Multivariate Analysis of Mixed Data: The R Package PCAmixdata

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Abstract

Mixed data arise when observations are described by a mixture of numerical and categorical variables. The R package PCAmixdata extends standard multivariate analysis methods to incorporate this type of data. The key techniques/methods included in the package are principal component analysis for mixed data (PCAmix), varimax-like orthogonal rotation for PCAmix, and multiple factor analysis for mixed multi-table data. This paper gives a synthetic presentation of the three algorithms with details to help the user understand graphical and numerical outputs of the corresponding R functions. The three main methods are illustrated on a real dataset composed of four data tables characterizing living conditions in different municipalities in the Gironde region of southwest France.

Keywords: mixture of numerical and categorical data, PCA, multiple correspondence analysis, multiple factor analysis, varimax rotation, R.

1 Introduction

Multivariate data analysis refers to descriptive statistical methods used to analyze data arising from more than one variable. These variables can be either numerical or categorical. For example, principal component analysis (PCA) handles numerical variables whereas multiple correspondence analysis (MCA) handles categorical variables. Multiple factor analysis (MFA; Escofier and Pagès, 1994; Abdi et al., 2013) works with multi-table data where the type of the variables can vary from one data table to the other but the variables should be of the same type within a given data table. Several existing R (R Core Team, 2017) packages implement standard multivariate analysis methods. These include **ade4** (Dray and Dufour, 2007; Dray et al., 2017), **FactoMineR** (Lê et al., 2008; Husson et al., 2017) or **ExPosition** (Beaton et al., 2014, 2013). However none of these are dedicated to multivariate analysis of mixed data where observations are described by a mixture of

numerical and categorical variables. The method of multivariate analysis that is usually available for mixed data is PCA. For instance the package **ade4** implements the method developed by Hill and Smith (1976) and the package **FactoMineR** implements that developed by Pagès (2004). The procedure PRINQUAL of the SAS statistical software (SAS Institute Inc., 2003) implements a method based on the work of Young et al. (1978). This procedure finds transformations of variables by using the method of alternating least squares to optimize properties of the transformed variables' covariance or correlation matrix. This procedure has the specificity to make a distinction between ordinal and nominal variables.

The R package PCAmixdata (Chavent et al., 2017) is dedicated to mixed data and provides three main functions: PCAmix (PCA of a mixture of numerical and categorical variables), PCArot (rotation after PCAmix) and MFAmix (multiple factor analysis of mixed multi-table data). Note that these functions make no distinction between ordinal and nominal variables. While PCA of mixed data can be found in other packages (with different implementations from PCAmix), the procedures PCArot (Chavent et al., 2012) and MFAmix are not implemented elsewhere. The procedure MFAmix proposed in this paper allows numerical and categorical variables to be combined within a single data table, something which is not possible with the standard MFA procedure. The package PCAmixdata also proposes functions to plot graphical outputs, predict scores for new observations of the principal components of PCAmix, PCArot and MFAmix, and project supplementary variables or levels (resp. supplementary groups of variables) on the maps of PCAmix (resp. MFAmix). These functions are implemented in the R package as S3 methods with generic names plot, predict and suppvar associated with the objects of class PCAmix, PCArot and MFAmix.

A real dataset called gironde is available in the package to illustrate the functions with simple examples. This dataset is made up of four data tables, each characterizing living conditions in 542 municipalities in the Gironde region in southwest France. This dataset was taken from the 2009 census database¹ of the French national institute of statistics and economic studies and from a topographic database² of the French national institute of geographic and forestry information. The first data table describes the 542 municipalities with 9 numerical variables relating to employment conditions. The second data table describes those municipalities with 5 variables (2 categorical and 3 numerical) relating to housing conditions, the third one with 9 categorical variables relating to services (restaurants, doctors, post offices,...) and the last one with 4 numerical variables relating to environmental conditions. A complete description of the 27 variables, divided into 4 groups (Employment, Housing, Services, Environment) is given in Appendix A.

The rest of the paper is organized as follows. Section 2 details the link between standard PCA and MCA via Generalized Singular Value Decomposition (GSVD). It demonstrates how MCA can be obtained from a single PCA with metrics, the cornerstone for merging standard PCA and MCA in PCAmix. Sections 3, 4 and 5 present respectively the PCAmix, PCArot and MFAmix methods with details for the interpretation of the associated graphical and numerical outputs. Each method is illustrated with the gironde dataset and the corresponding R code is provided.

¹http://www.insee.fr/fr/bases-de-donnees/

²http://professionnels.ign.fr/bdtopo

2 PCA with metrics

PCA with metrics is a generalization of the standard PCA method where metrics are used to introduce weights on the rows (observations) and on the columns (variables) of the data matrix. Standard PCA for numerical data and standard MCA for categorical data can be presented within this general framework so that the unique PCAmix procedure for a mixture of numerical and categorical data can easily be defined.

2.1 The general framework

Let **Z** be a real matrix of dimension $n \times p$. Let **N** (resp. **M**) be the diagonal matrix of the weights of the n rows (resp. the weights of the p columns).

Generalized Singular Value Decomposition. The GSVD of **Z** with metrics **N** on \mathbb{R}^n and **M** on \mathbb{R}^p gives the following decomposition:

$$\mathbf{Z} = \mathbf{U} \mathbf{\Lambda} \mathbf{V}^{\top},\tag{1}$$

where

- $\Lambda = \operatorname{diag}(\sqrt{\lambda_1}, \dots, \sqrt{\lambda_r})$ is the $r \times r$ diagonal matrix of the singular values of $\mathbf{Z}\mathbf{M}\mathbf{Z}^{\top}\mathbf{N}$ and $\mathbf{Z}^{\top}\mathbf{N}\mathbf{Z}\mathbf{M}$, and r denotes the rank of \mathbf{Z} ;
- **U** is the $n \times r$ matrix of the first r eigenvectors of $\mathbf{Z}\mathbf{M}\mathbf{Z}^{\top}\mathbf{N}$ such that $\mathbf{U}^{\top}\mathbf{N}\mathbf{U} = \mathbb{I}_r$, with \mathbb{I}_r the identity matrix of size r;
- **V** is the $p \times r$ matrix of the first r eigenvectors of $\mathbf{Z}^{\top} \mathbf{N} \mathbf{Z} \mathbf{M}$ such that $\mathbf{V}^{\top} \mathbf{M} \mathbf{V} = \mathbb{I}_r$.

Remark 1. The GSVD of **Z** can be obtained by performing the standard SVD of the matrix $\tilde{\mathbf{Z}} = \mathbf{N}^{1/2}\mathbf{Z}\mathbf{M}^{1/2}$, that is a GSVD with metrics \mathbb{I}_n on \mathbb{R}^n and \mathbb{I}_p on \mathbb{R}^p . It gives:

$$\tilde{\mathbf{Z}} = \tilde{\mathbf{U}}\tilde{\mathbf{\Lambda}}\tilde{\mathbf{V}}^{\top} \tag{2}$$

and transformation back to the original scale gives:

$$\Lambda = \tilde{\Lambda}, \quad \mathbf{U} = \mathbf{N}^{-1/2}\tilde{\mathbf{U}}, \quad \mathbf{V} = \mathbf{M}^{-1/2}\tilde{\mathbf{V}}.$$
 (3)

Principal Components. The n rows of \mathbf{Z} are projected with respect to the inner product matrix \mathbf{M} onto the axes spanned by the vectors $\mathbf{v}_1, \dots, \mathbf{v}_r$ of \mathbb{R}^p (columns of \mathbf{V}) found by solving the sequence (indexed by i) of optimization problems:

maximize
$$\|\mathbf{Z}\mathbf{M}\mathbf{v}_i\|_{\mathbf{N}}^2$$

subject to $\mathbf{v}_i^{\top}\mathbf{M}\mathbf{v}_j = 0 \quad \forall 1 \leq j < i,$
 $\mathbf{v}_i^{\top}\mathbf{M}\mathbf{v}_i = 1.$ (4)

The solutions $\mathbf{v}_1, \dots, \mathbf{v}_r$ are the eigenvectors of $\mathbf{Z}^\top \mathbf{N} \mathbf{Z} \mathbf{M}$, i.e., the right-singular vectors in (1).

The principal component scores (also called factor coordinates of the rows hereafter) are the coordinates of the projections of the n rows onto these r axes. Let \mathbf{F} denote the $n \times r$ matrix of the factor coordinates of the rows. By definition

$$\mathbf{F} = \mathbf{ZMV},\tag{5}$$

and we deduce from (1) that:

$$\mathbf{F} = \mathbf{U}\Lambda. \tag{6}$$

Let $\mathbf{f}_i = \mathbf{Z}\mathbf{M}\mathbf{v}_i$ denote a column of \mathbf{F} . The vector $\mathbf{f}_i \in \mathbb{R}^n$ is called the *i*th principal components (PC) and the solution of (4) gives $\|\mathbf{f}_i\|_{\mathbf{N}}^2 = \lambda_i$.

Loadings. The p columns of \mathbf{Z} are projected with respect to the inner product matrix \mathbf{N} onto the axes spanned by the vectors $\mathbf{u}_1, \ldots, \mathbf{u}_r$ of \mathbb{R}^n (columns of \mathbf{U}) found by solving the sequence (indexed by i) of optimization problems:

maximize
$$\|\mathbf{Z}^{\top} \mathbf{N} \mathbf{u}_i\|_{\mathbf{M}}^2$$

subject to $\mathbf{u}_i^{\top} \mathbf{N} \mathbf{u}_j = 0 \quad \forall 1 \leq j < i,$ $\mathbf{u}_i^{\top} \mathbf{N} \mathbf{u}_i = 1.$ (7)

The solutions $\mathbf{u}_1, \dots, \mathbf{u}_r$ are the eigenvectors of $\mathbf{Z}\mathbf{M}\mathbf{Z}^{\top}\mathbf{N}$, i.e., the left-singular vectors in (1). The loadings (also called factor coordinates of the columns hereafter) are the coordinates of the projections of the p columns onto these r axes. Let \mathbf{A} denote the $p \times r$ matrix of the factor coordinates of the columns. By definition

$$\mathbf{A} = \mathbf{Z}^{\mathsf{T}} \mathbf{N} \mathbf{U},\tag{8}$$

and we deduce from (1) that:

$$\mathbf{A} = \mathbf{V}\Lambda. \tag{9}$$

Let us denote $\mathbf{a}_i = \mathbf{Z}^{\top} \mathbf{N} \mathbf{u}_i$ a column of \mathbf{A} . The vector $\mathbf{a}_i \in \mathbb{R}^p$ is called the *i*th loadings vectors and the solution of (7) gives $\|\mathbf{a}_i\|_{\mathbf{M}}^2 = \lambda_i$.

Remark 2. Since $\tilde{\Lambda} = \Lambda$ in (2), it gives:

$$\lambda_i = \|\mathbf{a}_i\|_{\mathbf{M}}^2 = \|\tilde{\mathbf{a}}_i\|_{\mathbb{I}_n}^2$$

where $\tilde{\mathbf{a}}_i$ is the ith column of $\tilde{\mathbf{A}} = \tilde{\mathbf{V}}\tilde{\mathbf{\Lambda}}$. This result will be useful for the orthogonal rotation technique presented in Section 4.

2.2 Standard PCA and standard MCA

This section presents how standard PCA (for numerical data) and standard MCA (for categorical data) can be obtained from the GSVD of specific matrices \mathbf{Z} , \mathbf{N} , \mathbf{M} . In both cases, the numerical matrix \mathbf{Z} is obtained by pre-processing of the original data matrix \mathbf{X} and the matrix \mathbf{N} (resp. \mathbf{M}) is the diagonal matrix of the weights of the rows (resp. the columns) of \mathbf{Z} .

Standard PCA. The data table to be analyzed by PCA comprises n observations described by p numerical variables, and is represented by the $n \times p$ quantitative matrix \mathbf{X} . In the pre-processing step, the columns of \mathbf{X} are centered and normalized to construct the standardized matrix \mathbf{Z} (defined such that $\frac{1}{n}\mathbf{Z}^{\mathsf{T}}\mathbf{Z}$ is the linear correlation matrix). The n rows (observations) are usually weighted by $\frac{1}{n}$ and the p columns (variables) are weighted by 1. It gives $\mathbf{N} = \frac{1}{n}\mathbb{I}_n$ and $\mathbf{M} = \mathbb{I}_p$. The metric \mathbf{M} indicates that the distance between two observations is the standard euclidean distance between two rows of \mathbf{Z} . The total inertia of \mathbf{Z} is then equal to p. The matrix \mathbf{F} of the factor coordinates of the observations (principal components) and the matrix \mathbf{A} of the factor coordinates of the variables (loadings) are calculated directly from (6) and (9). The well-known properties of PCA are the following:

- Each loading a_{ji} (element of **A**) is the linear correlation between the numerical variable \mathbf{x}_j (the *j*th column of **X**) and the *i*th principal component \mathbf{f}_i (the *i*th column of **F**):

$$a_{ji} = \mathbf{z}_{i}^{\mathsf{T}} \mathbf{N} \mathbf{u}_{i} = r(\mathbf{x}_{j}, \mathbf{f}_{i}),$$
 (10)

where $\mathbf{u}_i = \frac{\mathbf{f}_i}{\lambda_i}$ is the *i*th standardized principal component and \mathbf{z}_j (resp. \mathbf{x}_j) is the *j*th column of \mathbf{Z} (resp. \mathbf{X}).

- Each eigenvalue λ_i is the variance of the *i*th principal component:

$$\lambda_i = \|\mathbf{f}_i\|_{\mathbf{N}}^2 = \operatorname{Var}(\mathbf{f}_i). \tag{11}$$

- Each eigenvalue λ_i is also the sum of the squared correlations between the p numerical variables and the ith principal component:

$$\lambda_i = \|\mathbf{a}_i\|_{\mathbf{M}}^2 = \sum_{j=1}^p r^2(\mathbf{x}_j, \mathbf{f}_i). \tag{12}$$

Standard MCA. The data table to be analyzed by MCA comprises n observations described by p categorical variables and it is represented by the $n \times p$ qualitative matrix \mathbf{X} . Each categorical variable has m_j levels and the sum of the m_j 's is equal to m. In the pre-processing step, each level is coded as a binary variable and the $n \times m$ indicator matrix \mathbf{G} is constructed. Usually MCA is performed by applying standard Correspondence Analysis (CA) to this indicator matrix. In CA the factor coordinates of the rows (observations) and the factor coordinates of the columns (levels) are obtained by applying PCA on two different matrices: the matrix of the row profiles and the matrix of the column profiles. Here, we provide different ways to calculate the factor coordinates of MCA by applying a single PCA with metrics to the indicator matrix \mathbf{G} .

Let **Z** now denote the centered indicator matrix **G**. The n rows (observations) are usually weighted by $\frac{1}{n}$ and the m columns (levels) are weighted by $\frac{n}{n_s}$, the inverse of the frequency of the level s, where n_s denotes the number of observations that belong to the sth level. It gives $\mathbf{N} = \frac{1}{n}\mathbb{I}_n$ and $\mathbf{M} = \operatorname{diag}(\frac{n}{n_s}, s = 1 \dots, m)$. This metric **M** indicates that the distance between two observations is a weighted euclidean distance similar to the χ^2 distance in CA. This distance gives more importance to rare levels. The total inertia of **Z** with this distance and the weights $\frac{1}{n}$ is equal to m - p. The GSVD of **Z** with these metrics allows a direct calculation using (6) the matrix **F** of the factor

coordinates of the observations (the principal components). The factor coordinates of the levels however are not obtained directly from the matrix \mathbf{A} defined in (9). Let \mathbf{A}^* denote the matrix of the factor coordinates of the levels. We define:

$$\mathbf{A}^* = \mathbf{MV}\mathbf{\Lambda} = \mathbf{MA}.\tag{13}$$

The usual properties of MCA are the following:

- Each coordinate a_{si}^* (element of \mathbf{A}^*) is the mean value of the (standardized) factor coordinates of the observations that belong to level s:

$$a_{si}^* = \frac{n}{n_s} a_{si} = \frac{n}{n_s} \mathbf{z}_s^{\mathsf{T}} \mathbf{N} \mathbf{u}_i = \bar{u}_i^s, \tag{14}$$

where \mathbf{z}_s is the sth column of \mathbf{Z} , $\mathbf{u}_i = \frac{\mathbf{f}_i}{\lambda_i}$ is the ith standardized principal component and \bar{u}_i^s is the mean value of the coordinates of \mathbf{u}_i associated with the observations that belong to level s.

- Each eigenvalue λ_i is the sum of the correlation ratios between the p categorical variables and the ith principal component (which is numerical):

$$\lambda_i = \|\mathbf{a}_i\|_{\mathbf{M}}^2 = \|\mathbf{a}_i^*\|_{\mathbf{M}^{-1}}^2 = \sum_{j=1}^p \eta^2(\mathbf{f}_i|\mathbf{x}_j).$$
 (15)

The correlation ratio $\eta^2(\mathbf{f}_i|\mathbf{x}_j)$ measures the part of the variance of \mathbf{f}_i explained by the categorical variable \mathbf{x}_i .

Remark 3. Compared to standard MCA method where correspondence analysis (CA) is applied to the indicator matrix, we can note that:

- the total inertia of \mathbf{Z} (based on the metrics \mathbf{M} and \mathbf{N}) is equal to m-p, whereas the total inertia in standard MCA is multiplied by p and is equal to p(m-p). This property is useful in PCA for mixed data to balance the inertia of the numerical data (equal to the number of numerical variables) and the inertia of the categorical data (equal now to the number of levels minus the number of categorical variables),
- the factor coordinates of the levels are the same. However, the eigenvalues are multiplied by p and factor coordinates of the observations are then multiplied by \sqrt{p} . This property has no impact since results are identical to within one multiplier coefficient.

3 PCA of a mixture of numerical and categorical data

Principal Component Analysis (PCA) methods dealing with a mixture of numerical and categorical variables already exist and have been implemented in the R packages ade4 (Dray and Dufour, 2007) and FactoMineR (Lê et al., 2008). In the package ade4, the dudi.hillsmith function implements the method developed by Hill and Smith (1976) and, in the package FactoMineR, the function FAMD implements the method developed by Pagès (2004). In the R package PCAmixdata, the function PCAmix implements an algorithm presented hereafter as a single PCA with metrics, i.e., based on a Generalized Singular Value Decomposition (GSVD) of pre-processed data. This algorithm includes naturally standard PCA and standard MCA as special cases.

3.1 The PCAmix algorithm

The data table to be analyzed by PCAmix comprises n observations described by p_1 numerical variables and p_2 categorical variables. It is represented by the $n \times p_1$ quantitative matrix \mathbf{X}_1 and the $n \times p_2$ qualitative matrix \mathbf{X}_2 . Let m denote the total number of levels of the p_2 categorical variables. The PCAmix algorithm merges PCA and MCA thanks to the general framework given in Section 2. The two first steps of PCAmix (pre-processing and factor coordinates processing) mimic this general framework with the numerical data matrix \mathbf{X}_1 and the qualitative data matrix \mathbf{X}_2 as inputs. The third step is dedicated to squared loading processing where squared loadings are defined as squared correlations for numerical variables and correlation ratios for categorical variables.

Step 1: pre-processing.

- 1. Build the real matrix $\mathbf{Z} = [\mathbf{Z}_1, \mathbf{Z}_2]$ of dimension $n \times (p_1 + m)$ where:
 - \hookrightarrow **Z**₁ is the standardized version of **X**₁ (as in standard PCA),
 - \hookrightarrow \mathbb{Z}_2 is the centered version of the indicator matrix \mathbb{G} of \mathbb{X}_2 (as in standard MCA).
- 2. Build the diagonal matrix **N** of the weights of the rows of **Z**. The *n* rows are often weighted by $\frac{1}{n}$, such that $\mathbf{N} = \frac{1}{n} \mathbb{I}_n$.
- 3. Build the diagonal matrix \mathbf{M} of the weights of the columns of \mathbf{Z} :
 - \hookrightarrow The first p_1 columns (corresponding to the numerical variables) are weighted by 1 (as in standard PCA).
 - \hookrightarrow The last m columns (corresponding to the levels of the categorical variables) are weighted by $\frac{n}{n_s}$ (as in standard MCA), where $n_s, s = 1, \ldots, m$ denotes the number of observations that belong to the sth level.

The metric

$$\mathbf{M} = \operatorname{diag}(1, \dots, 1, \frac{n}{n_1}, \dots, \frac{n}{n_m}) \tag{16}$$

indicates that the distance between two rows of \mathbf{Z} is a mixture of the simple euclidean distance used in PCA (for the first p_1 columns) and the weighted distance in the spirit of the χ^2 distance used in MCA (for the last m columns). The total inertia of \mathbf{Z} with this distance and the weights $\frac{1}{n}$ is equal to $p_1 + m - p_2$.

Step 2: factor coordinates processing.

1. The GSVD of \mathbf{Z} with metrics \mathbf{N} and \mathbf{M} gives the decomposition:

$$\mathbf{Z} = \mathbf{U} \mathbf{\Lambda} \mathbf{V}^{\top}$$

as defined in (1). Let r denote the rank of \mathbf{Z} .

2. The matrix of dimension $n \times r$ of the factor coordinates of the n observations is:

$$\mathbf{F} = \mathbf{ZMV},\tag{17}$$

or directly computed from the GSVD decomposition as:

$$\mathbf{F} = \mathbf{U}\mathbf{\Lambda}.\tag{18}$$

3. The matrix of dimension $(p_1 + m) \times r$ of the factor coordinates of the p_1 quantitative variables and the m levels of the p_2 categorical variables is:

$$\mathbf{A}^* = \mathbf{MV}\mathbf{\Lambda}.\tag{19}$$

The matrix \mathbf{A}^* is split as follows: $\mathbf{A}^* = \begin{bmatrix} \mathbf{A}_1^* \\ \mathbf{A}_2^* \end{bmatrix} \begin{cases} p_1 \\ m \end{cases}$ where

- \hookrightarrow \mathbf{A}_1^* contains the factor coordinates of the p_1 numerical variables,
- \hookrightarrow \mathbf{A}_2^* contains the factor coordinates of the m levels.

Step 3: squared loading processing. The squared loadings are defined as the contributions of the variables to the variance of the principal components. It was shown in Section 2.1 that $\operatorname{Var}(\mathbf{f}_i) = \lambda_i$ and that $\lambda_i = \|\mathbf{a}_i\|_{\mathbf{M}}^2 = \|\mathbf{a}_i^*\|_{\mathbf{M}^{-1}}^2$. The contributions can therefore be calculated directly from the matrix \mathbf{A} (or \mathbf{A}^*). Let c_{ji} denote the contribution of the variable \mathbf{x}_j (a column of \mathbf{X}_1 or \mathbf{X}_2) to the variance of the principal component \mathbf{f}_i . We have:

$$\begin{cases}
c_{ji} = a_{ji}^2 = a_{ji}^{*2} & \text{if the variable } \mathbf{x}_j \text{ is numerical,} \\
c_{ji} = \sum_{s \in I_j} \frac{n}{n_s} a_{si}^2 = \sum_{s \in I_j} \frac{n_s}{n} a_{si}^{*2} & \text{if the variable } \mathbf{x}_j \text{ is categorical,}
\end{cases}$$
(20)

where I_j is the set of indices of the levels of the categorical variable j. As usually the contribution of a categorical variable is the sum of the contributions of its levels. Note that the term squared loadings for categorical variables draws an analogy with squared loadings in PCA. The $(p_1 + p_2) \times r$ matrix of the squared loadings of the p_1 numerical variables and the p_2 categorical variables is denoted $\mathbf{C} = (c_{ji})$ hereafter.

Remark 4. If $q \le r$ dimensions are required by the user in PCAmix, the principal components are the q first columns of \mathbf{F} , the loadings vectors are the q first columns of \mathbf{A}^* and the squared loadings vectors are the q first columns of \mathbf{C} .

3.2 Graphical outputs of PCAmix

Principal component map. The function plot.PCAmix plots the observations, the numerical variables and the levels of the categorical variables according to their factor coordinates. The map of the observations (also called principal component map) gives an idea of the pattern of similarities between the observations. If two observations \mathbf{z}_k and $\mathbf{z}_{k'}$ (two rows of \mathbf{Z}) are well projected on the map, their distance in projection gives an idea of their distance in \mathbb{R}^{p_1+m} defined by

$$d_{\mathbf{M}}^2(\mathbf{z}_k,\mathbf{z}_{k'}) = (\mathbf{z}_k - \mathbf{z}_{k'})^{\top} \mathbf{M} (\mathbf{z}_k - \mathbf{z}_{k'})$$

where **M** is defined in (16). This squared distance can be interpreted as the squared euclidean distance calculated on the standardized numerical variables plus the squared χ^2 distance calculated on the levels of the categorical variables.

Correlations circle. The map of the quantitative variables, called the correlation circle, gives an idea of the pattern of linear links between the quantitative variables. If two columns \mathbf{z}_j and $\mathbf{z}_{j'}$ of \mathbf{Z}_1 corresponding to two quantitative variables \mathbf{x}_j and $\mathbf{x}_{j'}$ (two columns of \mathbf{X}_1) are well projected on the map, the cosine of their angle in projection gives an idea of their correlation in \mathbb{R}^n defined by

$$r(\mathbf{x}_j, \mathbf{x}_{j'}) = \mathbf{z}_j^{\top} \mathbf{N} \mathbf{z}_{j'}$$

with $\mathbf{N} = \frac{1}{n} \mathbb{I}_n$ in the usual case of observations weighted by $\frac{1}{n}$.

Level map. The level map gives an idea of the pattern of proximities between the levels of (different) categorical variables. If two levels \mathbf{z}_s and $\mathbf{z}_{s'}$ (two columns of the centered indicator matrix \mathbf{Z}_2) are well projected on the map, the distance when projected gives an idea of their distance in \mathbb{R}^n given by

$$d_{\mathbf{N}}^2(\mathbf{z}_s, \mathbf{z}_{s'}) = (\mathbf{z}_s - \mathbf{z}_{s'})^{\top} \mathbf{N} (\mathbf{z}_s - \mathbf{z}_{s'})$$

which can be interpreted as 1 minus the proportion of observations having both levels s and s'. With this distance two levels are similar if they are owned by the same observations.

Squared loading plot. Another graphical output available in plot.PCAmix is the plot of the variables (numerical and categorical) according to their squared loadings. The map of all the variables gives an idea of the pattern of links between the variables regardless of their type (quantitative or categorical). More precisely, it is easy to verify that the squared loading c_{ji} defined in (20) is equal to:

- the squared correlation $r^2(\mathbf{f}_i, \mathbf{x}_j)$ if the variable \mathbf{x}_j is numerical,
- the correlation ratio $\eta^2(\mathbf{f}_i|\mathbf{x}_j)$ if the variable \mathbf{x}_j is categorical.

Coordinates (between 0 and 1) of the variables on this plot measure the links (signless) between variables and principal components and can be used to interpret principal component maps.

Interpretation rules. The mathematical properties of the factor coordinates of standard PCA and standard MCA (see Section 2.2) are also applicable in PCAmix:

- the factor coordinates of the p_1 numerical variables (the p_1 first rows of \mathbf{A}^*) are correlations with the principal components (the columns of \mathbf{F}) as in PCA,
- the factor coordinates of the m levels (the m last rows of \mathbf{A}^*) are mean values of the (stan-dardized) factor coordinates of the observations that belong to these levels as in MCA.

These two properties are used to interpret the principal component map of the observations according to the correlation circle and according to the level map. The position (left, right, up, bottom) of the observations can be interpreted in terms of:

- numerical variables using the property indicating that coordinates on the correlation circle give correlations with PCs,
- levels of categorical variables using the property indicating that coordinates on the level map are barycenters of PC scores.

3.3 Prediction of PC scores with predict.PCAmix

A function to predict scores for new observations on the principal components can be helpful. For example:

- projecting new observations onto the principal component map of PCAmix,
- when the PCs are used as synthetic numerical variables replacing the original variables (quantitative or categorical) in a predictive model (regression or classification for instance).

More precisely, PCAmix computes new numerical variables called principal components that will "explain" or "extract" the largest part of the inertia of the data table \mathbf{Z} built from the original data tables \mathbf{X}_1 and \mathbf{X}_2 . The principal components (columns of \mathbf{F}) are by construction non correlated linear combinations of the columns of \mathbf{Z} and can be viewed as new synthetic numerical variables with:

- maximum dispersion: $\lambda_i = \|\mathbf{f}_i\|_{\mathbf{N}}^2 = \text{Var}(\mathbf{f}_i),$
- maximum link with the original variables:

$$\lambda_i = \|\mathbf{a}_i\|_{\mathbf{M}}^2 = \sum_{j=1}^{p_1} r^2(\mathbf{f}_i, \mathbf{x}_j) + \sum_{j=p_1+1}^{p_2} \eta^2(\mathbf{f}_i | \mathbf{x}_j).$$
 (21)

The *i*th principal component of PCAmix writes as a linear combination of the vectors $\mathbf{z}_1, \dots, \mathbf{z}_{p_1+m}$ (columns of \mathbf{Z}):

$$\mathbf{f}_i = \mathbf{Z} \mathbf{M} \mathbf{v}_i = \sum_{\ell=1}^{p_1} v_{\ell i} \mathbf{z}_{\ell} + \sum_{\ell=n_1+1}^{p_1+m} \frac{n}{n_{\ell}} v_{\ell i} \mathbf{z}_{\ell}.$$

It is then easy to write \mathbf{f}_i as a linear combination of the vectors $\mathbf{x}_1, \dots, \mathbf{x}_{p_1+m}$ (columns of $\mathbf{X} = (\mathbf{X}_1|\mathbf{G})$):

$$\mathbf{f}_i = \beta_{0i} + \sum_{\ell=1}^{p_1+m} \beta_{\ell i} \mathbf{x}_{\ell}, \tag{22}$$

with the coefficients defined as follows:

$$\beta_{0i} = -\sum_{\ell=1}^{p_1} v_{\ell i} \frac{\bar{\mathbf{x}}_{\ell}}{\hat{\sigma}_{\ell}} - \sum_{\ell=p_1+1}^{p_1+m} v_{\ell i},$$

$$\beta_{\ell i} = v_{\ell i} \frac{1}{\hat{\sigma}_{\ell}}, \text{ for } \ell = 1, \dots, p_1,$$

$$\beta_{\ell i} = v_{\ell i} \frac{n}{n_{\ell}}, \text{ for } \ell = p_1 + 1, \dots, p_1 + m,$$

where $\bar{\mathbf{x}}_{\ell}$ and $\hat{\sigma}_{\ell}$ are respectively the empirical mean and the standard deviation of the column \mathbf{x}_{ℓ} . The principal components are thereby written in (22) as a linear combination of the original numerical variables and of the original indicator vectors of the levels of the categorical variables. The function predict.PCAmix uses these coefficients to predict the scores (coordinates) of new observations on the $q \leq r$ first principal component (q is chosen by the user) of PCAmix.

3.4 Illustration of PCAmix

Let us now illustrate the procedure PCAmix with the data table housing of the dataset gironde. This data table contains n = 542 municipalities described on $p_1 = 3$ numerical variables and $p_2 = 2$ categorical with a total of m = 4 levels (see Appendix A for the description of the variables).

```
R> library("PCAmixdata")
```

- R> data("gironde")
- R> head(gironde\$housing)

	density	primaryres	houses	owners	council
ABZAC	131.70	88.77	inf 90%	64.23	sup 5%
AILLAS	21.21	87.52	sup 90%	77.12	inf 5%
AMBARES-ET-LAGRAVE	531.99	94.90	inf 90%	65.74	sup 5%
AMBES	101.21	93.79	sup 90%	66.54	sup 5%
ANDERNOS-LES-BAINS	551.87	62.14	inf 90%	71.54	inf 5%
ANGLADE	63.82	81.02	sup 90%	80.54	inf 5%

In order to explore the mixed data table housing, a principal component analysis is performed using the function PCAmix.

```
R> split <- splitmix(gironde$housing)
R> X1 <- split$X.quanti</pre>
```

R> X2 <- split\$X.quali

R> res.pcamix <- PCAmix(X.quanti=X1, X.quali=X2,rename.level=TRUE,graph=FALSE)</pre>

R> res.pcamix\$eig

Eigenvalue Proportion Cumulative

```
dim 1 2.5268771 50.537541 50.53754
dim 2 1.0692777 21.385553 71.92309
dim 3 0.6303253 12.606505 84.52960
dim 4 0.4230216 8.460432 92.99003
dim 5 0.3504984 7.009968 100.00000
```

Note that the function **splitmix** splits a mixed data matrix into two datasets: one with the numerical variables and one with the categorical variables.

The sum of the eigenvalues is equal to the total inertia $p_1 + m - p_2 = 5$ and the first two dimensions retrieve 71% of the total inertia. Let us visualize on these two dimensions the 4 different plots presented in Section 3.2.

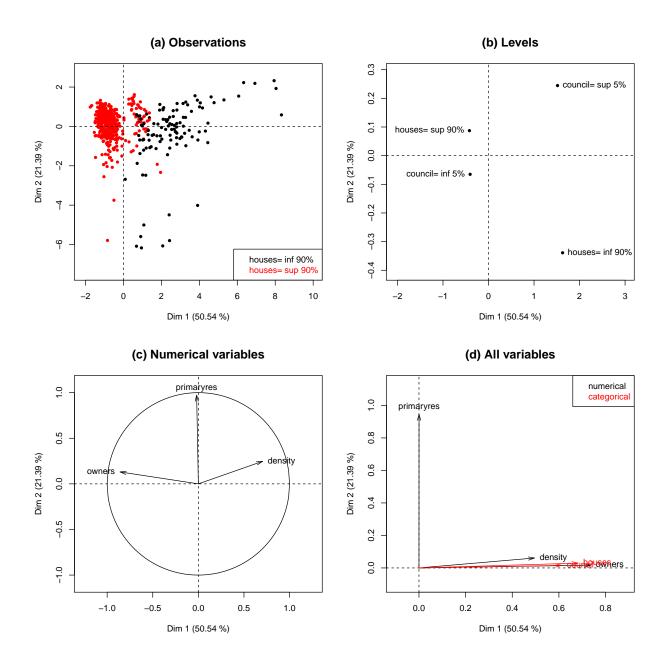


Figure 1: Graphical outputs of PCAmix applied to the data table housing.

Figure 1(a) shows the principal component map where the municipalities (the observations) are colored by their percentage of houses (less than 90%, more than 90%). The first dimension (left hand side) highlights municipalities with large proportions of privately-owned properties. The level map in Figure 1(b) confirms this interpretation and suggests that municipalities with a high proportion of houses (on the left) have a low percentage of council housing. The correlation circle in Figure 1(c) indicates that population density is negatively correlated with the percentage of home owners and that these two variables discriminate the municipalities on the first dimension.

Figure 1(d) plots the variables (categorical or numerical) using squared loadings as coordinates. For numerical variables, squared loadings are squared correlations and for categorical variables squared loadings are correlation ratios. In both cases, they measure the link between the variables and the principal components. One observes that the two numerical variables density and owners and the two categorical variables houses and council are linked to the first component. On the contrary, the variable primaryres is clearly orthogonal to these variables and associated to the second component. Note that these links show neither a positive nor a negative association, and the maps Figure 1(b) and Figure 1(c) are necessary for more precise interpretation.

In summary, municipalities on the right of the principal component map have a relatively high proportion of council housing and a small percentage of privately-owned houses, with most accommodation being rented. On the other hand, municipalities on the left hand side are mostly composed of home owners living in their primary residence. The percentage of primary residences also has a structuring role in the characterization of municipalities in this region of France by defining clearly the second dimension. Indeed the municipalities at the bottom of the map (those with small values on the second dimension) are sea resorts with many secondary residences. For instance the 10 municipalities with the smallest coordinates in the second dimension are well-known resorts on France's Atlantic coast:

<pre>R> sort(res.pcamix\$;</pre>		
VENDAYS-MONTALIVET	CARCANS	LACANAU
-6.171971	-6.087304	-6.070451
SOULAC-SUR-MER	GRAYAN-ET-L'HOPITAL	LEGE-CAP-FERRET
-5.802359	-5.791642	-5.596315
VERDON-SUR-MER	HOURTIN	ARCACHON
-5.008545	-4.493259	-4.013374
PORGE		
-3.751233		

Prediction and plot of scores for new observations. We will now illustrate how the function predict.PCAmix can be helpful in predicting the coordinates (scores) of observations not used in PCAmix. Here, 100 municipalities are sampled at random (test set) and the 442 remaining municipalities (training set) are used to perform PCAmix. The following R code shows how to predict the scores of the municipalities of the test set on the two first PCs obtained with the training set.

```
R> set.seed(10)
R> test <- sample(1:nrow(gironde$housing),100)</pre>
R> train.pcamix <- PCAmix(X1[-test,],X2[-test,],ndim=2,graph=FALSE)</pre>
R> pred <- predict(train.pcamix, X1[test,], X2[test,])</pre>
R> head(pred)
                                 dim1
                                              dim2
MAZION
                           -0.4120140
                                       0.03905247
FLAUJAGUES
                           -0.6881160 -0.33163728
                            0.7447583
LATRESNE
                                       0.65305517
SAINT-CHRISTOLY-DE-BLAYE -0.7006372 -0.33216807
BERSON
                           -1.1426625
                                       0.33607088
CHAMADELLE
                           -1.3781919
                                       0.24609791
```

These predicted coordinates can be used to plot the 100 supplementary municipalities on the principal component map of the other 442 municipalities (see Figure 2).

```
R> plot(train.pcamix,axes=c(1,2),label=FALSE,main="Observations map")
R> points(pred,col=2,pch=16)
R> legend("bottomright",legend = c("train","test"),fill=1:2,col=1:2)
```

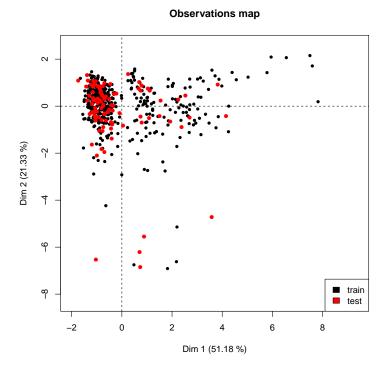


Figure 2: Projection of 100 supplementary municipalities (in red) on the PC map of the other 442 municipalities (in black).

Supplementary variables. The function supvar.PCAmix calculates the coordinates of supplementary variables (numerical or categorical) on the maps of PCAmix. More precisely this function builds an R object of class PCAmix including the supplementary coordinates. For instance let us consider the numerical variable building of the dataset environment and the categorical variable doctor of the dataset services as supplementary variables (see Appendix A for description of these two variables).

```
X1sup <- gironde$environment[,1,drop=FALSE]</pre>
R>
    X2sup <- gironde$services[,7,drop=FALSE]</pre>
R>
    res.sup <- supvar(res.pcamix,X1sup,X2sup,rename.level=TRUE)</pre>
    res.sup$quanti.sup$coord[,1:2,drop=FALSE]
R>
               dim1
                         dim2
building 0.6945295 0.1884711
    res.sup$levels.sup$coord[,1:2]
                      dim1
                                    dim2
doctor=0
               -0.44403187 -0.006224754
doctor=1 to 2 0.07592759 -0.112352412
doctor=3 or +
              1.11104073 0.099723319
```

The coordinates of the supplementary numerical variables building are still correlations. For instance, the correlation between building and the first PC is equal to 0.69. The coordinates of the levels of the supplementary categorical variables are still barycenters. For instance the coordinate -0.44 of the level doctor=0 is the mean value of the municipalities with 0 doctors on the first standardized PC. They are probably mostly left of the PC map. Graphical outputs including these supplementary variables and the original ones can be obtained as previously with the function plot.PCAmix, see Figure 3.

```
R> plot(res.sup,choice="cor",main="Numerical variables")
R> plot(res.sup,choice="levels",main="Levels",xlim=c(-2,2.5))
```

4 Orthogonal rotation in PCA of mixed data

It is common practice in PCA to apply a rotation procedure to the loadings to simplify interpretation of the principal components. The idea is to obtain either large (close to 1) or small (close to 0) loadings, in order to more clearly associate variables with the principal components. The well known varimax rotation procedure (Kaiser, 1958) is implemented in the R function varimax of the stats package but this procedure fits only for numerical data. The function PCArot of the package PCAmixdata implements a generalization of the varimax procedure to the case of mixed data (Chavent et al., 2012). The rotation procedure PCArot applies to the principal components of PCAmix to get either large or small squared loadings. Indeed in PCAmix the squared loadings are squared correlations for numerical variables and correlation ratios for categorical variables measuring then the link between the variables (numerical or categorical) and the principal components. The rotation procedure PCArot is therefore applied to the first q principal components of the procedure PCAmix where q is chosen by the user.

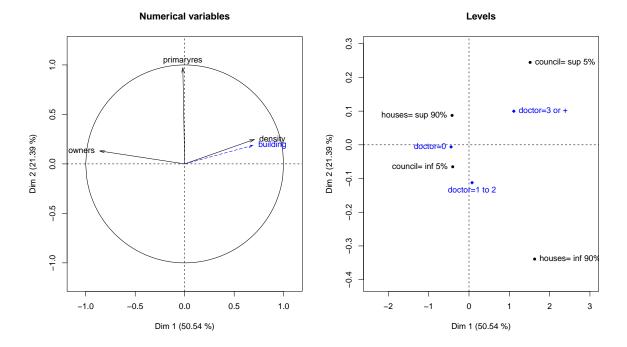


Figure 3: In blue, projection of the supplementary numerical variable building (left) and projection of the levels of the supplementary categorical variable doctor (right).

4.1 The PCArot algorithm

We have seen that PCAmix is essentially a GSVD:

$$\mathbf{Z} = \mathbf{U} \mathbf{\Lambda} \mathbf{V}^{\mathsf{T}},$$

defined in Section 2. The columns of \mathbf{U} are the standardized principal components (PCs) and the columns of $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}$ are the loading vectors. The PCArot procedure rotates the matrix \mathbf{U}_q of the q first standardized PCs and the matrix \mathbf{A}_q of the q first loading vectors.

Let **T** be a $q \times q$ orthonormal rotation matrix. Let $\mathbf{U}_{\text{rot}} = \mathbf{U}_q \mathbf{T}$ denote the matrix of the rotated standardized PCs and $\mathbf{A}_{\text{rot}} = \mathbf{A}_q \mathbf{T}$ denote the matrix of the rotated loading vectors. The squared loadings after rotation are then defined by:

$$\begin{cases}
c_{ji,\text{rot}} = a_{ji,\text{rot}}^2 & \text{if the variable } \mathbf{x}_j \text{ is numerical,} \\
c_{ji,\text{rot}} = \sum_{s \in I_j} \frac{n}{n_s} a_{si,\text{rot}}^2 & \text{if the variable } \mathbf{x}_j \text{ is categorical,}
\end{cases}$$
(23)

where I_j is the set of indices of the levels of the categorical variable j. They measure the links (squared correlations or correlation ratios) between the principal components after rotation and the variables.

The varimax rotation problem is then rephrased as

$$\max_{\mathbf{T}} \quad \{ f(\mathbf{T}) | \mathbf{T} \mathbf{T}^{\top} = \mathbf{T}^{\top} \mathbf{T} = \mathbb{I}_q \}, \tag{24}$$

where

$$f(\mathbf{T}) = \sum_{i=1}^{q} \sum_{j=1}^{p} (c_{ji,\text{rot}})^2 - \frac{1}{p} \sum_{i=1}^{q} \left(\sum_{j=1}^{p} c_{ji,\text{rot}} \right)^2.$$
 (25)

We have also seen in Remark 1 that PCAmix boils down to the standard SVD

$$\tilde{\mathbf{Z}} = \tilde{\mathbf{U}}\tilde{\boldsymbol{\Lambda}}\tilde{\mathbf{V}}^{\top}.$$

defined in (2). The rotation procedure proposed by (Chavent et al., 2012) uses the standard SVD of $\tilde{\mathbf{Z}}$ to optimize the objective function (25). Note that the equivalence between (25) and the objective function in (Chavent et al., 2012) can be obtained with Remark 2. The procedure implemented in the PCArot function is summarized in Appendix B.

Rotated factor coordinates processing.

1. The matrix of dimension $(p_1 + m) \times q$ of the rotated factor coordinates of the p_1 quantitative variables and the m levels of the p_2 categorical variables is:

$$\mathbf{A}_{\text{rot}}^* = \mathbf{M} \mathbf{A}_{\text{rot}} = \mathbf{M}^{1/2} \tilde{\mathbf{A}}_{\text{rot}}.$$
 (26)

$$\mathbf{A}_{\mathrm{rot}}^{*}$$
 is split as follows: $\mathbf{A}_{\mathrm{rot}}^{*} = \begin{bmatrix} \mathbf{A}_{1,\mathrm{rot}}^{*} \\ \mathbf{A}_{2,\mathrm{rot}}^{*} \end{bmatrix} \begin{array}{c} \} p_{1} \\ \} m \end{array}$ where

- $\hookrightarrow \mathbf{A}_{1,\mathrm{rot}}^*$ contains the rotated factor coordinates of the p_1 numerical variables,
- \hookrightarrow $\mathbf{A}^*_{2,\mathrm{rot}}$ contains the rotated factor coordinates of the m levels.
- 2. The variance $\lambda_{i,\text{rot}}$ of the *i*th rotated principal component is calculated as:

$$\lambda_{i,\text{rot}} = \|\mathbf{a}_{i,\text{rot}}\|_{\mathbf{M}}^2 = \|\tilde{\mathbf{a}}_{i,\text{rot}}\|_{\mathbb{I}_{p_1+m}}^2, \tag{27}$$

where $\mathbf{a}_{i,\text{rot}}$ (resp. $\tilde{\mathbf{a}}_{i,\text{rot}}$) is the *i*th column of \mathbf{A}_{rot} (resp. $\tilde{\mathbf{A}}_{\text{rot}}$).

Let $\Lambda_{\text{rot}} = \text{diag}(\sqrt{\lambda_{1,\text{rot}}}, \dots, \sqrt{\lambda_{q,\text{rot}}})$ denote the diagonal matrix of the standard deviations of the q rotated principal components.

3. The matrix of dimension $n \times q$ of the rotated factor coordinates of the n observations is:

$$\mathbf{F}_{\text{rot}} = \mathbf{U}_{\text{rot}} \Lambda_{\text{rot}} = \mathbf{N}^{-1/2} \tilde{\mathbf{U}}_{\text{rot}} \Lambda_{\text{rot}}.$$
 (28)

Remark 5. For numerical data, PCArot is the standard varimax procedure defined by Kaiser (1958) for rotation in PCA. For categorical data, PCArot is an orthogonal rotation procedure for Multiple Correspondence Analysis (MCA).

4.2 Graphical outputs of PCArot

The properties used to interpret the graphical outputs of PCAmix remain true after rotation:

- the rotated factor coordinates of the p_1 numerical variables (the p_1 first rows of $\mathbf{A}_{\text{rot}}^*$) are correlations with the rotated principal components (the columns of \mathbf{F}_{rot}),
- the rotated factor scores of the m levels (the m last rows of \mathbf{A}_{rot}^*) are mean values of the (standardized) rotated factor coordinates of the observations that belong these levels.

The contribution (squared loading) of the variable \mathbf{x}_j to the variance of the rotated principal component $\mathbf{f}_{i,\text{rot}}$ is calculated directly from the matrix $\tilde{\mathbf{A}}_{\text{rot}}$ with:

$$\begin{cases}
c_{ji,\text{rot}} = \tilde{a}_{ji,\text{rot}}^2 = r^2(\mathbf{f}_{i,\text{rot}}, \mathbf{x}_j) & \text{if the variable } \mathbf{x}_j \text{ is numerical,} \\
c_{ji,\text{rot}} = \sum_{s \in I_j} \tilde{a}_{si,\text{rot}}^2 = \eta^2(\mathbf{f}_{i,\text{rot}} | \mathbf{x}_j) & \text{if the variable } \mathbf{x}_j \text{ is categorical.}
\end{cases}$$
(29)

The squared loadings after rotation are then the squared correlation or correlation ratio between the variables and the rotated principal components.

The function plot.PCAmix presented Section 3.2 plots the observations, the numerical variables and the levels of the categorical variables according to their factor coordinates after rotation. It plots also the variables according to their squared loadings after rotation. The interpretation rules given in Section 3.2 remain true.

4.3 Prediction of rotated PC scores with predict.PCAmix

PCArot computes q new non correlated numerical variables called rotated principal components that will explain the same part of inertia than PCAmix but with simpler interpretation. Let us show that the rotated principal components (columns of \mathbf{F}_{rot}) are linear combination of the columns of \mathbf{Z} .

First it can be showed (see Appendix C) that:

$$\mathbf{F}_{\text{rot}} = \mathbf{Z}\mathbf{V}_{\text{rot}},\tag{30}$$

with

$$\mathbf{V}_{\text{rot}} = \mathbf{M}^{1/2} \tilde{\mathbf{V}}_{q} \tilde{\mathbf{\Lambda}}_{q}^{-1} \mathbf{T} \mathbf{\Lambda}_{\text{rot}}, \tag{31}$$

and

$$\mathbf{T} = \tilde{\mathbf{U}}_{a}^{\top} \tilde{\mathbf{U}}_{\text{rot}}.$$
 (32)

It follows that the *i*th rotated principal component $\mathbf{f}_{i,\text{rot}}$ of PCArot writes as a linear combination of the vectors $\mathbf{z}_1, \dots, \mathbf{z}_{p_1+m}$ (columns of \mathbf{Z}):

$$\mathbf{f}_{i,\text{rot}} = \mathbf{Z}\mathbf{v}_{i,\text{rot}} = \sum_{\ell=1}^{p_1+m} v_{\ell i,\text{rot}} \mathbf{z}_{\ell}.$$
(33)

It is then easy to write $\mathbf{f}_{i,\text{rot}}$ as a linear combination of the vectors $\mathbf{x}_1, \dots, \mathbf{x}_{p_1+m}$ (columns of $\mathbf{X} = (\mathbf{X}_1 | \mathbf{G})$):

$$\mathbf{f}_{i,\text{rot}} = \beta_{0i,\text{rot}} + \sum_{\ell=1}^{p_1+m} \beta_{\ell i,\text{rot}} \mathbf{x}_{\ell}, \tag{34}$$

with the coefficients

$$\beta_{0i,\text{rot}} = -\sum_{\ell=1}^{p_1} v_{\ell i,\text{rot}} \frac{\bar{\mathbf{x}}_{\ell}}{\hat{\sigma}_{\ell}} - \sum_{\ell=p_1+1}^{p_1+m} v_{\ell i,\text{rot}} \frac{n}{n_{\ell}} \bar{\mathbf{x}}_{\ell},$$

$$\beta_{\ell i,\text{rot}} = v_{\ell i,\text{rot}} \frac{1}{\hat{\sigma}_{\ell}}, \text{ for } \ell = 1, \dots, p_1,$$

$$\beta_{\ell i,\text{rot}} = v_{\ell i,\text{rot}} \frac{n}{n_{\ell}}, \text{ for } \ell = p_1 + 1, \dots, p_1 + m,$$

where $\bar{\mathbf{x}}_{\ell}$ and $\hat{\sigma}_{\ell}$ are respectively the empirical mean and the standard deviation of the column \mathbf{x}_{ℓ} . The rotated principal components are thereby in (34) linear combinations of the original numerical variables and of the original indicator vectors of the levels of the categorical variables. The function predict.PCAmix uses these coefficients to predict the scores (coordinates) of new observations on the q rotated principal component of PCArot.

4.4 Illustration of PCArot

Let us now illustrate the procedure PCArot with the mixed data table housing already used in Section 3.4. Let us first create a data frame without the first ten municipalities (used later for prediction purposes).

```
R> library("PCAmixdata")
R> data("gironde")
R> train <- gironde$housing[-c(1:10), ]</pre>
R> split <- splitmix(train)</pre>
R> X1 <- split$X.quanti
R> X2 <- split$X.quali
R> res.pcamix <- PCAmix(X.quanti=X1, X.quali=X2,rename.level=TRUE, graph=FALSE)
R> res.pcamix$eig
      Eigenvalue Proportion Cumulative
dim 1 2.5189342 50.378685
                              50.37868
dim 2 1.0781913 21.563825
                              71.94251
dim 3 0.6290897 12.581794
                              84.52430
dim 4 0.4269180
                   8.538361
                              93.06267
dim 5 0.3468667
                   6.937335 100.00000
```

The first q=3 principal components of PCAmix retrieve 84.5% of the total inertia. In order to improve the interpretation of these 3 components without adversely affecting the proportion of explained inertia we perform a rotation using the function PCArot.

The spread of the proportion of variance in the three dimensions is modified but the rotated principal components still contain 84.5% of the total inertia:

```
R> sum(res.pcarot$eig[,2])
[1] 84.5243
```

The rotation also modifies squared loadings with more clear association after rotation between the third principal component and the variable density. Indeed the squared correlation between density and the third PC is equal to 0.39 before rotation and increases to 0.9 after rotation.

R> res.pcarot\$sqload

	dim1.rot	dim2.rot	dim3.rot
density	0.04	0.01	0.90
primaryres	0.00	0.96	0.01
owners	0.48	0.03	0.25
houses	0.63	0.03	0.08
council	0.76	0.03	0.01

Because the rotation improves the interpretation of the third principal component, we plot the observations and the variables on the dimensions 1 and 3.

Figure 4 shows how the variable density is more clearly linked after rotation to the third principal component. Indeed, after rotation, the coordinates of the variable density on the y-axis is equal to 0.9 (the squared correlation between density and the 3rd rotated principal component). The municipalities at the top of the plot of the observations after rotation are then characterized by their population density. Note that the benefit of using rotation on this dataset is quite limited.

Prediction after rotation. Let us now predict the scores of the 10 first municipalities of the data table housing on the rotated principal components of PCArot.

```
R> test <- gironde$housing[1:10, ]
R> splitnew <- splitmix(test)
R> X1new <- splitnew$X.quanti
R> X2new<-splitnew$X.quali
R> pred.rot <- predict(object=res.pcarot, X.quanti=X1new, X.quali=X2new)</pre>
```

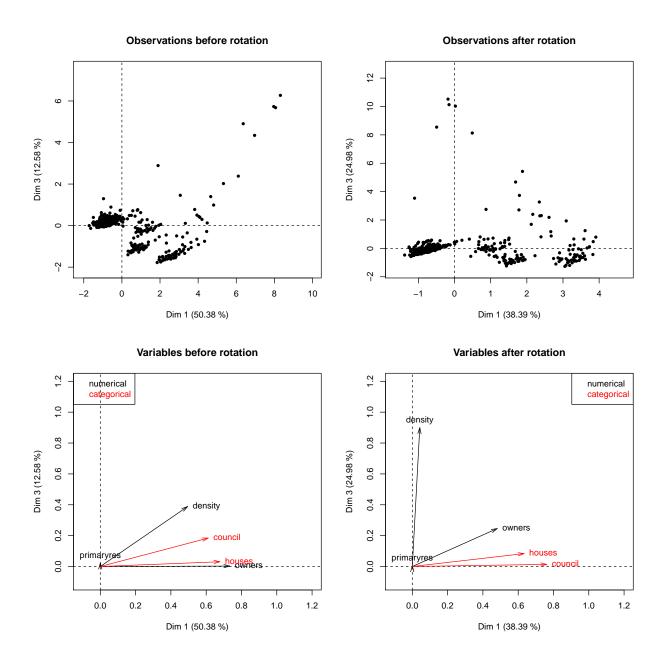


Figure 4: Graphical outputs of PCAmix applied to the data table housing (deprived of the 10 first rows) before rotation (left) and after rotation with PCArot (right).

R> pred.rot

```
dim2.rot
                     dim1.rot
                                             dim3.rot
ABZAC
                    3.2685436
                               0.3494533 -0.85177749
                   -0.7235629
AILLAS
                               0.1200285 -0.22254455
AMBARES-ET-LAGRAVE
                    2.8852451
                               0.9823515 -0.03451571
AMBES
                    1.7220716
                               1.1590890 -0.78227835
ANDERNOS-LES-BAINS
                    0.3423361 -2.6886415 0.90574890
ANGLADE
                   -0.9131248 -0.4514258 -0.20108349
ARBANATS
                   -0.6653760
                               0.4217893 0.13105217
ARBIS
                   -0.7668742
                               0.3099338 -0.23304721
ARCACHON
                    1.8825083 -4.4533014 2.36935740
ARCINS
                   -0.6896492 0.2060403 -0.09049882
```

These predicted coordinates can be used to plot the 10 supplementary municipalities on the rotated principal component map of the other 532 municipalities (Figure 5).

```
R> plot(res.pcarot,axes=c(1,3),label=FALSE,main="Observations map after rotation")
R> points(pred.rot[,c(1,3)],col=2,pch=16)
R> legend("topright",legend = c("train","test"),fill=1:2,col=1:2)
```

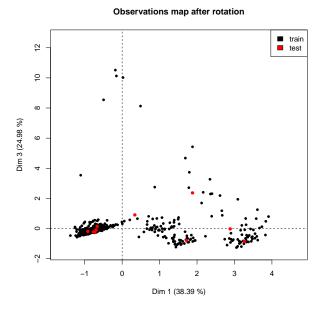


Figure 5: Projection of 10 supplementary municipalities (in red) on the map after rotation.

5 Multiple factor analysis of mixed data

Multiple factor analysis (Escofier and Pagès, 1994; Abdi et al., 2013) is a multivariate analysis method for multi-table data where observations are described by several groups of variables. The straightforward analysis obtained by concatenating all variables in a single data table has the

drawback to give more importance to groups with strong structure. The main idea in Multiple Factor Analysis (MFA) is therefore to give the same importance to each group by weighting each variable by the inverse of the variance of the first principal component of its group. In standard MFA, the nature of the variables (categorical or numerical) can vary from one group to another but the variables within a group must be of the same nature. The MFAmix procedure proposed in this paper works with mixed data even within a group.

5.1 The MFAmix algorithm

Here the p variables are separated into G groups. The types of variables within a group can be mixed. Each group is represented by a data matrix $\mathbf{X}^{(g)} = [\mathbf{X}_1^{(g)}, \mathbf{X}_2^{(g)}]$ where $\mathbf{X}_1^{(g)}$ (resp. $\mathbf{X}_2^{(g)}$) contains the numerical (resp. categorical) variables of group $g = 1, \ldots, G$. The numerical columns (resp. the categorical columns) of the matrices $\mathbf{X}^{(g)}$ are concatenated in a global numerical data matrix $\mathbf{X}_1 = [\mathbf{X}_1^{(1)}, \ldots, \mathbf{X}_1^{(G)}]$ (resp. a global categorical data matrix $\mathbf{X}_2 = [\mathbf{X}_2^{(1)}, \ldots, \mathbf{X}_2^{(G)}]$). Let \mathbf{Z} denote the matrix constructed with \mathbf{X}_1 and \mathbf{X}_2 as described in the pre-processing step of PCAmix in Section 3.1. The matrix \mathbf{Z} has then n rows and $p_1 + m$ columns where $p_1 = p_1^{(1)} + \ldots + p_1^{(G)}$ and $m = m^{(1)} + \ldots + m^{(G)}$. Each column of \mathbf{Z} is either a numerical variable (standardized) or the indicator vector of a level (centered). Let $\mathbf{N} = \frac{1}{n}\mathbb{I}_n$ and $\mathbf{M} = \operatorname{diag}(1, \ldots, 1, \frac{n}{n_1}, \ldots, \frac{n}{n_m})$ be the diagonal matrices of the weights of the rows and columns of \mathbf{Z} .

The MFAmix algorithm is a procedure where the first step modifies the weights of the columns of \mathbf{Z} to equilibrate the importance of the groups in a global PCAmix analysis.

Step 1: weighting step.

- 1. For g = 1, ..., G, compute the first eigenvalue $\lambda_1^{(g)}$ of PCAmix applied to $\mathbf{X}^{(g)}$.
- 2. Build the diagonal matrix **P** of the weights $\frac{1}{\lambda_1^{(t_k)}}$ where $t_k \in \{1, \dots, g, \dots, G\}$ denote the group of the kth column of **Z**.
- 3. Build the diagonal matrix **MP** of the new weights of the column of **Z**.

Step 2: re-weighted global PCAmix step.

1. The GSVD of **Z** with metrics **N** on \mathbb{R}^n and **MP** on \mathbb{R}^{p_1+m} gives:

$$\mathbf{Z} = \mathbf{U}_{\mathrm{mfa}} \boldsymbol{\Lambda}_{\mathrm{mfa}} \mathbf{V}_{\mathrm{mfa}}^{\top},$$

as defined in (1). Let r denote the rank of \mathbf{Z} .

2. The matrix of dimension $n \times r$ of the factor coordinates of the n observations is:

$$\mathbf{F}_{\mathrm{mfa}} = \mathbf{U}_{\mathrm{mfa}} \mathbf{\Lambda}_{\mathrm{mfa}}.\tag{35}$$

3. The matrix of dimension $(p_1+m)\times r$ of the factor coordinates of the p_1 quantitative variables and the m levels is:

$$\mathbf{A}_{\mathrm{mfa}}^* = \mathbf{M} \mathbf{V}_{\mathrm{mfa}} \mathbf{\Lambda}_{\mathrm{mfa}}. \tag{36}$$

The first p_1 rows contain the factor coordinates of the numerical variables and the following m rows contain the factor coordinates of the levels.

Step 3: squared loading processing. The squared loadings are the contributions of the p variables to the variance of the r principal components (columns of \mathbf{F}_{mfa}). It comes from Section 2.1 that the variance of the ith principal component $\mathbf{f}_{i,\text{mfa}}$ is $\text{Var}(\mathbf{f}_{i,\text{mfa}}) = \|\mathbf{a}_{i,\text{mfa}}\|_{\mathbf{MP}}^2$ where $\mathbf{a}_{i,\text{mfa}}$ is the ith loadings vector (column of $\mathbf{A}_{\text{mfa}} = \mathbf{V}_{\text{mfa}} \mathbf{\Lambda}_{\text{mfa}}$). The contribution $c_{ji,\text{mfa}}$ of the variable \mathbf{x}_j to the variance of the principal component $\mathbf{f}_{i,\text{mfa}}$ is then:

$$\begin{cases}
c_{ji,\text{mfa}} = \frac{1}{\lambda_1^{(t_j)}} a_{ji,\text{mfa}}^2 = \frac{1}{\lambda_1^{(t_j)}} a_{ji,\text{mfa}}^{*2} & \text{if the variable } \mathbf{x}_j \text{ is numerical,} \\
c_{ji,\text{mfa}} = \sum_{s \in I_j} \frac{1}{\lambda_1^{(t_s)}} \frac{n}{n_s} a_{si,\text{mfa}}^2 = \sum_{s \in I_j} \frac{1}{\lambda_1^{(t_s)}} \frac{n_s}{n} a_{si,\text{mfa}}^{*2} & \text{if the variable } \mathbf{x}_j \text{ is categorical,}
\end{cases}$$
(37)

where I_j is the set of indices of the levels of the categorical variable \mathbf{x}_j . Note that the contributions are no longer squared correlation or correlation ratios as previously in PCArot and PCAmix.

Remark 6. In general $q \le r$ dimensions are required by the user in MFAmix.

5.2 Graphical outputs of MFAmix

The graphical outputs of MFAmix are obtained with the function plot.MFAmix. The standard plots (observations, numerical variables and levels according to their factor coordinates) are interpreted with the same rules as in PCAmix (see Section 3.2) which remain true in MFAmix. The interpretation of the plot of the variables according to their squared loadings is however slightly different. Indeed, in MFAmix, squared loadings need to be interpreted as contributions and no longer as squared correlations or correlation ratios. The structure in groups of the variables allows to build in MFAmix new graphical outputs: plot of the groups, plot of the partial observations and plot of the partial axes.

Contribution of a group. The contribution of a variable is defined in (37). The contribution of a group g is therefore the sum of the contributions of all the variables of the group. The groups can then be plotted as points on a map using their contribution to the variance of the principal components.

Partial observations. The principal component map of the observations reveals the common structure through the groups, but it is not possible to see how each group "interprets" the principal component space. The visualization of an observation according to a specific group (called a partial observation) can be achieved by projecting the dataset of each group onto this space. This is done as follows:

- 1. For g = 1, ..., G, construct the matrix $\mathbf{Z}_{\text{part}}^{(g)}$ by putting to zero in \mathbf{Z} the values of the columns k such that $t_k \neq g$. The rows of $\mathbf{Z}_{\text{part}}^{(g)}$ are the partial observations for the group g.
- 2. For $q = 1, \ldots, G$, the factor coordinates of the partial observations are computed as:

$$\mathbf{F}_{\text{part}}^{(g)} = G \times \mathbf{Z}_{\text{part}}^{(g)} \mathbf{MPV}. \tag{38}$$

This matrix contains the coordinates of the orthogonal projections (with respect to the inner product matrix \mathbf{MP}) of the n rows of $\mathbf{Z}_{part}^{(g)}$ onto the axes spanned by the columns of \mathbf{V} (with the number of groups as multiplying factor).

The partial observations can then be plotted as supplementary points on the principal component map of the observations. Each observation has G partial observations and it can be shown that the observations are plotted at the barycenter of its G partial observations. To facilitate this interpretation, lines linking an observation with its partial observations are drawn on the map.

Partial axes. The MFAmix procedure is applied first PCAmix to the G separated data tables $\mathbf{X}^{(g)}$. The principal components $\mathbf{f}_i^{(g)}, i=1\dots q$ of these separate analyses are called the partial axes. Let $\mathbf{f}_{i,\text{mfa}}$ denote the ith principal component of the global analysis. The link between the separated analysis and the global analysis is explored by computing correlations between the principal components of each separated study and the principal components of the global study. The correlations $r(\mathbf{f}_i^{(g)}, \mathbf{f}_{i,\text{mfa}})$ are used as coordinates to plot the partial axes on a map.

5.3 Prediction of PC scores with predict.MFAmix

The $q \leq r$ principal components (PCs) are new numerical variables defined as a linear combination of the vectors $\mathbf{z}_1, \dots, \mathbf{z}_{p_1+m}$ (columns of \mathbf{Z}). For $i = 1, \dots, q$:

$$\mathbf{f}_{i,\text{mfa}} = \mathbf{ZMPv}_{i,\text{mfa}} = \sum_{\ell=1}^{p_1} \frac{1}{\lambda_1^{(t_\ell)}} v_{\ell i,\text{mfa}} \mathbf{z}_j + \sum_{\ell=p_1+1}^{p_1+m} \frac{1}{\lambda_1^{(t_\ell)}} \frac{n}{n_\ell} v_{\ell i,\text{mfa}} \mathbf{z}_\ell.$$

It is then easy to write $\mathbf{f}_{i,\text{mfa}}$ as a linear combination of the vectors $\mathbf{x}_1, \dots, \mathbf{x}_{p_1+m}$ (columns of $\mathbf{X} = (\mathbf{X}_1 | \mathbf{G})$) where \mathbf{G} is the indicator matrix of the m levels:

$$\mathbf{f}_{i,\text{mfa}} = \beta_{0i,\text{mfa}} + \sum_{\ell=1}^{p_1+m} \beta_{\ell i,\text{mfa}} \mathbf{x}_{\ell}, \tag{39}$$

with the coefficients

$$\beta_{0i,\text{mfa}} = -\sum_{\ell=1}^{p_1} \frac{1}{\lambda_1^{(t_\ell)}} v_{\ell i,\text{mfa}} \frac{\bar{\mathbf{x}}_\ell}{\hat{\sigma}_\ell} - \sum_{\ell=p_1+1}^{p_1+m} \frac{1}{\lambda_1^{(t_\ell)}} \frac{n}{n_\ell} v_{\ell i,\text{mfa}} \bar{\mathbf{x}},$$

$$\beta_{\ell i,\text{mfa}} = \frac{1}{\lambda_1^{(t_\ell)}} v_{\ell i,\text{mfa}} \frac{1}{\hat{\sigma}_\ell}, \text{ for } \ell = 1, \dots, p_1,$$

$$\beta_{\ell i,\text{mfa}} = \frac{1}{\lambda_1^{(t_\ell)}} \frac{n}{n_\ell} v_{\ell i,\text{mfa}}, \text{ for } \ell = p_1 + 1, \dots, p_1 + m,$$

where $\bar{\mathbf{x}}_{\ell}$ and $\hat{\sigma}_{\ell}$ are respectively the empirical mean and the standard deviation of the column \mathbf{x}_{ℓ} . The principal components are thereby written in (39) as a linear combination of the original numerical variables and of the original indicator vectors of the levels of the categorical variables. The function predict.MFAmix uses these coefficients to predict the scores (coordinates) of new observations on the $q \leq r$ first principal component of MFAmix (where q is chosen by the user).

5.4 Illustration of MFAmix

Let us now illustrate the procedure MFAmix with the 4 mixed data tables available in the dataset gironde. As introduced previously, this dataset describes 542 municipalities on 27 variables separated into 4 groups (Employment, Housing, Services, Environment). The dataset gironde is then a list of 4 data tables (one data table by group).

```
R> library("PCAmixdata")
R> data("gironde")
R> names(gironde)
[1] "employment" "housing" "services" "environment"
```

The four groups contain respectively 9, 5, 9 and 4 variables and the description of the variables of each data table is available in Appendix A.

The function MFAmix uses three main input arguments:

- data: the global data frame obtained by concatenation of the separated data tables,
- group: a vector of integer with the index of the group of each variable,
- name.group: a vector of character with the name of each group.

```
R> dat <- cbind(gironde$employment,gironde$housing,gironde$services,
gironde$environment)
R> index <- c(rep(1,9),rep(2,5),rep(3,9),rep(4,4))
R> names <- c("employment","housing","services","environment")
R> res.mfamix <- MFAmix(data=dat,groups=index,name.groups=names,
ndim=3,rename.level=TRUE,graph=FALSE)</pre>
```

The function MFAmix builds an object (of class MFAmix) which is a list with many numerical results described shortly with the print function.

The structure in groups of variables gives specific graphical outputs like the four maps of Figure 6.

Figure 6(a) is the correlation circle of the 16 numerical variables, colored according to their group membership. The coordinates of the variables on this map are correlations with the principal components of MFAmix. Because this map can be difficult to read due to multiple overlaying of the names of some variables, it can be useful to look at the numerical values of the coordinates available in the object res.MFAmix.

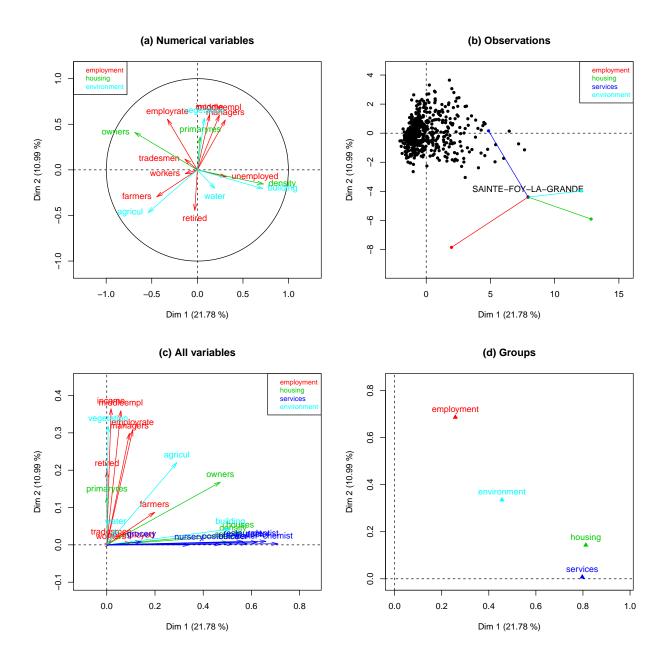


Figure 6: Some graphical outputs of MFAmix applied to the four data table of the dataset gironde.

This result gives the 4 numerical variables that are the most correlated (in absolute value) with the first principal component of MFAmix. The municipalities on the right hand side of the principal component map in Figure 6(b) have higher values for variables density and buildings, whereas municipalities to the left have higher values on the variables owners and agric.

To interpret the position of the municipalities at the top and bottom of Figure 6(b), the coordinates of the variables in the second dimension are useful.

This result gives the 5 variables that are the most correlated with the second principal component. The position (top or bottom) of the municipalities on the principal component map can then be interpreted with these variables.

For example, Figure 6(b) shows the municipality of SAINTE-FOY-LA-GRANDE plotted with its 4 partial representations (the four colored points linked to it with a line). The position of this municipality on the right of the map suggests a municipality with higher density of population, higher proportion of buildings, less owners and less agricultural land. Its position at the bottom of the map suggests smaller values on 4 variables of the group employment (managers, middleempl,employrate,income) and smaller values on the variable vegetation of the group environment.

But what about the 9 categorical variables of the group services. These variables naturally do not appear in the correlation circle but they appear in Figure 6(c) where all the variables are plotted according to their contributions to the principal components. This map shows that all the variables of the group services (dentist, dentist, nursery,...) contribute strongly to the first principal component. However it is not possible to know in which way. For instance the municipality SAINTE-FOY-LA-GRANDE which has a high score on the first principal component has more or less services than others? This information is given in Figure 7 where the levels of the categorical variables are plotted.



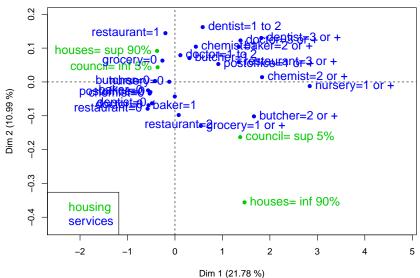


Figure 7: Plot of the levels of the 10 categorical variables after applying MFAmix.

The level map can be used with the barycentric property to interpret the map of the municipalities given Figure 6(b): the municipalities on the right are provided with more services than those on the left. The municipalities in the bottom right of the map (like SAINTE-FOY-LA-GRANDE) have more likely a smaller proportion of houses.

In summary, the municipality SAINTE-FOY-LA-GRANDE is a municipality with a good level of services, but with a fairly stagnant employment market and whose inhabitants are more likely to live in apartments than in other municipalities.

The last map Figure 6(d) is the plot of the groups according to their contributions to the first two principal components. This map confirms the previous interpretations of the principal components of MFAmix and the impact of the groups services and housing on the first dimension as well as the impact of the group employment on the second dimension.

Predicted scores for new observations. The scores of new observations can be obtained with the predict.MFAmix function. The municipality SAINTE-FOY-LA-GRANDE for instance can be considered as supplementary and plotted as an illustrative observation (test sample) on the map given in Figure 8 obtained with the n-1 remaining municipalities (training sample).

Supplementary groups. The supvar.MFAmix function calculates the coordinates of supplementary groups of variables on the maps of MFAmix. Let us for instance apply MFAmix with three groups (employment, services, environment) and add the group housing as a supplement.

Observations map

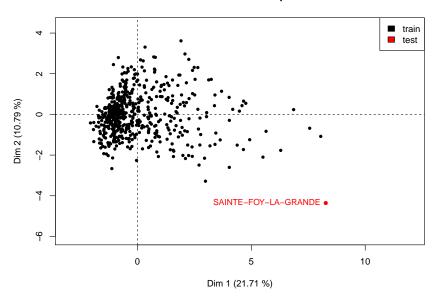


Figure 8: The municipality SAINTE-FOY-LA-GRANDE is plotted in supplementary in the graphical output of MFAmix.

6

Concluding remarks

R> plot(mfa.sup,choice="cor",coloring.var = "groups",

col.groups=c(2,4,5),col.groups.sup=3)

The multivariate analysis methods implemented in the R package PCAmixdata are presented in this paper in such a way that the theoretical details can be read separately from the R examples. Users interested in the practical aspects of the methods PCAmix, PCArot and MFAmix can reproduce the R code provided after each theoretical section, either with the dataset gironde (available in the package) or with their own data. Keys are also provided for the interpretation of most numerical results and graphical outputs.

The use of mixed data with other multivariate analysis methods is currently being studied. One example of this is orthogonal rotation of the principal component of MFAmix. Because MFAmix

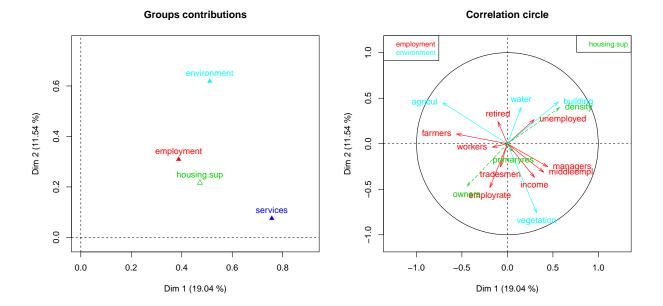


Figure 9: The group houses is plotted in supplementary in the graphical outputs of MFAmix.

is a re-weighted general PCAmix analysis, this implementation does not require many theoretical developments.

The development of a method of linear discriminant analysis compatible with mixed data is also under investigation.

Appendices

A The dataset gironde

B The iterative optimization step of PCArot

Let $\tilde{\mathbf{U}}_q$ (resp. $\tilde{\mathbf{A}}_q$) denote the matrix of the q first columns of $\tilde{\mathbf{U}}$ (resp. $\tilde{\mathbf{A}} = \tilde{\mathbf{\Lambda}}\tilde{\mathbf{V}}$).

- 1. Initialization: $\tilde{\mathbf{U}}_{\text{rot}} = \tilde{\mathbf{U}}_q$ and $\tilde{\mathbf{A}}_{\text{rot}} = \tilde{\mathbf{A}}_q$.
- 2. For each pair of dimensions (l,t), i.e., for $l=1,\ldots,q-1$ and $t=(l+1),\ldots,q$:
 - \hookrightarrow calculate the angle of rotation $\theta = \psi/4$ with:

$$\psi = \begin{cases} \arccos\left(\frac{h}{\sqrt{g^2 + h^2}}\right) & \text{if } g \ge 0, \\ -\arccos\left(\frac{b}{\sqrt{g^2 + h^2}}\right) & \text{if } g \le 0, \end{cases}$$

$$(40)$$

R_Names	Description	Group	Data type
farmers	Percentage of farmers	employment	Num
tradesmen	Percentage of tradesmen and shopkeepers	employment	Num
managers	Percentage of managers and executives	employment	Num
workers	Percentage of workers and employees	employment	Num
unemployed	Percentage of unemployed workers	employment	Num
middleemp	Percentage of middle-range employees	employment	Num
retired	Percentage of retired people	employment	Num
employrate	employment rate	employment	Num
income	Average income	employment	Num
density	Population density	housing	Num
primaryres	Percentage of primary residences	housing	Num
houses	Percentage of houses	housing	Categ
owners	Percentage of home owners living in their primary residence	housing	Num
council	Percentage of council housing	housing	Categ
butcher	Number of butchers	services	Categ
baker	Number of bakers	services	Categ
postoffice	Number of post offices	services	Categ
dentist	Number of dentists	services	Categ
grocery	Number of grocery stores	services	Categ
nursery	Number of child care day nurseries	services	Categ
doctor	Number of doctors	services	Categ
chemist	Number of chemists	services	Categ
restaurant	Number of restaurants	services	Categ
building	Percentage of buildings	environment	Num
water	Percentage of water	environment	Num
vegetation	Percentage of vegetation	environment	Num
agricul	Percentage of agricultural land	environment	Num

where g and h are given by:

$$g = 2p \sum_{j=1}^{p} \alpha_j \beta_j - 2 \sum_{j=1}^{p} \alpha_j \sum_{j=1}^{p} \beta_j,$$
(41)

$$h = p \sum_{j=1}^{p} (\alpha_j^2 - \beta_j^2) - \left(\sum_{j=1}^{p} \alpha_j\right)^2 + \left(\sum_{j=1}^{p} \beta_j\right)^2, \tag{42}$$

with p the total number of variables, and α_i and β_i defined by:

$$\alpha_j = \sum_{s \in I_j} (\tilde{a}_{sl,\text{rot}}^2 - \tilde{a}_{st,\text{rot}}^2) \quad \text{and} \quad \beta_j = 2 \sum_{s \in I_j} \tilde{a}_{sl,\text{rot}} \tilde{a}_{st,\text{rot}} . \tag{43}$$

Here, I_j is the set of row indices of $\tilde{\mathbf{A}}_{rot}$ associated with the levels of the variable j in the categorical case and $I_j = \{j\}$ in the numerical case.

- \hookrightarrow calculate the corresponding matrix of planar rotation $\mathbf{T}_2 = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$,
- \hookrightarrow update the matrices $\tilde{\mathbf{U}}_{\mathrm{rot}}$ and $\tilde{\mathbf{A}}_{\mathrm{rot}}$ by rotation of their l-th and t-th columns.
- 3. Repeat the previous step until the q(q-1)/2 successive rotations provide an angle of rotation θ equal to zero.

C Proof of (30)

The $q \times q$ rotation matrix **T** is such that

$$\tilde{\mathbf{U}}_{\rm rot} = \tilde{\mathbf{U}}_q \mathbf{T}.\tag{44}$$

By definition of $\tilde{\mathbf{U}}_q$, we have $\tilde{\mathbf{U}}_q^{\top}\tilde{\mathbf{U}}_q = \mathbb{I}_q$. It gives (32). By definition, $\tilde{\mathbf{F}}_{\text{rot}} = \tilde{\mathbf{U}}_{\text{rot}}\mathbf{\Lambda}_{\text{rot}}$. It gives $\tilde{\mathbf{F}}_{\text{rot}} = \tilde{\mathbf{U}}_q\mathbf{T}\mathbf{\Lambda}_{\text{rot}}$. The SVD decomposition $\tilde{\mathbf{Z}} = \tilde{\mathbf{U}}\tilde{\mathbf{\Lambda}}\tilde{\mathbf{V}}^{\top}$ gives $\tilde{\mathbf{U}}_q = \tilde{\mathbf{Z}}\tilde{\mathbf{V}}_q\tilde{\mathbf{\Lambda}}_q^{-1}$. Then $\tilde{\mathbf{F}}_{\text{rot}} = \tilde{\mathbf{Z}}\tilde{\mathbf{V}}_q\tilde{\mathbf{\Lambda}}_q^{-1}\mathbf{T}\mathbf{\Lambda}_{\text{rot}}$. With $\tilde{\mathbf{F}}_{\text{rot}} = \mathbf{N}^{1/2}\mathbf{F}_{\text{rot}}$ and $\tilde{\mathbf{Z}} = \mathbf{N}^{1/2}\mathbf{Z}\mathbf{M}^{1/2}$, it gives (30) and (31).

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