trillions of US dollars’ as previously stated. However, the countries are still those with the 15 highest [PPP GDPs](#) in US dollars during 2007 without adjusting for population size.
- The manual is updated with two new chapters included

VERSION 0.0-3

NOVEMBER 2008. Master's thesis version. Not publicly released.

- [Classification regions](#) in two canonical dimensions are now calculated explicitly, and classification regions are by default now calculated in two canonical dimensions. The `deldir` package ([Turner, 2007](#)) becomes a required package.
- A bug is fixed that very rarely caused the axes to be calibrated with values with 16 decimal places.
- A bug is fixed that resulted in a console error when [sample group means](#) were formatted before being displayed for the first time.
- The 'Report a bug' option is removed from the [Help](#) menu.
- The package help files are updated.

Technical

- A typographical error is corrected in the DESCRIPTION file.
- A more modern implementation of the [progress bar](#) is used.
- Work is done towards compatibility with Unix-alike. More work remains to be done.

VERSION 0.0-4

24 FEBRUARY 2009.

- A [Run](#) option, with shortcut 'R', is included in the [MDS](#) menu.
- The 'fly-by' in three-dimensional biplots is now disabled by default. It may be enabled via the [File](#) → [Options](#) dialogue box.
- The 'Distance metric' entry in the [Points](#) menu is renamed '[Dissimilarity metric](#)'.
- The 'Xbar' entry in the [export tab](#) of the [CVA](#) biplot is renamed 'XtrBar'. This object represents the matrix of sample group means of the transformed data matrix.
- 'RelMeanAbsErr' entries in the [export tab](#) are renamed 'MeanRelAbsErr'.
- Changes are made to the package help files, including correcting the units of the `Tel` variable of the `countries` data set. This variable measures the 'number of fixed line telephones per 1000 people' instead of 'per capita'.
- The manual is updated and reviewed.

Technical

- A `NAMESPACE` file is incorporated, and the DESCRIPTION file is updated. All features are now designed to work from the outset; there is no hierarchy of packages.
- A bug is fixed that occasionally resulted in the scroll bar of the [predictions tab](#) appearing at the centre of the table rather than at its right.
- A bug is fixed that occasionally resulted in the [kraal](#) being sized incorrectly.

VERSION 0.0-4.1

14 MARCH 2009.

- Due to the removal of the `xlsReadWrite` package ([Suter, Treetron and Switzerland, 2006](#)) from CRAN, the direct import of data from Excel 1997-2003 files has been deprecated. As an alternative mechanism, consider the `RODBC` package ([Lapsley and Ripley, 2009](#)).

CHAPTER B

KNOWN ISSUES

- The graphs in the [diagnostic tabs](#) occasionally do not show when the tabs are opened. Click to another tab and back.
- Interpolative circular non-linear biplots do not always initialise correctly in 3D. If this happens, first display a 3D predictive circular non-linear biplot.
- Extensive use of the [GUI](#) leads to memory leaks. If the system becomes noticeably slower, close the R console after saving, and re-open.

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