Multivariate analysis of mixed data: The PCAmixdata R package

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Multivariate analysis of a mixture of numerical and categorical data

Three main functions:

- Function `PCAmix` for principal component analysis (PCA) of mixed data.
  $\hookrightarrow$ Includes standard PCA and MCA (multiple component analysis) as special cases.
- Function `PCArot` for orthogonal rotation in PCAmix.
  $\hookrightarrow$ Includes standard varimax rotation and rotation in MCA as special cases.
- Function `MFAmix` for multiple factor analysis (MFA) for multiple-table mixed data.

https://github.com/chavent/PCAmixdata

Principal component analysis of mixed data

Several implementations already in R:

- Function `FAMD` in the R package **FactoMineR**.
  ↪ Implements the method designed by Pagès (2004).
- Function `dudi.mix` in the R package **ade4**.
  ↪ Implements the method of Hill & Smith (1976).
- Function `PCAmix` in the R package **PCAmixdata**.
  ↪ Implements a single PCA with metrics based on a GSVD of preprocessed data.

⇒ Three different coding scheme but identical numerical results.

A real data example

The `gironde` data are available in the package

```
library(PCAmixdata)
data(gironde)
```

- They characterize living conditions in Gironde, a southwest region in France.
- 542 cities are described with 27 variables separated into 4 groups (Employment, Housing, Services, Environment).

  $\hookrightarrow$ Four datatables

A mixed data type example

The datatable housing is mixed.

↪ 3 numerical and 2 categorical variables.

```
housing <- gironde$housing
```

```
head(housing)
```

```
##          density primaryres owners   houses council
## ABZAC        132          89     64  inf 90%  sup 5%
## AILLAS        21          88     77  sup 90%  inf 5%
## AMBARES      532          95     66  inf 90%  sup 5%
## AMBES        101          94     67  sup 90%  sup 5%
## ANDERNOS     552          62     72  inf 90%  inf 5%
## ANGLADE       64          81     81  sup 90%  inf 5%
```

Two data sets:

↪ a numerical data matrix $\mathbf{X}_1$ of dimension 542×3.

↪ a categorical data matrix $\mathbf{X}_2$ of dimension 542×2.

```
split<-splitmix(housing)
X1<-split$X.quanti
X2<-split$X.quali
```

```
head(X1)
```

```
##           density primaryres owners
## ABZAC         132          89     64
## AILLAS         21          88     77
## AMBARES       532          95     66
## AMBES         101          94     67
## ANDERNOS      552          62     72
## ANGLADE        64          81     81
```

```
head(X2)
```

```
##              houses council
## ABZAC     inf 90%  sup 5%
## AILLAS    sup 90%  inf 5%
## AMBARES   inf 90%  sup 5%
## AMBES     sup 90%  sup 5%
## ANDERNOS  inf 90%  inf 5%
## ANGLADE   sup 90%  inf 5%
```

The PCAmix method

An simple algorithm in three main steps

1. Preprocessing step.
2. GSVD (Generalized Singular Value Decomposition) step.
3. Scores and loadings processing step.

Some notations:

- Let $\mathbf{X}_1$ be a $n \times p_1$ **numerical** data matrix.
- Let $\mathbf{X}_2$ be a $n \times p_2$ **categorical** data matrix.
- Let m be the total number of levels of the categorical variables.

Preprocessing step

1. Build a **numerical data matrix** $\mathbf{Z} = (\mathbf{Z}_1|\mathbf{Z}_2)$ of dimension $n \times (p_1 + m)$ with:
   - $\hookrightarrow$ $\mathbf{Z}_1$ the standardized version of the matrix $\mathbf{X}_1$.
   - $\hookrightarrow$ $\mathbf{Z}_2$ the centered indicator matrix of the levels of $\mathbf{X}_2$.
2. Build the diagonal matrix $\mathbf{N}$ of the weights of the rows.
   - $\hookrightarrow$ The n rows are weighted by $\frac{1}{n}$.
3. Build the diagonal matrix $\mathbf{M}$ of the weights of the columns.
   - $\hookrightarrow$ The p_1 first columns are weighted by 1.
   - $\hookrightarrow$ The m last columns are weighted by $\frac{n}{n_s}$, with n_s the number of observations with level s.

$\hookrightarrow$ The total variance is $p_1 + m - p_2$.

GSVD step

The GSVD (Generalized Singular Value Decomposition) of $\mathbf{Z}$ with the metrics $\mathbf{N}$ and $\mathbf{M}$ gives the decompositon

$$\mathbf{Z} = \mathbf{U}\mathbf{D}\mathbf{V}^T \tag{1}$$

where

- $\mathbf{D} = \text{diag}(\sqrt{\lambda_1}, \ldots, \sqrt{\lambda_r})$ is the $r \times r$ diagonal matrix of the singular values of $\mathbf{Z}\mathbf{M}\mathbf{Z}^T\mathbf{N}$ and $\mathbf{Z}^T\mathbf{N}\mathbf{Z}\mathbf{M}$, and r denotes the rank of $\mathbf{Z}$;
- $\mathbf{U}$ is the $n \times r$ matrix of the first r eigenvectors of $\mathbf{Z}\mathbf{M}\mathbf{Z}^T\mathbf{N}$ such that $\mathbf{U}^T\mathbf{N}\mathbf{U} = \mathbb{I}_r$;
- $\mathbf{V}$ is the $p \times r$ matrix of the first r eigenvectors of $\mathbf{Z}^T\mathbf{N}\mathbf{Z}\mathbf{M}$ such that $\mathbf{V}^T\mathbf{M}\mathbf{V} = \mathbb{I}_r$.

Scores and loadings processing step

1. The principal coordinates of the rows are computed as:

$$\mathbf{F} = \mathbf{UD}.$$

$\hookrightarrow$ principal component scores of the observations,

2. The principal coordinates of the colums are computed as:

$$\mathbf{A} = \mathbf{MVD}.$$

$\hookrightarrow$ loadings of the numerical variables and of the levels of the caregorical variables,

$\hookrightarrow$ in standard PCA: $\mathbf{A} = \mathbf{VD}$.

The R function

```
args(PCAmix)


## function (X.quanti = NULL, X.quali = NULL, ndim = 5, rename.level = FALSE,
##     weight.col.quanti = NULL, weight.col.quali = NULL, graph = TRUE)
## NULL
```

```
PCAmix(X.quanti=X1,X.quali=X2,ndim=2,graph=FALSE)


##
## Call:
## PCAmix(X.quanti = X1, X.quali = X2, ndim = 2, graph = FALSE)
##
## Method = Principal Component of mixed data (PCAmix)
##
##
##      name      description
## [1,] "$eig"    "eigenvalues of the principal components (PC) "
## [2,] "$ind"    "results for the individuals (coord,contrib,cos2)"
## [3,] "$quanti" "results for the quantitative variables (coord,contrib,cos2)"
## [4,] "$levels" "results for the levels of the qualitative variables (coord,contrib,cos2)"
## [5,] "$quali"  "results for the qualitative variables (contrib,relative contrib)"
## [6,] "$sqload" "squared loadings"
## [7,] "$coef"   "coef of the linear combinations defining the PC"
```

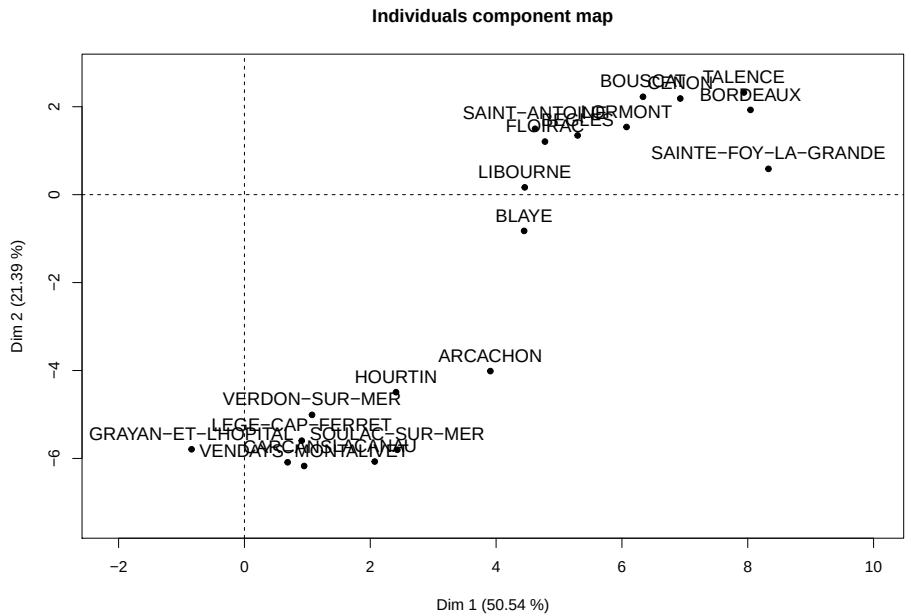
Scores of the observations

```
obj <- PCAmix(X.quanti=X1,X.quali=X2,
              ndim=2,rename.level = TRUE,graph=FALSE)
```

```
head(obj$ind$coord)
```

```
##           dim 1  dim 2
## ABZAC      2.36  0.024
## AILLAS    -0.88  0.123
## AMBARES    2.62  0.800
## AMBES      0.93  0.919
## ANDERNOS   1.18 -2.481
## ANGLADE   -1.01 -0.424
```

```
plot(obj,choice="ind",lim.contrib.plot = 1,cex=1.2)
```

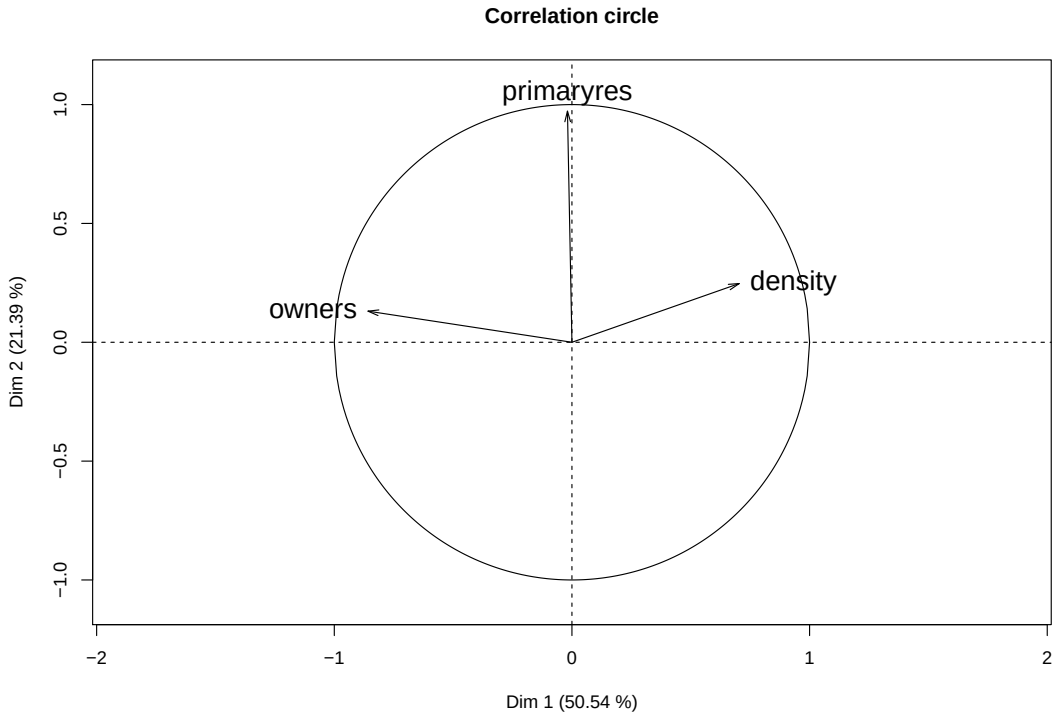


Scores of the numerical variables

```
head(obj$quanti.cor)
```

```
##              dim 1 dim 2
## density      0.704  0.25
## primaryres -0.019  0.97
## owners     -0.858  0.13
```

```
#Component map with factor scores of the numerical columns
plot(obj,choice="cor",cex=1.5)
```



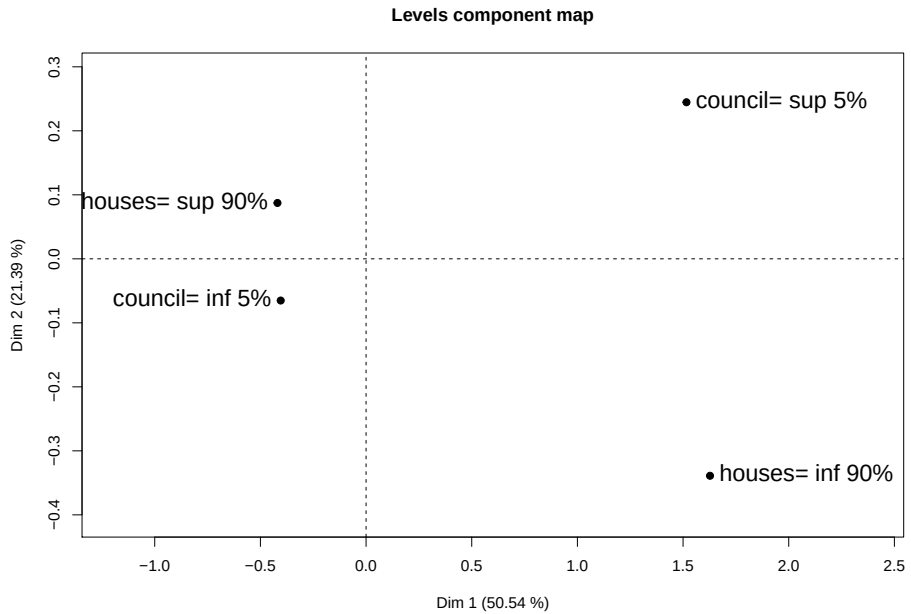
↪ The (non standardized) loadings are correlations.

Scores of the levels of the categorical variables

```
head(obj$categ.coord)
```

```
##                  dim 1  dim 2
## houses= inf 90%  1.63 -0.339
## houses= sup 90% -0.42  0.087
## council= inf 5% -0.40 -0.065
## council= sup 5%  1.52  0.245
```

```
plot(obj,choice="levels",cex=1.5,xlim=c(-1,2))
```



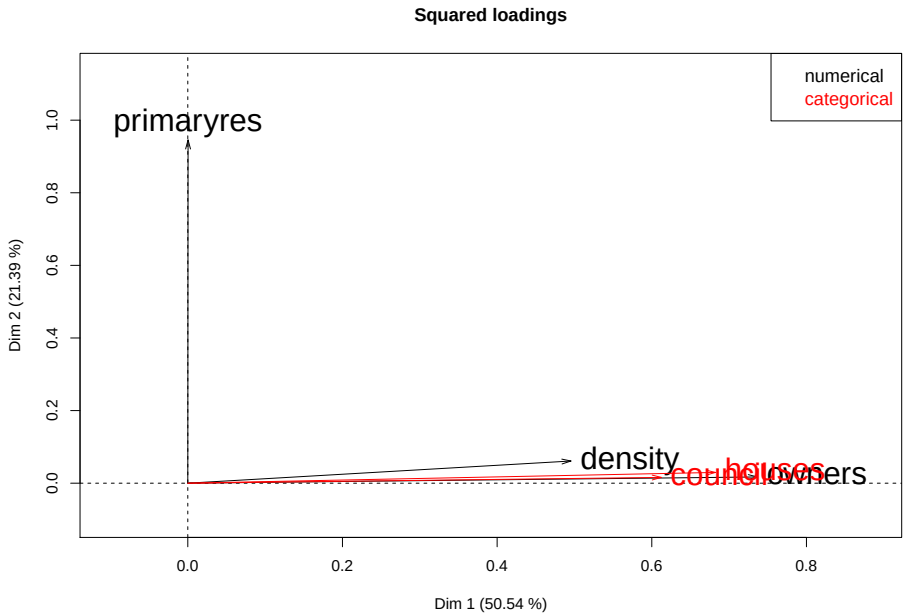
↪ The barycentric property is still verified.

Contributions of the variables

```
#contributions of the variables
head(obj$sqload)
```

```
##                dim 1 dim 2
## density      0.49550 0.061
## primaryres   0.00035 0.946
## owners       0.73651 0.017
## houses       0.68226 0.030
## council      0.61226 0.016
```

```
plot(obj,choice="sqload",coloring.var=TRUE,
     cex=2,posleg = "topright",cex.leg=1.2)
```



Squared loadings

The contribution $c_{j\alpha}$ of a variable j to the component α is:

$$\begin{cases} c_{j\alpha} = a_{j\alpha}^2 = \text{Squared correlation} & \text{if variable } j \text{ is numerical,} \\ c_{j\alpha} = \sum_{s \in I_j} \frac{n}{n_s} a_{s\alpha}^2 = \text{Correlation ratio} & \text{if variable } j \text{ is categorical.} \end{cases}$$

Principal components prediction

Each principal component $\mathbf{f}_\alpha$ writes as a linear combination of the columns of $\mathbf{X} = (\mathbf{X}_1|\mathbf{G})$ where $\mathbf{X}_1$ is the numerical data matrix and $\mathbf{G}$ is the indicator matrix of the levels of the matrix $\mathbf{X}_2$:

$$\mathbf{f}_\alpha = \beta_0 + \sum_{j=1}^{p_1+m} \beta_j \mathbf{x}_j$$

with:

$$\beta_0 = -\sum_{k=1}^{p_1} v_{k\alpha} \frac{\bar{\mathbf{x}}_k}{s_k} - \sum_{k=p_1+1}^{p_1+m} v_{k\alpha},$$

$$\beta_j = v_{j\alpha} \frac{1}{s_j}, \text{ for } j = 1, \ldots, p_1$$

$$\beta_j = v_{j\alpha} \frac{n}{n_j}, \text{ for } j = p_1 + 1, \ldots, p_1 + m$$

The method predict()

Coefficients of the PC found on the learning set (without the 5 first cities)

```
    test <- 1:5
    obj2 <- PCAmix(X1[-test,],X2[-test,],graph=FALSE,ndim=3)
    data.frame(obj2$coef)
```

```
##                dim1     dim2    dim3
##             3.64214 -9.02951  1.5950
## density     0.00086  0.00048  0.0015
## primaryres -0.00129  0.09355 -0.0179
## owners     -0.05065  0.01207 -0.0047
##  inf 90%    1.03579 -0.32092 -0.4617
##  sup 90%   -0.26076  0.08079  0.1162
##  inf 5%    -0.25129 -0.05706  0.2704
##  sup 5%     0.96441  0.21898 -1.0379
```

Scores of the 5 first cities on the principal components

```
    predict(obj2,X1[test,],X2[test,])
```

```
##           dim1   dim2   dim3
## ABZAC     2.39  0.011 -1.595
## AILLAS   -0.87  0.122  0.084
## AMBARES   2.65  0.795 -1.098
## AMBES     0.94  0.895 -1.164
## ANDERNOS  1.19 -2.466  0.800
```

Varimax type rotation in PCAmix

Let us introduce

- $\mathbf{T}$ an orthonormal rotation matrix: $\mathbf{T}\mathbf{T}' = \mathbf{T}'\mathbf{T} = \mathbf{I}_k$
- k is the number of dimensions in the rotation procedure

$\Rightarrow$ Rotate the axes of PCAmix so that variables appear more clearly associated with the principal components.

$\Rightarrow$ Association between variables and principal components are measured by the squared loadings : rotated squared loadings $\tilde{c}_{j\alpha}$ are squared correlations or correlation ratios.

$\Rightarrow$ The varimax function writes:

$$f(\mathbf{T}) = \sum_{\alpha=1}^{k}\sum_{j=1}^{p}(\tilde{c}_{j\alpha})^2 - \frac{1}{p}\sum_{\alpha=1}^{k}\left(\sum_{j=1}^{p}\tilde{c}_{j\alpha}\right)^2 . \qquad (2)$$

Find the optimal rotation matrix $\mathbf{T}$

The varimax rotation problem is formulated as

$$\max_{\mathbf{T}} \quad \{f(\mathbf{T}) | \mathbf{T}\mathbf{T}' = \mathbf{T}'\mathbf{T} = \mathbf{I}_k\}, \tag{3}$$

$\Rightarrow$ An iterative procedure based on successive planar rotations.

$\Rightarrow$ Direct solution for the optimal angle of rotation (Chavent & al. 2012).

$\Rightarrow$ Reduces to the Kaiser (1958) for numerical data.

$\Rightarrow$ Performs rotation in MCA for categorical data.

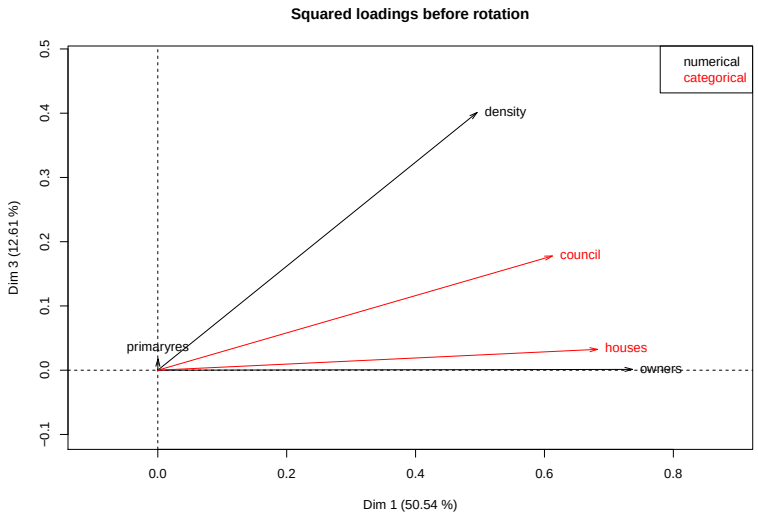
The R function

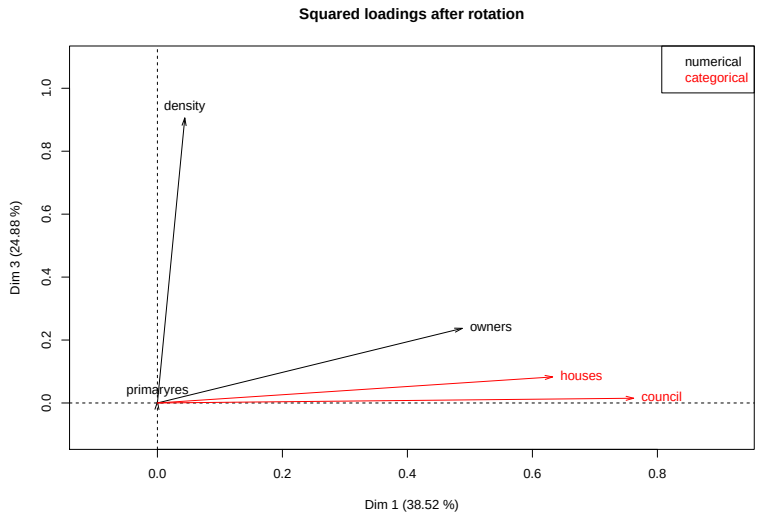
```
obj <- PCAmix(X.quanti=X1, X.quali=X2, rename.level=TRUE, graph=FALSE)
rot <- PCArot(obj,dim=3,graph=FALSE)
rot


##
## Call:
## PCArot(obj = obj, dim = 3, graph = FALSE)
##
## Method = rotation after Principal Component of mixed data (PCAmix)
## number of iterations:  4
##
##       name      description
##  [1,] "$eig"    "variances of the 'ndim' first dimensions after rotation"
##  [2,] "$ind"    "results for the individuals after rotation (coord)"
##  [3,] "$quanti" "results for the quantitative variables (coord) after rotation"
##  [4,] "$levels" "results for the levels of the qualitative variables (coord) after rotation"
##  [5,] "$quali"  "results for the qualitative variables (coord) after rotation "
##  [6,] "$sqload" "squared loadings after rotation"
##  [7,] "$coef"   "coef of the linear combinations defining the rotated PC"
##  [8,] "$theta"  "angle of rotation if 'dim'=2"
##  [9,] "$T"      "matrix of rotation"
```

The method plot()

```
plot(obj,choice="sqload",coloring.var=TRUE,
  leg=TRUE,axes=c(1,3), posleg="topright",
  main="Squared loadings before rotation")
```

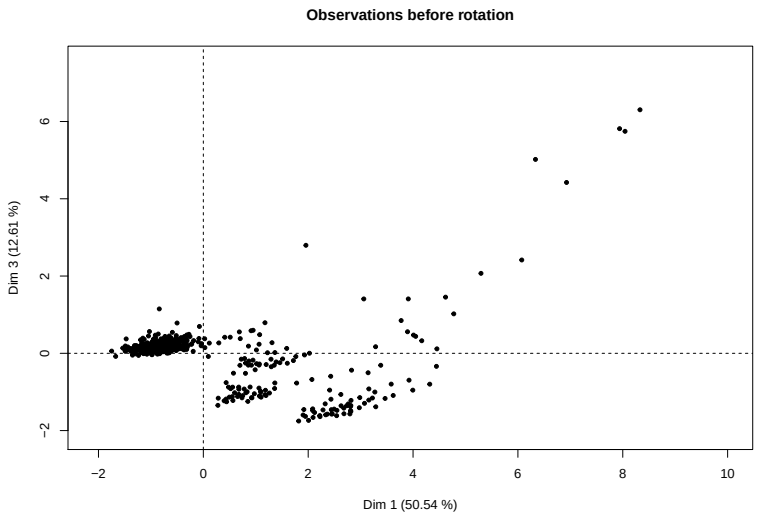
```
plot(rot,choice="sqload",coloring.var=TRUE,
  leg=TRUE,axes=c(1,3),posleg="topright",
  main="Squared loadings after rotation")
```



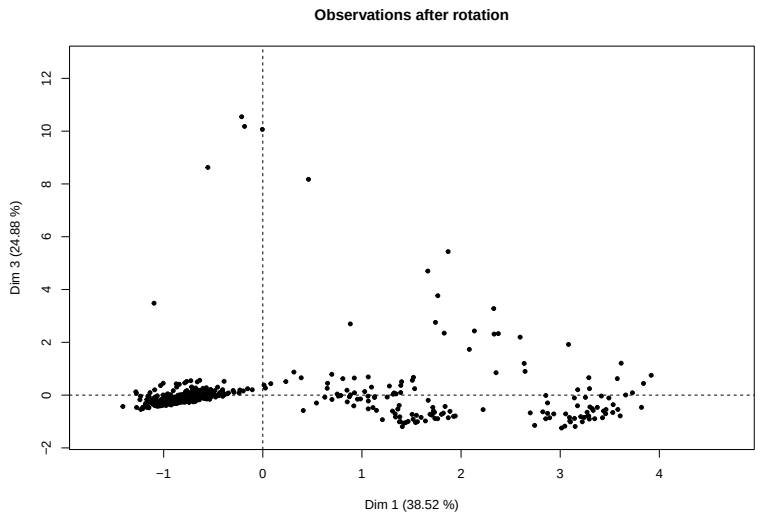


The method plot()

```
plot(obj,choice="ind",label=FALSE,axes=c(1,3),
  main="Observations before rotation")
```




```
plot(rot,choice="ind",label=FALSE,axes=c(1,3),
  main="Observations after rotation")
```



↪ Prediction of scores of new observations on the rotated principal components

The method predict()

Coefficients of the PC found on the learning set (without the 5 first cities)

```
    obj2 <- PCAmix(X1[-test,],X2[-test,],graph=FALSE)
    rot2 <- PCArot(obj2,dim=3,graph=FALSE)
    data.frame(rot2$coef)
```

```
##            dim1.rot dim2.rot dim3.rot
## const       2.00163 -9.3e+00   1.3741
## density    -0.00094  3.9e-05   0.0022
## primaryres  0.00688  9.6e-02  -0.0014
## owners     -0.03313  1.4e-02  -0.0228
##  inf 90%    1.23247 -2.2e-01  -0.1816
##  sup 90%   -0.31027  5.5e-02   0.0457
##  inf 5%    -0.44031 -1.2e-01   0.1958
##  sup 5%     1.68985  4.6e-01  -0.7514
```

Scores of the 5 first cities on the rotated principal components

```
    predict(rot2,X1[test,],X2[test,])
```

```
##          dim1.rot dim2.rot dim3.rot
## ABZAC        3.28     0.36   -0.865
## AILLAS      -0.72     0.12   -0.223
## AMBARES      2.90     0.98   -0.037
## AMBES        1.73     1.15   -0.764
## ANDERNOS     0.33    -2.64    0.868
```

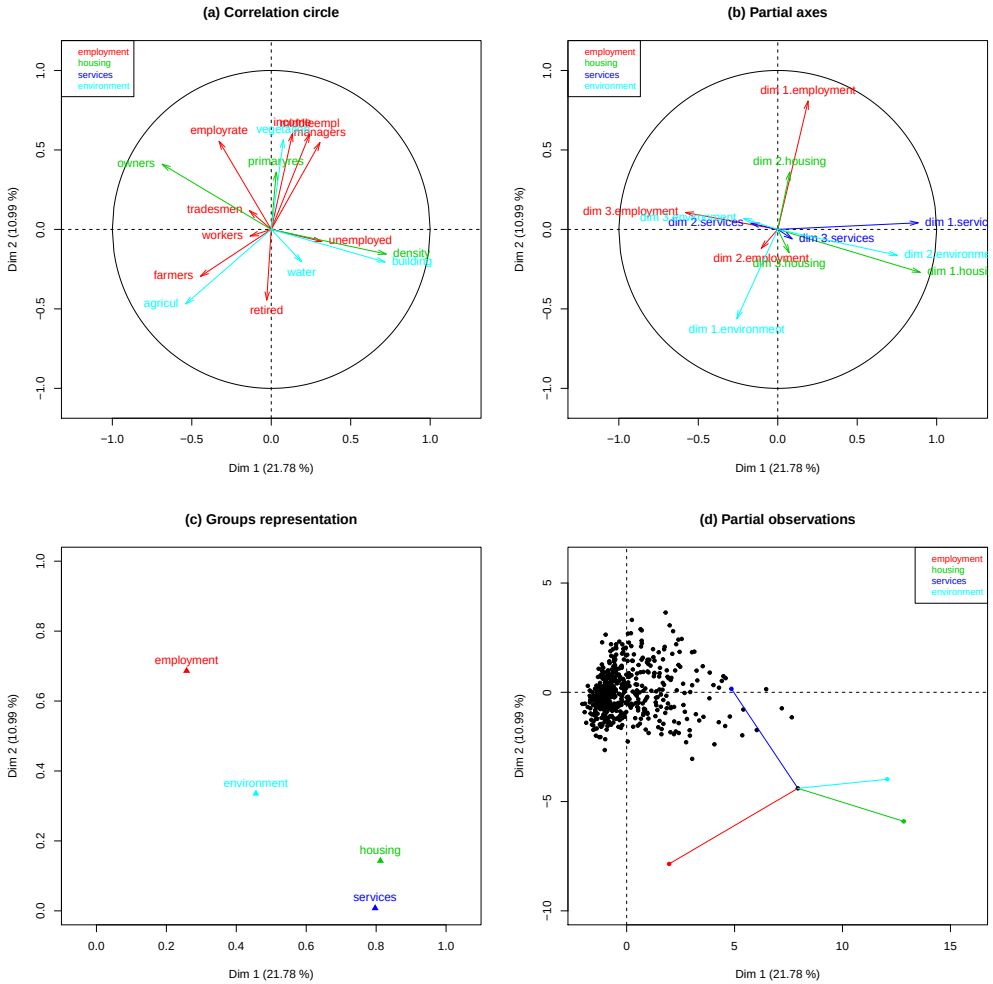
Multiple Factor Analysis for mixed data

- ⇒ Analyze a set of observations described by several groups of variables.
- ⇒ Make the importance of the groups comparable in the PCA analysis by introducing weights: the weight of a variable is the inverse of the variance of the first principal component of its group.
- ⇒ In the function MFA in the package `FactoMineR`, the nature of the variables (categorical or numerical) can vary from one group to another, but the variables should be of the same type within a given group.
- ⇒ MFAmix is able to handle mixed data within a group of variables.

The R function

```
dat<-cbind(gironde$employment,gironde$housing, gironde$services,gironde$environment)
#definition of the groups of variables
groupind<-c(rep(1,9),rep(2,5),rep(3,9),rep(4,4))
#names of the groups of variables
names<-c("employment","housing","services","environment")
#Perform MFAmix
obj3<-MFAmix(data=dat,groups=groupind,name.groups=names,ndim=3,rename.level=TRUE,graph=FALSE)
obj3


## **Results of the Multiple Factor Analysis for mixed data (MFAmix)**
## The analysis was performed on 542 individuals, described by 27 variables
## *Results are available in the following objects :
##
##       name                 description
##  [1,] "$eig"               "eigenvalues"
##  [2,] "$eig.separate"      "eigenvalues of the separate analyses"
##  [3,] "$separate.analyses" "separate analyses for each group of variables"
##  [4,] "$groups"            "results for all the groups"
##  [5,] "$partial.axes"      "results for the partial axes"
##  [6,] "$ind"               "results for the individuals"
##  [7,] "$ind.partial"       "results for the partial individuals"
##  [8,] "$quanti"            "results for the quantitative variables"
##  [9,] "$levels"            "results for the levels of the qualitative variables"
## [10,] "$quali"             "results for the qualitative variables"
## [11,] "$sqload"            "squared loadings"
## [12,] "$listvar.group"     "list of variables in each group"
## [13,] "$global.pca"        "results for the global PCA"
```

Some graphical output



Other packages working with mixed data

⇒ `ClustOfVar` for the clustering of variables.

⇒ `divclust` for the divisive and monothetic clustering of observations.

⇒ `ClustGeo` for the clustering with geographical constraints (very soon available for mixed data).

Some references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THANK YOU !