

Package ‘robCompositions’

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Description The package includes methods for imputation of compositional data including robust methods, methods to impute 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

NeedsCompilation yes

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robCompositions-package
Robust Estimation for Compositional Data.

Description

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
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License: GPL 2
LazyLoad: yes

Author(s)

Matthias Templ, Peter Filzmoser, Karel Hron,
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References

Aitchison, J. (1986) *The Statistical Analysis of Compositional Data* Monographs on Statistics and Applied Probability. Chapman & Hall Ltd., London (UK). 416p. \

Filzmoser, P., and Hron, K. (2008) Outlier detection for compositional data using robust methods. *Math. Geosciences*, **40** 233-248.

Filzmoser, P., Hron, K., Reimann, C. (2009) Principal Component Analysis for Compositional Data with Outliers. *Environmetrics*, **20** (6), 621–632.

P. Filzmoser, K. Hron, C. Reimann, R. Garrett (2009): Robust Factor Analysis for Compositional Data. *Computers and Geosciences*, **35** (9), 1854–1861.

Hron, K. and Templ, M. and Filzmoser, P. (2010) Imputation of missing values for compositional data using classical and robust methods *Computational Statistics and Data Analysis*, **54** (12), 3095–3107.

C. Reimann, P. Filzmoser, R.G. Garrett, and R. Dutter (2008): *Statistical Data Analysis Explained. Applied Environmental Statistics with R*. John Wiley and Sons, Chichester, 2008.

Examples

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

## iterative model based imputation
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

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
data(expenditures)
oD <- outCoDa(expenditures)
oD
plot(oD)

## transformations
data(arcticLake)
x <- arcticLake
x.alr <- addLR(x, 2)
y <- addLRinv(x.alr)
addLRinv(addLR(x, 3))
data(expenditures)
x <- expenditures
```

```

y <- addLRinv(addLR(x, 5))
head(x)
head(y)
addLRinv(x.alr, ivar=2, useClassInfo=FALSE)

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

require(MASS)
Sigma <- matrix(c(5.05,4.95,4.95,5.05), ncol=2, byrow=TRUE)
z <- isomLRinv(mvnorm(100, mu=c(0,2), Sigma=Sigma))

```

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))
```

Arguments

<code>x</code>	D-part compositional data
<code>ivar</code>	Rationing part

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:

<code>x.alr</code>	the transformed data
<code>varx</code>	the rationing variable
<code>ivar</code>	the index of the rationing variable, indicating the column number of the rationing variable in the data matrix <i>x</i>
<code>cnames</code>	the column names of <i>x</i>

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

Aitchison, J. (1986) *The Statistical Analysis of Compositional Data* Monographs on Statistics and Applied Probability. Chapman & Hall Ltd., London (UK). 416p.

See Also

[addLRinv](#), [isomLR](#)

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))
head(x)
head(y)
## --> absolute values are preserved as well.

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

addLRinv

Additive logistic transformaton

Description

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

Usage

```
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

Aitchison, J. (1986) *The Statistical Analysis of Compositional Data* Monographs on Statistics and Applied Probability. Chapman & Hall Ltd., London (UK). 416p.

See Also

[isomLRinv](#), [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))
head(x)
head(y)
## --> absolute values are preserved as well.

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

aDist	<i>Aitchison distance</i>
-------	---------------------------

Description

Computes the Aitchison distance between two observations or between two data sets.

Usage

```
aDist(x, y)
```

Arguments

x	a vector, matrix or data.frame
y	a vector, matrix or data.frame with equal dimension as x

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 and evaluate 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 is to compare two matrices.

The underlying code is written in C and allows a fast computation also for large data sets.

Value

The Aitchison distance between two compositions or between two data sets.

Author(s)

Matthias Templ

References

Aitchison, J. (1986) *The Statistical Analysis of Compositional Data* Monographs on Statistics and Applied Probability. Chapman and Hall Ltd., London (UK). 416p.

Aitchison, J. and Barcelo-Vidal, C. and Martin-Fernandez, J.A. and Pawlowsky-Glahn, V. (2000) Logratio analysis and compositional distance. *Mathematical Geology*, **32**, 271-275.

Hron, K. and Templ, M. and Filzmoser, P. (2010) Imputation of missing values for compositional data using classical and robust methods *Computational Statistics and Data Analysis*, vol 54 (12), pages 3095-3107.

See Also

[isomLR](#)

Examples

```
data(expenditures)
x <- xOrig <- expenditures
## Aitchison distance between the first 2 observations:
aDist(x[,1], x[,2])

## set some missing values:
x[1,3] <- x[3,5] <- x[2,4] <- x[5,3] <- x[8,3] <- NA

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

## calculate the relative Aitchison distance between xOrig and xImp:
aDist(xOrig, xImp)
```

adjust

Adjusting for original scale

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

Hron, K. and Templ, M. and Filzmoser, P. (2010) Imputation of missing values for compositional data using classical and robust methods *Computational Statistics and Data Analysis*, In Press, Corrected Proof, ISSN: 0167-9473, DOI:10.1016/j.csda.2009.11.023

See Also[impCoda](#)**Examples**

```

data(expenditures)
x <- expenditures
x[1,3] <- x[2,4] <- x[3,3] <- x[3,4] <- NA
xi <- impCoda(x)
x
xi$xImp
adjust(xi)$xImp

```

adtest

*Anderson-Darling Normality Tests***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](#).

Author(s)

Karel Hron, Matthias Templ

References

Anderson, T.W. and Darling, D.A. (1952) Asymptotic theory of certain goodness-of-fit criteria based on stochastic processes. *Annals of Mathematical Statistics*, **23** 193-212.

See Also

[adtestWrapper](#)

Examples

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

adtestWrapper

Wrapper for Anderson-Darling tests

Description

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

Usage

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

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.
robustEst	logical

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 normality.

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

Anderson, T.W. and Darling, D.A. (1952) *Asymptotic theory of certain goodness-of-fit criteria based on stochastic processes* Annals of Mathematical Statistics, **23** 193-212.

Aitchison, J. (1986) *The Statistical Analysis of Compositional Data* Monographs on Statistics and Applied Probability. Chapman & Hall Ltd., London (UK). 416p.

See Also

[adtest](#), [isomLR](#)

Examples

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

`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)
```

Format

A data frame with 39 observations on the following 3 variables.

`sand` numeric vector of percentages of sand

`silt` numeric vector of percentages of silt

`clay` numeric vector of percentages of clay

Details

The rows sum up to 100, except for rounding errors.

Source

Aitchison, J. (1986) *The Statistical Analysis of Compositional Data* Monographs on Statistics and Applied Probability. Chapman & Hall Ltd., London (UK). 416p.

Examples

```
data(arcticLake)
```

`cenLR`*Centred log-ratio transformation*

Description

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

Usage

```
cenLR(x)
```

Arguments

x multivariate data ideally of class data.frame or matrix

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

Aitchison, J. (1986) *The Statistical Analysis of Compositional Data* Monographs on Statistics and Applied Probability. Chapman & Hall Ltd., London (UK). 416p.

See Also

[cenLRinv](#), [addLR](#), [isomLR](#), [addLRinv](#), [isomLRinv](#)

Examples

```
data(expenditures)
eclr <- cenLR(expenditures)
inveclr <- cenLRinv(eclr)
head(expenditures)
head(inveclr)
head(isomLRinv(eclr$x.clr))
```

cenLRinv	<i>Inverse centred log-ratio transformation</i>
----------	---

Description

Applies the inverse centred log-ratio transformation.

Usage

```
cenLRinv(x, useClassInfo = TRUE)
```

Arguments

x	an object of class “clr”, “data.frame” or “matrix”
useClassInfo	if the object is of class “clr”, the useClassInfo is used to determine if the class information should be used. If yes, also absolute values may be preserved.

Value

the transformed data set.

Author(s)

Matthias Templ

References

Aitchison, J. (1986) *The Statistical Analysis of Compositional Data* Monographs on Statistics and Applied Probability. Chapman & Hall Ltd., London (UK). 416p.

See Also

[cenLR](#), [addLR](#), [isomLR](#), [addLRinv](#), [isomLRinv](#)

Examples

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

coffee	<i>Coffee data</i>
--------	--------------------

Description

27 commercially available coffee samples of different origins.

Usage

```
data(coffee)
```

Format

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

Metpyr Hydroxy-2-propanone

5-Met methylpyrazine

furfu methylfurfural

sort a character vector

Details

In the original data set, 15 volatile compounds (descriptors of coffee aroma) were selected for a statistical analysis. We selected only three compounds (compositional parts) Hydroxy-2-propanone, methylpyrazine and methylfurfural to allow for a visualization in a ternary diagram.

References

M.~Korhonov`a, K.~Hron, D.~Klimc`ikov`a, L.~Muller, P.~Bedn`ar, and P.~Bart`ak (2009) Coffee aroma - statistical analysis of compositional data. *Talanta*, 80(2): 710–715.

Examples

```
data(coffee)
```

constSum	<i>Constant sum</i>
----------	---------------------

Description

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

Usage

```
constSum(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

```
data(expenditures)
constSum(expenditures)
constSum(expenditures, 100)
```

daFisher

Discriminant analysis by Fisher Rule.

Description

Discriminant analysis by Fishers rule.

Usage

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

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”
plotScore	TRUE, if the scores should be plotted automatically.

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 loses 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
coda	coda

Author(s)

The code is was written by Peter Filzmoser. Minor modifications by Matthias Templ.

References

Filzmoser, P. and Hron, K. and Templ, M. (2009) Discriminant analysis for compositional data and robust parameter estimation. *Research Report SM-2009-3*, Vienna University of Technology, 27 pages.

Fisher, R. A. (1938) The statistical utilization of multiple measurements. *Annals of Eugenics*, 8:376-386.

Rao, C.R. (1948) The utilization of multiple measurements in problems of biological classification. *Journal of the Royal Statistical Society, Series B*, 10:159-203.

See Also

[Linda](#)

Examples

```
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))

#par(mfrow=c(1,2))
```

```
d1 <- daFisher(X,grp=grp,method="classical",coda=FALSE)
d2 <- daFisher(X,grp=grp,method="robust",coda=FALSE)
d2
```

expenditures	<i>Household expenditures data</i>
--------------	------------------------------------

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 with the following 5 variables.

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)

Details

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.

Source

Aitchison, J. (1986) *The Statistical Analysis of Compositional Data* Monographs on Statistics and Applied Probability. Chapman & Hall Ltd., London (UK). 416p.

Examples

```
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	<i>Mean consumption expenditures data.</i>
----------------	--

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.

Usage

```
data(expendituresEU)
```

Format

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

Food a numeric vector
Alcohol a numeric vector
Clothing a numeric vector
Housing a numeric vector
Furnishings a numeric vector
Health a numeric vector
Transport a numeric vector
Communications a numeric vector
Recreation a numeric vector
Education a numeric vector
Restaurants a numeric vector
Other a numeric vector

Source

Eurostat: [http://epp.eurostat.ec.europa.eu/statistics_explained/images/c/c2/Mean_consumption_expenditure_of_households,_2005\(PPS\).PNG](http://epp.eurostat.ec.europa.eu/statistics_explained/images/c/c2/Mean_consumption_expenditure_of_households,_2005(PPS).PNG)

References

Eurostat provides a website with the data:

http://epp.eurostat.ec.europa.eu/statistics_explained/index.php/Household_consumption_expenditure

Examples

```
data(expendituresEU)
```

gm	<i>geometric mean</i>
----	-----------------------

Description

This function calculates the geometric mean.

Usage

```
gm(x)
```

Arguments

x A numeric vector.

Details

Calculates the geometric mean of all positive entries of a vector.

Value

The geometric mean.

Author(s)

Matthias Templ

Examples

```
gm(runif(100))
```

haplogroups	<i>Haplogroups data.</i>
-------------	--------------------------

Description

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

Usage

```
data(haplogroups)
```

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)
```

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

```
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*.

Author(s)

Jiri Eichler

References

Hron, K. and Templ, M. and Filzmoser, P. (2010) Imputation of missing values for compositional data using classical and robust methods, *Computational Statistics and Data Analysis*, vol 54 (12), pages 3095-3107.

Martin-Fernandez, J.A. and Hron, K. and Templ, M. and Filzmoser, P. and Palarea-Albaladejo, J. (2012) Model-based replacement of rounded zeros in compositional data: Classical and robust approaches, *Computational Statistics*, 56 (2012), S. 2688 - 2704.

See Also

[impCoda](#), [impRZilr](#)

Examples

```
## see the compositionsGUI
```

impCoda

Imputation of missing values in compositional data

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 <code>==</code> "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.

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.

method 'roundedZero' is experimental. It imputes rounded zeros within our iterative framework.

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

Hron, K. and Templ, M. and Filzmoser, P. (2010) Imputation of missing values for compositional data using classical and robust methods *Computational Statistics and Data Analysis*, vol 54 (12), pages 3095-3107.

See Also

[impKNNa](#), [isomLR](#)

Examples

```
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
```

impKNNa

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

Aitchison, J. and Barcelo-Vidal, C. and Martin-Fernandez, J.A. and Pawlowsky-Glahn, V. (2000) Logratio analysis and compositional distance, *Mathematical Geology* 32(3):271-275.

Hron, K. and Templ, M. and Filzmoser, P. (2010) Imputation of missing values for compositional data using classical and robust methods *Computational Statistics and Data Analysis*, vol 54 (12), pages 3095-3107.

See Also

[impCoda](#)

Examples

```

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

```

impRZalr

alr EM-based Imputation for Rounded Zeros

Description

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

Usage

```

impRZalr(x, pos = ncol(x), dl = rep(0.05, ncol(x) - 1), eps = 1e-04,
maxit = 50, bruteforce=FALSE, method="lm", step=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

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

[impRZilr](#)

Examples

```
data(arcticLake)
x <- arcticLake
## generate rounded zeros artificially:
x[x[,1] < 5, 1] <- 0
x[x[,2] < 47, 2] <- 0
xia <- impRZalr(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

```
impRZilr(x, maxit = 10, eps = 0.1, method = "pls",
  dl = rep(0.05, ncol(x)), nComp="boot", bruteforce = FALSE,
  noisemethod="residuals", noise=FALSE, R=10, 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.
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 exceptionally 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".
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 iteratively imputes parts with rounded zeros whereas in each step (1) a 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

[impRZalr](#)

Examples

```
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
```

`isomLR`*Isometric log-ratio transformation*

Description

An isometric log-ratio transformation with a special choice of the balances according to Hron et al. (2010).

Usage`isomLR(x)`**Arguments**

`x` object of class `data.frame` or matrix with positive entries

Details

The `isomLR` transformation moves D -part compositional data from the simplex into a $(D-1)$ -dimensional real space isometrically. From this choice of the balances, all the relative information of the part x_1 from the remaining parts is separated. It is useful for estimating missing values in x_1 by regression of the remaining variables.

Value

The `isomLR` transformed data.

Author(s)

Karel Hron, Matthias Templ

References

Egozcue J.J., V. Pawlowsky-Glahn, G. Mateu-Figueras and C. Barcel' o-Vidal (2003) Isometric log-ratio transformations for compositional data analysis. *Mathematical Geology*, **35**(3) 279-300. \

Hron, K. and Templ, M. and Filzmoser, P. (2010) Imputation of missing values for compositional data using classical and robust methods *Computational Statistics and Data Analysis*, vol 54 (12), pages 3095-3107.

See Also

[isomLRinv](#)

Examples

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

data(expenditures)
isomLR(expenditures)
```

`isomLRinv`*Inverse isometric log-ratio transformation*

Description

The inverse transformation of 'isomLR()'.

Usage

```
isomLRinv(x.ilr)
```

Arguments

`x.ilr` data frame or matrix

Details

For details on the choice of the balances, please, see at the research report for which the link is given below.

Value

The transformed data.

Author(s)

Karel Hron

References

Egozcue J.J., V. Pawlowsky-Glahn, G. Mateu-Figueras and C. Barcel'ó-Vidal (2003) Isometric log-ratio transformations for compositional data analysis. *Mathematical Geology*, **35**(3) 279-300 \

Hron, K. and Templ, M. and Filzmoser, P. (2010) Imputation of missing values for compositional data using classical and robust methods *Computational Statistics and Data Analysis*, vol 54 (12), pages 3095-3107.

See Also

[isomLR](#)

Examples

```
require(MASS)
Sigma <- matrix(c(5.05,4.95,4.95,5.05), ncol=2, byrow=TRUE)
set.seed(123)
z <- mvrnorm(100, mu=c(0,2), Sigma=Sigma)
x <- isomLRinv(z)
head(x)
```

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

```
lmCoDaX(y, X, method = "robust")
ilrregression(X, y)
robilrregression(X, y)
```

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

Filzmoser, P., Hron, K., Thompson, K. (2012) Linear regression with compositional explanatory variables. *Journal of Applied Statistics*, 39, 1115-1128.

See Also[lm](#)**Examples**

```
## 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")
```

machineOperators	<i>Machine operators data set</i>
------------------	-----------------------------------

Description

The data set from Aitchison (1986), p. 382, contains compositions of eight-hour shifts of 27 machine operators. The parts represent proportions of shifts in each activity: high-quality production, low-quality production, machine setting and machine repair.

Usage

```
data(machineOperators)
```

Format

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

hqproduction high-quality production

lqproduction low-quality production

setting machine settings

repair machine repair

References

Aitchison, J. (1986) *The Statistical Analysis of Compositional Data* Monographs on Statistics and Applied Probability. Chapman & Hall Ltd., London (UK). 416p.

Examples

```
## maybe str(machineOperators) ; plot(machineOperators) ...
```

missPatterns *missing or zero pattern structure.*

Description

Analysis of the missing or 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

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)
```

orthbasis	<i>Orthonormal basis</i>
-----------	--------------------------

Description

Orthonormal basis from cenLR transformed data to isomLR transformed data.

Usage

```
orthbasis(D)
```

Arguments

D number of parts (variables)

Details

For the chosen balances for “isomLR”, 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

See Also

[isomLR](#), [cenLR](#)

Examples

```
data(expenditures)
V <- orthbasis(ncol(expenditures))
xcen <- cenLR(expenditures)$x.clr
xi <- as.matrix(xcen)
xi2 <- isomLR(expenditures)
all.equal(xi, xi2)
```

 outCoDa

Outlier detection for compositional data

Description

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

Usage

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

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 $(n+p+1)/2$).

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.

Value

mahaldist	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

- Egozcue J.J., V. Pawlowsky-Glahn, G. Mateu-Figueras and C. Barcel'ó-Vidal (2003) Isometric log-ratio transformations for compositional data analysis. *Mathematical Geology*, **35**(3) 279-300. \
- Filzmoser, P., and Hron, K. (2008) Outlier detection for compositional data using robust methods. *Math. Geosciences*, **40** 233-248.\
- Rousseeuw, P.J., Van Driessen, K. (1999) A fast algorithm for the minimum covariance determinant estimator. *Technometrics*, **41** 212-223.

See Also

[isomLR](#)

Examples

```
data(expenditures)
oD <- outCoDa(expenditures)
oD
```

pcaCoDa

Robust principal component analysis for compositional data

Description

This function applies robust principal component analysis for compositional data.

Usage

```
pcaCoDa(x, method = "robust", mult_comp=NULL)
```

Arguments

x	compositional data
method	either "robust" (default) or "standard"
mult_comp	a list of numeric vectors holding the indices of linked compositions

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)

K. Hron, P. Filzmoser, M. Templ

References

Filzmoser, P., Hron, K., Reimann, C. (2009) Principal Component Analysis for Compositional Data with Outliers. *Environmetrics*, **20**, 621-632.

See Also

[print.pcaCoDa](#), [plot.pcaCoDa](#)

Examples

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

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

pfa

Factor analysis for compositional data

Description

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

Usage

```
pfa(x, factors, 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
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 not 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 negative 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

- C. Reimann, P. Filzmoser, R.G. Garrett, and R. Dutter (2008): *Statistical Data Analysis Explained. Applied Environmental Statistics with R*. John Wiley and Sons, Chichester, 2008.
- P. Filzmoser, K. Hron, C. Reimann, R. Garrett (2009): Robust Factor Analysis for Compositional Data. *Computers and Geosciences*, **35** (9), 1854–1861.

Examples

```
data(expenditures)
x <- expenditures
res0 <- pfa(x, factors=1, covmat="cov")

## the following produce always the same result:
res1 <- pfa(x, factors=1, covmat="covMcd")
res2 <- pfa(x, factors=1, covmat=covMcd(isomLR(x))$cov)
res3 <- pfa(x, factors=1, covmat=covMcd(isomLR(x)))
```

phd

PhD Students in the EU

Description

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

Usage

```
data(phd)
```

Format

The format is: num [1:33, 1:8] 516.5 7.5 5.2 22.6 4.8 ... - attr(*, "dimnames")=List of 2 ..\$: chr [1:33] "EU" "Belgien" "Bulgarien" "Tschech.Rep."\$: chr [1:8] "Gesamtzahl der Doktoranden (in 1 000)" "maennlich" "weiblich" "Naturwissen-schaften, Mathematik, Informatik u. Ingenieurwesen" ...

Details

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

Source

http://epp.eurostat.ec.europa.eu/cache/ITY_PUBLIC/1-18092009-AP/DE/1-18092009-AP-DE.PDF

Examples

```
data(phd)
phdImputed <- impCoda(phd)$xOrig
```

plot.imp	<i>Plot method for objects of class imp</i>
----------	---

Description

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

Usage

```
## S3 method for class 'imp'
plot(x, ..., which = 1, ord = 1:ncol(x),
     colcomb = "misnonmiss", plotvars = NULL,
     col = c("skyblue", "red"), alpha = NULL,
     lty = par("lty"), xaxt = "s", xaxlabels = NULL,
     las = 3, interactive = TRUE, pch = c(1, 3),
     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=“misnonmiss”, observations with missings in any variable are highlighted. 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 <code>par(ask=.)</code> .
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

Aitchison, J. (1986) *The Statistical Analysis of Compositional Data* Monographs on Statistics and Applied Probability. Chapman & Hall Ltd., London (UK). 416p.

Wegman, E. J. (1990) *Hyperdimensional data analysis using parallel coordinates* Journal of the American Statistical Association 85, 664–675.

See Also

[impCoda](#), [impKNNa](#), [scatterplot.matrix](#)

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.outCoDa

plot method for outCoDa objects

Description

Plots the Mahalanobis distance.

Usage

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

Arguments

x	object from class 'outCoDa'
y	...
...	...

Details

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.

Author(s)

Matthias Templ

References

Filzmoser, P., and Hron, K. (2008) Outlier detection for compositional data using robust methods. *Math. Geosciences*, **40** 233-248.

See Also

[outCoDa](#)

Examples

```
data(expenditures)
oD <- outCoDa(expenditures)
oD
plot(oD)
```

plot.pcaCoDa	<i>Plot method</i>
--------------	--------------------

Description

Provides robust compositional biplots.

Usage

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

Arguments

x	object of class 'pcaCoDa'
y	...
...	...

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

References

Aitchison, J. and Greenacre, M. (2002). Biplots of compositional data. *Applied Statistics*, **51**, 375-392. \

Filzmoser, P., Hron, K., Reimann, C. (2009) Principal Component Analysis for Compositional Data with Outliers. *Environmetrics*, **20** (6), 621–632.

See Also

[pcaCoDa](#)

Examples

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

## 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="standard")
plot(pc, xlab=rownames(arcticLake))
```

print.adtestWrapper *print method for objects of class adtestWrapper*

Description

Provides a short print output as shown in the examples.

Usage

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

Arguments

```
x                    object of class 'adtestWrapper'
...                   ...
```

Details

Have a look at the example, it's self-explaining.

Value

nothing

Author(s)

Matthias Templ and Karel Hron

See Also

[adtestWrapper](#), [summary.adtestWrapper](#)

Examples

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

print.daFisher *print method for objects of class daFisher*

Description

Provides a print output of objects from class “daFisher” as shown in the examples.

Usage

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

Arguments

x	object of class ‘daFisher’
...	...

Details

Have a look at the example, it’s self-explaining.

Value

nothing

Author(s)

Matthias Templ

See Also

[daFisher](#)

Examples

```
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))
```

```
d1 <- daFisher(X,grp=grp,method="classical",coda=FALSE)
d2 <- daFisher(X,grp=grp,method="robust",coda=FALSE)
d2
```

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

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

Arguments

x	an object of class 'imp'
...	additional arguments passed trough

Value

None (invisible NULL).

Author(s)

Matthias Templ

See Also

[impCoda](#), [impKNNa](#)

Examples

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

print.outCoDa *print method for outCoDa objects*

Description

Gives a short information of the amount of outliers in objects of class 'outCoDa'.

Usage

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

Arguments

x	object of class 'ourCoDa'
...	...

Author(s)

Matthias Templ, Karel Hron

See Also

[outCoDa](#)

Examples

```
data(expenditures)  
oD <- outCoDa(expenditures)  
oD
```

print.pcaCoDa *Print method for pcaCoDa objects*

Description

Print method for objects of class 'pcaCoDa'.

Usage

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

Arguments

x	object of class 'pcaCoDa'
...	...

Value

Prints the (cummulative) percentages of explained variability for clr transformed data by principal component analysis.

Author(s)

M. Templ, K. Hron

See Also

[pcaCoDa](#), [plot.pcaCoDa](#)

Examples

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

robVariation	<i>Robust variation matrix</i>
--------------	--------------------------------

Description

Estimates the variation matrix with robust methods.

Usage

```
robVariation(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

Aitchison, J. (1986) *The Statistical Analysis of Compositional Data* Monographs on Statistics and Applied Probability. Chapman & Hall Ltd., London (UK). 416p.

Examples

```
data(expenditures)
robVariation(expenditures)
robVariation(expenditures, robust=FALSE)
```

skyeLavas

Aphyric skye lavas data

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.

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

Source

Aitchison, J. (1986) *The Statistical Analysis of Compositional Data* Monographs on Statistics and Applied Probability. Chapman & Hall Ltd., London (UK). 416p.

Examples

```
data(skyeLavas)
```

summary.adtestWrapper *summary method for objects of class adtestWrapper*

Description

Provides a summary as shown in the examples.

Usage

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

Arguments

object	object of class 'adtestWrapper'
...	additional arguments passed through

Details

A similar output is proposed by (Pawlowsky-Glahn, et al. (2008)). In addition to that, p-values are provided.

Value

a data frame including an information about the ilr-variables used (first column), the underlying test (second column), the test statistics (third column), the corresponding estimated p-values (fourth column) and an information about the rejection of the null hypothesis (last column).

Author(s)

Matthias Templ and Karel Hron

References

Pawlowsky-Glahn, V., Egozcue, J.J. and Tolosana-Delgado, R. (2008), *Lecture Notes on Compositional Data Analysis* Universitat de Girona, <http://dugi-doc.udg.edu/bitstream/10256/297/1/CoDa-book.pdf>

See Also

[adtestWrapper](#)

Examples

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

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

Description

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

Usage

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

Arguments

<code>object</code>	an object of class 'imp'
<code>...</code>	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)
```

ternaryDiag	<i>Ternary diagram</i>
-------------	------------------------

Description

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

Usage

```
ternaryDiag(x, name = colnames(x), 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
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>> <http://www.statistik.tuwien.ac.at/public/filz/>, Matthias Templ

References

C. Reimann, P. Filzmoser, R.G. Garrett, and R. Dutter: Statistical Data Analysis Explained. Applied Environmental Statistics with R. John Wiley and Sons, Chichester, 2008.

See Also

[ternary](#)

Examples

```
data(arcticLake)
ternaryDiag(arcticLake)

data(coffee)
x <- coffee[,1:3]
grp <- as.integer(factor(coffee[,4]))
ternaryDiag(x, col=grp, pch=grp)
ternaryDiag(x, grid=FALSE, col=grp, pch=grp)
legend("topright", 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	<i>Adds a line to a ternary diagram.</i>
-------------------	--

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.

Value

no values are returned.

Author(s)

Matthias Templ

See Also

[ternaryDiag](#)

Examples

```
data(coffee)
x <- coffee[,1:3]
ternaryDiag(x, grid=FALSE)
ternaryDiagAblines(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 trough.

Value

no values are returned.

Author(s)

Peter Filzmoser, Matthias Templ

See Also

[ternaryDiag](#)

Examples

```
data(coffee)
x <- coffee[,1:3]
ternaryDiag(x, grid=FALSE)
ternaryDiagEllipse(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

```
ternaryDiagPoints(x, ...)  
ternaryDiagLines(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

C. Reimann, P. Filzmoser, R.G. Garrett, and R. Dutter: Statistical Data Analysis Explained. Applied Environmental Statistics with R. John Wiley and Sons, Chichester, 2008.

See Also

[ternaryDiag](#)

Examples

```
data(coffee)  
x <- coffee[,1:3]  
ternaryDiag(x, grid=FALSE)  
ternaryDiagPoints(x+1, col="red", pch=2)
```


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