Package 'REPPlab'

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| REPPlab-package 2 coef.epplab 3 |
| EPPlab |
| EPPlabAgg |
| EPPlabOutlier 8 fitted.epplab 10 |
| pairs.epplab |
| plot.epplab |
| plot.epplabOutlier |

2 REPPlab-package

| | print.epplabOu | uner | | | | | | | | | | | | | | | | | | 16 |
|-------|-----------------|------|--|--|--|--|--|--|---|--|---|--|--|---|---|--|---|--|---|----|
|] | ReliabilityData | a | | | | | | | | | | | | | | | | | | 17 |
| 5 | screeplot.eppla | ıb | | | | | | | | | | | | | | | | | | 17 |
| 5 | summary.eppla | ıb | | | | | | | | | | | | | | | | | | 18 |
| | summary.eppla | | | | | | | | | | | | | | | | | | | |
| 1 | WhitenSVD . | | | | | | | | • | | • | | | • | • | | • | | • | 20 |
| Index | | | | | | | | | | | | | | | | | | | | 22 |

Description

An interface that gives access to the Java program 'EPP-lab' which implements several biologically inspired optimisation algorithms and several indices for Exploratory Projection Pursuit (PP). The objective of optimizing PP indices and projecting the data on the associated one-dimensional directions is to detect hidden structures such as clusters or outliers in (possibly high dimensional) data sets. The 'EPP-lab' sources and jar-files are available under https://github.com/fischuu/EPP-lab. For a detailed description of 'EPP-lab', see Larabi (2011).

Details

Package: REPPlab
Type: Package
Version: 0.9.6
Date: 2023-12-11
License: GPL
LazyLoad: yes

Author(s)

Daniel Fischer, Alain Berro, Klaus Nordhausen, Anne Ruiz-Gazen

Maintainer: Daniel Fischer <daniel.fischer@luke.fi>

References

Larabi Marie-Sainte, S., (2011), Biologically inspired algorithms for exploratory projection pursuit, PhD thesis, University of Toulouse.

Ruiz-Gazen, A., Larabi Marie-Sainte, S. and Berro, A. (2010), Detecting multivariate outliers using projection pursuit with particle swarm optimization, COMPSTAT2010, pp. 89-98.

coef.epplab 3

Berro, A., Larabi Marie-Sainte, S. and Ruiz-Gazen, A. (2010). Genetic algorithms and particle swarm optimization for exploratory projection pursuit. Annals of Mathematics and Artifcial Intelligence, 60, 153-178.

Larabi Marie-Sainte, S., Berro, A. and Ruiz-Gazen, A. (2010). An effcient optimization method for revealing local optima of projection pursuit indices. Swarm Intelligence, pp. 60-71.

coef.epplab

Extracts the Directions of an Epplab Object

Description

Extracts the found directions of an epplab object.

Usage

```
## S3 method for class 'epplab'
coef(object, which = 1:ncol(object$PPdir), ...)
```

Arguments

object Object of class epplab.

which Specifies which directions are extracted.

... Additional parameters.

Details

The coef function extracts the directions found from the EPPlab call.

Author(s)

Daniel Fischer

```
library(tourr)
data(olive)
res <- EPPlab(olive[,3:10],PPalg="PSO",PPindex="KurtosisMin",n.simu=10, maxiter=20)
coef(res)</pre>
```

4 EPPlab

EPPlab

Function for Exploratory Projection Pursuit.

Description

REPPlab optimizes a projection pursuit (PP) index using a Genetic Algorithm (GA) or one of two Particle Swarm Optimisation (PSO) algorithms over several runs, implemented in the Java program EPP-lab. One of the PSO algorithms is a classic one while the other one is a parameter-free extension called Tribes. The parameters of the algorithms (maxiter and individuals for GA and maxiter and particles for PSO) can be modified by the user. The PP indices are the well-known Friedman and Friedman-Tukey indices together with the kurtosis and a so-called discriminant index that is devoted to the detection of groups. At each run, the function finds a local optimum of the PP index and gives the associated projection direction and criterion value.

Usage

```
EPPlab(
    x,
    PPindex = "KurtosisMax",
    PPalg = "GA",
    n.simu = 20,
    sphere = FALSE,
    maxiter = NULL,
    individuals = NULL,
    particles = NULL,
    step_iter = 10,
    eps = 10^(-6)
)
```

Arguments

PPindex The used index, see details.

PPalg The used algorithm, see details.

n. simu Number of simulation runs.

sphere Logical, sphere the data. Default is FALSE, in which case the data is only standardized.

maxiter Maximum number of iterations.

individuals Size of the generated population in GA.

particles Number of generated particles in the standard PSO algorithm.

step_iter Convergence criterium parameter, see details. (Default: 10)
eps Convergence criterium parameter, see details. (Default: 10^(-6))

EPPlab 5

Details

The function always centers the data using colMeans and divides by the standard deviation. Sphering the data is optional. If sphering is requested the function WhitenSVD is used, which automatically tries to determine the rank of the data.

Currently the function provides the following projection pursuit indices: KurtosisMax, Discriminant, Friedman, FriedmanTukey, KurtosisMin.

Three algorithms can be used to find the projection directions. These are a Genetic Algorithm GA and two Particle Swarm Optimisation algorithms PSO and Tribe.

Since the algorithms might find local optima they are run several times. The function sorts the found directions according to the optimization criterion.

The different algorithms have different default settings. It is for GA: maxiter=50 and individuals=20. For PSO: maxiter=20 and particles=50. For Tribe: maxiter=20.

For GA, the size of the generated population is fixed by the user (individuals). The algorithm is based on a tournament section of three participants. It uses a 2-point crossover with a probability of 0.65 and the mutation operator is applied to all the individuals with a probability of 0.05. The termination criterion corresponds to the number of generations and is also fixed by the user (maxiter).

For PSO, the user can give the number of initial generated particles and also the maximum number of iterations. The other parameters are fixed following Clerc (2006) and using a "cosine" neighborhood adapted to PP for the PSO algorithm. For Tribes, only the maximum number of iterations needs to be fixed. The algorithm proposed by Cooren and Clerc (2009) and adapted to PP using a "cosine neighborhood" is used.

The algorithms stop as soon as one of the two following conditions holds: the maximum number of iterations is reached or the relative difference between the index value of the present iteration i and the value of iteration i-step_iter is less than eps. In the last situation, the algorithm is said to converge and EPPlab will return the number of iterations needed to attain convergence. If the convergence is not reached but the maximum number of iterations is attained, the function will return some warnings. The default values are 10 for step_iter and 1E-06 for eps. Note that if few runs have not converged this might not be problem and even non-converged projections might reveal some structure.

Value

A list with class 'epplab' containing the following components:

PPdir Matrix containing the PP directions as columns, see details.

PPindexVal Vector containing the objective criterion value of each run.

PPindex Name of the used projection index.

PPiter Vector containing the number of iterations of each run.

PPconv Boolean vector. Is TRUE if the run converged and FALSE else.

PPalg Name of the used algorithm.

maxiter Maximum number of iterations, as given in function call.

x Matrix containing the data (centered!).

sphere Logical

6 EPPlab

transform The transformation matrix from the whitening or standardization step.

backtransform The back-transformation matrix from the whitening or standardization step.

center The mean vector of the data

Author(s)

Daniel Fischer, Klaus Nordhausen

References

Larabi Marie-Sainte, S., (2011), Biologically inspired algorithms for exploratory projection pursuit, PhD thesis, University of Toulouse.

Ruiz-Gazen, A., Larabi Marie-Sainte, S. and Berro, A. (2010), Detecting multivariate outliers using projection pursuit with particle swarm optimization, COMPSTAT2010, pp. 89-98.

Berro, A., Larabi Marie-Sainte, S. and Ruiz-Gazen, A. (2010). Genetic algorithms and particle swarm optimization for exploratory projection pursuit. Annals of Mathematics and Artifcial Intelligence, 60, 153-178.

Larabi Marie-Sainte, S., Berro, A. and Ruiz-Gazen, A. (2010). An efficient optimization method for revealing local optima of projection pursuit indices. Swarm Intelligence, pp. 60-71.

Clerc, M. (2006). Particle Swarm Optimization. ISTE, Wiley.

Cooren, Y., Clerc, M. and Siarry, P. (2009). Performance evaluation of TRIBES, an adaptive particle swarm optimization algorithm. Swarm Intelligence, 3(2), 149-178.

```
library(tourr)
data(olive)
olivePP <- EPPlab(olive[,3:10],PPalg="PSO",PPindex="KurtosisMax",n.simu=5, maxiter=20)
summary(olivePP)

library(amap)
data(lubisch)
X <- lubisch[1:70,2:7]
rownames(X) <- lubisch[1:70,1]
res <- EPPlab(X,PPalg="PSO",PPindex="FriedmanTukey",n.simu=15, maxiter=20,sphere=TRUE)
print(res)
summary(res)
fitted(res)
plot(res)
pairs(res)
predict(res,data=lubisch[71:74,2:7])</pre>
```

EPPlabAgg 7

Description

Function that automatically aggregates the projection directions from one or more epplab objects. Three options are available on how to choose the final projection which can have a rank larger than one. The parameter x can either be a single object or a list of epplab objects. Options for method are inverse, sq.inverse and cumulative.

Usage

```
EPPlabAgg(x, method = "cumulative", percentage = 0.85)
```

Arguments

x An object of class epplab or a list of epplab objects.

method The type of method, see details. Options are inverse, sq.inverse and cumulative.

percentage Threshold for the relative eigenvalue sum to retain, see details.

Details

Denote $p_i, i=1,...,m$, the projection vectors contained in the list of epplab objects and $P_i, i=1,...,m$, the corresponding orthogonal projection matrices (each having rank one). The method cumulative is based on the eigenvalue decomposition of $P_w = \frac{1}{m} \sum_{i=1}^m P_i$ and transforms as 0 the eigenvectors such that the corresponding relative eigenvalues sum is at least percentage. The number of eigenvectors retained corresponds to the rank k and P is the corresponding orthogonal projection matrix. The methods inverse and sq. inverse are automatic rules to choose the number of eigenvectors to retain as implemented by the function AOP.

Value

A list with class 'epplabagg' containing the following components:

P The estimated average orthogonal projection matrix.

O An orthogonal matrix on which P is based upon.

k The rank of the average orthogonal projection matrix.

eigenvalues The relevant eigenvalues, see details. Only given if method="cumulative".

Author(s)

Daniel Fischer, Klaus Nordhausen, Anne Ruiz-Gazen

References

Liski, E., Nordhausen, K., Oja, H. and Ruiz-Gazen, A. (201?), Combining Linear Dimension Reduction Estimates, to appear in the Proceedings of ICORS 2015, pp. ??-??.

8 EPPlabOutlier

See Also

```
EPPlab, AOP
```

Examples

```
library(tourr)
data(olive)
# To keep the runtime short, maxiter and n.simu were chosen very
# small for demonstration purposes, real life applications would
# rather choose larger values, e.g. n.simu=100, maxiter=200
olivePP.kurt.max <-
  EPPlab(olive[,3:10],PPalg="PSO",PPindex="KurtosisMax",n.simu=10, maxiter=20)
olivePP.fried <-
  EPPlab(olive[,3:10],PPalg="PSO",PPindex="Friedman",n.simu=10, maxiter=20)
olivePPs <- list(olivePP.kurt.max, olivePP.fried)</pre>
EPPlabAgg(olivePP.kurt.max)$k
EPPlabAgg(olivePPs, "cum", 0.99)$k
pairs(olivePP.kurt.max$x %*% EPPlabAgg(olivePPs, "cum", 0.99)$0,
      col=olive[,2], pch=olive[,1])
olivAOP.sq <- EPPlabAgg(olivePPs, "inv")</pre>
oliveProj <- olivePP.kurt.max$x %*% olivAOP.sq$0
plot(density(oliveProj))
rug(oliveProj[olive$region==1],col=1)
rug(oliveProj[olive$region==2],col=2)
rug(oliveProj[olive$region==3],col=3)
```

EPPlabOutlier

Function to Find Outliers for an epplab Object

Description

Function to decide wether observations are considered outliers or not in specific projection directions of an epplab object.

Usage

```
EPPlabOutlier(x, which = 1:ncol(x\$PPdir), k = 3, location = mean, scale = sd)
```

EPPlabOutlier 9

Arguments

x An object of class epplab.

which The directions in which outliers should be searched. The default is to look at all.

k Numeric value to decide when an observation is considered an outlier or not.

Default is 3. See details.

location A function which gives the univariate location as an output. The default is mean.

scale A function which gives the univariate scale as an output. The default is sd.

Details

Denote $location_j$ as the location of the jth projection direction and analogously $scale_j$ as its scale. Then an observation x is an outlier in the jth projection direction, if $|x - location_j| \ge k \ scale_j$.

Naturally it is best to use for this purpose robust location and scale measures like median and mad for example.

Value

A list with class 'epplabOutlier' containing the following components:

outlier A matrix with only zeros and ones. A value of 1 classifies the observation as an

outlier in this projection direction.

k The factor k used.

location The name of the location estimator used.

scale The name of the scale estimator used.

PPindex The name of the PPindex used.

PPalg The name of the PPalg used.

Author(s)

Klaus Nordhausen

References

Ruiz-Gazen, A., Larabi Marie-Sainte, S. and Berro, A. (2010), Detecting multivariate outliers using projection pursuit with particle swarm optimization, COMPSTAT2010, pp. 89-98.

See Also

EPPlab

10 fitted.epplab

Examples

```
# creating data with 3 outliers
n <-300
p <- 10
X <- matrix(rnorm(n*p),ncol=p)
X[1,1] <- 9
X[2,4] <- 7
X[3,6] <- 8
# giving the data rownames, obs.1, obs.2 and obs.3 are the outliers.
rownames(X) <- paste("obs",1:n,sep=".")

PP<-EPPlab(X,PPalg="PSO",PPindex="KurtosisMax",n.simu=20, maxiter=20)
OUT<-EPPlabOutlier(PP, k = 3, location = median, scale = mad)
OUT</pre>
```

fitted.epplab

Calculates projections of the Data

Description

Calculates the projections of the data object onto the directions from an underlying ebblab object.

Usage

```
## S3 method for class 'epplab'
fitted(object, which = 1, ...)
```

Arguments

object Object of class epplab.which Onto which direction should the new data be projected.... Additional parameters

Details

The default projection direction is the direction with the best objective criterion.

Value

A matrix, having in each column the projection onto the direction of a certain run, and in each row the projected value.

Author(s)

Daniel Fischer

pairs.epplab 11

Examples

```
library(tourr)
data(olive)
res <- EPPlab(olive[,3:10],PPalg="PSO",PPindex="KurtosisMin",n.simu=10, maxiter=20)
# Projection to the best direction
fitted(res)
# Projection to the 1,2,5 best directions:
fitted(res,which=c(1,2,5))</pre>
```

pairs.epplab

Plots a Scatterplot Matrix for an epplab Object

Description

Plots a scatterplot matrix of fitted scores of an epplab object.

Usage

```
## S3 method for class 'epplab'
pairs(x, which = 1:10, ...)
```

Arguments

x Object of class epplab.
which Which simulation runs should be taken into account.
... Graphical parameters, see also par().

Details

The option which can restrict the output to certain simulation runs. In case of many simulations, this might improve the readability.

Author(s)

Daniel Fischer

```
library(tourr)
data(olive)
res <- EPPlab(olive[,3:10],PPalg="PSO",PPindex="KurtosisMin",n.simu=10, maxiter=20)
pairs(res)</pre>
```

12 plot.epplab

plot.epplab

Plot for an epplab Object

Description

The function offers three informative plots for an epplab object.

Usage

```
## $3 method for class 'epplab'
plot(
    x,
    type = "kernel",
    angles = "radiants",
    kernel = "biweight",
    which = 1:10,
    as.table = TRUE,
    ...
)
```

Arguments

| X | Object of class epplab. |
|----------|---|
| type | Type of plot, values are "kernel", "histogram" and "angles". |
| angles | Values are "degree" and "radiants", if type="angles". |
| kernel | Type of kernel, passed on to density. |
| which | Which simulation runs should be taken into account. |
| as.table | A logical flag that controls the order in which panels should be displayed. |
| | Graphical parameters, see also xyplot, densityplot and histogram. |

Details

The option which can restrict the output to certain simulation runs. In case of many simulations, this might improve the readability.

For type="kernel", the default, it plots a kernel density estimate for each of the chosen directions. In the case of type="histogram" the corresponding histograms. For type="angles" it plots the angles of the first chosen direction against all others. Whether the angles are given in degrees or radiants, depends on the value of angles.

Author(s)

Daniel Fischer, Klaus Nordhausen

See Also

```
xyplot, densityplot, histogram, density
```

plot.epplabOutlier 13

Examples

```
library(tourr)
data(olive)
res <- EPPlab(olive[,3:10],PPalg="PSO",PPindex="KurtosisMin",n.simu=10, maxiter=20)

# Plot with kernel estimator
plot(res)

# Just the best 5 and then 8
plot(res,which=c(1:5,8))

# Plot as histogram
plot(res,type="histogram")

# Plot an angles plot
plot(res,type="angles")</pre>
```

plot.epplabOutlier

Plot for an epplabOutlier Object

Description

Visualizes which observations are considered as outliers and how often for an epplabOutlier object.

Usage

```
## S3 method for class 'epplabOutlier'
plot(x, col = c("white", "black"), outlier = TRUE, xlab = "", ylab = "", ...)
```

Arguments

| x | Object of class epplabOutlier. |
|---------|--|
| col | Which colors should be used for non-outliers and outliers. Default is white and black. |
| outlier | Logical if only observations considered as outliers at least once should be plotted or all. Default is TRUE. xlab Possible x axis label. Default is none. ylab Possible x axis label. Default is none. |
| xlab | Sets the x-axis label. |
| ylab | Sets the y-axis label. |
| | Graphical parameters passed on to image. |

Author(s)

Daniel Fischer and Klaus Nordhausen

14 predict.epplab

See Also

```
EPPlabOutlier, image
```

Examples

```
# creating data with 3 outliers
n <-300
p <- 10
X <- matrix(rnorm(n*p),ncol=p)
X[1,1] <- 9
X[2,4] <- 7
X[3,6] <- 8
# giving the data rownames, obs.1, obs.2 and obs.3 are the outliers.
rownames(X) <- paste("obs",1:n,sep=".")

PP<-EPPlab(X,PPalg="PSO",PPindex="KurtosisMax",n.simu=20, maxiter=20)
OUT<-EPPlabOutlier(PP, k = 3, location = median, scale = mad)
plot(OUT)</pre>
```

predict.epplab

Calculates projections for a new Data Object

Description

Calculates the projections of a new data object onto the directions from an existing ebblab object.

Usage

```
## S3 method for class 'epplab'
predict(object, which = 1, data = NULL, ...)
```

Arguments

object Object of class epplab.

which Onto which direction should the new data be projected.

data The new data object
... Additional parameters

Details

The default projection direction is the direction with the best objective criterion. In case that no data is given to the function, the fitted scores for the original data will be returned.

Value

A matrix having in each column the projection onto the direction of a certain run and in each row the projected value.

print.epplab 15

Author(s)

Daniel Fischer

Examples

```
library(tourr)
data(olive)
res <- EPPlab(olive[,3:10], PPalg="PSO", PPindex="KurtosisMin", n.simu=10, maxiter=20)
newData <- matrix(rnorm(80), ncol=8)

# Projection on the best direction
predict(res, data=newData)

# Projection on the best 3 directions
predict(res, which=1:3, data=newData)

# Similar with function fitted() when no data is given:
predict(res)
fitted(res)</pre>
```

print.epplab

Print an epplab Object

Description

Prints an epplab object.

Usage

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

Arguments

x Object of class epplab.

... Additional parameters

Details

The print function displays the result with the best value in the objective criterion.

Author(s)

Daniel Fischer

print.epplabOutlier

Examples

```
library(tourr)
data(olive)
res <- EPPlab(olive[,3:10],PPalg="PSO",PPindex="KurtosisMin",n.simu=10, maxiter=20)
print(res)</pre>
```

Description

Prints an epplabOutlier object.

Usage

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

Arguments

x Object of class epplabOutlier.

... Additional parameters

Details

The print function displays only the outlier matrix from the epplabOutlier object.

Author(s)

Klaus Nordhausen

```
# creating data with 3 outliers
n <-300
p <- 10
X <- matrix(rnorm(n*p),ncol=p)
X[1,1] <- 9
X[2,4] <- 7
X[3,6] <- 8
# giving the data rownames, obs.1, obs.2 and obs.3 are the outliers.
rownames(X) <- paste("obs",1:n,sep=".")

PP<-EPPlab(X,PPalg="PSO",PPindex="KurtosisMax",n.simu=20, maxiter=20)
OUT<-EPPlabOutlier(PP, k = 3, location = median, scale = mad)
OUT</pre>
```

ReliabilityData 17

ReliabilityData

Reliability Data from an Industrial Context

Description

The data set contains 55 variables measured during the production process of 520 units. The problem for this data is to identify the produced items with a fault not detected by standard tests.

Format

A data frame with 520 observations on 55 variables.

Source

The data was anonymized to keep confidentiality.

Examples

```
data(ReliabilityData)
summary(ReliabilityData)
```

screeplot.epplab

Creating a Screeplot for an epplab Object

Description

Plots the objective criteria of an epplab object versus the simulation runs.

Usage

```
## S3 method for class 'epplab'
screeplot(
    x,
    type = "lines",
    which = 1:10,
    main = "",
    ylab = "Objective criterion",
    xlab = "Simulation run",
    ...
)
```

18 summary.epplab

Arguments

| X | Object of class epplab. |
|-------|---|
| type | Type of screeplot, values are "barplot" and "lines" |
| which | Which simulation runs should be taken into account |
| main | Main title of the plot |
| ylab | Y-axis label |
| xlab | X-axis label |
| | Graphical parameters, see also par() |

Details

The option which can restrict the output to certain simulation runs. In case of many simulations, this might improve the readability. The barplot option is often not meaningful, because the objective criteria are usually large and bars begin by default at zero.

Author(s)

Daniel Fischer

Examples

```
library(tourr)
data(olive)
res <- EPPlab(olive[,3:10],PPalg="PSO",PPindex="KurtosisMin",n.simu=10, maxiter=20)
screeplot(res)

# Pretty useless:
screeplot(res,type="barplot")
screeplot(res,which=1:5)</pre>
```

summary.epplab

Summarize an epplab Object

Description

Summarizes and prints an epplab object in an informative way.

Usage

```
## S3 method for class 'epplab'
summary(object, which = 1:10, digits = 4, ...)
```

summary.epplabOutlier 19

Arguments

| object | Object of class epplab. |
|--------|------------------------------------|
| which | Summary for which simulation runs |
| digits | Number of displayed decimal digits |
| | Additional parameters |

Details

The option which can restrict the output to certain simulation runs. In case of many simulations, this might improve the readability.

Author(s)

Daniel Fischer

Examples

```
library(tourr)
data(olive)
res <- EPPlab(olive[,3:10],PPalg="PSO",PPindex="KurtosisMin",n.simu=10, maxiter=20)
summary(res)</pre>
```

```
summary.epplabOutlier Summarize an epplabOutlier Object
```

Description

Summarizes and prints an epplabOutlier object in an informative way.

Usage

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

Arguments

```
object Object of class epplabOutlier.
... Additional parameters
```

Details

The main information provided here is a table with names of the observations which are considered outliers and in how many PP directions they are considered outliers. This function is useful if the data has been given row names.

20 WhitenSVD

Author(s)

Klaus Nordhausen

Examples

```
# creating data with 3 outliers
n <-300
p <- 10
X <- matrix(rnorm(n*p),ncol=p)
X[1,1] <- 9
X[2,4] <- 7
X[3,6] <- 8
# giving the data rownames, obs.1, obs.2 and obs.3 are the outliers.
rownames(X) <- paste("obs",1:n,sep=".")

PP<-EPPlab(X,PPalg="PSO",PPindex="KurtosisMax",n.simu=20, maxiter=20)
OUT<-EPPlabOutlier(PP, k = 3, location = median, scale = mad)
summary(OUT)</pre>
```

WhitenSVD

Whitening Data Using Singular Value Decomposition

Description

The function whitens a data matrix using the singular value decomposition.

Usage

```
WhitenSVD(x, tol = 1e-06)
```

Arguments

x A numeric data frame or data matrix with at least two rows.

Tolerance value to decide the rank of the data. See details for further information. If set to NULL it will be ignored.

Details

The function whitens the data so that the result has mean zero and identity covariance matrix using the function svd. The data can have here less observations than variables and svd will determine the rank of the data automatically as the number of singular values larger than the largest singular value times tol. If tol=NULL the rank is set to the number of singular values, which is not advised when one or more singular values are close to zero.

The output contains among others as attributes the singular values and the matrix needed to back-transform the whitened data to its original space.

WhitenSVD 21

Value

The whitened data.

Author(s)

Klaus Nordhausen

See Also

```
svd, cov, colMeans
```

```
# more observations than variables
X <- matrix(rnorm(200),ncol=4)
A <- WhitenSVD(X)
round(colMeans(A),4)
round(cov(A),4)
# how to backtransform
summary(sweep(A %*% (attr(A, "backtransform")), 2, attr(A, "center"), "+") - X)
# fewer observations than variables
Y <- cbind(rexp(4),runif(4),rnorm(4), runif(4), rnorm(4), rt(4,4))
B <- WhitenSVD(Y)
round(colMeans(B),4)
round(cov(B),4)
# how to backtransform
summary(sweep(B %*% (attr(B, "backtransform")), 2, attr(B, "center"), "+") - Y)</pre>
```

Index

| * datasets | density, <i>12</i> |
|---|---|
| ReliabilityData, 17 | densityplot, <i>12</i> |
| * hplot | EDD1-1- 4 0 0 |
| pairs.epplab, 11 | EPPlab, 4, 8, 9 |
| plot.epplab, 12 | EPPlabAgg, 7 |
| plot.epplabOutlier, 13 | EPPlabOutlier, 8, 14 |
| screeplot.epplab,17 | fitted, epplab-method (fitted.epplab), 10 |
| * methods | fitted-method (fitted.epplab), 10 |
| coef.epplab, 3 | fitted.epplab, 10 |
| fitted.epplab, 10 | Treed.eppias, 10 |
| pairs.epplab,11 | histogram, 12 |
| plot.epplab, 12 | 3 |
| plot.epplabOutlier, 13 | image, <i>13</i> , <i>14</i> |
| predict.epplab, 14 | |
| print.epplab, 15 | mad, 9 |
| print.epplabOutlier, 16 | mean, 9 |
| summary.epplab, 18 | median, 9 |
| summary.epplabOutlier,19 | |
| * multivariate | pairs, epplab-method (pairs.epplab), 11 |
| EPPlabAgg, 7 | pairs-method (pairs.epplab), 11 |
| EPPlabOutlier, 8 | pairs.epplab, 11 |
| REPPlab-package, 2 | plot, epplab-method (plot.epplab), 12 |
| WhitenSVD, 20 | plot,epplabOutlier-method |
| * print | (plot.epplabOutlier), 13 |
| coef.epplab, 3 | plot-method (plot.epplab), 12 |
| fitted.epplab, 10 | plot.epplab, 12 |
| predict.epplab, 14 | plot.epplabOutlier, 13 |
| print.epplab, 15 | <pre>predict,epplab-method(predict.epplab),</pre> |
| print.epplabOutlier, 16 | 14 |
| summary.epplab, 18 | predict-method (predict.epplab), 14 |
| summary.epplabOutlier, 19 | predict.epplab, 14 |
| , , , | print, epplab-method (print.epplab), 15 |
| AOP, 7, 8 | print,epplabOutlier-method |
| 7.01, 7, 7 | (print.epplabOutlier), 16 |
| <pre>coef,epplab-method(coef.epplab), 3</pre> | print-method (print.epplab), 15 |
| coef-method (coef.epplab), 3 | print.epplab, 15 |
| coef.epplab, 3 | print.epplabOutlier, 16 |
| colMeans, 5, 21 | PoliphilityData 17 |
| | ReliabilityData, 17 |
| cov, 21 | REPPlab-package, 2 |

INDEX 23