

# Package ‘robCompositions’

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**Title** Compositional Data Analysis

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MASS, mclust, sROC, tidyr, robustbase, VIM, zCompositions,  
reshape2, Rcpp

**Suggests** knitr, testthat

**VignetteBuilder** knitr

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

**Description** Methods for analysis of compositional data including robust methods (<doi:10.1007/978-3-319-96422-5>), imputation of missing values (<doi:10.1016/j.csda.2009.11.023>), methods to replace rounded zeros (<doi:10.1080/02664763.2017.1410524>, <doi:10.1016/j.chemolab.2016.04.011>, <doi:10.1016/j.csda.2012.02.012>), count zeros (<doi:10.1177/1471082X14535524>), methods to deal with essential zeros (<doi:10.1080/02664763.2016.1182135>), (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, functional data analysis and p-splines (<doi:10.1016/j.csda.2015.07.007>), contingency (<doi:10.1080/03610926.2013.824980>) and compositional tables (<doi:10.1111/sjos.12326>, <doi:10.1111/sjos.12223>, <doi:10.1080/02664763.2013.856871>) 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**Encoding** UTF-8**RoxygenNote** 7.0.0**NeedsCompilation** yes**Author** Matthias Templ [aut, cre] (<<https://orcid.org/0000-0002-8638-5276>>),

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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  
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

- 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 <- pivotCoordInv(mvrnorm(100, mu=c(0,2), Sigma=Sigma))
```

---

addLR	<i>Additive logratio coordinates</i>
-------	--------------------------------------

---

### Description

The additive logratio coordinates map 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 resulting coordinates
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 an inverse mapping 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](#), [pivotCoord](#)

**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

*Inverse additive logratio mapping*

---

**Description**

Inverse additive logratio mapping, 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 resulting compositional 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**

[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	<i>Aitchison distance</i>
-------	---------------------------

---

### Description

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

### Usage

```
aDist(x, y = NULL)
```

```
iproduct(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 compositional data. 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

- 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**[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:
x[1,3] <- x[3,5] <- x[2,4] <- x[5,3] <- x[8,3] <- NA

## impute the missing values:
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)

```

---

**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(pivotCoord(x[,1:2]))
adtest(pivotCoord(x[,1:3]))
adtest(pivotCoord(x))
adtest(pivotCoord(x[,1:2]), locscatt="robust")
```

---

adtestWrapper	<i>Wrapper for Anderson-Darling tests</i>
---------------	---

---

### 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)
```

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

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

### 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
...	additional parameters for print and summary passed through
object	an object of class adtestWrapper for the summary method

### 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.

A print and a summary method are implemented. The latter one provides a similar output is proposed 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**

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](#), [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**

Fiserova, E. and Hron, K. (2012). Statistical Inference in Orthogonal Regression for Three-Part Compositional Data Using a Linear Model with Type-II Constraints. *Communications in Statistics - Theory and Methods*, 41 (13-14), 2367-2385.

**Examples**

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

---

alcohol

*alcohol consumptions by country and type of alcohol*

---

**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**

Transferred from the World Health Organisation website.



**Examples**

```
data("alcohol")
str(alcohol)
summary(alcohol)
```

---

alcoholreg	<i>regional alcohol per capita (15+) consumption by WHO region</i>
------------	--

---

**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**

Transferred 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)
```

**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**

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

**Examples**

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

balances

*Balance calculation***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, resulting in orthonormal coordinates with respect to the Aitchison geometry of compositional data.

**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  $D \times (D-1)$  contrast matrix associated with the orthonormal basis, corresponding to the sequential binary partition (in clr coefficients).

**Author(s)**

Veronika Pintar, Karel Hron, Matthias Templ

**References**

(Egozcue, J.J., Pawłowsky-Glahn, V. (2005) Groups of parts and their balances in compositional data analysis. *Mathematical Geology*, 37 (7), 795-828.)

**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,-1,1),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)

```

---

biomarker

*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 wheter outlier diagnostic should be computed
plot	logical, indicating wheter Vstar values should be plotted
diag.plot	logical, indicating wheter 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 that 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 $V$ , $Vstar$ , 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 <code>diag=TRUE</code> )

**Author(s)**

Jan Walach

Jan Walach

**See Also**

[plot.biomarker](#)

**Examples**

```

# 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**

```

## 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

## 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

[pfa](#)

## Examples

```
data(expenditures)
res.rob <- pfa(expenditures, factors=2, scores = "regression")
biplot(res.rob)
```

---

biplot.pcaCoDa	<i>Biplot method</i>
----------------	----------------------

---

## Description

Provides robust compositional biplots.

## Usage

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

## Arguments

x	object of class 'pcaCoDa'
y	...
...	arguments passed to plot methods

## 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

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

## Examples

```
data(coffee)
p1 <- pcaCoDa(coffee[, -1])
p1
biplot(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="classical")
biplot(pc, xlabs=rownames(arcticLake))
```

---

bootnComp

*Bootstrap to find optimal number of components*

---

## Description

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

## Usage

```
bootnComp(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 `impRZilr`.

**Value**

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

**Author(s)**

Matthias Templ

**See Also**

[impRZilr](#)

**Examples**

```
## we refer to impRZilr()
```

---

cancer

*hospital discharges on cancer and distribution of age*

---

**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**

- country country
- year year
- p1 percentage of population with age below 15
- p2 percentage of population with age between 15 and 60
- p3 percentage of population with age above 60
- 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**

<http://www.ec.europa.eu/eurostat> and <http://unstats.un.org/unsd>

**References**

K. Hron, P. Filzmoser, K. Thompson (2012). Linear regression with compositional explanatory variables. *Journal of Applied Statistics*, Volume 39, Issue 5, 2012.

**Examples**

```
data(cancer)
str(cancer)
```

---

cancerMN	<i>malignant neoplasms cancer</i>
----------	-----------------------------------

---

**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 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 intergration by Matthias Templ <matthias.templ@tuwien.ac.at>

**Source**

<http://www.oecd.org>

## 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 compositional error distance

## Author(s)

Matthias Templ

## References

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

Templ, M., Hron, K., Filzmoser, P., Gardlo, A. (2016). Imputation of rounded zeros for high-dimensional compositional data. *Chemometrics and Intelligent Laboratory Systems*, 155, 183-190.

## See Also

[rdcm](#)

**Examples**

```

data(expenditures)
x <- expenditures
x[1,3] <- NA
xi <- impKNNa(x)$xImp
ced(expenditures, xi, ni = sum(is.na(x)))

```

---

cenLR

*Centred logratio coefficients*


---

**Description**

The centred logratio (clr) coefficients map 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 resulting clr coefficients, including

x.clr	clr coefficients
gm	the geometric means of the original compositional data.

**Note**

The resulting 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](#), [pivotCoord](#), [addLRinv](#), [pivotCoordInv](#)

**Examples**

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

---

cenLRinv

*Inverse centred logratio mapping*

---

**Description**

Applies the inverse centred logratio mapping.

**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 resulting compositional 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](#), [pivotCoord](#), [addLRinv](#), [pivotCoordInv](#)

## 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

**Cu** concentration in mg/kg  
**Eu\_INAA** concentration in mg/kg  
**Fe** concentration in mg/kg  
**Fe\_XRF** concentration in wt. percentage  
**Hf\_INAA** concentration in mg/kg  
**K** concentration in mg/kg  
**K\_XRF** concentration in wt. percentage  
**La** concentration in mg/kg  
**La\_INAA** concentration in mg/kg  
**Li** concentration in mg/kg  
**Lu\_INAA** concentration in mg/kg  
**Mg** concentration in mg/kg  
**Mg\_XRF** concentration in wt. percentage  
**Mn** concentration in mg/kg  
**Mn\_XRF** concentration in wt. percentage  
**Na** concentration in mg/kg  
**Na\_XRF** concentration in wt. percentage  
**Nd\_INAA** concentration in mg/kg  
**Ni** concentration in mg/kg  
**P** concentration in mg/kg  
**P\_XRF** concentration in wt. percentage  
**Pb** concentration in mg/kg  
**S** concentration in mg/kg  
**Sc** concentration in mg/kg  
**Sc\_INAA** concentration in mg/kg  
**Si** concentration in mg/kg  
**Si\_XRF** concentration in wt. percentage  
**Sm\_INAA** concentration in mg/kg  
**Sr** concentration in mg/kg  
**Th\_INAA** concentration in mg/kg  
**Ti** concentration in mg/kg  
**Ti\_XRF** concentration in wt. percentage  
**V** concentration in mg/kg  
**Y** concentration in mg/kg  
**Yb\_INAA** concentration in mg/kg  
**Zn** concentration in mg/kg  
**LOI** concentration in wt. percentage

**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

Kola Project (1993-1998)

### References

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

### See Also

[chorizon](#), [chorizonDL](#)

### Examples

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

### Description

Clustering in orthonormal coordinates or by using the Aitchison distance



**Usage**

```

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

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

```

**Arguments**

<code>x</code>	compositional data represented as a data.frame
<code>k</code>	number of clusters
<code>method</code>	clustering method. One of Mclust, cmeans, kmeansHartigan, cmeansUfcl, pam, clara, fanny, ward.D2, single, hclustComplete, average, mcquitty, median, centroid
<code>scale</code>	if orthonormal coordinates should be normalized.
<code>transformation</code>	default are the isometric logratio coordinates. Can only used when distMethod is not Aitchison.
<code>distMethod</code>	Distance measure to be used. If "Aitchison", then transformation should be "identity".
<code>iter.max</code>	parameter if kmeans is chosen. The maximum number of iterations allowed
<code>vals</code>	if cluster validity measures should be calculated
<code>alt</code>	a known partitioning can be provided (for special cluster validity measures)
<code>bic</code>	if TRUE then the BIC criteria is evaluated for each single cluster as validity measure
<code>verbose</code>	if TRUE additional print output is provided
<code>y</code>	the y coordinates of points in the plot, optional if x is an appropriate structure.
<code>...</code>	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 coordinates 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

M. Templ, P. Filzmoser, C. Reimann. Cluster analysis applied to regional geochemical data: Problems and possibilities. *Applied Geochemistry*, **23** (8), 2198–2213, 2008

Templ, M., Filzmoser, P., Reimann, C. (2008) *Cluster analysis applied to regional geochemical data: Problems and possibilities*, *Applied Geochemistry*, 23 (2008), pages 2198 - 2213.

### 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")

## Not run:
require(reshape2)
plot(rr)
plot(rr, normalized = TRUE)
plot(rr, normalized = TRUE, which.plot = "partMeans")

## End(Not run)
```

---

clustCoDa_qmode	<i>Q-mode cluster analysis for compositional parts</i>
-----------------	--

---

**Description**

Clustering 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**

Filzmoser, P., Hron, K. Templ, M. (2018) *Applied Compositional Data Analysis*, Springer, Cham.

**Examples**

```
data(expenditures)
x <- expenditures
c1 <- clustCoDa_qmode(x)
## Not run:
require(reshape2)
plot(c1)
c12 <- clustCoDa_qmode(x, method = "single")
plot(c12)

## End(Not run)
```

---

coffee

*coffee data set*

---

**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**

M. Korhonov'a, K. Hron, D. Klime'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)
str(coffee)
summary(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

```
compareMahal(x, imp = "KNNa")  
  
## S3 method for class 'mahal'  
plot(x, y, ...)
```

### Arguments

<code>x</code>	data frame or matrix
<code>imp</code>	imputation method
<code>y</code>	unused second argument for the plot method
<code>...</code>	additional arguments for plotting passed through

### Value

<code>df</code>	a data.frame containing the Mahalanobis distances from the estimation in sub-groups, the Mahalanobis distances from the imputation and covariance approach, an indicator specifying outliers and an indicator specifying the zero pattern
<code>df2</code>	a groupwise statistics.

### Author(s)

Matthias Templ, Karel Hron

### References

Templ, M., Hron, K., Filzmoser, P. (2017) Exploratory tools for outlier detection in compositional data with structural zeros". *Journal of Applied Statistics*, **44** (4), 734–752

### See Also

[impKNNa](#), [pivotCoord](#)

## Examples

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

---

constSum

*Constant sum*

---

## 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)
```

---

coord	<i>Coordinate representation of compositional tables</i>
-------	--

---

**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 can be considered as a two-factor composition, we refer to compositional tables. This function constructs orthonormal coordinates for compositional tables using the balances approach for given sequential binary partitions on rows and columns of the compositional table.

**Value**

Row and column balances and odds ratios as coordinate representations of the independence and interaction tables, respectively.

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

Facevicova, K., Hron, K., Todorov, V., Templ, M. (2018) General approach to coordinate representation of compositional tables. *Scandinavian Journal of Statistics*, 45(4), 879-899.

## Examples

```
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,-1),c(1,1,-1,0,0,0),c(1,-1,0,0,0,0),c(0,0,0,0,1,-1))
SBPr
result <- coord(x, SBPr,SBPc)
result
data(socExp)
```

---

corCoDa

*Correlations for compositional data*

---

## Description

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

## Usage

```
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. (2017) Correlation between compositional parts based on symmetric balances. *Mathematical Geosciences*, 49(6), 777-796.



**Examples**

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

---

cubeCoord	<i>Coordinate representation of a compositional cube and of a sample of compositional cubes</i>
-----------	---

---

**Description**

cubeCoord computes a system of orthonormal coordinates of a compositional cube. Computation of either pivot coordinates or a coordinate system based on the given SBP is possible.

Wrapper (cubeCoordWrapper): For each compositional cube in the sample cubeCoordWrapper computes a system of orthonormal coordinates and provide a simple descriptive analysis. Computation of either pivot coordinates or a coordinate system based on the given SBP is possible.

**Usage**

```
cubeCoord(  
  x,  
  row.factor = NULL,  
  col.factor = NULL,  
  slice.factor = NULL,  
  value = NULL,  
  SBPr = NULL,  
  SBPc = NULL,  
  SBPs = NULL,  
  pivot = FALSE,  
  print.res = FALSE  
)
```

```
cubeCoordWrapper(  
  X,  
  obs.ID = NULL,  
  row.factor = NULL,  
  col.factor = NULL,  
  slice.factor = NULL,  
  value = NULL,  
  SBPr = NULL,  
  SBPc = NULL,  
  SBPs = NULL,  
  pivot = FALSE,  
  test = FALSE,  
  n.boot = 1000  
)
```

**Arguments**

x	a data frame containing variables representing row, column and slice factors of the respective compositional cube and variable with the values of the composition.
row.factor	name of the variable representing the row factor. Needs to be stated with the quotation marks.
col.factor	name of the variable representing the column factor. Needs to be stated with the quotation marks.
slice.factor	name of the variable representing the slice factor. Needs to be stated with the quotation marks.
value	name of the variable representing the values of the composition. Needs to be stated with the quotation marks.
SBPr	an $I - 1 \times I$ array defining the sequential binary partition of the values of the row factor, where I is the number of the row factor levels. The values assigned in the given step to the + group are marked by 1, values from the - group by -1 and the rest by 0. If it is not provided, the pivot version of coordinates is constructed automatically.
SBPc	an $J - 1 \times J$ array defining the sequential binary partition of the values of the column factor, where J is the number of the column factor levels. The values assigned in the given step to the + group are marked by 1, values from the - group by -1 and the rest by 0. If it is not provided, the pivot version of coordinates is constructed automatically.
SBPs	an $K - 1 \times K$ array defining the sequential binary partition of the values of the slice factor, where K is the number of the slice factor levels. The values assigned in the given step to the + group are marked by 1, values from the - group by -1 and the rest by 0. If it is not provided, the pivot version of coordinates is constructed automatically.
pivot	logical, default is FALSE. If TRUE, or one of the SBPs is not defined, its pivot version is used.
print.res	logical, default is FALSE. If TRUE, the output is displayed in the Console.
X	a data frame containing variables representing row, column and slice factors of the respective compositional cubes, variable with the values of the composition and variable distinguishing the observations.
obs.ID	name of the variable distinguishing the observations. Needs to be stated with the quotation marks.
test	logical, default is FALSE. If TRUE, the bootstrap analysis of coordinates is provided.
n.boot	number of bootstrap samples.

**Details**

## cubeCoord

This transformation moves the IJK-part compositional cubes from the simplex into a (IJK-1)-dimensional real space isometrically with respect to its three-factorial nature.

Wrapper (cubeCoordWrapper): Each of  $n$  IJK-part compositional cubes from the sample is with respect to its three-factorial nature isometrically transformed from the simplex into a  $(IJK-1)$ -dimensional real space. Sample mean values and standard deviations are computed and using bootstrap an estimate of 95 % confidence interval is given.

### Value

Coordinates	an array of orthonormal coordinates.
Grap.rep	graphical representation of the coordinates. Parts denoted by + form the groups in the numerator of the respective computational formula, parts - form the denominator and parts . are not involved in the given coordinate.
Row.balances	an array of row balances.
Column.balances	an array of column balances.
Slice.balances	an array of slice balances.
Row.column.OR	an array of row-column OR coordinates.
Row.slice.OR	an array of row-slice OR coordinates.
Column.slice.OR	an array of column-slice OR coordinates.
Row.col.slice.OR	an array of coordinates describing the mutual interaction between all three factors.
Contrast.matrix	contrast matrix.
Log.ratios	an array of pure log-ratios between groups of parts without the normalizing constant.
Coda.cube	cube form of the given composition.
Bootstrap	array of sample means, standard deviations and bootstrap confidence intervals.
Cubes	Cube form of the given compositions.

### Author(s)

Kamila Facevicova

### References

Facevicova, K., Filzmoser, P. and K. Hron (2019) Compositional Cubes: Three-factorial Compositional Data. Under review.

### See Also

[tabCoord](#) [tabCoordWrapper](#)

## Examples

```
#####
### Coordinate representation of a CoDa Cube
## Not run:
### example from Fa\v cevico\v'a (2019)
data(employment2)
CZE <- employment2[which(employment2$Country == 'CZE'), ]

# pivot coordinates
cubeCoord(CZE, "Sex", 'Contract', "Age", 'Value')

# coordinates with given SBP

r <- t(c(1,-1))
c <- t(c(1,-1))
s <- rbind(c(1,-1,-1), c(0,1,-1))

cubeCoord(CZE, "Sex", 'Contract', "Age", 'Value', r,c,s)

## End(Not run)

#####
### Analysis of a sample of CoDa Cubes
## Not run:
### example from Fa\v cevico\v'a (2019)
data(employment2)
### Compositional tables approach,
### analysis of the relative structure.
### An example from Facevi\v cov\v'a (2019)

# pivot coordinates
cubeCoordWrapper(employment2, 'Country', 'Sex', 'Contract', 'Age', 'Value',
test=TRUE)

# coordinates with given SBP (defined in the paper)

r <- t(c(1,-1))
c <- t(c(1,-1))
s <- rbind(c(1,-1,-1), c(0,1,-1))

res <- cubeCoordWrapper(employment2, 'Country', 'Sex', 'Contract',
"Age", 'Value', r,c,s, test=TRUE)

### Classical approach,
### generalized linear mixed effect model.

library(lme4)
employment2$y <- round(employment2$Value*1000)
glmer(y~Sex*Age*Contract+(1|Country),data=employment2,family=poisson)

### other relations within cube (in the log-ratio form)
### e.g. ratio between women and man in the group FT, 15to24
```

```
### and ratio between age groups 15to24 and 55plus

# transformation matrix
T <- rbind(c(1,rep(0,5), -1, rep(0,5)), c(rep(c(1/4,0,-1/4), 4)))
T

## End(Not run)
```

---

daCoDa

*Linear and quadratic discriminant analysis for compositional data.*


---

### Description

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

### Usage

```
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

Compositional data are expressed in orthonormal (ilr) coordinates (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 coordinates and clr coefficients. 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

Filzmoser, P., Hron, K., Templ, M. (2012) Discriminant analysis for compositional data and robust parameter estimation. *Computational Statistics*, 27(4), 585-604.

## See Also

[LdaClassic](#), [Linda](#), [QdaClassic](#), [QdaCov](#)

## Examples

```
## 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)
```

## Description

Discriminant analysis by Fishers rule using the logratio approach to compositional data.

**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 loses its optimality in case of deviations from normality.

The classical Fisher discriminant rule is invariant to ilr coordinates and clr coefficients. 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**

Filzmoser, P. and Hron, K. and Templ, M. (2012) Discriminant analysis for compositional data and robust parameter estimation. *Computational Statistics*, 27(4), 585-604.

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**

```
## 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))

#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 = "RnavGraph")
# exclude zeros (alternatively impute them if
```



```

# the detection limit is known using imprZilr()
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 <- daFisher(x, grp, method = "robust")
res
summary(res)
predict(res, newdata = x)
res <- daFisher(x,grp, plotScore = TRUE, method = "robust")

# 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 capital 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**

Eurostat, <http://ec.europa.eu/eurostat/data>

**Examples**

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

---

educFM	<i>education level of father (F) and mother (M)</i>
--------	---

---

**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**

```
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**

from Eurostat, <http://ec.europa.eu/eurostat/>

**Examples**

```
data(educFM)
str(educFM)
```

---

election	<i>election data</i>
----------	----------------------

---

**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 (GRUNE), 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**

Eurostat, <http://ec.europa.eu/eurostat/data>

**Examples**

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

---

electionATbp

*Austrian presidential election data*

---

**Description**

Results the Austrian presidential election in October 2016.

**Usage**

```
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**

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

---

employment	<i>employment in different countries by gender and status.</i>
------------	--

---

**Description**

employment in different countries by gender and status.

**Usage**

```
data(employment)
```

**Format**

A three-dimensional table

**Examples**

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

---

employment2	<i>Employment in different countries by Sex, Age, Contract, Value</i>
-------------	---

---

**Description**

Estimated number of employees in 42 countries in 2015, distributed according to gender (Women/Men), age (15-24, 25-54, 55+) and type of contract (Full- and part-time).

**Usage**

```
data(employment2)
```

**Format**

A data.frame with 504 rows and 5 columns.

## Details

For each country in the sample, an estimated number of employees in the year 2015 was available, divided according to gender and age of employees and the type of the contract. The data form a sample of 42 cubes with two rows (gender), two columns (type) of contract) and three slices (age), which allow for a deeper analysis of the overall employment structure, not just from the perspective of each factor separately, but also from the perspective of the relations/interactions between them. Thorough analysis of the sample is described in Facevicova (2019).

- CountryCountry
- Sexgender, males (M) and females (F)
- Ageage class, young (category 15 - 24), middle-aged (25 - 54) and older (55+) employees
- Contractfactor, defining the type of contract, full-time (FT) and part-time (PT) contracts
- ValueNumber of employees in the given category (in thousands)

## Author(s)

Kamila Facevicova

## Source

<http://stats.oecd.org>

## References

Facevicova, K., Filzmoser, P. and K. Hron (2019) Compositional Cubes: Three-factorial Compositional Data. Under review.

## Examples

```
data(employment2)
head(employment2)
```

---

employment\_df

*Employment in different countries by gender and status.*

---

## Description

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

## Usage

```
data(employment_df)
```

**Format**

A data.frame with 132 rows and 4 columns.

**Examples**

```
data(employment_df)
head(employment_df)
```

---

expenditures	<i>synthetic household expenditures toy data set</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 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**

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      *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
- Housinga numeric vector
- Furnishingsa numeric vector
- Healtha numeric vector
- Transporta numeric vector
- Communicationa numeric vector
- Recreationa numeric vector
- Educationa numeric vector
- Restaurantsa numeric vector
- Othera numeric vector

**Source**

Eurostat

**Examples**

```
data(expendituresEU)
```



---

`GDPsatis`*GDP satisfaction*

---

**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**

from Eurostat, <http://ec.europa.eu/eurostat/>

**Examples**

```
data(GDPsatis)  
str(GDPsatis)
```

---

gemas

*GEMAS geochemical data set*

---

### **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 calcium (in mg/kg)
- Cr Concentration of chromium (in mg/kg)
- Fe Concentration of iron (in mg/kg)
- K Concentration of potassium (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

Reimann, C., Birke, M., Demetriades, A., Filzmoser, P. & O'Connor, P. (Editors), 2014. Chemistry of Europe's agricultural soils - Part A: Methodology and interpretation of the GEMAS data set. Geologisches Jahrbuch (Reihe B 102), Schweizerbarth, Hannover, 528 pp. + DVD Reimann, C., Birke, M., Demetriades, A., Filzmoser, P. & O'Connor, P. (Editors), 2014. Chemistry of Europe's agricultural soils - Part B: General background information and further analysis of the GEMAS data set. Geologisches Jahrbuch (Reihe B 103), Schweizerbarth, Hannover, 352 pp.

#### 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)
```

---

gjovik

*gjovik*

---

**Description**

Gjovik geochemical data set

**Format**

A data frame with 615 observations and 63 variables.

- ID a numeric vector
- MAT type of material
- mE32wgs longitude
- mN32wgs latitude
- XCOO X coordinates
- YCOO Y coordinates
- ALT altitute
- kmNS some distance north-south
- kmSN some distance south-north
- LITHO lithologies
- Ag a numeric vector
- Al a numeric vector
- As a numeric vector
- Au a numeric vector
- B a numeric vector
- Ba a numeric vector
- Be a numeric vector
- Bi a numeric vector
- Ca a numeric vector
- Cd a numeric vector
- Ce a numeric vector
- Co a numeric vector
- Cr a numeric vector
- Cs a numeric vector
- Cu a numeric vector
- Fe a numeric vector
- Ga a numeric vector
- Ge a numeric vector

- Hf a numeric vector
- Hg a numeric vector
- In a numeric vector
- K a numeric vector
- La a numeric vector
- Li a numeric vector
- Mg a numeric vector
- Mn a numeric vector
- Mo a numeric vector
- Na a numeric vector
- Nb a numeric vector
- Ni a numeric vector
- P a numeric vector
- Pb a numeric vector
- Pd a numeric vector
- Pt a numeric vector
- Rb a numeric vector
- Re a numeric vector
- S a numeric vector
- Sb a numeric vector
- Sc a numeric vector
- Se a numeric vector
- Sn a numeric vector
- Sr a numeric vector
- Ta a numeric vector
- Te a numeric vector
- Th a numeric vector
- Ti a numeric vector
- Tl a numeric vector
- U a numeric vector
- V a numeric vector
- W a numeric vector
- Y a numeric vector
- Zn a numeric vector
- Zr a numeric vector

**Details**

Geochemical data set. 41 sample sites have been investigated. At each site, 15 different sample materials have been collected and analyzed for the concentration of more than 40 chemical elements. Soil: CHO - C horizon, OHO - O horizon. Mushroom: LAC - milkcap. Plant: BIL - birch leaves, BLE - blueberry leaves, BLU - blueberry twigs, BTW - birch twigs, CLE - cowberry leaves, COW - cowberry twigs, EQU - horsetail, FER - fern, HYL - terrestrial moss, PIB - pine bark, SNE - spruce needles, SPR - spruce twigs.

**Author(s)**

Peter Filzmoser, Dominika Miksova

**References**

C. Reimann, P. Englmaier, B. Flem, O.A. Eggen, T.E. Finne, M. Andersson & P. Filzmoser (2018). The response of 12 different plant materials and one mushroom to Mo and Pb mineralization along a 100-km transect in southern central Norway. *Geochemistry: Exploration, Environment, Analysis*, 18(3), 204-215.

**Examples**

```
data(gjovik)
str(gjovik)
```

---

gm	<i>gmean</i>
----	--------------

---

**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	<i>Geometric mean</i>
-----------	-----------------------

---

**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[1, ]))
gmean(arcticLake)
gmean(arcticLake, margin = 1)
gmean(arcticLake, margin = 2)
gmean(arcticLake, margin = 3)
```

---

govexp

*government spending*

---

## 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 in 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

*haplogroups data.*

---

### 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](http://www.eupedia.com/europe/european_y-dna_haplogroups.shtml)

### Examples

```
data(haplogroups)
```

---

 ilr.2x2

*ilr coordinates in 2x2 compositional tables*


---

**Description**

ilr coordinates of original, independent and interaction compositional 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 “book”.

**Value**

The ilr coordinates

**Author(s)**

Kamila Facevicova, Matthias Templ

**References**

Facevicova, K., Hron, K., Todorov, V., Guo, D., Templ, M. (2014). Logratio approach to statistical analysis of 2x2 compositional tables. *Journal of Applied Statistics*, 41 (5), 944–958.

**Examples**

```
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 coordinates 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`.

**References**

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

Martin-Fernandez, J.A., Hron, K., Templ, M., Filzmoser, P., Palarea-Albaladejo, J. (2012) Model-based replacement of rounded zeros in compositional data: Classical and robust approaches, *Computational Statistics*, 56 (2012), 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 ==\$ "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 'ItsReg': 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. 'ItsReg2': 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**

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

**See Also**

[impKNNa](#), [pivotCoord](#)

**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	“Aichison” 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	depricated. 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

<code>xOrig</code>	Original data frame or matrix
<code>xImp</code>	Imputed data
<code>w</code>	Amount of imputed values
<code>wind</code>	Index of the missing values in the data
<code>metric</code>	Metric used

### Author(s)

Matthias Templ

### References

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

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

**References**

Palarea-Albaladejo, J., Martin-Fernandez, J.A. Gomez-Garcia, J. (2007) A parametric approach for dealing with compositional rounded zeros. *Mathematical Geology*, 39(7), 625-645.

**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 <- 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 coordinates with a special choice of balances.

**Usage**

```
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 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".
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 considered as missing not at random missing values.

The algorithm iteratively imputes parts with rounded zeros whereas in each step (1) compositional data are expressed in pivot coordinates (2) tobit regression is applied (3) the rounded zeros are replaced by the expected values (4) the corresponding inverse ilr mapping 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

**References**

Martin-Fernandez, J.A., Hron, K., Templ, M., Filzmoser, P., Palarea-Albaladejo, J. (2012) Model-based replacement of rounded zeros in compositional data: Classical and robust approaches. *Computational Statistics and Data Analysis*, 56 (9), 2688-2704.

Templ, M., Hron, K., Filzmoser, P., Gardlo, A. (2016) Imputation of rounded zeros for high-dimensional compositional data. *Chemometrics and Intelligent Laboratory Systems*, 155, 183-190.

**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
```

---

imputeBDLs

*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 coordinates with a 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 bootstraped 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) compositional data are expressed in pivot coordinates (2) tobit regression is applied (3) the rounded zeros are replaced by the expected values (4) the corresponding inverse ilr mapping 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

- Templ, M., Hron, K., Filzmoser, P., Gardlo, A. (2016). Imputation of rounded zeros for high-dimensional compositional data. *Chemometrics and Intelligent Laboratory Systems*, 155, 183-190.
- Chen, J., Zhang, X., Hron, K., Templ, M., Li, S. (2018). Regression imputation with Q-mode clustering for rounded zero replacement in high-dimensional compositional data. *Journal of Applied Statistics*, 45 (11), 2067-2080.

### See Also

[imputeBDLs](#)

**Examples**

```

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}
## Not run:
# under dontrun because of long execution time
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)
## 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[x[,i] < dl[i], i] <- 0
}
ni <- sum(x==0, na.rm=TRUE)
ni/(ncol(x)*nrow(x)) * 100
dl[seq(2, ncol(x), 2)] <- 0
replaced_lm <- imputeBDLs(x, dl=dl, eps=1, method="lm",
  verbose=FALSE, R=50, variation=TRUE)$x
replaced_lmrob <- imputeBDLs(x, dl=dl, eps=1, method="lmrob",
  verbose=FALSE, R=50, variation=TRUE)$x
replaced_plsfull <- imputeBDLs(x, dl=dl, eps=1,
  method="pls", verbose=FALSE, R=50,
  variation=FALSE)$x

## End(Not run)

```

---

imputeUDLs	<i>Imputation of values above an upper detection limit in compositional data</i>
------------	--

---

### Description

Parametric replacement of values above upper detection limit for compositional data using classical and robust methods (possibly also the pls method) based on ilr-transformations with special choice of balances.

### Usage

```
imputeUDLs(
  x,
  maxit = 10,
  eps = 0.1,
  method = "lm",
  dl = NULL,
  variation = TRUE,
  nPred = NULL,
  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", "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 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".
correction	normal or density
verbose	additional print output during calculations.

### Details

#### imputeUDLs

An imputation method for right-censored compositional data. Statistical analysis is not possible with values reported in data, for example as ">10000". These values are replaced using tobit regression.

The algorithm iteratively imputes parts with values above upper detection limit whereas in each step (1) compositional data are expressed in pivot coordinates (2) tobit regression is applied (3) the values above upper detection limit are replaced by the expected values (4) the corresponding inverse ilr mapping is applied. After all parts are imputed, the algorithm starts again until the imputations only change marginally.

### Value

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

### Author(s)

Peter Filzmoser, Dominika Miksova based on function imputeBDLs code from Matthias Templ

### References

- Martin-Fernandez, J.A., Hron K., Templ, M., Filzmoser, P. and Palarea-Albaladejo, J. (2012). Model-based replacement of rounded zeros in compositional data: Classical and robust approaches. *Computational Statistics and Data Analysis*, 56, 2688-2704.
- Templ, M. and Hron, K. and Filzmoser and Gardlo, A. (2016). Imputation of rounded zeros for high-dimensional compositional data. *Chemometrics and Intelligent Laboratory Systems*, 155, 183-190.



**See Also**

[imputeBDLs](#)

**Examples**

```
data(gemas) # read data
dat <- gemas[gemas$COUNTRY=="HEL",c(12:29)]
UDL <- apply(dat,2,max)
names(UDL) <- names(dat)
UDL["Mn"] <- quantile(dat[, "Mn"], probs = 0.8) # UDL present only in one variable
whichudl <- dat[, "Mn"] > UDL["Mn"]
# classical method
imp.lm <- dat
imp.lm[whichudl, "Mn"] <- Inf
res.lm <- imputeUDLs(imp.lm, dl=UDL, method="lm", variation=TRUE)
imp.lm <- res.lm$x
```

---

ind2x2

*Independence 2x2 compositional table*


---

**Description**

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

**Usage**

```
ind2x2(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 independence tables should be estimated.
pTabMethod	'classical' that is function <code>prop.table()</code> from package <code>base</code> 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

Facevicova, K., Hron, K., Todorov, V., Guo, D., Templ, M. (2014). Logratio approach to statistical analysis of 2x2 compositional tables. *Journal of Applied Statistics*, 41 (5), 944–958.

## Examples

```
data(employment)
ind2x2(employment)
```

---

indTab	<i>Independence table</i>
--------	---------------------------

---

## Description

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

## Usage

```
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.
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.

## Details

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

## Value

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

## Author(s)

Matthias Templ

## References

Egozcue, J.J., Pawlowsky-Glahn, V., Templ, M., Hron, K. (2015) Independence in contingency tables using simplicial geometry. *Communications in Statistics - Theory and Methods*, 44 (18), 3978–3996.

## Examples

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

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

## End(Not run)
```

---

instw                                    *value added, output and input for different ISIC codes and countries.*

---

## Description

- ctct
- isicISIC classification, Rev 3.2
- VValue added
- OUToutput
- INPinput
- IS03country code
- mhtmht

## Usage

```
data(instw)
```

## Format

A data.frame with 1555 rows and 7 columns.

## Examples

```
data(instw)
head(instw)
```

---

int2x2	<i>Interaction 2x2 table</i>
--------	------------------------------

---

### 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 independence tables should be estimated.
pTabMethod	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.

### Value

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

### Author(s)

Kamila Facevicova, Matthias Templ

### References

Facevicova, K., Hron, K., Todorov, V., Guo, D., Templ, M. (2014). Logratio approach to statistical analysis of 2x2 compositional tables. *Journal of Applied Statistics*, 41 (5), 944–958.

### Examples

```
data(employment)
int2x2(employment)
```

---

intArray	<i>Interaction array</i>
----------	--------------------------

---

**Description**

Estimates the interaction compositional table with normalization for further analysis according to Egozcue et al. (2015)

**Usage**

```
intArray(x)
```

**Arguments**

x                    an object of class “intTab”

**Details**

Estimates the interaction table using its ilr coordinates.

**Value**

The interaction array

**Author(s)**

Matthias Templ

**References**

Egozcue, J.J., Pawlowsky-Glahn, V., Templ, M., Hron, K. (2015) Independence in contingency tables using simplicial geometry. *Communications in Statistics - Theory and Methods*, 44 (18), 3978–3996.

**See Also**

[intTab](#)

**Examples**

```
data(precipitation)
tab1prob <- prop.table(precipitation)
tab1 <- indTab(precipitation)
tabINT <- intTab(tab1prob, tab1)
intArray(tabINT)
```

---

intTab	<i>Interaction table</i>
--------	--------------------------

---

### Description

Estimates the interaction table based on clr and inverse clr coefficients.

### Usage

```
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 marginals.

### 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

Egozcue, J.J., Pawlowsky-Glahn, V., Templ, M., Hron, K. (2015) Independence in contingency tables using simplicial geometry. *Communications in Statistics - Theory and Methods*, 44 (18), 3978–3996.

### Examples

```
data(precipitation)
tab1prob <- prop.table(precipitation)
tab1 <- indTab(precipitation)
intTab(tab1prob, tab1)
```

---

is.equivalent	<i>equivalence class</i>
---------------	--------------------------

---

**Description**

Checks if two vectors or two data frames are from the same equivalence class

**Usage**

```
is.equivalent(x, y, tolerance = .Machine$double.eps^0.5)
```

**Arguments**

x	either a numeric vector, or a data.frame containing such vectors.
y	either a numeric vector, or a data.frame containing such vectors.
tolerance	numeric $\geq 0$ . Differences smaller than tolerance are not considered.

**Value**

logical TRUE if the two vectors are from the same equivalence class.

**Author(s)**

Matthias Templ

**References**

Filzmoser, P., Hron, K., Templ, M. (2018) *Applied Compositional Data Analysis*. Springer, Cham.

**See Also**

[all.equal](#)

**Examples**

```
is.equivalent(1:10, 1:10*2)
is.equivalent(1:10, 1:10+1)
data(expenditures)
x <- expenditures
is.equivalent(x, constSum(x))
y <- x
y[1,1] <- x[1,1]+1
is.equivalent(y, constSum(x))
```

---

isic32	<i>ISIC codes by name</i>
--------	---------------------------

---

**Description**

- code ISIC code, Rev 3.2
- description Description of ISIC codes

**Usage**

```
data(isic32)
```

**Format**

A data.frame with 24 rows and 2 columns.

**Examples**

```
data(instw)
instw
```

---

laborForce	<i>labour force by status in employment</i>
------------	---

---

**Description**

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

**Format**

A data set on 124 compositions on 9 variables.

**Details**

- country country
- year 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**

<http://unstats.un.org/unsd/demographic/products/indwm/tab5c.htm>

**References**

K. Hron, P. Filzmoser, K. Thompson (2012). Linear regression with compositional explanatory variables. *Journal of Applied Statistics*, Volume 39, Issue 5, 2012.

**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**

<http://www.ec.europa.eu/eurostat> and <http://unstats.un.org/unsd>

**References**

K. Hron, P. Filzmoser, K. Thompson (2012). Linear regression with compositional explanatory variables. *Journal of Applied Statistics*, Volume 39, Issue 5, 2012.

**Examples**

```
data(lifeExpGdp)
str(lifeExpGdp)
```

---

 lmCoDaX

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

---

**Description**

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

**Usage**

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

**Arguments**

<code>y</code>	The response which should be non-compositional
<code>X</code>	The compositional predictors as a matrix, data.frame or numeric vector
<code>method</code>	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 pivot coordinates is used.

**Value**

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

**Author(s)**

Peter Filzmoser

## References

Filzmoser, P., Hron, K., Thompsonc, 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</i>
------------------	--------------------------

---

## 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

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.

## Author(s)

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

## References

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

## Examples

```
data(machineOperators)
str(machineOperators)
summary(machineOperators)
rowSums(machineOperators)
```

---

manu\_abs

*Distribution of manufacturing output*

---

## Description

The data consists of values of the manufacturing output in 42 countries in 2009. The output, given in national currencies, is structured according to the 3-digit ISIC category and its components. Thorough analysis of the sample is described in Facevicova (2018).

## Usage

```
data(manu_abs)
```

## Format

A data frame with 630 observations of 4 variables.

## Details

- country Country
- isic 3-digit ISIC category. The categories are 151 processed meat, fish, fruit, vegetables, fats; 152 Dairy products; 153 Grain mill products, starches, animal feeds; 154 Other food products and 155 Beverages.
- output The output components are Labour, Surplus and Input.
- value Value of manufacturing output in the national currency

## Author(s)

Kamila Facevicova

## Source

Elaboration based on the INDSTAT 4 database (UNIDO 2012a), see also UNIDO, 2012b. UNIDO (2012a), INDSTAT 4 Industrial Statistics Database at 3- and 4-digit level of ISIC Revision 3 and 4. Vienna. Available from <http://stat.unido.org>. UNIDO (2012b) International Yearbook of Industrial Statistics, Edward Elgar Publishing Ltd, UK.

## References

Facevicova, K., Hron, K., Todorov, V. and M. Templ (2018) General approach to coordinate representation of compositional tables. *Scandinavian Journal of Statistics*, 45(4).

## Examples

```
data(manu_abs)

### Compositional tables approach
### analysis of the relative structure

result <- tabCoordWrapper(manu_abs, obs.ID='country', row.factor = 'output',
  col.factor = 'isic', value='value', test = TRUE)

result$Bootstrap

### Classical approach
### generalized linear mixed effect model
## Not run:
library(lme4)
m <- glmer(value~output*as.factor(isic)+(1|country),
  data=manu_abs, family=poisson)
summary(m)

## End(Not run)
```

---

mca

*metabolomics mca data set*

---

## 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(mca)
```

## 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

Najdekr L., Gardlo A., Madrova L., Friedeckyy D., Janeckova H., Correa E.S., Goodacre R., Adam T., Oxidized phosphatidylcholines suggest oxidative stress in patients with medium-chain acyl-CoA dehydrogenase deficiency, *Talanta* 139, 2015, 62-66.

## Examples

```
data(mcad)
str(mcad)
```

---

missPatterns	<i>missing or zero pattern structure.</i>
--------------	---

---

## 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**

Eurostat, <http://ec.europa.eu/eurostat/data>

**Examples**

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

---

mortality\_tab

*mortality table*

---

**Description**

Mortality data by gender, unknown year

**Usage**

```
data(mortality_tab)
```

**Format**

A table

**Details**

- femalemortality rates for females by age groups
- malemortality rates for males by age groups

**Author(s)**

Matthias Templ

**Examples**

```
data(mortality_tab)
mortality_tab
```



---

nutrients

*nutrient contents*

---

### **Description**

Nutrients on more than 40 components and 965 generic food products

### **Usage**

```
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
- carbohydratescarbohydrates in gram per 100g edible portion
- starch starch in gram per 100g edible portion
- sugars sugars in gram per 100g edible portion
- 'diatar\_ fibres 'diatar fibres in gram per 100g edible portion
- fat fat in gram per 100g edible portion
- cholesterol cholesterolin 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 microgram 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 microgram per 100g edible portion
- niacin niacin in milligram per 100g edible portion
- folate folate in microgram 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 microgram 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])
```

---

nutrients_branded	<i>nutrient contents (branded)</i>
-------------------	------------------------------------

---

## 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 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-naehwerttabelle/>

**References**

<http://www.sge-ssn.ch/shop/produkt/schweizer-naehwerttabelle/>

**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
```

---

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, 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 in isometric logratio coordinates. 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**

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., Pawlowsky-Glahn, V., Mateu-Figueras, G., Barcelo-Vidal, C. (2003) Isometric logratio 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**

[pivotCoord](#)

**Examples**

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

---

payments

*special payments*

---

### 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 colar workers
- spay\_bc special payments for blue colar 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**

```
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**

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

## 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 expressed in isometric logratio coordinates. 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 isometric logratio coordinates are 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)**

Karel Hron, Peter Filzmoser, Matthias Templ and a contribution for dimnames in external variables by Amelia Landre.

**References**

Filzmoser, P., Hron, K., Reimann, C. (2009) Principal component analysis for compositional data with outliers. *Environmetrics*, **20**, 621-632.

Kynclova, P., Filzmoser, P., Hron, K. (2016) Compositional biplots including external non-compositional variables. *Statistics: A Journal of Theoretical and Applied Statistics*, **50**, 1132-1148.

**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.cla <- pcaCoDa(arcticLake, method="classical")
biplot(res.cla)

## 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)
```

```
res <- pcaCoDa(election[,1:6], method="classical", external=election[,7:8])
res
biplot(res, scale=0)
```

---

perturbation

*Perturbation and powering*

---

## 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

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

## 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**

```
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 no 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
res.rob <- pfa(x, factors=1)
res.cla <- pfa(x, factors=1, robust=FALSE)

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

---

phd

*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
- human phd students in human sciences including teaching
- health phd students in health and life sciences
- agriculture phd students in agriculture

### Source

Eurostat

### 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.

### 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**

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.

### **Examples**

```
data("phd_totals")  
str(phd_totals)
```

---

pivotCoord                      *Pivot coordinates and their inverse*

---

### Description

Pivot coordinates as a special case of isometric logratio coordinates and their inverse mapping.

### 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 may occur. Only available for method "pivot".
method	pivot takes the method described in the description. Method "symm" uses symmetric pivot coordinates (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**

Pivot coordinates map D-part compositional data from the simplex into a (D-1)-dimensional real space isometrically. From our choice of pivot coordinates, all the relative information about one of parts (or about two parts) is aggregated in the first coordinate (or in the first two coordinates in case of symmetric pivot coordinates, respectively).

**Value**

The data represented in pivot coordinates

**Author(s)**

Matthias Templ, Karel Hron, Peter Filzmoser

**References**

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

Filzmoser, P., Hron, K., Templ, M. (2018) *Applied Compositional Data Analysis*. Springer, Cham.

**Examples**

```
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 pivot coordinates)
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 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 <a href="#">par</a> ).
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 <a href="#">par</a> ).
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 <a href="#">par(ask=.)</a> .
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](#)**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**

```
## 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**

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

**See Also**

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

**Examples**

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

---

`plot.smoothSpl`

*plot smoothSpl*

---

**Description**

plot densities of objects of class `smoothSpl`

**Usage**

```
## S3 method for class 'smoothSpl'
plot(x, y, ..., by = 1, n = 10, index = NULL)
```

**Arguments**

<code>x</code>	class <code>smoothSpl</code> object
<code>y</code>	ignored
<code>...</code>	further arguments passed by
<code>by</code>	stepsize
<code>n</code>	length of sequence to plot
<code>index</code>	optionally the sequence instead of <code>by</code> and <code>n</code>

---

precipitation	<i>24-hour precipitation</i>
---------------	------------------------------

---

**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**

- springnumeric vector on counts for different level of precipitation
- summernumeric vector on counts for different level of precipitation
- autumnnumeric vector on counts for different level of precipitation
- winternumeric vector on counts for different level of precipitation

**Author(s)**

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

**References**

Romero R, Guijarro J A, Ramis C, Alonso S (1998). A 30-years (1964-93) daily rainfall data base for the Spanish Mediterranean regions: first exploratory study. *International Journal of Climatology* 18, 541-560.

**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**

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

**Arguments**

<code>x</code>	an object of class 'imp'
<code>...</code>	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  
## Not run:  
xi <- impCoda(expenditures)  
xi  
summary(xi)  
plot(xi, 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)
```

---

pTab	<i>Propability table</i>
------	--------------------------

---

**Description**

Calculates the propability table using different methods

**Usage**

```
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 probablity table

**Author(s)**

Matthias Templ

**References**

Egozcue, J.J., Pawlowsky-Glahn, V., Templ, M., Hron, K. (2015) Independence in contingency tables using simplicial geometry. *Communications in Statistics - Theory and Methods*, 44 (18), 3978–3996.

**Examples**

```
data(precipitation)
pTab(precipitation)
pTab(precipitation, method = "dirichlet")
```



---

rcodes	<i>codes for UNIDO tables</i>
--------	-------------------------------

---

**Description**

- ISOCNISO CN codes
- OPERATOROperator
- ADESCCountry
- CCODECountry code
- CDESCCountry destination
- ACODECountry destination code

**Usage**

```
data(rcodes)
```

**Format**

A data.frame with 2717 rows and 6 columns.

**Examples**

```
data(rcodes)
str(rcodes)
```

---

rdcm	<i>relative difference between covariance matrices</i>
------	--

---

**Description**

The sample covariance matrices are computed from compositions expressed in the same isometric logratio coordinates.

**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**

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.

Templ, M. and Hron, K. and Filzmoser and Gardlo, A. (2016). Imputation of rounded zeros for high-dimensional compositional data. *Chemometrics and Intelligent Laboratory Systems*, 155, 183-190.

**See Also**

[rdcm](#)

**Examples**

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

---

rSDev

*Relative simplicial deviance*

---

**Description**

Relative simplicial deviance

**Usage**

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

**Arguments**

x                    a propability table  
y                    an interaction table

**Value**

The relative simplicial deviance

**Author(s)**

Matthias Templ

**References**

Egozcue, J.J., Pawlowsky-Glahn, V., Templ, M., Hron, K. (2015) Independence in contingency tables using simplicial geometry. *Communications in Statistics - Theory and Methods*, 44 (18), 3978–3996.

**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 = "multinom")
```

**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 “hstest” containing the following components:

- statisticthe value of the relative simplicial deviance (test statistic).
- methoda character string indicating what type of rSDev.test was performed.
- p.valuethe p-value for the test.

**Author(s)**

Matthias Templ, Karel Hron

**References**

Egozcue, J.J., Pawlowsky-Glahn, V., Templ, M., Hron, K. (2015) Independence in contingency tables using simplicial geometry. *Communications in Statistics - Theory and Methods*, 44 (18), 3978–3996.

**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

Juan Jose Egozcuea, Vera Pawlowsky-Glahn, Matthias Templ, Karel Hron (2015) Independence in Contingency Tables Using Simplicial Geometry. *Communications in Statistics - Theory and Methods*, Vol. 44 (18), 3978–3996. DOI:10.1080/03610926.2013.824980

## Examples

```
data(precipitation)
tab1prob <- prop.table(precipitation)
SDev(tab1prob)
```

---

skyeLavas	<i>aphyric skye lavas data</i>
-----------	--------------------------------

---

## 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 Na<sub>2</sub>O+K<sub>2</sub>O
- iron a numeric vector of percentages of Fe<sub>2</sub>O<sub>3</sub>
- magnesium a numeric vector of percentages of MgO

## Author(s)

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

## References

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

## Examples

```
data(skyeLavas)
str(skyeLavas)
summary(skyeLavas)
rowSums(skyeLavas)
```

smoothSplines

*Estimate density from histogram***Description**

Given raw (discretized) distributional observations, smoothSplines computes the density function that 'best' fits data, in a trade-off between smooth and least squares approximation, using B-spline basis functions.

**Usage**

```
smoothSplines(
  k,
  l,
  alpha,
  data,
  xcp,
  knots,
  weights = matrix(1, dim(data)[1], dim(data)[2]),
  num_points = 100,
  prior = "default",
  cores = 1,
  fast = 0
)
```

**Arguments**

k	smoothing splines degree
l	order of derivative in the penalization term
alpha	weight for penalization
data	an object of class "matrix" containing data to be smoothed, row by row
xcp	vector of control points
knots	either vector of knots for the splines or a integer for the number of equispaced knots
weights	matrix of weights. If not given, all data points will be weighted the same.
num_points	number of points of the grid where to evaluate the density estimated
prior	prior used for zero-replacements. This must be one of "perks", "jeffreys", "bayes_laplace", "sq" or "default"
cores	number of cores for parallel execution, if the option was enabled before installing the package
fast	1 if maximal performance is required (print statements suppressed), 0 otherwise

## Details

The original discretized densities are not directly smoothed, but instead the centred logratio transformation is first applied, to deal with the unit integral constraint related to density functions.

Then the constrained variational problem is set. This minimization problem for the optimal density is a compromise between staying close to the given data, at the corresponding xcp, and obtaining a smooth function. The non-smoothness measure takes into account the  $l$ th derivative, while the fidelity term is weighed by  $\alpha$ .

The solution is a natural spline. The vector of its coefficients is obtained by the minimum norm solution of a linear system. The resulting splines can be either back-transformed to the original Bayes space of density functions (in order to provide their smoothed counterparts for visualization and interpretation purposes), or retained for further statistical analysis in the clr space.

## Value

An object of class `smoothSpl`, containing among the other the following variables:

<code>bspline</code>	each row is the vector of B-spline coefficients
<code>Y</code>	the values of the smoothed curve, for the grid given
<code>Y_clr</code>	the values of the smoothed curve, in the clr setting, for the grid given

## References

J. Machalova, K. Hron & G.S. Monti (2016): Preprocessing of centred logratio transformed density functions using smoothing splines. *Journal of Applied Statistics*, 43:8, 1419-1435.

## Examples

```
SepalLengthCm <- iris$Sepal.Length
Species <- iris$Species

iris1 <- SepalLengthCm[iris$Species==levels(iris$Species)[1]]
h1 <- hist(iris1, nclass = 12, plot = FALSE)

midx1 <- h1$mids
midy1 <- matrix(h1$density, nrow=1, ncol = length(h1$density), byrow=TRUE)
knots <- 7
sol1 <- smoothSplines(k=3,l=2,alpha=1000,midy1,midx1,knots)
plot(sol1)

h1 <- hist(iris1, freq = FALSE, nclass = 12, xlab = "Sepal Length [cm]", main = "Iris setosa")
# black line: kernel method; red line: smoothSplines result
lines(density(iris1), col = "black", lwd = 1.5)
xx1 <- seq(sol1$Xcp[1],tail(sol1$Xcp,n=1),length.out = sol1$NumPoints)
lines(xx1,sol1$Y[1,], col = 'red', lwd = 2)
```

---

smoothSplinesVal      *Estimate density from histogram - for different alpha*

---

### Description

As [smoothSplines](#), `smoothSplinesVal` computes the density function that 'best' fits discretized distributional data, using B-spline basis functions, for different alpha. Comparing and choosing an appropriate alpha is the ultimate goal.

### Usage

```
smoothSplinesVal(
  k,
  l,
  alpha,
  data,
  xcp,
  knots,
  weights = matrix(1, dim(data)[1], dim(data)[2]),
  prior = "default",
  cores = 1
)
```

### Arguments

<code>k</code>	smoothing splines degree
<code>l</code>	order of derivative in the penalization term
<code>alpha</code>	vector of weights for penalization
<code>data</code>	an object of class "matrix" containing data to be smoothed, row by row
<code>xcp</code>	vector of control points
<code>knots</code>	either vector of knots for the splines or a integer for the number of equispaced knots
<code>weights</code>	matrix of weights. If not gives, all data points will be weighted the same.
<code>prior</code>	prior used for zero-replacements. This must be one of "perks", "jeffreys", "bayes_laplace", "sq" or "default"
<code>cores</code>	number of cores for parallel execution

### Details

See [smoothSplines](#) for the description of the algorithm.



**Value**

A list of three objects:

alpha	the values of alpha
J	the values of the functional evaluated in the minimizing
CV-error	the values of the leave-one-out CV-error

**References**

J. Machalova, K. Hron & G.S. Monti (2016): Preprocessing of centred logratio transformed density functions using smoothing splines. *Journal of Applied Statistics*, 43:8, 1419-1435.

**Examples**

```
SepalLengthCm <- iris$Sepal.Length
Species <- iris$Species

iris1 <- SepalLengthCm[iris$Species==levels(iris$Species)[1]]
h1 <- hist(iris1, nclass = 12, plot = FALSE)

midx1 <- h1$mids
midy1 <- matrix(h1$density, nrow=1, ncol = length(h1$density), byrow=TRUE)
knots <- 7
sol1 <- smoothSplinesVal(k=3,l=2,alpha=10^seq(-4,4,by=1),midy1,midx1,knots,cores=1)
```

---

socExp	<i>social expenditures</i>
--------	----------------------------

---

**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**

```
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**

Egozcue, J.J., Pawlowsky-Glahn, V., Templ, M., Hron, K. (2015) Independence in contingency tables using simplicial geometry. *Communications in Statistics - Theory and Methods*, 44 (18), 3978–3996.

**Examples**

```
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**

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

**Arguments**

<code>object</code>	an object of class 'imp'
<code>...</code>	additional arguments passed through

**Details**

Note that this function will be enhanced with more sophisticated methods in future versions of the package. It is very rudimentary 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)
```

---

tabCoord	<i>Coordinate representation of compositional tables and a sample of compositional tables</i>
----------	---

---

### Description

tabCoord computes a system of orthonormal coordinates of a compositional table. Computation of either pivot coordinates or a coordinate system based on the given SBP is possible.

tabCoordWrapper: For each compositional table in the sample tabCoordWrapper computes a system of orthonormal coordinates and provide a simple descriptive analysis. Computation of either pivot coordinates or a coordinate system based on the given SBP is possible.

### Usage

```
tabCoord(
  x = NULL,
  row.factor = NULL,
  col.factor = NULL,
  value = NULL,
  SBPr = NULL,
  SBPc = NULL,
  pivot = FALSE,
  print.res = FALSE
)
```

```
tabCoordWrapper(
  X,
  obs.ID = NULL,
  row.factor = NULL,
  col.factor = NULL,
  value = NULL,
  SBPr = NULL,
  SBPc = NULL,
  pivot = FALSE,
  test = FALSE,
  n.boot = 1000
)
```

### Arguments

x	a data frame containing variables representing row and column factors of the respective compositional table and variable with the values of the composition.
row.factor	name of the variable representing the row factor. Needs to be stated with the quotation marks.
col.factor	name of the variable representing the column factor. Needs to be stated with the quotation marks.

value	name of the variable representing the values of the composition. Needs to be stated with the quotation marks.
SBPr	an $I - 1 \times I$ array defining the sequential binary partition of the values of the row factor, where I is the number of the row factor levels. The values assigned in the given step to the + group are marked by 1, values from the - group by -1 and the rest by 0. If it is not provided, the pivot version of coordinates is constructed automatically.
SBPc	an $J - 1 \times J$ array defining the sequential binary partition of the values of the column factor, where J is the number of the column factor levels. The values assigned in the given step to the + group are marked by 1, values from the - group by -1 and the rest by 0. If it is not provided, the pivot version of coordinates is constructed automatically.
pivot	logical, default is FALSE. If TRUE, or one of the SBPs is not defined, its pivot version is used.
print.res	logical, default is FALSE. If TRUE, the output is displayed in the Console.
X	a data frame containing variables representing row and column factors of the respective compositional tables, variable with the values of the composition and variable distinguishing the observations.
obs.ID	name of the variable distinguishing the observations. Needs to be stated with the quotation marks.
test	logical, default is FALSE. If TRUE, the bootstrap analysis of coordinates is provided.
n.boot	number of bootstrap samples.

### Details

#### tabCoord

This transformation moves the IJ-part compositional tables from the simplex into a (IJ-1)-dimensional real space isometrically with respect to its two-factorial nature. The coordinate system is formed by two types of coordinates - balances and log odds-ratios.

tabCoordWrapper: Each of n IJ-part compositional tables from the sample is with respect to its two-factorial nature isometrically transformed from the simplex into a (IJ-1)-dimensional real space. Sample mean values and standard deviations are computed and using bootstrap an estimate of 95 % confidence interval is given.

### Value

Coordinates	an array of orthonormal coordinates.
Grap.rep	graphical representation of the coordinates. Parts denoted by + form the groups in the numerator of the respective computational formula, parts - form the denominator and parts . are not involved in the given coordinate.
Ind.coord	an array of row and column balances. Coordinate representation of the independent part of the table.
Int.coord	an array of OR coordinates. Coordinate representation of the interactive part of the table.

Contrast.matrix	contrast matrix.
Log.ratios	an array of pure log-ratios between groups of parts without the normalizing constant.
Coda.table	table form of the given composition.
Bootstrap	array of sample means, standard deviations and bootstrap confidence intervals.
Tables	Table form of the given compositions.

**Author(s)**

Kamila Facevicova

**References**

Facevicova, K., Hron, K., Todorov, V. and M. Templ (2018) General approach to coordinate representation of compositional tables. *Scandinavian Journal of Statistics*, 45(4), 879–899.

**See Also**

[cubeCoord](#) [cubeCoordWrapper](#)

**Examples**

```
#####
### Coordinate representation of a CoDa Table

# example from Fa\v cevicov\`a (2018):
data(manu_abs)
manu_USA <- manu_abs[which(manu_abs$country=='USA'),]
manu_USA$output <- factor(manu_USA$output, levels=c('LAB', 'SUR', 'INP'))

# pivot coordinates
tabCoord(manu_USA, row.factor = 'output', col.factor = 'isic', value='value')

# SBPs defined in paper
r <- rbind(c(-1,-1,1), c(-1,1,0))
c <- rbind(c(-1,-1,-1,-1,1), c(-1,-1,-1,1,0), c(-1,-1,1,0,0), c(-1,1,0,0,0))
tabCoord(manu_USA, row.factor = 'output', col.factor = 'isic', value='value', SBPr=r, SBPc=c)

#####
### Analysis of a sample of CoDa Tables

# example from Fa\v cevicov\`a (2018):
data(manu_abs)

### Compositional tables approach,
### analysis of the relative structure.
### An example from Facevi\v cov\`a (2018)

manu_abs$output <- factor(manu_abs$output, levels=c('LAB', 'SUR', 'INP'))
```

```

# pivot coordinates
tabCoordWrapper(manu_abs, obs.ID='country',
row.factor = 'output', col.factor = 'isic', value='value')

# SBPs defined in paper
r <- rbind(c(-1,-1,1), c(-1,1,0))
c <- rbind(c(-1,-1,-1,-1,1), c(-1,-1,-1,1,0),
c(-1,-1,1,0,0), c(-1,1,0,0,0))
tabCoordWrapper(manu_abs, obs.ID='country',row.factor = 'output',
col.factor = 'isic', value='value', SBPr=r, SBPc=c, test=TRUE)

### Classical approach,
### generalized linear mixed effect model.

## Not run:
library(lme4)
glmer(value~output*as.factor(isic)+(1|country),data=manu_abs,family=poisson)

## End(Not run)

```

---

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/>

**References**

OECD (2017), Teaching staff (indicator). doi: 10.1787/6a32426b-en (Accessed on 27 March 2017)

**Examples**

```
data(teachingStuff)
str(teachingStuff)
```

---

ternaryDiag

*Ternary diagram*

---

**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),
  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 indicates 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

### References

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

### 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("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      *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.

**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 trough.

**Value**

no values are returned.

**Author(s)**

Peter Filzmoser, Matthias Templ

**See Also**

[ternaryDiag](#)

**Examples**

```
data(coffee)
x <- coffee[,2:4]
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, ...)
```

**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[,2:4]
ternaryDiag(x, grid=FALSE)
ternaryDiagPoints(x+1, col="red", pch=2)
```

---

trondelagC

*regional geochemical survey of soil C in Norway*

---

**Description**

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

**Usage**

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)
- 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)
- Ti Concentration of titanium (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 km<sup>2</sup>.

### Author(s)

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

### References

C.Reimann, J.Schilling, D.Roberts, K.Fabian. A regional-scale geochemical survey of soil C horizon samples in Nord-Trondelag, Central Norway. Geology and mineral potential, *Applied Geochemistry* 61 (2015) 192-205.

### Examples

```
data(trondelagC)
str(trondelagC)
```

---

trondelag0

*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(trondelag0)
```

### 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 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)
- 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)
- Ti Concentration of titanium (in mg/kg)
- Tl Concentration of thallium (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 km<sup>2</sup>.

**Author(s)**

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

**References**

C.Reimann, J.Schilling, D.Roberts, K.Fabian. A regional-scale geochemical survey of soil C horizon samples in Nord-Trondelag, Central Norway. Geology and mineral potential, *Applied Geochemistry* 61 (2015) 192-205.

**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

**Source**

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

**References**

OECD (2017), Youth not in employment, education or training (NEET) (indicator). doi: 10.1787/72d1033a-en (Accessed on 27 March 2017)

**Examples**

```
data(unemployed)
str(unemployed)
```

---

variation

*Robust and classical variation matrix*

---

**Description**

Estimates the variation matrix with robust methods.

**Usage**

```
variation(x, method = "robustPivot")
```

**Arguments**

x	data frame or matrix with positive entries
method	method used for estimating covariances. See details.

**Details**

The variation matrix is estimated for a given compositional data set. Instead of using the classical standard deviations the minimum covariance estimator is used (`covMcd`) is used when parameter `robust` is set to `TRUE`.

For method `robustPivot` formula 5.8. of the book (see second reference) is used. Here robust (mcd-based) covariance estimation is done on pivot coordinates. Method `robustPairwise` uses a mcd covariance estimation on pairwise log-ratios. Methods `Pivot` (see second reference) and `Pairwise` (see first reference) are the non-robust counterparts. Naturally, `Pivot` and `Pairwise` gives the same results, but the computational time is much less for method `Pairwise`.

**Value**

The (robust) variation matrix.

**Author(s)**

Karel Hron, Matthias Templ

## References

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

# Filzmoser, P., Hron, K., Templ, M. (2018) *Applied Compositional Data Analysis*. Springer, Cham.

## Examples

```
data(expenditures)
variation(expenditures) # default is method "robustPivot"
variation(expenditures, method = "Pivot")
variation(expenditures, method = "robustPairwise")
variation(expenditures, method = "Pairwise") # same results as Pivot
```

---

zeroOut	<i>Detection of outliers of zero-inflated data</i>
---------	--

---

## 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

```
### Installing and loading required packages
data(expenditures)
```

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