Package ‘robCompositions’

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Type Package

Title Robust Estimation for Compositional Data

Version 2.0.8

Date 2018-05-29

Depends R (>= 3.0.0), robustbase, ggplot2, data.table, e1071, pls

LinkingTo Rcpp

Imports car, rrcov, cluster, cvTools, fpc, GGally, kernlab, MASS, mclust, Rcpp, sROC, VIM, zCompositions

Suggests knitr

VignetteBuilder knitr

Maintainer Matthias Templ <matthias.templ@gmail.com>

Description Methods for analysis of compositional data including robust methods, imputation, methods to replace rounded zeros, (robust) outlier detection for compositional data, (robust) principal component analysis for compositional data, (robust) factor analysis for compositional data, (robust) discriminant analysis for compositional data (Fisher rule), robust regression with compositional predictors and (robust) Anderson-Darling normality tests for compositional data as well as popular log-ratio transformations (addLR, cenLR, isomLR, and their inverse transformations). In addition, visualisation and diagnostic tools are implemented as well as high and low-level plot functions for the ternary diagram.

License GPL (>= 2)

LazyLoad yes

LazyData true

RoxygenNote 6.0.1

NeedsCompilation yes

Author Matthias Templ [aut, cre],
   Karel Hron [aut],
   Peter Filzmoser [aut],
   Petra Kynclova [ctb],
   Jan Walach [ctb],
Veronika Pintar [ctb],
Jiajia Chen [ctb]

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The package contains methods for imputation of compositional data including robust methods, (robust) outlier detection for compositional data, (robust) principal component analysis for compositional data, (robust) factor analysis for compositional data, (robust) discriminant analysis (Fisher rule) and (robust) Anderson-Darling normality tests for compositional data as well as popular log-ratio transformations (alr, clr, ilr, and their inverse transformations).

Details

Package: robCompositions
Type: Package
Version: 1.3.3
Date: 2009-11-28
License: GPL 2
LazyLoad: yes

Author(s)

Matthias Templ, Peter Filzmoser, Karel Hron,
Maintainer: Matthias Templ <templ@tuwien.ac.at>
References


Examples

```r
## k nearest neighbor imputation
data(expenditures)
expenditures[1,3]
expenditures[1,3] <- NA
impKNNa(expenditures)$Imp[1,3]

## iterative model based imputation
data(expenditures)
x <- expenditures
x[1,3]
x[1,3] <- NA
xi <- impCoda(x)$Imp
xi[1,3]
s1 <- sum(xi[1,-3])
impS <- sum(xi[1,-3])
xi[,3] * s1/impS

xi <- impKNNa(expenditures)
xi
summary(xi)
## Not run: plot(xi, which=1)
plot(xi, which=2)
plot(xi, which=3)

## pca
data(expenditures)
p1 <- pcaCoDa(expenditures)
p1
plot(p1)
```

## outlier detection
addLR

Additive log-ratio transformation

Description

The additive log-ratio transformation moves D-part compositional data from the simplex into a (D-1)-dimensional real space.

Usage

```
addLR(x, ivar = ncol(x), base = exp(1))
```

Arguments

- **x**: D-part compositional data
- **ivar**: Rationing part
- **base**: a positive or complex number: the base with respect to which logarithms are computed. Defaults to `exp(1)`. 

Details
The compositional parts are divided by the rationing part before the logarithm is taken.

Value
A list of class “alr” which includes the following content:

- `x.alr`: the transformed data
- `varx`: the rationing variable
- `ivar`: the index of the rationing variable, indicating the column number of the rationing variable in the data matrix `x`
- `cnames`: the column names of `x`

The additional information such as `cnames` or `ivar` is useful when a back-transformation is applied on the `same` data set.

Author(s)
Matthias Templ

References

See Also
`addLRinv`, `pivotCoord`

Examples
```r
data(arcticLake)
x <- arcticLake
x.alr <- addLR(x, 2)
y <- addLRinv(x.alr)
## This exactly fulfills:
addLRinv(addLR(x, 3))
data(expenditures)
x <- expenditures
y <- addLRinv(addLR(x, 5))
head(x)
head(y)
## --> absolute values are preserved as well.

## preserve only the ratios:
addLRinv(x.alr, ivar=2, useClassInfo=FALSE)
```
addLRinv

Additive logistic transformation

**Description**

Inverse additive log-ratio transformation, often called additive logistic transformation.

**Usage**

```r
addLRinv(x, cnames = NULL, ivar = NULL, useClassInfo = TRUE)
```

**Arguments**

- **x**
  - data set, object of class “alr”, “matrix” or “data.frame”
- **cnames**
  - column names. If the object is of class “alr” the column names are chosen from therein.
- **ivar**
  - index of the rationing part. If the object is of class “alr” the column names are chosen from therein. If not and ivar is not provided by the user, it is assumed that the rationing part was the last column of the data in the simplex.
- **useClassInfo**
  - if FALSE, the class information of object x is not used.

**Details**

The function allows also to preserve absolute values when class info is provided. Otherwise only the relative information is preserved.

**Value**

the transformed data matrix

**Author(s)**

Matthias Templ

**References**


**See Also**

`pivotCoordInv`, `cenLRinv`, `cenLR`, `addLR`
Examples

data(arcticLake)
x <- arcticLake
x/alr <- addLR(x, 2)
y <- addLRinv(x/alr)
## This exactly fulfills:
addLRinv(addLR(x, 3))
data(expenditures)
x <- expenditures
y <- addLRinv(addLR(x, 5, 2))
head(x)
head(y)
## --> absolute values are preserved as well.

## preserve only the ratios:
addLRinv(x/alr, ivar=2, useClassInfo=FALSE)

---

**aDist**

*Aitchison distance*

Description

Computes the Aitchison distance between two observations, between two data sets or within observations of one data set.

Usage

\[
aDist(x, y = \text{NULL})
\]

\[
\text{iprod}(x, y)
\]

Arguments

- **x**: a vector, matrix or data.frame
- **y**: a vector, matrix or data.frame with equal dimension as x or NULL.

Details

This distance measure accounts for the relative scale property of the Aitchison distance. It measures the distance between two compositions if x and y are vectors. It evaluates the sum of the distances between x and y for each row of x and y if x and y are matrices or data frames. It computes a n times n distance matrix (with n the number of observations/compositions) if only x is provided.

The underlying code is partly written in C and allows a fast computation also for large data sets whenever y is supplied.
Value

The Aitchison distance between two compositions or between two data sets, or a distance matrix in case codey is not supplied.

Author(s)

Matthias Templ, Bernhard Meindl

References


See Also

pivotCoord

Examples

data(expenditures)
x <- xOrig <- expenditures
## Aitchison distance between two 2 observations:
adist(x[1, ], x[2, ])

## Aitchison distance of x:
adist(x)

## Example of distances between matrices:
## set some missing values:

## impute them:
xImp <- impCoda(x, method="ltsReg")$xImp

## calculate the relative Aitchison distance between xOrig and xImp:
/adist(xOrig, xImp)

data("expenditures")
adist(expenditures)
x <- expenditures[, 1]
y <- expenditures[, 2]
adist(x, y)
adist(expenditures, expenditures)
Description

Results from the model based iterative methods provides the results in another scale (but the ratios are still the same). This function rescale the output to the original scale.

Usage

adjust(x)

Arguments

x object from class ‘imp’

Details

It is self-explaining if you try the examples.

Value

The object of class ‘imp’ but with the adjusted imputed data.

Author(s)

Matthias Templ

References


See Also

impCoda

Examples

data(expenditures)
x <- expenditures
xi <- impCoda(x)
x xi$xImp
adjust(xi)$xImp
Description

This function provides three kinds of Anderson-Darling Normality Tests (Anderson and Darling, 1952).

Usage

\[
adtest(x, R = 1000, locscatt = "standard")
\]

Arguments

- `x` either a numeric vector, or a data.frame, or a matrix
- `R` Number of Monte Carlo simulations to obtain p-values
- `locscatt` standard for classical estimates of mean and (co)variance. robust for robust estimates using `covMcd()` from package robustbase

Details

Three version of the test are implemented (univariate, angle and radius test) and it depends on the data which test is chosen.

If the data is univariate the univariate Anderson-Darling test for normality is applied.

If the data is bivariate the angle Anderson-Darling test for normality is performed out.

If the data is multivariate the radius Anderson-Darling test for normality is used.

If `locscatt` is equal to “robust” then within the procedure, robust estimates of mean and covariance are provided using `covMcd()` from package robustbase.

To provide estimates for the corresponding p-values, i.e. to compute the probability of obtaining a result at least as extreme as the one that was actually observed under the null hypothesis, we use Monte Carlo techniques where we check how often the statistic of the underlying data is more extreme than statistics obtained from simulated normal distributed data with the same (column-wise-) mean(s) and (co)variance.

Value

- `statistic` The result of the corresponding test statistic
- `method` The chosen method (univariate, angle or radius)
- `p.value` p-value

Note

These functions are use by `adtestWrapper`. 
**adtestWrapper**

**Description**

A set of Anderson-Darling tests (Anderson and Darling, 1952) are applied as proposed by Aitchison (Aichison, 1986).

**Usage**

```r
adtestWrapper(x, alpha = 0.05, R = 1000, robustEst = FALSE)
```

### Examples

```r
adtest(rnorm(100))
data(machineOperators)
x <- machineOperators
adtest(pivotCoord(x[,1:2]))
adtest(pivotCoord(x[,1:3]))
adtest(pivotCoord(x))
adtest(pivotCoord(x[,1:2]), locscatt="robust")
```

**Arguments**

- `x` : compositional data of class data.frame or matrix
- `alpha` : significance level
- `R` : Number of Monte Carlo simulations in order to provide p-values.

**Author(s)**

Karel Hron, Matthias Templ

**References**


**See Also**

`adtestWrapper`
Details

First, the data is transformed using the ‘ilr’-transformation. After applying this transformation
- all (D-1)-dimensional marginal, univariate distributions are tested using the univariate Anderson-
  Darling test for normality.
- all 0.5 (D-1)(D-2)-dimensional bivariate angle distributions are tested using the Anderson-Darling
  angle test for normality.
- the (D-1)-dimensional radius distribution is tested using the Anderson-Darling radius test for nor-
  mality.

A print and a summary method are implemented. The latter one provides a similar output is pro-
posed by (Pawlowsky-Glahn, et al. (2008). In addition to that, p-values are provided.

Value

- `res` a list including each test result
- `check` information about the rejection of the null hypothesis
- `alpha` the underlying significance level
- `info` further information which is used by the print and summary method.
- `est` “standard” for standard estimation and “robust” for robust estimation

Author(s)

Matthias Templ and Karel Hron

References


Aitchison, J. (1986) The Statistical Analysis of Compositional Data Monographs on Statistics and

See Also

adtest, pivotCoord

Examples

data(machineOperators)
a <- adtestWrapper(machineOperators, R=50) # choose higher value of R
a
summary(a)
ageCatWorld  

child, middle and elderly population

Description

Percentages of childs, middle generation and elderly population in 195 countries.

Usage

data(ageCatWorld)

Format

A data frame with 195 rows and 4 variables

Details

- <15 Percentage of people with age below 15
- 15-60 Percentage of people with age between 15 and 60
- 60+ Percentage of people with age above 60
- country country of origin

The rows sum up to 100.

Author(s)

extracted by Karel Hron and Eva Fiserova, implemented by Matthias Templ

References


Examples

data(ageCatWorld)
str(ageCatWorld)
summary(ageCatWorld)
rowSums(ageCatWorld[, 1:3])
ternaryDiag(ageCatWorld[, 1:3])
plot(pivotCoord(ageCatWorld[, 1:3]))
Description

- **country** Country
- **year** Year
- **beer** Consumption of pure alcohol on beer (in percentages)
- **wine** Consumption of pure alcohol on wine (in percentages)
- **spirits** Consumption of pure alcohol on spirits (in percentages)
- **other** Consumption of pure alcohol on other beverages (in percentages)

Usage

data(alcohol)

Format

A data frame with 193 rows and 6 variables

Author(s)

Matthias Templ <matthias.templ@tuwien.ac.at>

Source

Transfered from the World Health Organisation website.

Examples

data("alcohol")
str(alcohol)
summary(alcohol)
alcoholreg  

regional alcohol per capita (15+) consumption by WHO region

Description

- country Country
- year Year
- recorded Recorded alcohol consumption
- unrecorded Unrecorded alcohol consumption

Usage

data(alcoholreg)

Format

A data frame with 6 rows and 4 variables

Author(s)

Matthias Templ <matthias.templ@tuwien.ac.at>

Source

Transfered from the World Health Organisation website.

Examples

data("alcoholreg")
alcoholreg

arcticLake  

arctic lake sediment data

Description

Sand, silt, clay compositions of 39 sediment samples at different water depths in an Arctic lake. This data set can be found on page 359 of the Aitchison book (see reference).

Usage

data(arcticLake)
balances

Format
A data frame with 39 rows and 3 variables

Details
- sand numeric vector of percentages of sand
- silt numeric vector of percentages of silt
- clay numeric vector of percentages of clay
  The rows sum up to 100, except for rounding errors.

Author(s)
Matthias Templ <matthias.templ@tuwien.ac.at>

References

Examples

data(arcticLake)
str(arcticLake)
summary(arcticLake)
rowSums(arcticLake)
ternaryDiag(arcticLake)
plot(pivotCoord(arcticLake))

<table>
<thead>
<tr>
<th>balances</th>
<th>Balance calculation</th>
</tr>
</thead>
</table>

Description
Given a D-dimensional compositional data set and a sequential binary partition, the function bal calculates the balances in order to express the given data in the (D-1)-dimensional real space.

Usage
balances(x, y)

Arguments
- x data frame or matrix, typically compositional data
- y binary partition
**Details**

The sequential binary partition constructs an orthonormal basis in the (D-1)-dimensional hyperplane in real space.

**Value**

balances

The balances represent orthonormal coordinates which allow an interpretation in sense of groups of compositional parts. Output is a matrix, the D-1 columns contain balance coordinates of the observations in the rows.

V

A DxD(D-1) contrast matrix associated with the orthonormal basis, corresponding to the sequential binary partition (in clr coordinates).

**Author(s)**

Veronika Pintar, Karel Hron, Matthias Templ

**References**


**Examples**

data(expenditures, package = "robCompositions")
y1 <- data.frame(c(1,1,1,-1,-1),c(1,-1,-1,0,0), c(0,+1,-1,0,0),c(0,0,0,+1,-1))
y2 <- data.frame(c(1,-1,1,-1,-1),c(1,0,-1,0,0), c(1,-1,-1,-1),c(0,-1,0,1,0))
y3 <- data.frame(c(1,1,1,-1,-1),c(-1,-1,-1,+1,0), c(-1,-1,+1,0,0),c(-1,1,0,0,0))
y4 <- data.frame(c(1,1,1,-1,-1),c(0,0,0,-1,1), c(-1,-1,+1,0,0),c(-1,1,0,0,0))
y5 <- data.frame(c(1,1,1,-1,-1),c(-1,-1,+1,0,0), c(0,0,0,-1,1),c(-1,1,0,0,0))
b1 <- balances(expenditures, y1)
b2 <- balances(expenditures, y5)
b1$balances
b2$balances
data(machineOperators)
sbp <- data.frame(c(1,1,-1,-1),c(-1,+1,0,0), c(0,0,+1,-1))
balances(machineOperators, sbp)
balZav

New average symmetric coordinates

Description

New average symmetric coordinates

Usage

balZav(x)

Arguments

x composition data

Value

Z.av A matrix of new average symmetric coordinates.

Author(s)

Petra Kynclova

biomarker

Description

The function for identification of biomarkers and outlier diagnostics as described in paper "Robust biomarker identification in a two-class problem based on pairwise log-ratios"

Usage

biomarker(x, cut = qnorm(0.975, 0, 1), g1, g2, type = "tau", diag = TRUE, plot = FALSE, diag.plot = FALSE)

## S3 method for class 'biomarker'
plot(x, cut = qnorm(0.975, 0, 1), type = "Vstar", ...)

## S3 method for class 'biomarker'
print(x, ...)

## S3 method for class 'biomarker'
summary(object, ...)
**Arguments**

- **x**
  - data frame
- **cut**
  - cut-off value, initially set as 0.975 quantile of standard normal distribution
- **g1**
  - vector with locations of observations of group 1
- **g2**
  - vector with locations of observations of group 2
- **type**
  - type of estimation of the variation matrix. Possible values are "sd", "mad" and "tau", representing Standard deviation, Median absolute deviation and Tau estimator of scale
- **diag**
  - logical, indicating whether outlier diagnostic should be computed
- **plot**
  - logical, indicating whether Vstar values should be plotted
- **diag.plot**
  - logical, indicating whether outlier diagnostic plot should be made
- **...**
  - further arguments can be passed through
- **object**
  - object of class biomarker

**Details**

Robust biomarker identification and outlier diagnostics

The method computes variation matrices separately with observations from both groups and also together with all observations. Then, \( V \) statistics is then computed and normalized. The variables, for which according \( V^* \) values are bigger than the cut-off value are considered as biomarkers.

**Value**

The function returns object of type "biomarker". Functions `print`, `plot` and `summary` are available.

- **biom.ident**
  - List of \( V \), \( V^* \), biomarkers
- **V**
  - Values of \( V \) statistics
- **Vstar**
  - Normalizes values of \( V \) statistics (\( V^* \) values))
- **biomarkers**
  - Logical value, indicating if certain variable was identified as biomarker
- **diag**
  - Outlier diagnostics (returned only if `diag=TRUE`)

**Author(s)**

Jan Walach

**See Also**

`plot.biomarker`
Examples

```r
# Data simulation
set.seed(4523)
n <- 40; p <- 50
r <- runif(p, min = 1, max = 10)
conc <- runif(p, min = 0, max = 1)*5+matrix(1,p,1)*5
a <- conc*r
S <- rnorm(n,0,0.3) %*% t(rep(1,p))
B <- matrix(rnorm(n*p,0,0.8),n,p)
R <- rep(1,n) %*% t(r)
M <- matrix(rnorm(n*p,0,0.021),n,p)
# Fifth observation is an outlier
M[5,] <- M[5,]*3 + sample(c(0.5,-0.5),replace=TRUE,p)
C <- rep(1,n) %*% t(conc)
C[1:20,c(2,15,28,40)] <- C[1:20,c(2,15,28,40)]+matrix(1,20,4)*1.8
X <- (1-S)*(C*R+B)*exp(M)
# Biomarker identification
b <- biomarker(X, g1 = 1:20, g2 = 21:40, type = "tau")
```

---

**biplot.factanal**  
**Biplot method**

**Description**

Provides robust compositional biplots.

**Usage**

```r
## S3 method for class 'factanal'
biplot(x, ...)
```

**Arguments**

- `x`  
  object of class ‘factanal’

- `...`  

**Details**

The robust compositional biplot according to Aitchison and Greenacre (2002), computed from resulting (robust) loadings and scores, is performed.

**Value**

The robust compositional biplot.

**Author(s)**

M. Templ, K. Hron
biplot.pcaCoDa

References

See Also
pfa

Examples
\begin{verbatim}
data(expenditures)
res.rob <- pfa(expenditures, factors=2, scores = "regression")
biplot(res.rob)
\end{verbatim}

Description
Provides robust compositional biplots.

Usage
\begin{verbatim}
## S3 method for class 'pcaCoDa'
biplot(x, y, ...)
\end{verbatim}

Arguments
\begin{description}
\item[x] object of class `pcaCoDa`
\item[y] ...
\item[...] arguments passed to plot methods
\end{description}

Details
The robust compositional biplot according to Aitchison and Greenacre (2002), computed from (robust) loadings and scores resulting from *pcaCoDa*, is performed.

Value
The robust compositional biplot.

Author(s)
M. Templ, K. Hron
References


See Also

`pcaCoDa, plot.pcaCoDa`

Examples

```r
data(coffee)
p1 <- pcaCoDa(coffee[, -1])
p1
biplot(p1)
```

```r
## with labels for the scores:
data(arcticLake)
rownames(arcticLake) <- paste(sample(letters[1:26], nrow(arcticLake), replace=TRUE),
                               1:nrow(arcticLake), sep="")
pc <- pcaCoDa(arcticLake, method="classical")
biplot(pc, xlabs=rownames(arcticLake))
```

---

**boonComp**

*Bootstrap to find optimal number of components*

Description

Combined bootstrap and cross validation procedure to find optimal number of PLS components

Usage

```r
boonComp(X, y, R = 99, plotting = FALSE)
```

Arguments

- `X` predictors as a matrix
- `y` response
- `R` number of bootstrap replicates
- `plotting` if TRUE, a diagnostic plot is drawn for each bootstrap replicate
Details

Heavily used internally in function \texttt{impRZilr}.

Value

Including other information in a list, the optimal number of components

Author(s)

Matthias Templ

See Also

\texttt{impRZilr}

Examples

\begin{verbatim}
## we refer to impRZilr()
\end{verbatim}

\begin{verbatim}
cancer

hospital discharges on cancer and distribution of age

<table>
<thead>
<tr>
<th>cancer</th>
</tr>
</thead>
<tbody>
<tr>
<td>hospital discharges on cancer and distribution of age</td>
</tr>
</tbody>
</table>

Description

Hospital discharges of in-patients on neoplasms (cancer) per 100,000 inhabitants (year 2007) and population age structure.

Format

A data set on 24 compositions on 6 variables.

Details

- \texttt{country}
- \texttt{year}
- \texttt{p1} percentage of population with age below 15
- \texttt{p2} percentage of population with age between 15 and 60
- \texttt{p3} percentage of population with age above 60
- \texttt{discharges} hospital discharges of in-patients on neoplasms (cancer) per 100,000 inhabitants

The response (discharges) is provided for the European Union countries (except Greece, Hungary and Malta) by Eurostat. As explanatory variables we use the age structure of the population in the same countries (year 2008). The age structure consists of three parts, age smaller than 15, age between 15 and 60 and age above 60 years, and they are expressed as percentages on the overall population in the countries. The data are provided by the United Nations Statistics Division.
Author(s)
conversion to R by Karel Hron and Matthias Templ <matthias.templ@tuwien.ac.at>

Source

References

Examples

data(cancer)
str(cancer)

---

cancerMN    malignant neoplasms cancer

Description
Two main types of malignant neoplasms cancer affecting colon and lung, respectively, in male and female populations. For this purpose population data (2012) from 35 OECD countries were collected.

Format
A data set on 35 compositional tables on 4 parts (row-wise sorted cells) and 5 variables.

Details
- country
- females-colon number of colon cancer cases in female population
- females-lung number of lung cancer cases in female population
- males-colon number of colon cancer cases in male population
- males-lung number of lung cancer cases in male population

The data are obtained from the OECD website.

Author(s)
conversion to R by Karel Hron and integration by Matthias Templ <matthias.templ@tuwien.ac.at>

Source
http://www.oecd.org
ced

Examples

data(cancerMN)
head(cancerMN)
rowSums(cancerMN[, 2:5])

ced                      compositional error deviation

Description
Normalized Aitchison distance between two data sets

Usage
ced(x, y, ni)

Arguments
x      matrix or data frame
y      matrix or data frame of the same size as x
ni     normalization parameter. See details below.

Details
This function has been mainly written for procedures that evaluate imputation or replacement of rounded zeros. The ni parameter can thus, e.g. be used for expressing the number of rounded zeros.

Value
the compositiona error distance

Author(s)
Matthias Templ

References

See Also
rdcm
Description

The cenLR transformation moves D-part compositional data from the simplex into a D-dimensional real space.

Usage

cenLR(x, base = exp(1))

Arguments

  x        multivariate data ideally of class data.frame or matrix
  base     a positive or complex number: the base with respect to which logarithms are computed. Defaults to exp(1).

Details

  Each composition is divided by the geometric mean of its parts before the logarithm is taken.

Value

  The transformed data, including

  x.clr       clr transformed data
  gm          the geometric means of the original composition.

Note

  The resulting transformed data set is singular by definition.

Author(s)

  Matthias Templ

References

See Also

cenLRinv, addLR, pivotCoord, addLRinv, pivotCoordInv

Examples

data(expenditures)
eclr <- cenLR(expenditures)
inveclr <- cenLRinv(eclr)
head(expenditures)
head(inveclr)
head(pivotCoordInv(eclr$x$clr))
Examples

data(expenditures)
eclr <- cenLR(expenditures, 2)
inveclr <- cenLRinv(eclr)
head(expenditures)
head(inveclr)
head(cenLRinv(eclr$x.clr))

chorizonDL

C-horizon of the Kola data with rounded zeros

Description

This data set is almost the same as chorizon data set in package mvoutlier and chorizonDL, except that values below the detection limit are coded as zeros, and detection limits provided as attributes to the data set and less variables are included.

Format

A data frame with 606 observations on the following 62 variables.

*ID  a numeric vector
XCOO  a numeric vector
YCOO  a numeric vector
Ag  concentration in mg/kg
Al  concentration in mg/kg
Al_XRF  concentration in wt. percentage
As  concentration in mg/kg
Ba  concentration in mg/kg
Ba_INAA  concentration in mg/kg
Be  concentration in mg/kg
Bi  concentration in mg/kg
Ca  concentration in mg/kg
Ca_XRF  concentration in wt. percentage
Cd  concentration in mg/kg
Ce_INAA  concentration in mg/kg
Co  concentration in mg/kg
Co_INAA  concentration in mg/kg
Cr  concentration in mg/kg
Cr_INAA  concentration in mg/kg
<table>
<thead>
<tr>
<th>Element</th>
<th>Concentration Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Eu_INAA</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Fe</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Fe_XRF</td>
<td>concentration in wt. percentage</td>
</tr>
<tr>
<td>Hf_INAA</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>K</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>K_XRF</td>
<td>concentration in wt. percentage</td>
</tr>
<tr>
<td>La</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>La_INAA</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Li</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Lu_INAA</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Mg</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Mg_XRF</td>
<td>concentration in wt. percentage</td>
</tr>
<tr>
<td>Mn</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Mn_XRF</td>
<td>concentration in wt. percentage</td>
</tr>
<tr>
<td>Na</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Na_XRF</td>
<td>concentration in wt. percentage</td>
</tr>
<tr>
<td>Nd_INAA</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Ni</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>P</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>P_XRF</td>
<td>concentration in wt. percentage</td>
</tr>
<tr>
<td>Pb</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>S</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Sc</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Sc_INAA</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Si</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Si_XRF</td>
<td>concentration in wt. percentage</td>
</tr>
<tr>
<td>Sm_INAA</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Sr</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Th_INAA</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Ti</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Ti_XRF</td>
<td>concentration in wt. percentage</td>
</tr>
<tr>
<td>V</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Y</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Yb_INAA</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>Zn</td>
<td>concentration in mg/kg</td>
</tr>
<tr>
<td>LOI</td>
<td>concentration in wt. percentage</td>
</tr>
</tbody>
</table>
**clustCoDa**

- **pH** ph value
- **ELEV** elevation
- **COUN** country
- **ASP** a numeric vector
- **TOPC** a numeric vector
- **LITO** information on lithography

**Note**

For a more detailed description of this data set, see *chorizon* in package *mvoutlier*.

**Source**


**References**


**See Also**

*chorizon, chorizondL*

**Examples**

```r
data(chorizondL, package = "robCompositions")
dim(chorizondL)
colnames(chorizondL)
zeroPatterns(chorizondL)
```

---

**clustCoDa**  
*Cluster analysis for compositional data*

**Description**

Clustering in orthonormal coordinates or by using the Aitchison distance

**Usage**

```r
clustCoDa(x, k = NULL, method = "Mclust", scale = "robust",
          transformation = "pivotCoord", distMethod = NULL, iter.max = 100,
          vals = TRUE, alt = NULL, bic = NULL, verbose = TRUE)
```

```r
## S3 method for class 'clustCoDa'
plot(x, y, ..., normalized = FALSE,
     which.plot = "clusterMeans", measure = "silwidths")
```
**Arguments**

- **x**: compositional data represented as a data.frame
- **k**: number of clusters
- **method**: clustering method. One of Mclust, cmeans, kmeansHartigan, cmeansUfcl, pam, clara, fanny, ward.D2, single, hclustComplete, average, mcquitty, median, centroid
- **scale**: If orthonormal coordinates should be normalized.
- **transformation**: default is the isometric log-ratio transformation. Can only used when distMethod is not Aitchison.
- **distMethod**: Distance measure to be used. If “Aitchison”, then transformation should be “identity”.
- **iter.max**: parameter if kmeans is chosen. The maximum number of iterations allowed
- **vals**: if cluster validity measures should be calculated
- **alt**: a known partitioning can be provided (for special cluster validity measures)
- **bic**: if TRUE then the BIC criteria is evaluated for each single cluster as validity measure
- **verbose**: if TRUE additional print output is provided
- **y**: the y coordinates of points in the plot, optional if x is an appropriate structure.
- **NNN**: additional parameters for print method passed through
- **normalized**: results gets normalized before plotting. Normalization is done by z-transformation applied on each variable.
- **which.plot**: currently the only plot. Plot of cluster centers.
- **measure**: cluster validity measure to be considered for which.plot equals “partMeans”

**Details**

The compositional data set is either internally represented by orthonormal coordiantes before a cluster algorithm is applied, or - depending on the choice of parameters - the Aitchison distance is used.

**Value**

all relevant information such as cluster centers, cluster memberships, and cluster statistics.

**Author(s)**

Matthias Templ (accessing the basic features of hclust, Mclust, kmeans, etc. that are all written by others)

**References**


Examples

data(expenditures)
x <- expenditures
rr <- clustCoDa(x, k=6, scale = "robust", transformation = "pivotCoord")
rr2 <- clustCoDa(x, k=6, distMethod = "Aitchison", scale = "none",
    transformation = "identity")
rr3 <- clustCoDa(x, k=6, distMethod = "Aitchison", method = "single",
    transformation = "identity", scale = "none")
plot(rr)
plot(rr, normalized = TRUE)
plot(rr, normalized = TRUE, which.plot = "partMeans")

Description

Clustering in using the variation matrix of compositional parts

Usage

clustCoDa_qmode(x, method = "ward.D2")

Arguments

x  compositional data represented as a data.frame
method  hclust method

Value

a hclust object

Author(s)

Matthias Templ (accessing the basic features of hclust that are all written by other authors)

References


Examples

data(expenditures)
x <- expenditures
c1 <- clustCoDa_qmode(x)
plot(c1)
c12 <- clustCoDa_qmode(x, method = "single")
plot(c12)
### Description

30 commercially available coffee samples of different origins.

### Usage

data(coffee)

### Format

A data frame with 30 observations and 7 variables.

### Details

- sort sort of coffee
- acit acetic acid
- metpyr methylpyrazine
- furfu furfural
- furfualc furfuryl alcohol
- dimeth 2,6 dimethylpyrazine
- met5 5-methylfurfural

In the original data set, 15 volatile compounds (descriptors of coffee aroma) were selected for a statistical analysis. We selected six compounds (compositional parts) on three sorts of coffee.

### Author(s)

Matthias Templ <matthias.templ@tuwien.ac.at>, Karel Hron

### References


### Examples

data(coffee)
str(coffee)
supply(coffee)
compareMahal

Compares Mahalanobis distances from two approaches

Description

Mahalanobis distances are calculated for each zero pattern. Two approaches are used. The first one estimates Mahalanobis distance for observations belonging to one each zero pattern each. The second method uses a more sophisticated approach described below.

Usage

```r
compareMahal(x, imp = "KNNa")
```

```r
## S3 method for class 'mahal'
plot(x, y, ...)
```

Arguments

- `x`: data frame or matrix
- `imp`: imputation method
- `y`: unused second argument for the plot method
- `...`: additional arguments for plotting passed through

Value

- `df`: a data frame containing the Mahalanobis distances from the estimation in subgroups, the Mahalanobis distances from the imputation and covariance approach, an indicator specifying outliers and an indicator specifying the zero pattern
- `df2`: a groupwise statistics.

Author(s)

Matthias Templ, Karel Hron

References


See Also

`impKNNa`, `pivotCoord`
**Examples**

```r
data(arcticLake)
  # generate some zeros
  arcticLake[1:10, 1] <- 0
  arcticLake[11:20, 2] <- 0
  m <- compareMahal(arcticLake)
  plot(m)
```

---

**Description**

Closes compositions to sum up to a given constant (default 1), by dividing each part of a composition by its row sum.

**Usage**

```r
costSum(x, const = 1, na.rm = TRUE)
```

**Arguments**

- `x`: multivariate data ideally of class data.frame or matrix
- `const`: constant, the default equals 1.
- `na.rm`: removing missing values.

**Value**

The data for which the row sums are equal to `const`.

**Author(s)**

Matthias Templ

**Examples**

```r
data(expenditures)
costSum(expenditures)
costSum(expenditures, 100)
```
coord  

Coordinate representation of CoDa tables

Description

General approach to orthonormal coordinates for compositional tables

Usage

coord(x, SBPr, SBPc)

## S3 method for class 'coord'
print(x, ...)

Arguments

x  an object of class “table”, “data.frame” or “matrix”
SBPr sequential binary partition for rows
SBPc sequential binary partition for columns
... further arguments passed to the print function

Details

A contingency or propability table is by definition a compositional data set. This approach consider the related special properties of compositional tables. It constructs orthonomal coordinates for compositional tables using the isometric log-ratio approach for given sequential binary partitions on rows and columns.

Value

Row and column balances, odds ratios, particularly

row_balances  row balances
row_bin  binary partition for rows
col_balances  column balances
col_bin  binary partition for columns
odds_ratios_coord  odds ratio coordinates

Author(s)

Kamila Facevicova, and minor adaption by Matthias Templ

References

Kamila Facevicova, Karel Hron, Valentin Todorov, Matthias Templ (201x) General approach to coordinate representation of compositional tables. Submitted to JRSS B.
Examples

```r
x <- rbind(c(1,5,3,6,8,4), c(6,4,9,5,8,12), c(15,2,68,42,11,6),
           c(20,15,4,6,23,8), c(11,20,35,26,44,8))
x
SBPc <- rbind(c(1,1,1,1,-1,-1), c(1,-1,-1,1,0,0), c(0,1,1,1,0,0),
              c(0,1,-1,0,0,0), c(0,0,0,0,1,-1))
SBPc
SBPr <- rbind(c(1,1,1,-1,-1), c(1,1,-1,0,0), c(1,-1,0,0,0), c(0,0,0,1,-1))
SBPr
result <- coord(x, SBPr, SBPc)
result
data(socExp)
```

Description

This function computes correlation coefficients between compositional parts based on symmetric balances.

Usage

```r
corcoda(x, ...)
```

Arguments

- `x`: a matrix or data frame with compositional data
- `...`: additional arguments for the function `cor`

Value

A compositional correlation matrix.

Author(s)

Petra Kynclova

References

Kynclova, P., Hron, K., Filzmoser, P. Correlation between compositional parts based on symmetric balances. Submitted to *Mathematical Geosciences*. 
**Examples**

```r
data(expenditures)
corCoDa(expenditures)
x <- arcticLake
corCoDa(x)
```

---

**Description**

Linear and quadratic discriminant analysis for compositional data using either robust or classical estimation.

**Usage**

```r
daCoDa(x, grp, coda = TRUE, method = "classical", rule = "linear", ...)
```

**Arguments**

- `x`: a matrix or data frame containing the explanatory variables
- `grp`: grouping variable: a factor specifying the class for each observation.
- `coda`: TRUE, when the underlying data are compositions.
- `method`: "classical" or "robust"
- `rule`: a character, either "linear" (the default) or "quadratic".
- `...`: additional arguments for the functions passed through

**Details**

An ilr-transformation is applied to compositional data (if `coda==TRUE`). For linear discriminant analysis the functions LdaClassic (classical) and Linda (robust) from the package rrcov are used. Similarly, quadratic discriminant analysis uses the functions QdaClassic and QdaCov (robust) from the same package.

The classical linear and quadratic discriminant rules are invariant to ilr and clr transformations. The robust rules are invariant to ilr transformations if affine equivariant robust estimators of location and covariance are taken.

**Value**

An S4 object of class LdaClassic, Linda, QdaClassic or QdaCov. See package rrcov for details.

**Author(s)**

Jutta Gamper
References


See Also

LdaClassic, Linda, QdaClassic, QdaCov

Examples

```r
## toy data (non-compositional)
require(MASS)
x1 <- mvrnorm(20,c(0,0,0),diag(3))
x2 <- mvrnorm(30,c(3,0,0),diag(3))
x3 <- mvrnorm(40,c(0,3,0),diag(3))
X <- rbind(x1,x2,x3)
grp=c(rep(1,20),rep(2,30),rep(3,40))
clas1 <- daCoDa(X, grp, coda=FALSE, method = "classical", rule="linear")
summary(clas1)
## predict runs only with newest verison of rrcov
## Not run:
predict(clas1)

## End(Not run)
# specify different prior probabilities
clas2 <- daCoDa(X, grp, coda=FALSE, prior=c(1/3, 1/3, 1/3))
summary(clas2)

## compositional data
data(coffee)
x <- coffee[coffee$sort!="robusta",2:7]
group <- droplevels(coffee$sort[coffee$sort!="robusta"])
cof.cla <- daCoDa(x, group, method="classical", rule="quadratic")
cof.rob <- daCoDa(x, group, method="robust", rule="quadratic")
## predict runs only with newest verison of rrcov
## Not run:
predict(cof.cla)@ct
predict(cof.rob)@ct

## End(Not run)
```

**daFisher**

*Discriminant analysis by Fisher Rule.*

**Description**

Discriminant analysis by Fishers rule using CoDa methods.
Usage

daFisher(x, grp, coda = TRUE, method = "classical", plotScore = FALSE, 
...)

## S3 method for class 'daFisher'
print(x, ...)

## S3 method for class 'daFisher'
predict(object, ..., newdata)

## S3 method for class 'daFisher'
summary(object, ...)

Arguments

x            a matrix or data frame containing the explanatory variables (training set)
grp          grouping variable: a factor specifying the class for each observation.
coda         TRUE, when the underlying data are compositions.
method        "classical" or "robust" estimation.
plotScore     TRUE, if the scores should be plotted automatically.
...           additional arguments for the print method passed through
object        object of class “daFisher”
newdata       new data in the appropriate form (CoDa, etc)

Details

The Fisher rule leads only to linear boundaries. However, this method allows for dimension reduction and thus for a better visualization of the separation boundaries. For the Fisher discriminant rule (Fisher, 1938; Rao, 1948) the assumption of normal distribution of the groups is not explicitly required, although the method looses its optimality in case of deviations from normality.

The classical Fisher discriminant rule is invariant to ilr and clr transformations. The robust rule is invariant to ilr transformations if affine equivariant robust estimators of location and covariance are taken.

Robustification is done (method “robust”) by estimating the columnwise means and the covariance by the Minimum Covariance Estimator.

Value

an object of class “daFisher” including the following elements

B            Between variance of the groups
W            Within variance of the groups
loadings     loadings
scores       fisher scores
mc           table indicating misclassifications
mcrate     misclassification rate
coda       coda
grp        grouping
grppred    predicted groups
xc          xc
meanj      meanj
cv          cv
pj          pj
meanov    meanov
fdiscr     fdiscr

Author(s)

Peter Filzmoser, Matthias Templ.

References


See Also

Linda

Examples

```r
## toy data (non-compositional)
require(MASS)
x1 <- mvrnorm(20,c(0,0,0),diag(3))
x2 <- mvrnorm(20,c(3,0,0),diag(3))
x3 <- mvrnorm(20,c(0,3,0),diag(3))
X <- rbind(x1,x2,x3)
grp=c(rep(1,20),rep(2,20),rep(3,20))

#par(mfrow=c(1,2))
d1 <- daFisher(X,grp=grp,method="classical",coda=FALSE)
d2 <- daFisher(X,grp=grp,method="robust",coda=FALSE)
d2
summary(d2)
predict(d2, newdata = X)

## example with olive data:
## Not run:
```
data(olive, package = "RnaiveGraph")
# exclude zeros (alternatively impute them if
# the detection limit is known using impRZlr())
ind <- which(olive == 0, arr.ind = TRUE)[,1]
olives <- olive[-ind, ,]
x <- olives[, 4:10]
grp <- olives$Region # 3 groups
res <- daFisher(x, grp)
res
summary(res)
res <- daFisher(x, grp, plotScore = TRUE)
res
summary(res)
predict(res, newdata = x)
res <- daFisher(x, grp, plotScore = TRUE, method = "robust")
res
summary(res)
predict(res, newdata = x)

# 9 regions
grp <- olives$Area
res <- daFisher(x, grp, plotScore = TRUE)
res
summary(res)
predict(res, newdata = x)

## End(Not run)

economy economic indicators

Description
Household and government consumptions, gross captial formation and import and exports of goods
and services.

Usage
data(economy)

Format
A data frame with 30 observations and 7 variables

Details
- country  country name
- country2 country name, short version
- HHconsumption Household and NPISH final consumption expenditure
- GOVconsumption Final consumption expenditure of general government


- capital  Gross capital formation  
- exports  Exports of goods and services  
- imports  Imports of goods and services  

**Author(s)**

Peter Filzmoser, Matthias Templ <matthias.templ@tuwien.ac.at>

**References**


**Examples**

```r
data(economy)
str(economy)
```

---

**educFM**  
*education level of father (F) and mother (M)*

**Description**

Education level of father (F) and mother (M) in percentages of low (l), medium (m), and high (h) of 31 countries in Europe.

**Usage**

```r
data(educFM)
```

**Format**

A data frame with 31 observations and 8 variables

**Details**

- country  community code
- F.l  percentage of females with low education level
- F.m  percentage of females with medium education level
- F.h  percentage of females with high education level
- F.l  percentage of males with low education level
- F.m  percentage of males with medium education level
- F.h  percentage of males with high education level
Author(s)

Peter Filzmoser, Matthias Templ

Source


Examples

data(election)
str(election)

Description

Results of a election in Germany 2013 in different federal states

Usage

data(election)

Format

A data frame with 16 observations and 8 variables

Details

Votes for the political parties in the elections (compositional variables), and their relation to the unemployment rate and the average monthly income (external non-compositional variables). Votes are for the Christian Democratic Union and Christian Social Union of Bavaria, also called The Union (CDU/CSU), Social Democratic Party (SDP), The Left (DIE LINKE), Alliance ’90/The Greens (GRUENE), Free Democratic Party (FDP) and the rest of the parties participated in the elections (other parties). The votes are examined in absolute values (number of valid votes). The unemployment in the federal states is reported in percentages, and the average monthly income in Euros.

- CDU_CSU Christian Democratic Union and Christian Social Union of Bavaria, also called The Union
- SDP Social Democratic Party
- GRUENE Alliance ’90/The Greens
- FDP Free Democratic Party
- DIE_LINKE The Left
- other_parties Votes for the rest of the parties participated in the elections
- unemployment Unemployment in the federal states in percentages
- income Average monthly income in Euros
**Author(s)**
Petra Klynclova, Matthias Templ

**Source**
German Federal Statistical Office

**References**

**Examples**

```r
data(election)
str(election)
```

---

**Description**
Results the Austrian presidential election in October 2016.

**Usage**

```r
data(electionATbp)
```

**Format**
A data frame with 2202 observations and 10 variables

**Details**
Votes for the candidates Hofer and Van der Bellen.

- **gkz** Community code
- **name** Name of the community
- **eligible** eligible votes
- **votes_total** total votes
- **votes_invalid** invalid votes
- **votes_valid** valid votes
- **hofer_total** votes for Hofer
- **hofer_perc** votes for Hofer in percentages
- **vanderbellen_total** votes for Van der Bellen
- **vanderbellen_perc** votes for Van der Bellen in percentages
Author(s)

Peter Filzmoser

Source

OpenData Austria, https://www.data.gv.at/

Examples

```r
data(electionATbp)
str(electionATbp)
```

<table>
<thead>
<tr>
<th>employment</th>
<th>employment in different countries by gender and status.</th>
</tr>
</thead>
</table>

Description

employment in different countries by gender and status.

Usage

```r
data(employment)
```

Format

A three-dimensional table

Examples

```r
data(employment)
str(employment)
employment
```

<table>
<thead>
<tr>
<th>employment_df</th>
<th>Employment in different countries by gender and status.</th>
</tr>
</thead>
</table>

Description

- genderfactor
- statusfactor, defining if part or full time work
- countrycountry
- valueemployment
expenditures

Usage

data(employment_df)

Format

A data.frame with 132 rows and 4 columns.

Examples

data(employment_df)
head(employment_df)

---

expenditures

Synthetic household expenditures toy data set

---

Description

This data set from Aitchison (1986), p. 395, describes household expenditures (in former Hong Kong dollars) on five commodity groups.

Usage

data(expenditures)

Format

A data frame with 20 observations on the following 5 variables.

Details

- housing  housing (including fuel and light)
- foodstuffs  foodstuffs
- alcohol  alcohol and tobacco
- other  other goods (including clothing, footwear and durable goods)
- services  services (including transport and vehicles)

This data set contains household expenditures on five commodity groups of 20 single men. The variables represent housing (including fuel and light), foodstuff, alcohol and tobacco, other goods (including clothing, footwear and durable goods) and services (including transport and vehicles). Thus they represent the ratios of the men’s income spent on the mentioned expenditures.

Author(s)

Matthias Templ <matthias.templ@tuwien.ac.at>, Karel Hron
References


Examples

```r
data(expenditures)
## imputing a missing value in the data set using k-nearest neighbor imputation:
expenditures[1,3]
expenditures[1,3] <- NA
impKNNa(expenditures)$xImp[1,3]
```

| expendituresEU | mean consumption expenditures data. |

Description

Mean consumption expenditure of households at EU-level. The final consumption expenditure of households encompasses all domestic costs (by residents and non-residents) for individual needs.

Format

A data frame with 27 observations on the following 12 variables.

- Fooda numeric vector
- Alcohola numeric vector
- Clothinga numeric vector
- Housingsa numeric vector
- Furnishingsa numeric vector
- Healtha numeric vector
- Transporta numeric vector
- Communicationsa numeric vector
- Recreationa numeric vector
- Educationa numeric vector
- Restaurantsa numeric vector
- Othera numeric vector

Source

Eurostat

 Examples

```r
data(expendituresEU)
```
**Description**

Satisfaction of GDP in 31 countries. The GDP is measured per capita from the year 2012.

**Usage**

`data(GDPsatis)`

**Format**

A data frame with 31 observations and 8 variables

**Details**

- `country` community code
- `gdp` GDP per capita in 2012
- `very.bad` satisfaction very bad
- `bad` satisfaction bad
- `moderately.bad` satisfaction moderately bad
- `moderately.good` satisfaction moderately good
- `good` satisfaction good
- `very.good` satisfaction very good

**Author(s)**

Peter Filzmoser, Matthias Templ

**Source**


**Examples**

```r
data(GDPsatis)
str(GDPsatis)
```
Description

Geochemical data set on agricultural and grazing land soil

Usage

data(gemas)

Format

A data frame with 2108 observations and 30 variables

Details

- COUNTRY country name
- longitude longitude in WGS84
- latitude latitude in WGS84
- Xcoord UTM zone east
- Ycoord UTM zone north
- MeanTempAnnual mean temperature
- AnnPrec Annual mean precipitation
- soilclass soil class
- sand sand
- silt silt
- clay clay
- Al Concentration of aluminum (in mg/kg)
- Ba Concentration of barium (in mg/kg)
- Ca Concentration of calzium (in mg/kg)
- Cr Concentration of chromium (in mg/kg)
- Fe Concentration of iron (in mg/kg)
- K Concentration of pottasium (in mg/kg)
- Mg Concentration of magnesium (in mg/kg)
- Mn Concentration of manganese (in mg/kg)
- Na Concentration of sodium (in mg/kg)
- Nb Concentration of niobium (in mg/kg)
- Ni Concentration of nickel (in mg/kg)
- P Concentration of phosphorus (in mg/kg)
• Si  Concentration of silicium (in mg/kg)
• Sr  Concentration of strontium (in mg/kg)
• Ti  Concentration of titanium (in mg/kg)
• V   Concentration of vanadium (in mg/kg)
• Y   Concentration of yttrium (in mg/kg)
• Zn  Concentration of zinc (in mg/kg)
• Zr  Concentration of zirconium (in mg/kg)
• LOI Loss on ignition (in wt-percent)

The sampling, at a density of 1 site/2500 sq. km, was completed at the beginning of 2009 by collecting 2211 samples of agricultural soil (Ap-horizon, 0-20 cm, regularly ploughed fields), and 2118 samples from land under permanent grass cover (grazing land soil, 0-10 cm), according to an agreed field protocol. All GEMAS project samples were shipped to Slovakia for sample preparation, where they were air dried, sieved to <2 mm using a nylon screen, homogenised and split to subsamples for analysis. They were analysed for a large number of chemical elements. In this sample, the main elements by X-ray fluorescence are included as well as the composition on sand, silt, clay.

Author(s)

GEMAS is a cooperation project between the EuroGeoSurveys Geochemistry Expert Group and Eurometaux. Integration in R, Peter Filzmoser and Matthias Templ.

References


Examples

data(gemas)
str(gemas)
## sample sites
## Not run:
require(ggmap)
map <- get_map("europe", source = "stamen", maptype = "watercolor", zoom=4)
ggmap(map) + geom_point(aes(x=longitude, y=latitude), data=gemas)
map <- get_map("europe", zoom=4)
ggmap(map) + geom_point(aes(x=longitude, y=latitude), data=gemas, size=0.8)

## End(Not run)
Description

This function calculates the geometric mean.

Usage

gm(x)

Arguments

x a vector

Details

gm calculates the geometric mean for all positive entries of a vector. Please note that there is a faster version available implemented with Rcpp but it currently do not pass CRAN checks cause of use of Rcpp11 features. This C++ version accounts for over- and underflows. It is placed in inst/doc

Author(s)

Matthias Templ

Examples

gm(c(3,5,3,6,7))

gmean_sum

Description

Computes the geometric mean(s) of a numeric vector, matrix or data.frame

Usage

gmean_sum(x, margin = NULL)

gmean(x, margin = NULL)

Arguments

x matrix or data.frame with numeric entries
margin a vector giving the subscripts which the function will be applied over, 1 indicates rows, 2 indicates columns, 3 indicates all values.
Details

gmean_sum calculates the totals based on geometric means while gmean calculates geometric means on rows (margin = 1), on columns (margin = 2), or on all values (margin = 3)

Value

geometric means (if gmean is used) or totals (if gmean_sum is used)

Author(s)

Matthias Templ

Examples

data("precipitation")
gmean_sum(precipitation)
gmean_sum(precipitation, margin = 2)
gmean_sum(precipitation, margin = 1)
gmean_sum(precipitation, margin = 3)
addmargins(precipitation)
addmargins(precipitation, FUN = gmean_sum)
addmargins(precipitation, FUN = mean)
addmargins(precipitation, FUN = gmean)

data("arcticLake", package = "robCompositions")
gmean(arcticLake$sand)
gmean(as.numeric(arcticLake[, ]))
gmean(arcticLake)
gmean(arcticLake, margin = 1)
gmean(arcticLake, margin = 2)
gmean(arcticLake, margin = 3)

Description

Government expenditures based on COFOG categories

Format

A (tidy) data frame with 5140 observations on the following 4 variables.

- country  Country of origin
- category  The COFOG expenditures are divided into the following ten categories: general public services; defence; public order and safety; economic affairs; environmental protection; housing and community amenities; health; recreation, culture and religion; education; and social protection.
- year  Year
- value  COFOG spendings/expenditures
Details

The general government sector consists of central, state and local governments, and the social security funds controlled by these units. The data are based on the system of national accounts, a set of internationally agreed concepts, definitions, classifications and rules for national accounting. The classification of functions of government (COFOG) is used as classification system. The central government spending by category is measured as a percentage of total expenditures.

Author(s)

translated from https://data.oecd.org/ and restructured by Matthias Templ

Source

OECD: https://data.oecd.org/

Examples

data(govexp)
str(govexp)

---

haplogroups

Description

Distribution of European Y-chromosome DNA (Y-DNA) haplogroups by region in percentage.

Format

A data frame with 38 observations on the following 12 variables.

- I1 pre-Germanic (Nordic)
- I2b pre-Celto-Germanic
- I2a1 Sardinian, Basque
- I2a2 Dinaric, Danubian
- N1c1 Uralo-Finnic, Baltic, Siberian
- R1a Balto-Slavic, Mycenaean Greek, Macedonia
- R1b Italic, Celtic, Germanic; Hitite, Armenian
- G2a Caucasian, Greco-Anatolien
- E1b1b North and Eastern Afrika, Near Eastern, Balkanic
- J2 Mesopotamian, Minoan Greek, Phoenician
- J1 Semitic (Arabic, Jewish)
- T Near-Eastern, Egyptian, Ethiopian, Arabic
Details
Human Y-chromosome DNA can be divided in genealogical groups sharing a common ancestor, called haplogroups.

Source
Eupedia: http://www.eupedia.com/europe/european_y-dna_haplogroups.shtml

Examples

data(haplogroups)

| ilr.2x2 | ilr coordinates in 2x2 tables |

Description
ilr coordinates of original, independent and interaction table using SBP1 and SBP2

Usage
ilr.2x2(x, margin = 1, type = "independence", version = "book")

Arguments

x a 2x2 table

margin for 2x2 tables available for a whole set of another dimension. For example, if 2x2 tables are available for every country.

type choose between “independence” or “interaction” table

version the version used in the “paper” below or the version of the upcoming “book”.

Value
The ilr coordinates

Author(s)
Kamila Facevicova, Matthias Templ

References
Examples

```r
data(employment)
ilr.2x2(employment[, "AUT"])
ilr.2x2(employment[, "AUT"], version = "paper")
ilr.2x2(employment, margin = 3, version = "paper")
ilr.2x2(employment[, "AUT"], type = "interaction")
```

---

**impAll**

Replacement of rounded zeros and missing values.

**Description**

Parametric replacement of rounded zeros and missing values for compositional data using classical and robust methods based on ilr-transformations with special choice of balances. Values under detection limit should be saved with the negative value of the detection limit (per variable). Missing values should be coded as NA.

**Usage**

```r
impAll(x)
```

**Arguments**

- `x`: data frame

**Details**

This is a wrapper function that calls `impRZilr()` for the replacement of zeros and `impCoda` for the imputation of missing values sequentially. The detection limit is automatically derived from negative numbers in the data set.

**Value**

The imputed data set.

**Note**

This function is mainly used by the compositionsGUI.

**References**


Description

This function offers different methods for the imputation of missing values in compositional data. Missing values are initialized with proper values. Then iterative algorithms try to find better estimations for the former missing values.

Usage

```
impCoda(x, maxit = 10, eps = 0.5, method = "ltsReg", closed = FALSE,
init = "KNN", k = 5, dl = rep(0.05, ncol(x)), noise = 0.1,
bruteforce = FALSE)
```

Arguments

- **x**: data frame or matrix
- **maxit**: maximum number of iterations
- **eps**: convergence criteria
- **method**: imputation method
- **closed**: imputation of transformed data (using ilr transformation) or in the original space (closed equals TRUE)
- **init**: method for initializing missing values
- **k**: number of nearest neighbors (if init == "KNN")
- **dl**: detection limit(s), only important for the imputation of rounded zeros
- **noise**: amount of adding random noise to predictors after convergency
- **bruteforce**: if TRUE, imputations over dl are set to dl. If FALSE, truncated (Tobit) regression is applied.

Examples

```
## see the compositionsGUI
```

See Also

`impCoda, impRZilr`
Details

eps: The algorithm is finished as soon as the imputed values stabilize, i.e. until the sum of Aitchison distances from the present and previous iteration changes only marginally (eps).

method: Several different methods can be chosen, such as ‘ltsReg’: least trimmed squares regression is used within the iterative procedure. ‘lm’: least squares regression is used within the iterative procedure. ‘classical’: principal component analysis is used within the iterative procedure. ‘ltsReg2’: least trimmed squares regression is used within the iterative procedure. The imputed values are perturbed in the direction of the predictor by values drawn from a normal distribution with mean and standard deviation related to the corresponding residuals and multiplied by noise.

Value

- `xOrig`: Original data frame or matrix
- `xImp`: Imputed data
- `criteria`: Sum of the Aitchison distances from the present and previous iteration
- `iter`: Number of iterations
- `maxit`: Maximum number of iterations
- `w`: Amount of imputed values
- `wind`: Index of the missing values in the data

Author(s)

Matthias Templ, Karel Hron

References


See Also

- `impKNNa`, `pivotCoord`

Examples

```r
data(expenditures)
x <- expenditures
x[1,3]
x[1,3] <- NA
xi <- impCoda(x)$xImp
xi[1,3]
s1 <- sum(x[1,-3])
impS <- sum(xi[1,-3])
xi[,3] * s1/impS
```
Imputation of missing values in compositional data using knn methods

Description

This function offers several k-nearest neighbor methods for the imputation of missing values in compositional data.

Usage

impKNNa(x, method = "knn", k = 3, metric = "Aitchison", agg = "median", primitive = FALSE, normknn = TRUE, das = FALSE, adj = "median")

Arguments

- x: data frame or matrix
- method: method (at the moment, only “knn” can be used)
- k: number of nearest neighbors chosen for imputation
- metric: “Aitchison” or “Euclidean”
- agg: “median” or “mean”, for the aggregation of the nearest neighbors
- primitive: if TRUE, a more enhanced search for the $k$-nearest neighbors is obtained (see details)
- normknn: An adjustment of the imputed values is performed if TRUE
- das: deprecated. if TRUE, the definition of the Aitchison distance, based on simple logratios of the compositional part, is used (Aitchison, 2000) to calculate distances between observations. if FALSE, a version using the clr transformation is used.
- adj: either ‘median’ (default) or ‘sum’ can be chosen for the adjustment of the nearest neighbors, see Hron et al., 2010.

Details

The Aitchison metric should be chosen when dealing with compositional data, the Euclidean metric otherwise.

If primitive == FALSE, a sequential search for the $k$-nearest neighbors is applied for every missing value where all information corresponding to the non-missing cells plus the information in the variable to be imputed plus some additional information is available. If primitive == TRUE, a search of the $k$-nearest neighbors among observations is applied where in addition to the variable to be imputed any further cells are non-missing.

If normknn is TRUE (preferred option) the imputed cells from a nearest neighbor method are adjusted with special adjustment factors (more details can be found online (see the references)).
### Value

- **xOrig**: Original data frame or matrix
- **xImp**: Imputed data
- **w**: Amount of imputed values
- **wind**: Index of the missing values in the data
- **metric**: Metric used

### Author(s)

Matthias Templ

### References


### See Also

- `impCoda`

### Examples

```r
data(expenditures)
x <- expenditures
x[1,3]
x[1,3] <- NA
xi <- impKNNa(x)$xImp
xi[1,3]
```

### Description

A modified EM alr-algorithm for replacing rounded zeros in compositional data sets.

### Usage

```r
impRZalr(x, pos = ncol(x), dl = rep(0.05, ncol(x) - 1), eps = 1e-04,
maxit = 50, bruteforce = FALSE, method = "lm", step = FALSE,
nComp = "boot", R = 10, verbose = FALSE)
```
Arguments

- **x**: Compositional data
- **pos**: Position of the rationing variable for alr transformation
- **dl**: Detection limit for each part
- **eps**: Convergence criteria
- **maxit**: Maximum number of iterations
- **bruteforce**: If TRUE, imputations over dl are set to dl. If FALSE, truncated (Tobit) regression is applied.
- **method**: Either “lm” (default) or “MM”
- **step**: If TRUE, a stepwise (AIC) procedure is applied when fitting models
- **nComp**: If determined, it fixes the number of pls components. If “boot”, the number of pls components are estimated using a bootstrapped cross validation approach.
- **R**: number of bootstrap samples for the determination of pls components. Only important for method “pls”.
- **verbose**: Additional print output during calculations.

Details

Statistical analysis of compositional data including zeros runs into problems, because log-ratios cannot be applied. Usually, rounded zeros are considered as missing not at random missing values. The algorithm first applies an additive log-ratio transformation to the compositions. Then the rounded zeros are imputed using a modified EM algorithm.

Value

- **xOrig**: Original data frame or matrix
- **xImp**: Imputed data
- **wind**: Index of the missing values in the data
- **iter**: Number of iterations
- **eps**: eps

Author(s)

Matthias Templ and Karel Hron

See Also

impRZalr
Examples

```r
data(arcticLake)
x <- arcticLake
## generate rounded zeros artificially:
x[x[,1] < 5, 1] <- 0
x[x[,2] < 47, 2] <- 0
xia <- impRZIlr(x, pos=3, dl=c(5,47), eps=0.05)
xia$xImp
```

---

**impRZIlr**

*EM-based replacement of rounded zeros in compositional data*

---

**Description**

Parametric replacement of rounded zeros for compositional data using classical and robust methods based on ilr-transformations with special choice of balances.

**Usage**

```r
impRZIlr(x, maxit = 10, eps = 0.1, method = "pls", dl = rep(0.05, ncol(x)), variation = FALSE, nComp = "boot", bruteforce = FALSE, noisemethod = "residuals", noise = FALSE, R = 10, correction = "normal", verbose = FALSE)
```

**Arguments**

- **x**: data.frame or matrix
- **maxit**: maximum number of iterations
- **eps**: convergency criteria
- **method**: either “lm”, “MM” or “pls”
- **dl**: Detection limit for each variable. zero for variables with variables that have no detection limit problems.
- **variation**: matrix is used to first select number of parts
- **nComp**: if determined, it fixes the number of pls components. If “boot”, the number of pls components are estimated using a bootstraped cross validation approach.
- **bruteforce**: sets imputed values above the detection limit to the detection limit. Replacement above the detection limit are only excepcionally occur due to numerical instabili-
- **noisemethod**: adding noise to imputed values. Experimental
- **noise**: TRUE to activate noise (experimental)
- **R**: number of bootstrap samples for the determination of pls components. Only important for method “pls”.
- **correction**: normal or density
- **verbose**: additional print output during calculations.
Details

Statistical analysis of compositional data including zeros runs into problems, because log-ratios cannot be applied. Usually, rounded zeros are considerer as missing not at random missing values.

The algorithm iteratively imputes parts with rounded zeros whereas in each step (1) an specific ilr transformation is applied (2) tobit regression is applied (3) the rounded zeros are replaced by the expected values (4) the corresponding inverse ilr transformation is applied. After all parts are imputed, the algorithm starts again until the imputations do not change.

Value

| x | imputed data |
| criteria | change between last and second last iteration |
| iter | number of iterations |
| maxit | maximum number of iterations |
| wind | index of zeros |
| nComp | number of components for method pls |
| method | chosen method |

Author(s)

Matthias Templ and Peter Filzmoser

See Also

imprzilr

Examples

```r
data(arcticLake)
x <- arcticLake
## generate rounded zeros artificially:
x[x[,1] < 5, 1] <- 0
x[x[,2] < 44, 2] <- 0
xia <- impRZilr(x, dl=c(5,44,0), eps=0.01, method="lm")
xia$x
```

Description

EM-based replacement of rounded zeros in compositional data

Parametric replacement of rounded zeros for compositional data using classical and robust methods based on ilr-transformations with special choice of balances.
Usage

imputeBDLs(x, maxit = 10, eps = 0.1, method = "subPLS", dl = rep(0.05, ncol(x)), variation = TRUE, nPred = NULL, nComp = "boot", bruteforce = FALSE, noisemethod = "residuals", noise = FALSE, R = 10, correction = "normal", verbose = FALSE, test = FALSE)

adjustImputed(xImp, xOrig, wind)

checkData(x, dl)

## S3 method for class 'replaced'
print(x, ...)

Arguments

x data.frame or matrix
maxit maximum number of iterations
eps convergency criteria
method either "lm", "lmrob" or "pls"
dl Detection limit for each variable. zero for variables with variables that have no detection limit problems.
variation, if TRUE those predictors are chosen in each step, who’s variation is lowest to the predictor.
nPred, if determined and variation equals TRUE, it fixes the number of predictors
nComp if determined, it fixes the number of pls components. If “boot”, the number of pls components are estimated using a bootstrapped cross validation approach.
bruteforce sets imputed values above the detection limit to the detection limit. Replacement above the detection limit are only exeptionally occur due to numerical instabilities. The default is FALSE!
noisemethod adding noise to imputed values. Experimental
noise TRUE to activate noise (experimental)
R number of bootstrap samples for the determination of pls components. Only important for method “pls”.
correction normal or density
verbose additional print output during calculations.
test an internal test situation (this parameter will be deleted soon)
xImp imputed data set
xOrig original data set
wind index matrix of rounded zeros
... further arguments passed through the print function
Details

Statistical analysis of compositional data including zeros runs into problems, because log-ratios cannot be applied. Usually, rounded zeros are considered as missing not at random missing values.

The algorithm iteratively imputes parts with rounded zeros whereas in each step (1) an specific ilr transformation is applied (2) tobit regression is applied (3) the rounded zeros are replaced by the expected values (4) the corresponding inverse ilr transformation is applied. After all parts are imputed, the algorithm starts again until the imputations do not change.

Value

x  imputed data
criteria change between last and second last iteration
iter number of iterations
maxit maximum number of iterations
wind index of zeros
nComp number of components for method pls
method chosen method

Author(s)

Matthias Templ, method subPLS from Jiajia Chen

References


See Also

`imputeBDLs`

Examples

```r
p <- 10
n <- 50
k <- 2
T <- matrix(rnorm(n*k), ncol=k)
B <- matrix(runif(p*k,-1,1),ncol=k)
X <- T %*% t(B)
E <- matrix(rnorm(n*p, 0,0.1), ncol=p)
XE <- X + E
data <- data.frame(pivotCoordInv(XE))
```
col <- ncol(data)
row <- nrow(data)
DL <- matrix(rep(0), ncol=col, nrow=1)
for(j in seq(1, col, 2))
{DL[j] <- quantile(data[,j], probs=0.06, na.rm=FALSE)}

for(j in 1:col)
{data[data[,j]<DL[j],j] <- 0}

imp <- imputeBDLs(data, dl=DL, maxit=10, eps=0.1, R=10, method="subPLS")
imp
imp <- imputeBDLs(data, dl=DL, maxit=10, eps=0.1, R=10, method="pls", variation = FALSE)
imp
imp <- imputeBDLs(data, dl=DL, maxit=10, eps=0.1, R=10, method="lm")
imp
imp <- imputeBDLs(data, dl=DL, maxit=10, eps=0.1, R=10, method="lmrob")
imp

data(mcad)
# Not run:
# longer computation times...
# generate rounded zeros artificially:
x <- mcad
x <- x[1:25, 2:ncol(x)]
dl <- apply(x, 2, quantile, 0.1)
for(i in seq(1, ncol(x), 2)){
  x[,i] < dl[i], i] <- 0
}

ni <- sum(x==0, na.rm=TRUE)
ni/(ncol(x)*nrow(x)) * 100
ndl[seq(2, ncol(x), 2)] <- 0
replaced_lm <- imputeBDLs(x, dl=ndl, eps=1, method="lm",
                          verbose=FALSE, R=50, variation=TRUE)$x
replaced_lmrob <- imputeBDLs(x, dl=ndl, eps=1, method="lmrob",
                          verbose=FALSE, R=50, variation=TRUE)$x
replaced_plsfull <- imputeBDLs(x, dl=ndl, eps=1,
                              method="pls", verbose=FALSE, R=50,
                              variation=FALSE)$x

# End(Not run)

---

**Description**

Estimates the expected frequencies from an 2x2 table under the null hypotheses of independence.
Usage

\texttt{ind2x2(x, margin = 3, pTabMethod = c("dirichlet", "half", "classical"))}

Arguments

\begin{description}
\item \textit{x} \hspace{1cm} a 2x2 table
\item \textit{margin} \hspace{1cm} if multidimensional table (larger than 2-dimensional), then the margin determines on which dimension the independence tables should be estimated.
\item \textit{pTabMethod} \hspace{1cm} ‘classical’ that is function \texttt{prop.table()} from package base or method “half” that add 1/2 to each cell to avoid zero problems.
\end{description}

Value

The independence table(s) with either relative or absolute frequencies.

Author(s)

Kamila Facevicova, Matthias Templ

References


Examples

\begin{verbatim}
data(employment)
ind2x2(employment)
\end{verbatim}

---

\texttt{indTab} \hspace{1cm} \textit{Independence table}

Description

Estimates the expected frequencies from an m-way table under the null hypotheses of independence.

Usage

\texttt{indTab(x, margin = c("gmean_sum", "sum"), frequency = c("relative", "absolute"), pTabMethod = c("dirichlet", "half", "classical"))}
Arguments

x: an object of class table

margin: determines how the margins of the table should be estimated (default via geometric mean margins)

frequency: indicates whether absolute or relative frequencies should be computed.

propMethod: to estimate the probability table. Default is ‘dirichlet’. Other available methods: ‘classical’ that is function prop.table() from package base or method “half” that add 1/2 to each cell to avoid zero problems.

Details

Because of the compositional nature of probability tables, the independence tables should be estimated using geometric margins.

Value

The independence table(s) with either relative or absolute frequencies.

Author(s)

Matthias Templ

References


Examples

data(precipitation)
tab1 <- indTab(precipitation)
tab1
sum(tab1)

## Not run:
data("PreSex", package = "vcd")
indTab(PreSex)

## End(Not run)
Description

- ctct
- isicISIC classification, Rev 3.2
- VAvalue added
- OUToutput
- INPinput
- IS03country code
- nhtmht

Usage

data(instw)

Format

A data.frame with 1555 rows and 7 columns.

Examples

data(instw)
head(instw)

int2x2  Interaction 2x2 table

Description

Estimates the interactions from an 2x2 table under the null hypotheses of independence.

Usage

int2x2(x, margin = 3, pTabMethod = c("dirichlet", "half", "classical"))

Arguments

- x  a 2x2 table
- margin if multidimensional table (larger than 2-dimensional), then the margin determines on which dimension the independene tables should be estimated.
- pTabMethod to estimate the propability table. Default is ‘dirichlet’. Other available methods: ‘classical’ that is function prop.table() from package base or method “half” that add 1/2 to each cell to avoid zero problems.
Value
The independence table(s) with either relative or absolute frequencies.

Author(s)
Kamila Facevicova, Matthias Templ

References

Examples
```r
data(employment)
int2x2(employment)
```

---

**Description**
Estimates the interaction array

**Usage**
```r
intArray(x)
```

**Arguments**
x an object of class “intTab”

**Details**
Estimates the interaction array using an ilr transformation of the interaction table.

**Value**
The interaction array

**Author(s)**
Matthias Templ
References

See Also
intTab

Examples
```r
data(precipitation)
tablprob <- prop.table(precipitation)
tabl <- intTab(precipitation)
tablINT <- intTab(tablprob, tabl)
tIntArray(tablINT)
```

intTab

*Interaction table*

Description
Estimates the interaction table based on clr and inverse clr transformations.

Usage
```r
intTab(x, y, frequencies = c("relative", "absolute"))
```

Arguments
- `x`: an object of class `table`.
- `y`: the corresponding independence table which is of class “intTab”.
- `frequencies`: indicates whether absolute or relative frequencies should be computed.

Details
Because of the compositional nature of probability tables, the independence tables should be estimated using geometric margins.

Value
- `intTab`: The interaction table(s) with either relative or absolute frequencies.
- `signs`: The sign illustrates if there is an excess of probability (plus), or a deficit (minus) regarding to the estimated probability table and the independence table in the clr space.

Author(s)
Matthias Templ
References

Examples
data(precipitation)
tab\prob \leftarrow \text{prop.table(precipitation)}
tab\ind \leftarrow \text{indTab(precipitation)}
intTab(tab\prob, tab\ind)

isic32
*ISIC codes by name*

Description
- codeISIC code, Rev 3.2
- descriptionDescription of ISIC codes

Usage
data(isic32)

Format
A data.frame with 24 rows and 2 columns.

Examples
data(instw)
instw

laborForce
*labour force by status in employment*

Description
Labour force by status in employment for 124 countries, latest update: December 2009

Format
A data set on 124 compositions on 9 variables.
lifeExpGdp

Details

- country
- year
- employeesW percentage female employees
- employeesM percentage male employees
- employersW percentage female employers
- employersM percentage male employers
- ownW percentage female own-account workers and contributing family workers
- ownM percentage male own-account workers and contributing family workers
- source HS: household or labour force survey. OE: official estimates. PC: population census

Author(s)

conversion to R by Karel Hron and Matthias Templ <matthias.templ@tuwien.ac.at>

Source


References


Examples

data(laborForce)
str(laborForce)

lifeExpGdp

life expectancy and GDP (2008) for EU-countries

Description

Social-economic data for compositional regression.

Format

A data set on 27 compositions on 9 variables.
Details

- country country
- agriculture GDP on agriculture, hunting, forestry, fishing (ISIC A-B, x1)
- manufacture GDP on mining, manufacturing, utilities (ISIC C-E, x2)
- construction GDP on construction (ISIC F, x3)
- wholesales GDP on wholesale, retail trade, restaurants and hotels (ISIC G-H, x4)
- transport GDP on transport, storage and communication (ISIC I, x5)
- other GDP on other activities (ISIC J-P, x6)
- lifeExpMen life expectancy for men and women
- lifeExpWomen life expectancy for men and women

Author(s)

conversion to R by Karel Hron and Matthias Templ <matthias.templ@tuwien.ac.at>

Source


References


Examples

data(lifeExpGdp)
str(lifeExpGdp)

```r
lmCoDaX
```

*Classical and robust regression of non-compositional response on compositional predictors*

Description

Delivers appropriate inference for regression of y on a compositional matrix X.

Usage

```r
lmCoDaX(y, X, method = "robust")
```
Arguments

y The response which should be non-compositional
X The compositional predictors as a matrix, data.frame or numeric vector
method If robust, LTS-regression is applied, while with method equals “classical”, the conventional least squares regression is applied.

Details

Compositional explanatory variables should not be directly used in a linear regression model because any inference statistic can become misleading. While various approaches for this problem were proposed, here an approach based on the isometric logratio (ilr) transformation is used.

Value

An object of class ‘lts’ or ‘lm’ and two summary objects.

Author(s)

Peter Filzmoser

References


See Also

lm

Examples

```r
## How the total household expenditures in EU Member
## States depend on relative contributions of
## single household expenditures:
data(expendituresEU)
y <- as.numeric(apply(expendituresEU, 1, sum))
lmCoDaX(y, expendituresEU, method = "classical")
lmCoDaX(y, expendituresEU, method = "robust")
```
Description

Compositions of eight-hour shifts of 27 machine operators

Usage

data(machineOperators)

Format

A data frame with 27 observations on the following 4 variables.

Details

- hqproduction high-quality production
- lqproduction low-quality production
- setting machine settings
- repair machine repair


Author(s)

Matthias Templ <matthias.templ@tuwien.ac.at>

References


Examples

data(machineOperators)
str(machineOperators)
summary(machineOperators)
rowSums(machineOperators)
**Description**

The aim of the experiment was to ascertain novel biomarkers of MCAD (Medium chain acyl-CoA dehydrogenase) deficiency. The data consists of 25 patients and 25 controls and the analysis was done by LC-MS. Rows represent patients and controls and columns represent chemical entities with their quantity.

**Usage**

data(mcad)

**Format**

A data frame with 50 observations and 279 variables

**Details**

- **group** patient group
- . . . the remaining variables columns are represented by m/z which are chemical characterizations of individual chemical components on exact mass measurements.

**References**


**Examples**

data(mcad)
str(mcad)

---

**Description**

Analysis of the missing or the zero patterns structure of a data set.
Usage

missPatterns(x)

zeroPatterns(x)

Arguments

x a data frame or matrix.

Details

Here, one pattern defines those observations that have the same structure regarding their missingness or zeros. For all patterns a summary is calculated.

Value

groups List of the different patterns and the observation numbers for each pattern
cn the names of the patterns coded as vectors of 0-1’s
tabcomb the pattern structure - all combinations of zeros or missings in the variables

tabcombPlus the pattern structure - all combinations of zeros or missings in the variables including the size of those combinations/patterns, i.e. the number of observations that belongs to each pattern.

rsum the number of zeros or missing values in each row of the data set.

rindex the index of zeros or missing values in each row of the data set

Author(s)

Matthias Templ. The code is based on a previous version from Andreas Alfons and Matthias Templ from package VIM

See Also

aggr

Examples

data(expenditures)
## set NA’s artificial:
expenditures[expenditures < 300] <- NA
## detect the NA structure:
missPatterns(expenditures)
mortality

mortality and life expectancy in the EU

Description

- country  country name
- country2  country name, short version
- sex  gender
- lifeExpectancy  life expectancy
- infectious  certain infectious and parasitic diseases (A00-B99)
- neoplasms  malignant neoplasms (C00-C97)
- endocrine  endocrine nutritional and metabolic diseases (E00-E90)
- mental  mental and behavioural disorders (F00-F99)
- nervous  diseases of the nervous system and the sense organs (G00-H95)
- circulatory  diseases of the circulatory system (I00-I99)
- respiratory  diseases of the respiratory system (J00-J99)
- digestive  diseases of the digestive system (K00-K93)

Usage

data(mortality)

Format

A data frame with 60 observations and 12 variables

Author(s)

Peter Filzmoser, Matthias Templ <matthias.templ@tuwien.ac.at>

References


Examples

data(mortality)
str(mortality)
## totals (mortality)
aggregate(mortality[,5:ncol(mortality)],
  list(mortality$country2), sum)
### mortality_tab

**Description**

Mortality data by gender, unknown year

**Usage**

```r
data(mortality_tab)
```

**Format**

A table

**Details**

- female mortality rates for females by age groups
- male mortality rates for males by age groups

**Author(s)**

Matthias Templ

**Examples**

```r
data(mortality_tab)
mortality_tab
```

### nutrients

**Description**

Nutrients on more than 40 components and 965 generic food products

**Usage**

```r
data(nutrients)
```

**Format**

A data frame with 965 observations on the following 50 variables.
Details

• ID  ID, for internal use
• ID_V4  ID V4, for internal use
• ID_SwissFIR  ID, for internal use
• name_D  Name in German
• name_F  Name in French
• name_I  Name in Italian
• name_E  Name in Spanish
• category_D  Category name in German
• category_F  Category name in French
• category_I  Category name in Italy
• category_E  Category name in Spanish
• gravity  specific gravity
• 'energy_kJ  'energy in kJ per 100g edible portion
• energy_kcal  energy in kcal per 100g edible portion
• protein  protein in gram per 100g edible portion
• alcohol  alcohol in gram per 100g edible portion
• water  water in gram per 100g edible portion
• carbohydrates  carbohydrates in gram per 100g edible portion
• starch  starch in gram per 100g edible portion
• sugars  sugars in gram per 100g edible portion
• 'dietar_fibres  'dietar fibres in gram per 100g edible portion
• fat  fat in gram per 100g edible portion
• cholesterol  cholesterol in milligram per 100g edible portion
• fattyacids_monounsaturated  fatty acids monounsaturated in gram per 100g edible portion
• fattyacids_saturated  fatty acids saturated in gram per 100g edible portion
• fatty_acids_polyunsaturated  fatty acids polyunsaturated in gram per 100g edible portion
• vitaminA  vitamin A in retinol equivalent per 100g edible portion
• 'all-trans_retinol_equivalents  'all trans-retinol equivalents in gram per 100g edible portion
• 'beta-carotene-activity  'beta-carotene activity in beta-carotene equivalent per 100g edible portion
• 'beta-carotene  'beta-carotene in micogram per 100g edible portion
• vitaminB1  vitamin B1 in milligram per 100g edible portion
• vitaminB2  vitamin B2 in milligram per 100g edible portion
• vitaminB6  vitamin B6 in milligram per 100g edible portion
• vitaminB12  vitamin B12 in micogram per 100g edible portion
• niacin  niacin in milligram per 100g edible portion
• folate  folate in micogram per 100g edible portion
• pantothenic_acid  pantothenic acid in milligram per 100g edible portion
• vitaminC  vitamin C in milligram per 100g edible portion
• vitaminD  vitamin D in micogram per 100g edible portion
• vitaminE  vitamin E in alpha-tocopherol equivalent per 100g edible portion
• Na  Sodium in milligram per 100g edible portion
• K  Potassium in milligram per 100g edible portion
• Cl  Chloride
• Ca  Calcium
• Mg  Magnesium
• P  Phosphorus
• Fe  Iron
• I  Iodide in milligram per 100g edible portion
• Zn  Zink
• unit  a factor with levels per 100g edible portion per 100ml food volume

Author(s)
Translated from the Swiss nutrition data base by Matthias Templ <matthias.templ@tuwien.ac.at>

Source
From the Swiss nutrition data base 2015 (second edition), see http://www.sge-ssn.ch/shop/produkt/schweizer-naehrwerttabelle/

References
http://www.sge-ssn.ch/shop/produkt/schweizer-naehrwerttabelle/

Examples

data(nutrients)
str(nutrients)
head(nutrients[, 41:49])
Description

Nutrients on more than 10 components and 9618 branded food products

Usage

data(nutrients_branded)

Format

A data frame with 9618 observations on the following 18 variables.

Details

- name_D  name (in German)
- category_D  factor specifying the category names
- category_F  factor specifying the category names
- category_I  factor specifying the category names
- category_E  factor specifying the category names
- gravity  specific gravity
- energy_kJ  energy in kJ
- ‘energy_kcal’  energy in kcal
- protein  protein in gram
- alcohol  alcohol in gram
- water  water in gram
- carbohydrates_available  available carbohydrates in gram
- sugars  sugars in gram
- dietary_fibres  dietary fibres in gram
- fat_total  total fat in gram
- fatty_acids_saturated  saturated acids fat in gram
- Na  Sodium in gram
- unit  a factor with levels per 100g edible portion per 100ml food volume

Author(s)

Translated from the Swiss nutrition database by Matthias Templ <matthias.templ@tuwien.ac.at>
Source
From the Swiss nutrition data base 2015 (second edition), see http://www.sge-ssn.ch/shop/produkt/schweizer-naehrwerttabelle/

References
http://www.sge-ssn.ch/shop/produkt/schweizer-naehrwerttabelle/

Examples

data(nutrients_branded)
str(nutrients_branded)

------
orthbasis Orthonormal basis

Description
Orthonormal basis from cenLR transformed data to pivotCoord transformed data.

Usage
orthbasis(D)

Arguments
D number of parts (variables)

Details
For the chosen balances for “pivotCoord”, this is the orthonormal basis that transfers the data from centered logratio to isometric logratio.

Value
the orthonormal basis.

Author(s)
Karel Hron, Matthias Templ. Some code lines of this function are a copy from function gsi.buildilr from

See Also
pivotCoord, cenLR
Examples

data(expenditures)
V <- orthbasis(ncol(expenditures))
xcen <- cenLR(expenditures)$x.clr
xi <- as.matrix(xcen) %*% V$V
xi
xi2 <- pivotCoord(expenditures)
xi2

Description

Outlier detection for compositional data using standard and robust statistical methods.

Usage

outCoDa(x, quantile = 0.975, method = "robust", h = 1/2, coda = TRUE)

# S3 method for class 'outCoDa'
print(x, ...)

# S3 method for class 'outCoDa'
plot(x, y, ..., which = 1)

Arguments

x compositional data
quantile quantile, corresponding to a significance level, is used as a cut-off value for outlier identification: observations with larger (squared) robust Mahalanobis distance are considered as potential outliers.
method either "robust" (default) or "standard"
h the size of the subsets for the robust covariance estimation according the MCD-estimator for which the determinant is minimized (the default is (n+p+1)/2).
coda if TRUE, data transformed to coordinate representation before outlier detection.
... additional parameters for print and plot method passed through
y unused second plot argument for the plot method
which 1 ... MD against index 2 ... distance-distance plot
Details

The outlier detection procedure is based on (robust) Mahalanobis distances after a isometric logratio transformation of the data. Observations with squared Mahalanobis distance greater equal a certain quantile of the Chi-squared distribution are marked as outliers.

If method “robust” is chosen, the outlier detection is based on the homogeneous majority of the compositional data set. If method “standard” is used, standard measures of location and scatter are applied during the outlier detection procedure.

plot method: the Mahalanobis distance are plotted against the index. The dashed line indicates the \((1 - \alpha)\) quantile of the Chi-squared distribution. Observations with Mahalanobis distance greater than this quantile could be considered as compositional outliers.

Value

- **mahaDist**: resulting Mahalanobis distance
- **limit**: quantile of the Chi-squared distribution
- **outlierIndex**: logical vector indicating outliers and non-outliers
- **method**: method used

Note

It is highly recommended to use the robust version of the procedure.

Author(s)

Matthias Templ, Karel Hron

References


See Also

- `pivotCoord`

Examples

```r
data(expenditures)
oD <- outCoDa(expenditures)
oD
## providing a function:
oD <- outCoDa(expenditures, coda = log)
```
Description

Payments splitted by different NACE categories and kind of employment in Austria 2004

Usage

data(payments)

Format

A data frame with 535 rows and 11 variables

Details

- nace  NACE classification, 2 digits
- oenace_2008  Corresponding Austrian NACE classification (in German)
- year  year
- month  month
- localunit  local unit ID
- spay  special payments (total)
- spay_wc  special payments for white collar workers
- spay_bc  special payments for blue collar workers
- spay_traintrade  special payments for trainees in trade business
- spay_home  special payments for home workers
- spay_traincomm  special payments for trainees in commercial business

Author(s)

Matthias Templ <matthias.templ@tuwien.ac.at>

Source

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Examples

```r
data(payments)
str(payments)
summary(payments)
```

---

**pcaCoDa**  
*Robust principal component analysis for compositional data*

---

**Description**

This function applies robust principal component analysis for compositional data.

**Usage**

```r
pcacoda(x, method = "robust", mult_comp = NULL, external = NULL)
```

```r
## S3 method for class 'pcacoda'
print(x, ...)

## S3 method for class 'pcacoda'
summary(object, ...)
```

**Arguments**

- `x`  
  compositional data
- `method`  
  must be either “robust” (default) or “classical”
- `mult_comp`  
  a list of numeric vectors holding the indices of linked compositions
- `external`  
  external non-compositional variables
- `...`  
  additional parameters for print method passed through
- `object`  
  object of class pcaCoDa

**Details**

The compositional data set is transformed using the ilr transformation. Afterwards, robust principal component analysis is performed. Resulting loadings and scores are back-transformed to the clr space where the compositional biplot can be shown.

`mult_comp` is used when there are more than one group of compositional parts in the data. To give an illustrative example, lets assume that one variable group measures angles of the inner ear-bones of animals which sum up to 100 and another one having percentages of a whole on the thickness of the inner ear-bones included. Then two groups of variables exists which are both compositional parts. The ilr-transformation is then internally applied to each group independently whenever the `mult_comp` is set correctly.
Value

scores  scores in clr space
loadings  loadings in clr space
eigenvalues  eigenvalues of the clr covariance matrix
method  method
princompOutputClr  output of princomp needed in plot.pcaCoDa

Author(s)


References


See Also

print.pcaCoDa, summary.pcaCoDa, biplot.pcaCoDa, plot.pcaCoDa

Examples

data(arcticLake)

## robust estimation (default):
res.rob <- pcaCoDa(arcticLake)
res.rob
summary(res.rob)
plot(res.rob)

## classical estimation:
res.cl <- pcaCoDa(arcticLake, method="classical")
biplot(res.cl)

## just for illustration how to set the mult_comp argument:
data(expenditures)
p1 <- pcaCoDa(expenditures, mult_comp=list(c(1,2,3),c(4,5)))
p1

## example with external variables:
data(election)
# transform external variables
election$unemployment <- log((election$unemployment/100)/(1-election$unemployment/100))
election$income <- scale(election$income)
perturbation

Description
Perturbation and powering for two compositions.

Usage
perturbation(x, y)

powering(x, a)

Arguments

x  (compositional) vector containing positive values
y  (compositional) vector containing positive values or NULL for powering
a  constant, numeric vector of length 1

Value
Result of perturbation or powering

Author(s)
Matthias Templ

References

Examples
data(expenditures)
x <- expenditures[1 ,]
y <- expenditures[2, ]
perturbation(x, y)
powering(x, 2)
**Description**

Computes the principal factor analysis of the input data which are transformed and centered first.

**Usage**

```r
pfa(x, factors, robust = TRUE, data = NULL, covmat = NULL, n.obs = NA,
     subset, na.action, start = NULL, scores = c("none", "regression",
     "Bartlett"), rotation = "varimax", maxiter = 5, control = NULL, ...)
```

**Arguments**

- `x`: (robustly) scaled input data
- `factors`: number of factors
- `robust`: default value is TRUE
- `data`: default value is NULL
- `covmat`: (robustly) computed covariance or correlation matrix
- `n.obs`: number of observations
- `subset`: if a subset is used
- `na.action`: what to do with NA values
- `start`: starting values
- `scores`: which method should be used to calculate the scores
- `rotation`: if a rotation should be made
- `maxiter`: maximum number of iterations
- `control`: default value is NULL
- `...`: arguments for creating a list

**Details**

The main difference to usual implementations is that uniquenesses are nor longer of diagonal form. This kind of factor analysis is designed for centered log-ratio transformed compositional data. However, if the covariance is not specified, the covariance is estimated from isometric log-ratio transformed data internally, but the data used for factor analysis are backtransformed to the clr space (see Filzmoser et al., 2009).
**Value**

- **loadings**: A matrix of loadings, one column for each factor. The factors are ordered in decreasing order of sums of squares of loadings.
- **uniqueness**: uniqueness
- **correlation**: correlation matrix
- **criteria**: The results of the optimization: the value of the negativ log-likelihood and information of the iterations used.
- **factors**: the factors
- **dof**: degrees of freedom
- **method**: “principal”
- **n.obs**: number of observations if available, or NA
- **call**: The matched call.
- **STATISTIC, PVAL**: The significance-test statistic and p-value, if they can be computed

**Author(s)**

Peter Filzmoser, Karel Hron, Matthias Templ

**References**


**Examples**

data(expenditures)
x <- expenditures
res.rob <- pfa(x, factors=1)
res.cla <- pfa(x, factors=1, robust=FALSE)

```r
# the following produce always the same result:
res1 <- pfa(x, factors=1, covmat="covMcd")
res2 <- pfa(x, factors=1, covmat=covMcd(pivotCoord(x))$cov)
res3 <- pfa(x, factors=1, covmat=covMcd(pivotCoord(x)))
```
PhD students in the EU

Description

PhD students in Europe based on the standard classification system splitted by different kind of studies (given as percentages).

Format

A data set on 32 compositions and 11 variables.

Details

Due to unknown reasons the rowSums of the percentages is not always 100.

- country country of origin (German)
- countryEN country of origin (English)
- country2 country of origin, 2-digits
- total total phd students (in 1.000)
- male male phd students (in 1.000)
- female total phd students (in 1.000)
- technical phd students in natural and technical sciences
- socio-economic-low phd students in social sciences, economic sciences and law sciences
- health phd students in health and life sciences
- agriculture phd students in agriculture

Source

Eurostat

References


Examples

data(phd)
str(phd)
phd_totals

PhD students in the EU (totals)

Description
PhD students in Europe by different kind of studies.

Format
A data set on 29 compositions and 5 variables.

Details
- technical phd students in natural and technical sciences
- socio-economic-low phd students in social sciences, economic sciences and law sciences
- human phd students in human sciences including teaching
- health phd students in health and life sciences
- agriculture phd students in agriculture

Source
Eurostat

References

Examples

data("phd_totals")
str(phd_totals)
pivotCoord  

Pivot coordinates and their inverse

Description

Isometric log-ratio transformations and it’s inverse transformation with a special choice of balances.

Usage

pivotCoord(x, pivotvar = 1, fast = FALSE, method = "pivot",  
base = exp(1), norm = "orthonormal")

isomLR(x, fast = FALSE, base = exp(1), norm = "sqrt((D-i)/(D-i+1))")

isomLRinv(x)

pivotCoordInv(x, norm = "orthonormal")

isomLRp(x, fast = FALSE, base = exp(1), norm = "sqrt((D-i)/(D-i+1))")

isomLRinvp(x)

Arguments

x  
object of class data.frame or matrix. Positive values only.

pivotvar  
pivotal variable. If any other number than 1, the data are resorted in that sense that the pivotvar is shifted to the first part.

fast  
if TRUE, it is approx. 10 times faster but numerical problems in case of high-dimensional data numerical instabilities may occur. Only available for method “pivot”.

method  
pivot takes the method described in the description. Method "symm" uses symmetric balances (parameters pivotvar and norm have then no effect)

base  
a positive or complex number: the base with respect to which logarithms are computed. Defaults to exp(1).

norm  
if FALSE then the normalizing constant is not used, if TRUE sqrt((D-i)/(D-i+1)) is used (default). The user can also specify a self-defined constant.

Details

This transformation moves D-part compositional data from the simplex into a (D-1)-dimensional real space isometrically. From our choice of (pivot) balances, all the relative information of one part is separated from the remaining parts.

Value

The data represented in pivot coordinates
**Author(s)**

Matthias Templ, Karel Hron, Peter Filzmoser

**References**


**Examples**

```r
require(MASS)
Sigma <- matrix(c(5.05,4.95,4.95,5.05), ncol=2, byrow=TRUE)
z <- pivotCoordInv(mvrnorm(100, mu=c(0,2), Sigma=Sigma))

data(expenditures)
## first variable as pivot variable
pivotCoord(expenditures)
## third variable as pivot variable
pivotCoord(expenditures, 3)

x <- exp(mvrnorm(2000, mu=rep(1,10), diag(10)))
system.time(pivotCoord(x))
system.time(pivotCoord(x, fast=TRUE))

## without normalizing constant
pivotCoord(expenditures, norm = "orthogonal") # or:
pivotCoord(expenditures, norm = "1")
## other normalization
pivotCoord(expenditures, norm = "-sqrt((D-i)/(D-i+1))")

# symmetric balances (results in 2-dim symmetric balances)
pivotCoord(expenditures, method = "symm")
```

**plot.imp**

Plot method for objects of class `imp`

**Description**

This function provides several diagnostic plots for the imputed data set in order to see how the imputated values are distributed in comparison with the original data values.
plot.imp

Usage

## S3 method for class 'imp'
plot(x, ..., which = 1L, ord = 1L:ncol(x),
colcomb = "missnonmiss", plotvars = NULL, col = c("skyblue", "red"),
alpha = NULL, lty = par("lty"), xaxt = "s", xaxlabels = NULL,
las = 3L, interactive = TRUE, pch = c(1L, 3L), ask = prod(par("mfcol")) <
length(which) & dev.interactive(), center = FALSE, scale = FALSE,
id = FALSE, seg.l = 0.02, seg1 = TRUE)

Arguments

x          object of class ‘imp’
...         other parameters to be passed through to plotting functions.
which       if a subset of the plots is required, specify a subset of the numbers 1:3.
ord         determines the ordering of the variables
colcomb     if colcomb = "missnonmiss", observations with missings in any variable are high-
            lighted. Otherwise, observations with missings in any of the variables specified
            by colcomb are highlighted in the parallel coordinate plot.
plotvars    Parameter for the parallel coordinate plot. A vector giving the variables to be
            plotted. If NULL (the default), all variables are plotted.
col         a vector of length two giving the colors to be used in the plot. The second color
            will be used for highlighting.
alpha       a numeric value between 0 and 1 giving the level of transparency of the colors,
            or NULL. This can be used to prevent overplotting.
lty         a vector of length two giving the line types. The second line type will be used
            for the highlighted observations. If a single value is supplied, it will be used for
            both non-highlighted and highlighted observations.
xaxt        the x-axis type (see par).
xaxlabels   a character vector containing the labels for the x-axis. If NULL, the column
            names of x will be used.
las         the style of axis labels (see par).
interactive  a logical indicating whether the variables to be used for highlighting can be
            selected interactively (see ‘Details’).
pch         a vector of length two giving the symbol of the plotting points. The symbol will
            be used for the highlighted observations. If a single value is supplied, it will be used
            for both non-highlighted and highlighted observations.
ask          logical; if TRUE, the user is asked before each plot, see par(ask=).
center       logical, indicates if the data should be centered prior plotting the ternary plot.
scale        logical, indicates if the data should be centered prior plotting the ternary plot.
id           reads the position of the graphics pointer when the (first) mouse button is pressed
            and returns the corresponding index of the observation. (only used by the ternary
            plot)
seg.l        length of the plotting symbol (spikes) for the ternary plot.
seg1         if TRUE, the spikes of the plotting symbol are justified.
Details

The first plot (which == 1) is a multiple scatterplot where for the imputed values another plot symbol and color is used in order to highlight them. Currently, the ggpairs functions from the GGally package is used.

Plot 2 is a parallel coordinate plot in which imputed values in certain variables are highlighted. In parallel coordinate plots, the variables are represented by parallel axes. Each observation of the scaled data is shown as a line. If interactive is TRUE, the variables to be used for highlighting can be selected interactively. Observations which includes imputed values in any of the selected variables will be highlighted. A variable can be added to the selection by clicking on a coordinate axis. If a variable is already selected, clicking on its coordinate axis will remove it from the selection. Clicking anywhere outside the plot region quits the interactive session.

Plot 3 shows a ternary diagram in which imputed values are highlighted, i.e. those spikes of the chosen plotting symbol are colored in red for which of the values are missing in the unimputed data set.

Value

None (invisible NULL).

Author(s)

Matthias Templ

References


See Also

*impCoda, impKNNa*

Examples

data(expenditures)
expenditures[1,3]
expenditures[1,3] <- NA
xi <- impKNNa(expenditures)
xi
summary(xi)
## Not run: plot(xi, which=1)
plot(xi, which=2)
plot(xi, which=3)
plot(xi, which=3, seg1=FALSE)
plot.pcaCoDa  

Plot method

Description

Provides a screeplot for (robust) compositional principal components analysis.

Usage

```r
## S3 method for class 'pcaCoDa'
plot(x, y, ...)
```

Arguments

- `x` object of class `pcaCoDa`
- `y` ...
- `...` ...

Value

The robust compositional screeplot.

Author(s)

M. Templ, K. Hron

References


See Also

`pcaCoDa, biplot.pcaCoDa`

Examples

```r
data(coffee)
p1 <- pcaCoDa(coffee[, -1])
plot(p1)
plot(p1, type="lines")
```
Description

table containing counts for 24-hour precipitation for season at the rain-gouge.

Usage

data(precipitation)

Format

A table with 4 rows and 6 columns

Details

- spring numeric vector on counts for different level of precipitation
- summer numeric vector on counts for different level of precipitation
- autumn numeric vector on counts for different level of precipitation
- winter numeric vector on counts for different level of precipitation

Author(s)

Matthias Templ <matthias.templ@tuwien.ac.at>

References


Examples

data(precipitation)
precipitation
str(precipitation)
print.imp  Print method for objects of class imp

Description

The function returns a few information about how many missing values are imputed and possible other information about the amount of iterations, for example.

Usage

```r
## S3 method for class 'imp'
print(x, ...)
```

Arguments

- `x`: an object of class ‘imp’
- `...`: additional arguments passed through

Value

None (invisible NULL).

Author(s)

Matthias Templ

See Also

`impCoda`, `impKNNa`

Examples

```r
data(expenditures)
expenditures[1,3] <- NA
## Not run:
x1 <- impCoda(expenditures)
x1
summary(x1)
plot(x1, which=1:2)

## End(Not run)
```
production

production splitted by nationality on enterprise level

Description

• nace  NACE classification, 2 digits
• oenace_2008  Corresponding Austrian NACE classification (in German)
• year year
• month month
• enterprise enterprise ID
• total total ...
• home home ...
• EU EU ...
• non-EU non-EU ...

Usage

data(production)

Format

A data frame with 535 rows and 9 variables

Author(s)

Matthias Templ <matthias.templ@tuwien.ac.at>

Source

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Examples

data(production)
str(production)
summary(production)
**Description**

Calculates the probability table using different methods

**Usage**

```r
pTab(x, method = "dirichlet", alpha = 1/length(as.numeric(x)))
```

**Arguments**

- `x`: an object of class `table`
- `method`: default is ‘`dirichlet`’. Other available methods: ‘`classical`’ that is function `prop.table()` from package base or method “half” that add 1/2 to each cell to avoid zero problems.
- `alpha`: constant used for method ‘`dirichlet`’

**Value**

The probability table

**Author(s)**

Matthias Templ

**References**


**Examples**

```r
data(precipitation)
pTab(precipitation)
pTab(precipitation, method = "dirichlet")
```
rcodes  codes for UNIDO tables

Description

- ISOCN ISO CON codes
- OPERATOR Operator
- ADESC Country
- CODE Country code
- CDESC Country destination
- ACODE Country destination code

Usage

data(rcodes)

Format

A data.frame with 2717 rows and 6 columns.

Examples

data(rcodes)
str(rcodes)

rdcm  relative difference between covariance matrices

Description

The sample covariance matrices are computed with the same isometric transformed observations.

Usage

rdcm(x, y)

Arguments

x  matrix or data frame
y  matrix or data frame of the same size as x.

Details

The difference in covariance structure is based on the Euclidean distance between both covariance estimations.
**Value**

the error measures value

**Author(s)**

Matthias Templ

**References**


**See Also**

`rdcm`

**Examples**

```r
data(expenditures)
x <- expenditures
x[1,3] <- NA
xi <- impKNNa(x)$xImp
rdcm(expenditures, xi)
```

<table>
<thead>
<tr>
<th>rSdev</th>
<th>Relative simplicial deviance</th>
</tr>
</thead>
</table>

**Description**

Relative simplicial deviance

**Usage**

```r
rSDev(x, y)
```

**Arguments**

- `x` a probability table
- `y` an interaction table

**Value**

The relative simplicial deviance
Author(s)
Matthias Templ

References

Examples
data(precipitation)
tabprob <- prop.table(precipitation)
tabind <- indTab(precipitation)
tabint <- intTab(tabprob, tabind)
rsdev(tabprob, tabint$intTab)

rsDev.test Relative simplicial deviance tests

Description
Monte Carlo based contingency table tests considering the compositional approach to contingency tables.

Usage
rsDev.test(x, R = 999, method = "rmultinom")

Arguments
x matrix, data.frame or table
R an integer specifying the number of replicates used in the Monte Carlo test.
method either “rmultinom” (default) or “permutation”.

Details
Method “rmultinom” generate multinomially distributed samples from the independent probability table, which is estimated from x using geometric mean marginals. The relative simplicial deviance of the original data are then compared to the generated ones.

Method “permutation” permutes the entries of x and compares the relative simplicial deviance estimated from the original data to the ones of the permuted data (the independence table is unchanged and originates on x).

Method “rmultinom” should be preferred, while method “permutation” can be used for comparisons.
Value
A list with class "htest" containing the following components:

• statistic the value of the relative simplicial deviance (test statistic).
• method a character string indicating what type of rSDev.test was performed.
• p.value the p-value for the test.

Author(s)
Matthias Templ, Karel Hron

References

See Also
rSDev

Examples

data(precipitation)
rsDev.test(precipitation)

SDev Simplicial deviance

Description
Simplicial deviance

Usage
SDev(x)

Arguments
x a propability table

Value
The simplicial deviance

Author(s)
Matthias Templ
References

Examples
data(precipitation)
tablprob <- prop.table(precipitation)
SDev(tablprob)

<table>
<thead>
<tr>
<th>skyelavas</th>
<th>aphyric skye lavas data</th>
</tr>
</thead>
</table>

Description
AFM compositions of 23 aphyric Skye lavas. This data set can be found on page 360 of the Aitchison book (see reference).

Usage
data(skyelavas)

Format
A data frame with 23 observations on the following 3 variables.

Details
• sodium-potassium a numeric vector of percentages of Na2O+K2O
• iron a numeric vector of percentages of Fe2O3
• magnesium a numeric vector of percentages of MgO

Author(s)
Matthias Templ <matthias.templ@tuwien.ac.at>

References

Examples
data(skyelavas)
str(skyelavas)
summary(skyelavas)
rowSums(skyelavas)
Description

Social expenditures according to source (public or private) and three important branches (health, old age, incapacity related) in selected OECD countries in 2010. Expenditures are always provided in the respective currency.

Usage

data(socExp)

Format

A data frame with 20 observations on the following 8 variables (country + currency + row-wise sorted cells of 2x3 compositional table).

Details

• country Country of origin
• currency Currency unit (in Million)
• health-public Health from the public
• old-public Old age expenditures from the public
• incap-public Incapacity related expenditures from the public
• health-private Health from private sources
• old-private Old age expenditures from private sources
• incap-private Incapacity related expenditures from private sources

Author(s)

conversion to R by Karel Hron Karel Hron and modifications by Matthias Templ <matthias.templ@tuwien.ac.at>

References

OECD, http://www.oecd.org

Examples

data(socExp)
str(socExp)
rowSums(socExp[, 3:ncol(socExp)])
**stats**

*Classical estimates for tables*

**Description**

Some standard/classical (non-compositional) statistics

**Usage**

```r
stats(x, margins = NULL, statistics = c("phi", "cramer", "chisq", "yates"),
      maggr = mean)
```

**Arguments**

- **x**: a data.frame, matrix or table
- **margins**: margins
- **statistics**: statistics of interest
- **maggr**: a function for calculating the mean margins of a table, default is the arithmetic mean

**Details**

statistics 'phi' is the values of the table divided by the product of margins. 'cramer' normalize these values according to the dimension of the table. 'chisq' are the expected values according to Pearson while 'yates' according to Yates.

For the `maggr` function argument, arithmetic means (`mean`) should be chosen to obtain the classical results. Any other user-provided functions should be take with care since the classical estimations relies on the arithmetic mean.

**Value**

List containing all statistics

**Author(s)**

Matthias Templ

**References**

Examples

```r
data(precipitation)
tab1 <- indTab(precipitation)
stats(precipitation)
stats(precipitation, statistics = "cramer")
stats(precipitation, statistics = "chisq")
stats(precipitation, statistics = "yates")

## take with care
## (the provided statistics are not designed for that case):
stats(precipitation, statistics = "chisq", maggr = gmean)
```

**summary.imp**  
*Summary method for objects of class imp*

**Description**

A short comparison of the original data and the imputed data is given.

**Usage**

```r
## S3 method for class 'imp'
summary(object, ...)
```

**Arguments**

- `object` an object of class ‘imp’
- `...` additional arguments passed trough

**Details**

Note that this function will be enhanced with more sophisticated methods in future versions of the package. It is very rudimental in its present form.

**Value**

None (invisible NULL).

**Author(s)**

Matthias Templ

**See Also**

`impCoda`, `impKNNa`
Examples

data(expenditures)
expenditures[1,3]
expenditures[1,3] <- NA
xi <- impKNNa(expenditures)
xi
summary(xi)
# plot(xi, which=1:2)

teachingStuff               teaching stuff

Description

Teaching stuff in selected countries

Format

A (tidy) data frame with 1216 observations on the following 4 variables.

- country  Country of origin
- subject  school type: primary, lower secondary, higher secondary and tertiary
- year     Year
- value    Number of stuff

Details

Teaching staff include professional personnel directly involved in teaching students, including classroom teachers, special education teachers and other teachers who work with students as a whole class, in small groups, or in one-to-one teaching. Teaching staff also include department chairs of whose duties include some teaching, but it does not include non-professional personnel who support teachers in providing instruction to students, such as teachers’ aides and other paraprofessional personnel. Academic staff include personnel whose primary assignment is instruction, research or public service, holding an academic rank with such titles as professor, associate professor, assistant professor, instructor, lecturer, or the equivalent of any of these academic ranks. The category includes personnel with other titles (e.g. dean, director, associate dean, assistant dean, chair or head of department), if their principal activity is instruction or research.

Author(s)

translated from https://data.oecd.org/ and restructured by Matthias Templ

Source

OECD: https://data.oecd.org/
ternaryDiag

References


Examples

data(teachingStuff)
str(teachingStuff)

---

ternaryDiag  Ternary diagram

Description

This plot shows the relative proportions of three variables (compositional parts) in one diagramm. Before plotting, the data are scaled.

Usage

ternaryDiag(x, name = colnames(x), text = NULL, grid = TRUE,
gridCol = grey(0.6), mcex = 1.2, line = "none", robust = TRUE,
group = NULL, tol = 0.975, ...)

Arguments

x  matrix or data.frame with 3 columns
name  names of the variables
text  default NULL, text for each point can be provided
grid  if TRUE a grid is plotted additionally in the ternary diagram
gridCol  color for the grid lines
mcex  label size
line  may be set to “none”, “pca”, “regression”, “regressionconf”, “regressionpred”, “ellipse”, “lda”
robust  if line equals TRUE, it dedicates if a robust estimation is applied or not.
group  if line equals “da”, it determines the grouping variable
tol  if line equals “ellipse”, it determines the parameter for the tolerance ellipse
...  further parameters, see, e.g., par()

Details

The relative proportions of each variable are plotted.

Author(s)

Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>>, Matthias Templ
ternaryDiagAbline

References


See Also
ternary

Examples

data(arcticLake)
ternaryDiag(arcticLake)

data(coffee)
x <- coffee[,2:4]
grp <- as.integer(coffee[,1])
ternaryDiag(x, col=grp, pch=grp)
ternaryDiag(x, grid=FALSE, col=grp, pch=grp)
legend("topleft", legend=unique(coffee[,4]), pch=1:2, col=1:2)

ternaryDiag(x, grid=FALSE, col=grp, pch=grp, line="ellipse", tol=c(0.975,0.9), lty=2)
ternaryDiag(x, grid=FALSE, line="pca")
ternaryDiag(x, grid=FALSE, col=grp, pch=grp, line="pca", lty=2, lwd=2)

ternaryDiagAbline Adds a line to a ternary diagram.

Description

A low-level plot function which adds a line to a high-level ternary diagram.

Usage

ternaryDiagAbline(x, ...)

Arguments

x Two-dimensional data set in isometric log-ratio transformed space.

... Additional graphical parameters passed through.

Details

This is a small utility function which helps to add a line in a ternary plot from two given points in an isometric transformed space.
ternaryDiagEllipse

Value
   no values are returned.

Author(s)
   Matthias Templ

See Also
   ternaryDiag

Examples

   data(coffee)
   x <- coffee[,2:4]
   ternaryDiag(x, grid=FALSE)
   ternaryDiagAbline(data.frame(z1=c(0.01,0.5), z2=c(0.4,0.8)), col="red")

ternaryDiagEllipse   Adds tolerance ellipses to a ternary diagram.

Description
   Low-level plot function which add tolerance ellipses to a high-level plot of a ternary diagram.

Usage
   ternaryDiagEllipse(x, tolerance = c(0.9, 0.95, 0.975), locscatt = "MCD",
                       ...

Arguments
   x     Three-part composition. Object of class “matrix” or “data.frame”.
   tolerance  Determines the amount of observations with Mahalanobis distance larger than
               the drawn ellipse, scaled to one.
   locscatt  Method for estimating the mean and covariance.
   ...     Additional arguments passed through.

Value
   no values are returned.

Author(s)
   Peter Filzmoser, Matthias Templ
ternaryDiagPoints

See Also
ternaryDiag

Examples

```r
data(coffee)
x <- coffee[,2:4]
ternaryDiag(x, grid=FALSE)
ternaryDiagEllipses(x)
  ## or directly:
ternaryDiag(x, grid=FALSE, line="ellipse")
```

ternaryDiagPoints  

Add points or lines to a given ternary diagram.

Description

Low-level plot function to add points or lines to a ternary high-level plot.

Usage

```r
ternaryDiagPoints(x, ...)
```

Arguments

- `x` Three-dimensional composition given as an object of class “matrix” or “data.frame”.
- `...` Additional graphical parameters passed through.

Value

no values are returned.

Author(s)

Matthias Templ

References


See Also
ternaryDiag
Examples

```r
data(coffee)
x <- coffee[,2:4]
ternaryDiag(x, grid=FALSE)
ternaryDiagPoints(x+1, col="red", pch=2)
```

---

### Description

A regional-scale geochemical survey of C horizon samples in Nord-Trøndelag, Central Norway

### Usage

```r
data(trondelagC)
```

### Format

A data frame with 754 observations and 70 variables

### Details

- `X.S.ID` ID
- `X.Loc_ID` ID
- `longitude` longitude in WGS84
- `latitude` latitude in WGS84
- `E32wgs` UTM zone east
- `N32wgs` UTM zone north
- `X.Medium`
- `Ag` Concentration of silver (in mg/kg)
- `Al` Concentration of aluminum (in mg/kg)
- `As` Concentration of arsenic (in mg/kg)
- `Au` Concentration of gold (in mg/kg)
- `B` Concentration of boron (in mg/kg)
- `Ba` Concentration of barium (in mg/kg)
- `Be` Concentration of beryllium (in mg/kg)
- `Bi` Concentration of bismuth (in mg/kg)
- `Ca` Concentration of calcium (in mg/kg)
- `Cd` Concentration of cadmium (in mg/kg)
- Ce  Concentration of cerium (in mg/kg)
- Co  Concentration of cobalt (in mg/kg)
- Cr  Concentration of chromium (in mg/kg)
- Cs  Concentration of cesium (in mg/kg)
- Cu  Concentration of copper (in mg/kg)
- Fe  Concentration of iron (in mg/kg)
- Ga  Concentration of gallium (in mg/kg)
- Ge  Concentration of germanium (in mg/kg)
- Hf  Concentration of hafnium (in mg/kg)
- Hg  Concentration of mercury (in mg/kg)
- In  Concentration of indium (in mg/kg)
- K  Concentration of potassium (in mg/kg)
- La  Concentration of lanthanum (in mg/kg)
- Li  Concentration of lithium (in mg/kg)
- Mg  Concentration of magnesium (in mg/kg)
- Mn  Concentration of manganese (in mg/kg)
- Mo  Concentration of molybdenum (in mg/kg)
- Na  Concentration of sodium (in mg/kg)
- Nb  Concentration of niobium (in mg/kg)
- Ni  Concentration of nickel (in mg/kg)
- P  Concentration of phosphorus (in mg/kg)
- Pb  Concentration of lead (in mg/kg)
- Pb204  Concentration of lead, 204 neutrons (in mg/kg)
- Pb206  Concentration of lead, 206 neutrons (in mg/kg)
- Pb207  Concentration of lead, 207 neutrons (in mg/kg)
- Pb208  Concentration of lead, 208 neutrons (in mg/kg)
- X6_7Pb  Concentration of lead (in mg/kg)
- X7_8Pb  Concentration of lead (in mg/kg)
- X6_4Pb  Concentration of lead (in mg/kg)
- X7_4Pb  Concentration of lead (in mg/kg)
- X8_4Pb  Concentration of lead (in mg/kg)
- Pd  Concentration of palladium (in mg/kg)
- Pt  Concentration of platinum (in mg/kg)
- Rb  Concentration of rubidium (in mg/kg)
- Re  Concentration of rhenium (in mg/kg)
- S  Concentration of sulfur (in mg/kg)
- Sb  Concentration of antimony (in mg/kg)
The samples were analysed using aqua regia extraction. Sampling was based on a 6.6km grid, i.e. 1 sample site/36 km².

Author(s)

NGU, http://www.ngu.no, transferred to R by Matthias Templ <matthias.templ@tuwien.ac.at>

References


Examples

data(trondelago)
str(trondelago)

trondelago  regional geochemical survey of soil O in Norway

Description

A regional-scale geochemical survey of O horizon samples in Nord-Trondelag, Central Norway

Usage

data(trondelago)
Format

A data frame with 754 observations and 70 variables

Details

- `X.Loc_ID` ID
- `LITHO` Rock type
- `longitude` longitude in WGS84
- `latitude` latitude in WGS84
- `E32wgs` UTM zone east
- `N32wgs` UTM zone north
- `X.Medium` a numeric vector
- `Alt_masl` a numeric vector
- `LOI_480` Loss on ignition
- `pH` Numeric scale used to specify the acidity or alkalinity of an aqueous solution
- `Ag` Concentration of silver (in mg/kg)
- `Al` Concentration of aluminum (in mg/kg)
- `As` Concentration of arsenic (in mg/kg)
- `Au` Concentration of gold (in mg/kg)
- `B` Concentration of boron (in mg/kg)
- `Ba` Concentration of barium (in mg/kg)
- `Be` Concentration of beryllium (in mg/kg)
- `Bi` Concentration of bismuth (in mg/kg)
- `Ca` Concentration of calcium (in mg/kg)
- `Cd` Concentration of cadmium (in mg/kg)
- `Ce` Concentration of cerium (in mg/kg)
- `Co` Concentration of cobalt (in mg/kg)
- `Cr` Concentration of chromium (in mg/kg)
- `Cs` Concentration of cesium (in mg/kg)
- `Cu` Concentration of copper (in mg/kg)
- `Fe` Concentration of iron (in mg/kg)
- `Ga` Concentration of gallium (in mg/kg)
- `Ge` Concentration of germanium (in mg/kg)
- `Hf` Concentration of hafnium (in mg/kg)
- `Hg` Concentration of mercury (in mg/kg)
- `In` Concentration of indium (in mg/kg)
- `K` Concentration of potassium (in mg/kg)
- `La` Concentration of lanthanum (in mg/kg)
• Li Concentration of lithium (in mg/kg)
• Mg Concentration of magnesium (in mg/kg)
• Mn Concentration of manganese (in mg/kg)
• Mo Concentration of molybdenum (in mg/kg)
• Na Concentration of sodium (in mg/kg)
• Nb Concentration of niobium (in mg/kg)
• Ni Concentration of nickel (in mg/kg)
• P Concentration of phosphorus (in mg/kg)
• Pb Concentration of lead (in mg/kg)
• Pb204 Concentration of lead, 204 neutrons (in mg/kg)
• Pb206 Concentration of lead, 206 neutrons (in mg/kg)
• Pb207 Concentration of lead, 207 neutrons (in mg/kg)
• Pb208 Concentration of lead, 208 neutrons (in mg/kg)
• X6_7Pb Concentration of lead (in mg/kg)
• X7_8Pb Concentration of lead (in mg/kg)
• X6_4Pb Concentration of lead (in mg/kg)
• X7_4Pb Concentration of lead (in mg/kg)
• X8_4Pb Concentration of lead (in mg/kg)
• Pd Concentration of palladium (in mg/kg)
• Pt Concentration of platium (in mg/kg)
• Rb Concentration of rubidium (in mg/kg)
• Re Concentration of rhenium (in mg/kg)
• S Concentration of sulfur (in mg/kg)
• Sb Concentration of antimony (in mg/kg)
• Sc Concentration of scandium (in mg/kg)
• Se Concentration of selenium (in mg/kg)
• Sn Concentration of tin (in mg/kg)
• Sr Concentration of strontium (in mg/kg)
• Ta Concentration of tantalum (in mg/kg)
• Te Concentration of tellurium (in mg/kg)
• Th Concentration of thorium (in mg/kg)
• Tl Concentration of thalium (in mg/kg)
• U Concentration of uranium (in mg/kg)
• V Concentration of vanadium (in mg/kg)
• W Concentration of tungsten (in mg/kg)
• Y Concentration of yttrium (in mg/kg)
• Zn Concentration of zinc (in mg/kg)
• Zr Concentration of zirconium (in mg/kg)

The samples were analysed using aqua regia extraction. Sampling was based on a 6.6km grid, i.e. 1 sample site/36 km2.
Author(s)

NGU, http://www.ngu.no, transferred to R by Matthias Templ <matthias.templ@tuwien.ac.at>

References


Examples

data(trondelag0)
str(trondelag0)

unemployed    unemployed of young people

Description

Youth not in employment, education or training (NEET) in 43 countries from 1997 till 2015

Format

A (tidy) data frame with 1216 observations on the following 4 variables.

• country  Country of origin
• age  age group
• year  Year
• value  percentage of unemployed

Details

This indicator presents the share of young people who are not in employment, education or training (NEET), as a percentage of the total number of young people in the corresponding age group, by gender. Young people in education include those attending part-time or full-time education, but exclude those in non-formal education and in educational activities of very short duration. Employment is defined according to the OECD/ILO Guidelines and covers all those who have been in paid work for at least one hour in the reference week of the survey or were temporarily absent from such work. Therefore NEET youth can be either unemployed or inactive and not involved in education or training. Young people who are neither in employment nor in education or training are at risk of becoming socially excluded - individuals with income below the poverty-line and lacking the skills to improve their economic situation.

Author(s)

translated from https://data.oecd.org/ and restructured by Matthias Templ
variation

Source

OECD: https://data.oecd.org/

References


Examples

data(unemployed)
str(unemployed)

<table>
<thead>
<tr>
<th>variation</th>
<th>Robust and classical variation matrix</th>
</tr>
</thead>
</table>

Description

Estimates the variation matrix with robust methods.

Usage

variation(x, robust = TRUE)

Arguments

x data frame or matrix with positive entries
robust if FALSE, standard measures are used.

Details

The variation matrix is estimated for a given compositional data set. Instead of using the classical standard deviations the mad is used when parameter robust is set to TRUE.

Value

The (robust) variation matrix.

Author(s)

Matthias Templ

References

Examples

data(expenditures)
variation(expenditures)
variation(expenditures, robust=FALSE)

zeroOut  Detection of outliers of zero-inflated data

Description

detects outliers in compositional zero-inflated data

Usage

zeroOut(x, impute = "knn")

Arguments

  x  a data frame
  impute  imputation method internally used

Details

XXX

Value

XXX

Author(s)

  Matthias Templ

Examples

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