

Package ‘ToolsForCoDa’

July 21, 2025

Type Package

Title Multivariate Tools for Compositional Data Analysis

Version 1.1.0

Date 2025-01-09

Author Jan Graffelman [aut, cre]

Maintainer Jan Graffelman <jan.graffelman@upc.edu>

Depends R (>= 1.8.0), MASS, calibrate, Correlplot

Description Provides functions for multivariate analysis with compositional data. Includes a function for doing compositional canonical correlation analysis. This analysis requires two data matrices of compositions, which can be adequately transformed and used as entries in a specialized program for canonical correlation analysis, that is able to deal with singular covariance matrices. The methodology is described in Graffelman et al. (2017) <doi:10.1101/144584>. Functions for log-ratio principal component analysis with condition number computations and log-ratio discriminant analysis have been added to the package.

License GPL (>= 2)

URL <https://www.r-project.org>, <http://www-eio.upc.edu/~jan/>

Suggests knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

Repository CRAN

Date/Publication 2025-01-09 11:00:05 UTC

Contents

Artificial	2
bentonites	2
canocov	3
cen	5
clrmat	6
largest.kappas	6
lrcco	7

lrllda	9
lrpca	10
PinotNoir	11
ternaryplot	12
tr	13
Tubb	14
Index	15

Artificial	<i>Two sets of 3-part compositions</i>
------------	--

Description

The list object `Artificial` contains two data frames of 3-part compositions. The data refer to the example in Section 3.1 of Graffelman et al. (2017)

Usage

```
data(Artificial)
```

Format

A list containing two data frames containing 100 observations.

Source

Laird, N. M. and Lange, C. Table 7.11, p. 124

References

Graffelman, J., Pawlowsky-Glahn, V., Egozcue, J.J. and Buccianti, A. (2017) Compositional Canonical Correlation Analysis.

bentonites	<i>Isotopic and chemical compositions of bentonites</i>
------------	---

Description

The data consists of 14 geological samples from the US with their major oxide composition (SiO₂, Al₂O₃, Fe₂O₃, MnO, MgO, CaO, K₂O, Na₂O and H₂O+) and delta Deuterium and delta-18-Oxygen (dD,d18O).

Usage

```
data("bentonites")
```

Format

A data frame with 14 observations on the following 11 variables.

Si a numeric vector
 Al a numeric vector
 Fe a numeric vector
 Mn a numeric vector
 Mg a numeric vector
 Ca a numeric vector
 K a numeric vector
 Na a numeric vector
 H2O a numeric vector
 dD a numeric vector
 d18O a numeric vector

Source

Cadrin, A.A.J (1995), Tables 1 and 2. Reyment, R. A. and Savazzi, E. (1999), pp. 220-222.

References

Cadrin, A.A.J., Kyser, T.K., Caldwell, W.G.E. and Longstaffe, F.J. (1995) Isotopic and chemical compositions of bentonites as paleoenvironmental indicators of the Cretaceous Western Interior Seaway Palaeogeography, Palaeoclimatology, Palaeoecology 119 pp. 301–320.
 Reyment, R. A. and Savazzi, E. (1999) Aspects of Multivariate Statistical Analysis in Geology, Elsevier Science B.V., Amsterdam.

Examples

```
data(bentonites)
```

canocov

Canonical correlation analysis.

Description

Function canocov performs a canonical correlation analysis. It operates on raw data matrices, which are only centered in the program. It uses generalized inverses and can deal with structurally singular covariance matrices.

Usage

```
canocov(X, Y)
```

Arguments

X	The n times p X matrix of observations
Y	The n times q Y matrix of observations

Details

canocov computes the solution by a singular value decomposition of the transformed between set covariance matrix.

Value

Returns a list with the following results

ccor	the canonical correlations
A	canonical weights of the X variables
B	canonical weights of the Y variables
U	canonical X variates
V	canonical Y variates
Fs	biplot markers for X variables (standard coordinates)
Gs	biplot markers for Y variables (standard coordinates)
Fp	biplot markers for X variables (principal coordinates)
Gp	biplot markers for Y variables (principal coordinates)
Rxu	canonical loadings, (correlations X variables, canonical X variates)
Rxv	canonical loadings, (correlations X variables, canonical Y variates)
Ryu	canonical loadings, (correlations Y variables, canonical X variates)
Ryv	canonical loadings, (correlations Y variables, canonical Y variates)
Sxu	covariance X variables, canonical X variates
Sxv	covariance X variables, canonical Y variates
Syu	covariance Y variables, canonical X variates
Syv	covariance Y variables, canonical Y variates
fitRxy	goodness of fit of the between-set correlation matrix
fitXs	adequacy coefficients of X variables
fitXp	redundancy coefficients of X variables
fitYs	adequacy coefficients of Y variables
fitYp	redundancy coefficients of Y variables

Author(s)

Jan Graffelman <jan.graffelman@upc.edu>

References

- Hotelling, H. (1935) The most predictable criterion. *Journal of Educational Psychology* (26) pp. 139-142.
- Hotelling, H. (1936) Relations between two sets of variates. *Biometrika* (28) pp. 321-377.
- Johnson, R. A. and Wichern, D. W. (2002) *Applied Multivariate Statistical Analysis*. New Jersey: Prentice Hall.

See Also

[cancor](#)

Examples

```
set.seed(123)
X <- matrix(runif(75),ncol=3)
Y <- matrix(runif(75),ncol=3)
cca.results <- canocov(X,Y)
```

cen	<i>centring of a data matrix</i>
-----	----------------------------------

Description

centres the columns of a matrix to mean zero.

Usage

```
cen(X,w=rep(1,nrow(X))/nrow(X))
```

Arguments

X	a raw data matrix.
w	a vector of case weights.

Value

returns a matrix

Author(s)

Jan Graffelman (jan.graffelman@upc.edu)

Examples

```
X<-matrix(runif(10),ncol=2)
Y<-cen(X)
print(Y)
```

clrmat	<i>Centred log-ratio transformation</i>
--------	---

Description

Program clrmat calculates the centred log-ratio transformation for a matrix of compositions.

Usage

```
clrmat(X)
```

Arguments

X	A matrix of compositions
---	--------------------------

Value

A matrix containing the transformed data

Author(s)

Jan Graffelman <jan.graffelman@upc.edu>

Examples

```
data(Artificial)
Xsim.com <- Artificial$Xsim.com
Xclr <- clrmat(Xsim.com)
```

largest.kappas	<i>Calculate condition indices for subcompositions</i>
----------------	--

Description

Function largest.kappas calculates the condition numbers for all subcompositions of a given size, for a particular compositional data set.

Usage

```
largest.kappas(Xcom, nparts = 3, sizetoplist = 10)
```

Arguments

Xcom	A data matrix with compositions in rows
nparts	The number of parts for the subcompositions to be analysed.
sizetoplist	The length of the list of the "best" subcompositions

Details

Log-ratio PCA is executed for each subcomposition, and the resulting eigenvalues and eigenvectors are stored.

Value

A data frame with an ordered list of subcompositions

Author(s)

Jan Graffelman (jan.graffelman@upc.edu)

Examples

```
X <- matrix(runif(600),ncol=6)
Xcom <- X/rowSums(X)
Results <- largest.kappas(Xcom)
```

lrcco

Logratio Canonical Correlation Analysis

Description

Function lrcco is a wrapper function around canocov. It performs logratio canonical correlation analysis (LR-CCO) accepting two compositional data matrices as input.

Usage

```
lrcco(X, Y)
```

Arguments

X	The matrix of X compositions
Y	The matrix of Y compositions

Details

Matrices X and Y are assumed to contain positive elements only, and there rows sum to one.

Value

Returns a list with the following results

ccor	the canonical correlations
A	canonical weights of the X variables
B	canonical weights of the Y variables
U	canonical X variates

V	canonical Y variates
Fs	biplot markers for X variables (standard coordinates)
Gs	biplot markers for Y variables (standard coordinates)
Fp	biplot markers for X variables (principal coordinates)
Gp	biplot markers for Y variables (principal coordinates)
Rxu	canonical loadings, (correlations X variables, canonical X variates)
Rxv	canonical loadings, (correlations X variables, canonical Y variates)
Ryu	canonical loadings, (correlations Y variables, canonical X variates)
Ryv	canonical loadings, (correlations Y variables, canonical Y variates)
Sxu	covariance X variables, canonical X variates
Sxv	covariance X variables, canonical Y variates
Syu	covariance Y variables, canonical X variates
Syv	covariance Y variables, canonical Y variates
fitRxy	goodness of fit of the between-set correlation matrix
fitXs	adequacy coefficients of X variables
fitXp	redundancy coefficients of X variables
fitYs	adequacy coefficients of Y variables
fitYp	redundancy coefficients of Y variables

Author(s)

Jan Graffelman <jan.graffelman@upc.edu>

References

- Hotelling, H. (1935) The most predictable criterion. *Journal of Educational Psychology* (26) pp. 139-142.
- Hotelling, H. (1936) Relations between two sets of variates. *Biometrika* (28) pp. 321-377.
- Johnson, R. A. and Wichern, D. W. (2002) *Applied Multivariate Statistical Analysis*. New Jersey: Prentice Hall.
- Graffelman, J. and Pawlowsky-Glahn, V. and Egozcue, J.J. and Buccianti, A. (2018) Exploration of geochemical data with compositional canonical biplots, *Journal of Geochemical Exploration* 194, pp. 120–133. doi:[10.1016/j.gexplo.2018.07.014](https://doi.org/10.1016/j.gexplo.2018.07.014)

See Also

[cancor](#), [canocov](#)

Examples

```
set.seed(123)
X <- matrix(runif(75),ncol=3)
Y <- matrix(runif(75),ncol=3)
Xc <- X/rowSums(X) # create compositions by closure
Yc <- Y/rowSums(Y)
out.lrcco <- lrcco(X,Y)
```

lrllda

*Logratio Linear Discriminant Analysis***Description**

Function `lrllda` implements logratio linear discriminant analysis for compositional data, using the centred logratio transformation (clr)

Usage

```
lrllda(Xtrain, group, Xtest = NULL, divisorn = FALSE, verbose = FALSE)
```

Arguments

<code>Xtrain</code>	A compositional data set, the training data for logratio-LDA.
<code>group</code>	A categorical variable defining the groups.
<code>Xtest</code>	A compositional data set for which group prediction is sought (the test data). If no test data is supplied, the training data itself is classified.
<code>divisorn</code>	Use divisor "n" (<code>divisorn=TRUE</code>) in the calculation of covariance or use "n-1" (<code>divisorn=TRUE</code>)
<code>verbose</code>	Print output (<code>verbose = TRUE</code>) or not.

Details

Function `lrllda` uses the centred logratio transformation, which produces a singular covariance matrix. This singularity is dealt with by using a generalized inverse. When test data is supplied via argument `Xtest`, the scores of the linear classifier, the poster probabilities and the predicted classes are calculated for the test data. If no test data is supplied, these quantities are calculated for the training data.

Value

<code>LD</code>	Scores on the linear classifier for the test observations. These are also the biplot coordinates of the individuals.
<code>Fp</code>	Biplot coordinates of the group means.
<code>Gs</code>	Biplot coordinates of the variables.
<code>Sp</code>	Pooled covariance matrix.
<code>Mc</code>	Matrix of centred clr mean vectors, one row for each group.
<code>S.list</code>	Covariance matrices of each group.
<code>la</code>	Vector of eigenvalues.
<code>pred</code>	Predicted class for the test observations.
<code>CM</code>	The confusion matrix.
<code>gsize</code>	Sample size of each group.

Mc1r Matrix of mean vectors for clr coordinates, one row for each group.
 prob.posterior Vector of posterior probabilities.
 decom Table with decomposition of variability as expressed by the eigenvalues.

Author(s)

Jan Graffelman (jan.graffelman@upc.edu)

See Also

[lrpca](#), [lrllda](#)

Examples

```
data(Tubb)
sampleid <- Tubb$Sample
site <- factor(Tubb$site)
Oxides <- as.matrix(Tubb[,2:10])
rownames(Oxides) <- sampleid
Oxides <- Oxides/rowSums(Oxides)
out.lda <- lrllda(Oxides,site,verbose=FALSE)
```

lrpca

Logratio principal component analysis with condition indices

Description

Function `lrpca` performs logratio principal component analysis. It returns the variance decomposition, principal components, biplot coordinates and a table with condition indices.

Usage

```
lrpca(Xcom)
```

Arguments

Xcom A matrix with compositions in its rows

Details

Calculations are based on the singular value decompositon of the clr transformed compositions.

Value

Fp	matrix with principal components
Fs	matrix with standardized principal components
Gp	biplot markers for parts (principal coordinates)
Gs	biplot markers for parts (standard coordinates)
La	eigenvalues
D	singular values
decom	table with variance decomposition
kappalist	table with condition indices and eigenvectors

Author(s)

Jan Graffelman (jan.graffelman@upc.edu)

See Also

[princomp](#)

Examples

```
data(bentonites)
Ben <- bentonites[,1:8]
Ben.com <- Ben/rowSums(Ben)
out.lrpca <- lrpca(Ben.com)
```

PinotNoir

Chemical composition of Pinot Noir wines

Description

Dataframe `PinotNoir` contains the composition of 17 chemical components for 37 Pinot Noir wines, as well as an Aroma evaluation.

Usage

```
data("PinotNoir")
```

Format

A data frame with 37 observations on the following 18 variables.

Cd Cadmium
 Mo Molybdenum
 Mn Manganese
 Ni Nickel

Cu Copper
Al Aluminium
Ba Barium
Cr Chromium
Sr Strontium
Pb Lead
B Boron
Mg Magnesium
Si Silicon
Na Sodium
Ca Calcium
P Phosphorus
K Potassium
Aroma Aroma evaluation

Source

[doi:10.1016/S00032670\(00\)842452](https://doi.org/10.1016/S00032670(00)842452)

References

Frank, I.E. and Kowalski, B.R. (1984) Prediction of Wine Quality and Geographic Origin from Chemical Measurements by Partial Least-Squares Regression Modeling. *Analytica Chimica Acta* 162, pp. 241–251 [doi:10.1016/S00032670\(00\)842452](https://doi.org/10.1016/S00032670(00)842452)

Examples

```
data(PinotNoir)
```

ternaryplot

Create a Ternary Plot for three-part Compositions

Description

Function ternaryplot accepts a matrix of three part compositions or non-negative counts and presents these in a ternary diagram.

Usage

```
ternaryplot(X, vertexlab = colnames(X), vertex.cex = 1, pch = 19, addpoints = TRUE,  
            grid = FALSE, gridlabels = TRUE, ...)
```

Arguments

X	A matrix of counts or compositions with three columns
vertexlab	Labels for the vertices of the ternary diagram
vertex.cex	Character expansion factor for vertex labels
pch	Plotting character for the compositions
addpoints	Show the compositions addpoints=TRUE or not
grid	Place a grid over the ternary diagram
gridlabels	Place grid labels or not
...	Additional arguments for the points function

Value

NULL

Author(s)

Jan Graffelman (jan.graffelman@upc.edu)

Examples

```
data("Artificial")
Xsim.com <- Artificial$Xsim.com
colnames(Xsim.com) <- paste("X",1:3,sep="")
ternaryplot(Xsim.com)
```

tr	<i>Compute the trace of a matrix</i>
----	--------------------------------------

Description

tr computes the trace of a matrix.

Usage

```
tr(X)
```

Arguments

X	a (square) matrix
---	-------------------

Value

the trace (a scalar)

Author(s)

Jan Graffelman (jan.graffelman@upc.edu)

Examples

```
X <- matrix(runif(25),ncol=5)
print(X)
print(tr(X))
```

Tubb

Romano-British pottery oxides

Description

A dataframe with the major oxide composition of pottery found at Romano-British kiln sites in Wales, Gloucester and the New Forest as determined by atomic absorption.

Usage

```
data("Tubb")
```

Format

A data frame with 48 observations on the following 11 variables.

Sample Sample identifier

Al2O3 Aluminium oxide

Fe2O3 Iron (III) oxide

MgO Magnesium oxide

CaO Calcium oxide

Na2O Sodium oxide

K2O Potassium oxide

TiO2 Titanium dioxide

MnO Manganese oxide

BaO Barium oxide

site Geographical region of the sample. G=Gloucester, NF=New Forest, W=Wales.

References

Tubb, A., Parker, A.J. and Nickless, G. (1980) The analysis of Romano-British pottery by atomic absorption spectrophotometry. *Archaeometry* 22(2) pp. 153–171.

Examples

```
data(Tubb)
```

Index

- * **algebra**
 - tr, [13](#)
- * **aplot**
 - ternaryplot, [12](#)
- * **array**
 - tr, [13](#)
- * **datasets**
 - Artificial, [2](#)
 - bentonites, [2](#)
 - PinotNoir, [11](#)
 - Tubb, [14](#)
- * **multivariate**
 - canocov, [3](#)
 - cen, [5](#)
 - clrmat, [6](#)
 - largest.kappas, [6](#)
 - lrcco, [7](#)
 - lrllda, [9](#)
 - lrpca, [10](#)

Artificial, [2](#)

bentonites, [2](#)

cancor, [5](#), [8](#)

canocov, [3](#), [8](#)

cen, [5](#)

clrmat, [6](#)

largest.kappas, [6](#)

lrcco, [7](#)

lrllda, [9](#), [10](#)

lrpca, [10](#), [10](#)

PinotNoir, [11](#)

princomp, [11](#)

ternaryplot, [12](#)

tr, [13](#)

Tubb, [14](#)