Package 'ssMRCD'

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Type Package

Title Spatially Smoothed MRCD Estimator

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Description Estimation of the Spatially Smoothed Minimum Regularized Determinant (ssMRCD) estimator and its usage in an ssMRCD-based outlier detection method as described in Puchhammer and Filzmoser (2023) <doi:10.1080/10618600.2023.2277875> and for sparse robust PCA for multi-source data described in Puchhammer, Wilms and Filzmoser (2024) <doi:10.48550/arXiv.2407.16299>. Included are also complementary visualization and parameter tuning tools.

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align_PC

Description

Aligns loadings per neighborhood for better visualization and comparison. Different options are available.

Usage

align_PC(PC, N, p, type = "largest", vec = NULL)

Arguments

PC	matrix of loadings of size Np x k
Ν	integer, number of groups/neighborhoods
р	integer, number of variables
type	<pre>character indicating how loadings are aligned (see details), options are "largest", "maxvar", "nonzero", "mean", "scalar", "none".</pre>
vec	NULL or vector containing vectors for type "scalar"

Details

For input type possible values are "largest", "maxvar", "nonzero", "mean", "scalar". For option "maxvar" the variable with the highest absolute value in the loading is scaled to be positive (per neighborhood, per loading). For option "nonzero" the variable with largest distance to zero in the entries is scaled to be positive (per neighborhood, per loading). For option "scalar" the variable is scaled in a way, that the scalar product between the loading and the respective part of vec is positive (per neighborhood, per loading). If vec is of size p times k, the same vector is used for all neighborhoods. Option "mean" is option "scalar" with vec being the mean of the loadings per variable across neighborhoods. Option "largest" scales the largest absolute value to be positive per neighborhood and per PC. Option "none" does nothing and returns PC.

Value

Returns a matrix of loadings of size Np times k.

biplot.PCAloc

Description

Biplot for PCAloc

Usage

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

Arguments

х	object of class PCAloc.
	other input arguments, see details.

Details

Additional parameters that can be given to the function are:

shape	point shape
size	point size
alpha	transparency
color	either "variable" or "groups" indication how points should be coloured.

Value

Returns version of biplot for PCAloc object.

```
# set seed
set.seed(236)
# make data
data = matrix(rnorm(2000), ncol = 4)
groups = sample(1:10, 500, replace = TRUE)
W = time_weights(N = 10, c(3,2,1))
# calculate covariance matrices
covs = ssMRCD(data, groups = groups, weights = W, lambda = 0.3)
```

contamination_random

contamination_random Contamination Through Swapping

Description

This function swaps observations completely random in order to introduce contamination in the data. Used in parameter_tuning.

Usage

contamination_random(cont, data)

Arguments

cont	numeric, amount of contamination in data.
data	data whose observations should be switched.

Value

A matrix with switched observations.

```
# set seed
set.seed(1)
# get data
data(weatherAUT2021)
# switch 5% of observations
contamination_random(cont = 0.05, data = weatherAUT2021[,1:6])
```

eval_objective

Description

Objective function value for local sparse PCA

Usage

eval_objective(PC, eta, gamma, COVS)

Arguments

PC	vectorised component to evaluate.
eta	degree of sparsity.
gamma	distribution of sparsity between groupwise ($\gamma=1)$ and entrywise ($\gamma=0)$ sparsity.
COVS	list of covariance matrices used for PCA

Value

Returns value of the objective function for given v.

Examples

explained_var Explained Variance summarized over Groups

Description

Explained Variance summarized over Groups

Usage

```
explained_var(COVS, PC, k, type = "scaled", cor = FALSE, gamma = 0.5)
```

geo_weights

Arguments

COVS	list of covariance matrices
PC	matrix-like object holding the loadings of length np
k	which component should be evaluated
type	character, either "scaled" for scaling using the extremes solutions or "percent" as percentage of overall variance.
cor	logical, if COVS is a correlation matrix or not
gamma	scalar between 0 and 1 indicatig distribution of sparsity.

Value

Returns scalar

Examples

```
S1 = matrix(c(1, 0.9, 0.8, 0.5,
              0.9, 1.1, 0.7, 0.4,
              0.8, 0.7, 1.5, 0.2,
              0.5, 0.4, 0.2, 1), ncol = 4)
S2 = t(S1)%*% S1
S2 = S2/2
explained_var(COVS = list(S1, S2),
              PC = c(1,0,0,0,sqrt(2),0,0,-sqrt(2)),
              k = 1,
              cor = FALSE,
              gamma = 0.5)
explained_var(COVS = list(cov2cor(S1), cov2cor(S2)),
              PC = c(1,0,0,0,sqrt(2),0,0,-sqrt(2)),
              k = 1,
              cor = TRUE,
              gamma = 0.5)
```

geo.	_weights	Inver

nverse Geographic Weight Matrix

Description

Calculates a inverse-distance based weight matrix for the function ssMRCD (see details).

Usage

geo_weights(coordinates, groups)

Arguments

coordinates	matrix of coordinates of observations.
groups	vector of neighborhood groups.

Details

First, the centers (means of the coordinates given) c_i of each neighborhood is calculated. Then, the Euclidean distance between the centers is calculated and the weight is based on the inverse distance between two neighborhoods,

$$w_{ij} = \frac{1}{dist(c_i, c_j)}$$

It is scaled according to a weight matrix.

Value

Returns a weighting matrix W and the coordinates of the centers per neighborhood centersN.

See Also

rescale_weights

Examples

```
coordinates = matrix(rnorm(1000), ncol = 2, nrow = 500)
groups = sample(1:5, 500, replace = TRUE)
geo_weights(coordinates, groups)
```

groups_gridbased Creates Grid-Based Neighborhood Structure

Description

This function creates a grid-based neighborhood structure for the ssMRCD function using cut-off values for two coordinate axis.

Usage

```
groups_gridbased(x, y, cutx, cuty)
```

Arguments

х	vector of first coordinate of data set.
У	vector of second coordinate of data set.
cutx	cut-offs for first coordinate.
cuty	cut-offs for second coordinate.

Value

Returns a neighborhood assignment vector for the coordinates x and y.

Examples

local_outliers_ssMRCD Local Outlier Detection Technique based on ssMRCD

Description

This function applies the local outlier detection method based on the spatially smoothed MRCD estimator developed in Puchhammer and Filzmoser (2023).

Usage

```
local_outliers_ssMRCD(
   data,
   coords,
   groups,
   lambda,
   weights = NULL,
   k = NULL,
   dist = NULL
)
```

Arguments

data	data matrix with measured values.
coords	matrix of coordinates of observations.
groups	vector of neighborhood assignments.
lambda	scalar used for spatial smoothing (see also ssMRCD).
weights	weight matrix used in ssMRCD.
k	integer, if given the k nearest neighbors per observations are used to calculate next distances. Default value is $k = NULL$.

dist	scalar, if given the neighbors closer than given distance are used for next dis-
	tances. If dist is given, dist is used, otherwise k is used.

Value

Returns an object of class "locOuts" with following components:

outliers	indices of found outliers.
next_distance	vector of next distances for all observations.
cutoff	upper fence of adjusted boxplot (see adjbox) used as cutoff value for next distances.
coords	matrix of observation coordinates.
data	matrix of observation values.
groups	vector of neighborhood assignments.
k,dist	specifications regarding neighbor comparisons.
centersN	coordinates of centers of neighborhoods.
matneighbor	matrix storing information which observations where used to calculate next distance for each observation (j
ssMRCD	object of class "ssMRCD" and output of ssMRCD covariance estimation.

References

Puchhammer P. and Filzmoser P. (2023): Spatially smoothed robust covariance estimation for local outlier detection. doi:10.48550/arXiv.2305.05371

See Also

See also functions ssMRCD, plot.locOuts, summary.locOuts.

objective_matrix

outs

k = 10)

objective_matrix Calculation of Objective Function

Description

Calculation of the value of the objective function for the ssMRCD for a given list of matrices, lambda and a weighting matrix according to formula (3) in Puchhammer and Filzmoser (2023).

Usage

```
objective_matrix(matrix_list, lambda, weights)
```

Arguments

matrix_list	a list of matrices K_i
lambda	scalar smoothing parameter
weights	matrix of weights

Value

Returns the value of the objective function using matrices K_i .

References

Puchhammer P. and Filzmoser P. (2023): Spatially smoothed robust covariance estimation for local outlier detection. doi:10.48550/arXiv.2305.05371

```
# construct matrices
k1 = matrix(c(1,2,3,4), nrow = 2)
k2 = matrix(c(1,3,5,7), nrow = 2)
# construct weighting matrix
W = matrix(c(0, 1, 1, 0), nrow = 2)
objective_matrix(list(k1, k2), 0.5, W)
```

parameter_tuning

Description

This function provides insight into the effects of different parameter settings.

Usage

```
parameter_tuning(
    data,
    coords,
    groups,
    lambda = c(0, 0.25, 0.5, 0.75, 0.9),
    weights = NULL,
    k = NULL,
    dist = NULL,
    cont = 0.05,
    repetitions = 5
)
```

Arguments

data	matrix with observations.
coords	matrix of coordinates of these observations.
groups	numeric vector, the neighborhood structure that should be used for ssMRCD.
lambda	scalar, the smoothing parameter.
weights	weighting matrix used in ssMRCD.
k	vector of possible k-values to evaluate.
dist	vector of possible dist-values to evaluate.
cont	level of contamination, between 0 and 1.
repetitions	number of repetitions wanted to have a good picture of the best parameter com- bination.

Value

Returns a matrix of average false-negative rate (FNR) values and the total number of outliers found by the method as aproxy for the false-positive rate. Be aware that the FNR does not take into account that there are also natural outliers included in the data set that might or might not be found. Also a plot is returned representing these average. The best parameter selection depends on the goal of the analysis.

plot.locOuts

Examples

```
# get data set
data("weatherAUT2021")
# make neighborhood assignments
cut_lon = c(9:16, 18)
cut_lat = c(46, 47, 47.5, 48, 49)
N = ssMRCD::groups_gridbased(weatherAUT2021$lon, weatherAUT2021$lat, cut_lon, cut_lat)
table(N)
N[N == 2] = 1
N[N == 3] = 4
N[N == 5] = 4
N[N == 6] = 7
N[N == 11] = 15
N = as.numeric(as.factor(N))
# tune parameters
set.seed(123)
parameter_tuning(data = weatherAUT2021[, 1:6 ],
                 coords = weatherAUT2021[, c("lon", "lat")],
                 groups = N,
                 lambda = c(0.5, 0.75),
                 k = c(10),
                 repetitions = 1)
```

plot.locOuts	Diagnostic Plots for Local Outlier Detection
--------------	--

Description

This function plots different diagnostic plots for local outlier detection. It can be applied to an object of class "locOuts" which is the output of the function local_outliers_ssMRCD.

Usage

```
## S3 method for class 'locOuts'
plot(
    x,
    type = c("hist", "spatial", "lines", "3D"),
    colour = "all",
    focus = NULL,
    pos = NULL,
    alpha = 0.3,
    data = NULL,
    add_map = TRUE,
    ...
)
```

Arguments

x	a locOuts object obtained by the function local_outliers_ssMRCD.
type	<pre>vector containing the types of plots that should be plotted, possible values c("hist", "spatial", "lines", "3D").</pre>
colour	character specifying the color scheme (see details). Possible values "all", "onlyOuts", "outScore".
focus	an integer being the index of the observation whose neighborhood should be analysed more closely.
pos	integer specifying the position of the text "cut-off" in the histogram (see par).
alpha	scalar specifying the transparency level of the points plotted for plot type "spatial", "3D" and "lines".
data	optional data frame or matrix used for plot of type "line". Will be used to plot lines based scaled data instead of the data used for local outlier detection.
add_map	TRUE if a map should be plotted along the line plot (type = "lines").
	further parameters passed on to base-R plotting functions.

Details

Regarding the parameter type the value "hist" corresponds to a plot of the histogram of the next distances together with the used cutoff-value. When using "spatial" the coordinates of each observation are plotted and colorized according to the color setting. The "lines" plot is used with the index focus of one observation whose out/inlyingness to its neighborhood should by plotted. The whole data set is scaled to the range [0,1] and the scaled value of the selected observation and its neighbors are plotted. Outliers are plotted in orange. The "3D" setting leads to a 3D-plot using the colour setting as height. The view can be adapted using the parameters theta and phi.

For the colour setting possible values are "all" (all next distances are used and colored in an orange palette), "onlyOuts" (only outliers are plotted in orange, inliers are plotted in grey) and "outScore" (the next distance divided by the cutoff value is used to colourize the points; inliers are colorized in blue, outliers in orange).

Value

Returns plots regarding next distances and spatial context.

See Also

local_outliers_ssMRCD

```
# set seed
set.seed(1)
# make locOuts object
data = matrix(rnorm(2000), ncol = 4)
coords = matrix(rnorm(1000), ncol = 2)
```

plot.PCAloc Plotting method PCAloc object

Description

Plotting method PCAloc object

Usage

```
## S3 method for class 'PCAloc'
plot(
    x,
    type = c("loadings", "screeplot", "scores", "score_distances", "biplot"),
    ...
)
```

Arguments

Х	object of class PCAloc
type	character indicating the type of plot, see details.
	further arguments passed down.

Value

Returns plots in ggplot2.

```
# set seed
set.seed(236)
# create data and setup
data = matrix(rnorm(2000), ncol = 4)
```

```
plot.ssMRCD
```

Plot Method for ssMRCD Object

Description

Plots diagnostics for function output of ssMRCD regarding convergence behavior and the resulting covariances matrices.

Usage

```
## S3 method for class 'ssMRCD'
plot(
    x,
    type = c("convergence", "ellipses"),
    centersN = NULL,
    colour_scheme = "none",
    xlim_upper = 9,
    manual_rescale = 1,
    legend = TRUE,
    xlim = NULL,
    ylim = NULL,
    ...
)
```

Arguments

х	object of class "ssMRCD".
type	type of plot, possible values are "convergence" and "ellipses". See details.

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plot.ssMRCD

for plot type "ellipses" a matrix specifying the positions of the centers of the covariance estimation centers, see also geo_weights.
coloring scheme used for plot type "ellipses", either "trace" or "regularity" or "none".
numeric giving the upper x limit for plot type "convergence".
for plot type "ellipses" numeric used to re-scale ellipse sizes.
logical, if color legend should be included.
vector of xlim (see par).
vector of ylim (see par).
further plotting parameters.

Details

For type = "convergence" a plot is produced displaying the convergence behaviour. Each line represents a different initial value used for the c-step iteration. On the x-axis the iteration step is plotted with the corresponding value of the objective function. Not monotonically lines are plotted in red.

For type = "ellipses" and more than a 2-dimensional data setting plotting the exact tolerance ellipse is not possible anymore. Instead the two eigenvectors with highest eigenvalue from the MCD used on the full data set without neighborhood assignments are taken and used as axis for the tolerance ellipses of the ssMRCD covariance estimators. The tolerance ellipse for the global MCD covariance is plotted in grey in the upper left corner. It is possible to set the colour scheme to "trace" to see the overall amount of variability and compare the plotted covariance and the real trace to see how much variance is not plotted. For "regularity" the regularization of each covariance is shown.

Value

Returns plots of the ssMRCD methodology and results.

See Also

ssMRCD, summary.ssMRCD,local_outliers_ssMRCD, plot.locOuts

```
# set seed
set.seed(1)
# create data set
data = matrix(rnorm(2000), ncol = 4)
coords = matrix(rnorm(1000), ncol = 2)
groups = sample(1:10, 500, replace = TRUE)
lambda = 0.3
```

```
# calculate ssMRCD by using the local outlier detection method
outs = local_outliers_ssMRCD(data = data,
```

```
coords = coords,
groups = groups,
lambda = lambda,
k = 10)
# plot ssMRCD object included in outs
plot(x = outs$ssMRCD,
centersN = outs$centersN,
colour_scheme = "trace",
legend = FALSE)
```

plot_loadings Plots of loadings of PCAloc object

Description

Plots of loadings of PCAloc object

Usage

plot_loadings(object, ...)

Arguments

object	object of class PCAloc
	other input arguments, see details.

Details

Additional parameters that can be given to the function are:

text	logical if values should be added as text.
size	point size.
tolerance	tolerance for rounding to zero.
k	integer, which component scores should be plotted.
groupnames	names of groups.
varnames	names of variables.
textrotate	angle of text rotation, if included.

plot_scores

Value

Returns loading heatmap for component k.

Examples

plot_scores Plots of score distribution

Description

Plots of score distribution

Usage

```
plot_scores(X, PC, groups, ssMRCD, ...)
```

Arguments

Х	data matrix.
PC	loadings from PCA.
groups	vector containing group assignments.
ssMRCD	ssMRCD object.
	other input arguments, see details.

Details

Additional parameters that can be given to the function are:

shape	point shape
size	point size
alpha	transparency
k	integer, which component scores should be plotted

Value

Returns histograms of scores for component k.

Examples

```
# set seed
set.seed(236)
data = matrix(rnorm(2000), ncol = 4)
groups = sample(1:10, 500, replace = TRUE)
W = time_weights(N = 10, c(3, 2, 1))
# calculate covariance matrices
covs = ssMRCD(data, groups = groups, weights = W, lambda = 0.3)
# sparse PCA
pca = sparsePCAloc(eta = 0.3, gamma = 0.7, cor = FALSE, COVS = covs$MRCDcov,
             n_max = 1000, increase_rho = list(TRUE, 50, 1), trace = FALSE)
# plot score distances
plot_scores(PC = pca$PC,
            groups = groups,
            X = data,
            ssMRCD = covs,
            k = 1,
            alpha = 0.4,
            shape = 16,
            size = 2)
```

plot_score_distances Distance-distance plot of scores of PCA

Description

Distance-distance plot of scores of PCA

Usage

```
plot_score_distances(X, PC, groups, ssMRCD, k, ...)
```

Arguments

Х	data matrix.
PC	loadings from PCA.
groups	vector containing group assignments.
ssMRCD	ssMRCD object.
k	integer of how many components should be used.
	other input arguments, see details.

Details

Additional parameters that can be given to the function are:

shape	point shape
size	point size
alpha	transparency

Value

Returns distance-distance plot of orthogonal and score distance.

```
# set seed
set.seed(236)
data = matrix(rnorm(2000), ncol = 4)
groups = sample(1:10, 500, replace = TRUE)
W = time_weights(N = 10, c(3,2,1))
# calculate covariance matrices
covs = ssMRCD(data, groups = groups, weights = W, lambda = 0.3)
# sparse PCA
pca = sparsePCAloc(eta = 0.3, gamma = 0.7, cor = FALSE, COVS = covs$MRCDcov,
             n_max = 1000, increase_rho = list(TRUE, 50, 1), trace = FALSE)
# plot score distances
plot_score_distances(PC = pca$PC,
                     groups = groups,
                     X = data,
                     ssMRCD = covs,
                     k = 2,
                     alpha = 0.4,
                     shape = 16,
                     size = 2)
```

rescale_weights Rescale Weight Matrix

Description

Given a matrix with values for neighborhood influences the function rescales the matrix in order to get an appropriate weight matrix used for the function ssMRCD.

Usage

rescale_weights(W)

Arguments

W

weight matrix with diagonals equal to zero and at least one positive entry per row.

Value

An appropriately scaled weight matrix.

See Also

ssMRCD, local_outliers_ssMRCD, geo_weights

Examples

residuals.ssMRCD Extracting Residuals from Local Fit

Description

Extracting Residuals from Local Fit

Usage

```
## S3 method for class 'ssMRCD'
residuals(object, ...)
```

Arguments

object	ssMRCD object, see ssMRCD.
	see details

Details

Other input variables are:

remove_outliers	logical (default FALSE). If TRUE, only residuals from not outlying observations are calculated. If FALSE
Х	matrix of new data, if data from the ssMRCD object is used.
groups	vector of groups for new data, if NULL data from the ssMRCD object is used.
mean	logical (default FALSE), specifying if mean of trimmed observations is returned or all residuals.

If X and groups are provided, alpha is set to one and all residuals are used. If remove_outliers is TRUE, alpha is set to 1 automatically.

Value

Returns either all residuals or the mean of the residual norms lower than the alpha-Quantile.

```
# create data set
x1 = matrix(runif(200), ncol = 2)
x2 = matrix(rnorm(200), ncol = 2)
x = list(x1, x2)
# create weighting matrix
W = matrix(c(0, 1, 1, 0), ncol = 2)
# calculate ssMRCD
localCovs = ssMRCD(x, weights = W, lambda = 0.5)
# residuals of model
residuals(localCovs, remove_outliers = TRUE, mean = FALSE)
# residuals of new data
residuals(localCovs,
X = matrix(rnorm(20), ncol = 2, nrow = 10),
groups = rep(2, 10),
mean =TRUE)
```

restructure_as_list Restructure Data Matrix as List

Description

This function restructures neighborhood information given by a data matrix containing all information and one neighborhood assignment vector. It returns a list of data matrices used in ssMRCD.

Usage

```
restructure_as_list(data, groups)
```

Arguments

data	data matrix with all observations.
groups	numeric neighborhood assignment vector.

Value

Returns a list containing the observations per neighborhood assignment. The list is sorted according to the order of the first appearance in the groups vector.

Examples

data matrix
data = matrix(rnorm(n = 3000), ncol = 3)
N_assign = sample(x = 1:10, size = 1000, replace = TRUE)

```
restructure_as_list(data, N_assign)
```

scale_ssMRCD Scale Data Locally

Description

Scale Data Locally

Usage

```
scale_ssMRCD(
   ssMRCD,
   X = NULL,
   groups = NULL,
   multivariate = FALSE,
   center_only = FALSE
)
```

scores

Arguments

ssMRCD	ssMRCD object, see ssMRCD
Х	matrix, new data to scale with ssMRCD estimation.
groups	vector, group assignments of new data X.
multivariate	logical, TRUE if multivariate structure should be used. Otherwise, univariate variances from the ssMRCD estimator is used.
center_only	logical, if TRUE observations are only centered.

Value

Returns matrix of observations. If X = NULL X from the ssMRCD object is used and sorted according to group numbering.

See Also

ssMRCD

Examples

```
# create data set
x1 = matrix(runif(200), ncol = 2)
x2 = matrix(rnorm(200), ncol = 2)
x = list(x1, x2)
# create weighting matrix
W = matrix(c(0, 1, 1, 0), ncol = 2)
# calculate ssMRCD
localCovs = ssMRCD(x, weights = W, lambda = 0.5)
# scale used data
scale_ssMRCD(localCovs,
     multivariate = TRUE)
# scale new data
scale_ssMRCD(localCovs,
      X = matrix(rnorm(20), ncol = 2, nrow = 10),
      groups = rep(2, 10),
     multivariate =TRUE)
```

```
scores
```

Calculate Scores for local sparse PCA

Description

Calculate Scores for local sparse PCA

Usage

scores(X, PC, groups, ssMRCD = NULL)

Arguments

Х	data set as matrix.
PC	loading matrix.
groups	vector of grouping structure (numeric).
ssMRCD	ssMRCD object used for scaling X. If NULL no scaling and centering is performed.

Value

Returns a list with scores and univariately and locally centered and scaled observations.

See Also

ssMRCD, scale_ssMRCD

Examples

scores.OD

Orthogonal Distances for PCAloc

Description

Orthogonal Distances for PCAloc

scores.SD

Usage

scores.OD(X, PC, groups, ssMRCD)

Arguments

Х	data matrix of observations.
PC	loadings of sparse local PCA.
groups	grouping vector for locality.
ssMRCD	ssMRCD object used for PCA calculation.

Value

Returns vector of orthogonal distances of observations.

See Also

scores.SD, sparsePCAloc, scale_ssMRCD

Examples

groups = rep(c(1,2), each = 100), ssMRCD = loccovs)

scores.SD

Score Distances for PCAloc

Description

Score Distances for PCAloc

Usage

scores.SD(X, PC, groups, ssMRCD)

Arguments

Х	data matrix of observations.
PC	loadings of sparse local PCA.
groups	grouping vector for locality.
ssMRCD	ssMRCD object used for PCA calculation.

Value

Returns vector of score distances of observations.

See Also

scores.OD, sparsePCAloc, scale_ssMRCD

Examples

groups = rep(c(1,2), each = 100), ssMRCD = loccovs)

screeplot.PCAloc Screeplot for PCAloc

Description

Screeplot for PCAloc

screeplot.PCAloc

Usage

S3 method for class 'PCAloc'
screeplot(x, ...)

Arguments

х	object of class PCAloc.
	other input arguments, see details.

Details

Additional parameters that can be given to the function are:

text	logical if text should be plotted
size	text size
cutoff	cutoff line for scree plot
groupnames	name of groups
textrotate	angle of text, if text is plotted.

Value

Returns version of scree plot and cumulative explained variance per group for PCAloc object.

select_smoothing

Description

The optimal smoothing value for the ssMRCD estimator is based on the residuals and the trimmed mean of the norm.

Usage

```
select_smoothing(
   X,
   groups,
   weights,
   lambda = seq(0, 1, 0.1),
   TM = NULL,
   alpha = 0.75,
   seed = 123436,
   return_all = TRUE,
   cores = 1
)
```

Arguments

Х	data matrix containing observations.
groups	grouping vector corresponding to X.
weights	weight matrix for groups, see rescale_weights, and geo_weights.
lambda	vector of parameter values for smoothing, between 0 and 1.
ТМ	target matrix, if not given MCD (or MRCD if non regular) is used with default values and alpha.
alpha	percentage of outliers to be expected.
seed	seed for ssMRCD calculations.
return_all	logical, if FALSE the function returns only the optimal lambda.
cores	integer, number of cores used for parallel computing.

Value

lambda_opt	optimal lambda for smoothing.
COVS	ssMRCD object with optimal parameter setting.
plot	plot for optimal parameter setting.
residuals	mean of norm of residuals for varying lambda.

Examples

```
# create data set
x1 = matrix(runif(200), ncol = 2)
x2 = matrix(rnorm(200), ncol = 2)
# create weighting matrix
W = matrix(c(0, 1, 1, 0), ncol = 2)
select_smoothing (X = rbind(x1, x2),
    groups = rep(c(1,2), each = 100),
    weights = W,
    lambda = seq(0, 1, 0.1),
    return_all = TRUE,
    cores = 1)
```

select_sparsity Optimal Sparsity Parameter Selection for PCA

Description

Optimal Sparsity Parameter Selection for PCA

Usage

```
select_sparsity(
 COVS,
 k = 1,
  rho = NULL,
  cor = FALSE,
 eta = seq(0, 5, by = 0.2),
  gamma = seq(0, 1, 0.05),
  eps_threshold = 0.001,
  eps_root = 0.1,
  eps_ADMM = 1e-04,
  n_{max} = 300,
  adjust_eta = FALSE,
  cores = 1,
  increase_rho = list(TRUE, 100, 1),
  convergence_plot = FALSE,
  trace = FALSE,
  stop.sparse = TRUE
)
```

Arguments

COVS	list of covariance or correlation matrices.	
k	number of components to be returned.	
rho	penalty parameter for ADMM.	
cor	logical, if starting values for covariances or correlation matrices should be used.	
eta	vector of possible values for degree of sparsity.	
gamma	vector of possible values for distribution of sparsity. If only one value is pro- vided, the optimal eta is calculated.	
eps_threshold	tolerance for thresholding.	
eps_root	tolerance for root finder.	
eps_ADMM	tolerance for ADMM iterations.	
n_max	maximal number of ADMM iterations.	
adjust_eta	if eta should be adjusted for further components.	
cores	number of cores for parallel computing.	
increase_rho	list of settings for improved automated calculation and convergence. See De- tails.	
convergence_plot		
	logical, if convergence plot should be plotted. Not applicable for cores > 1.	
trace	logical, if messages should be displayed. Not applicable for cores > 1.	
stop.sparse	calculate if AUC should be calculated for PCAs until full sparsity is reached (TRUE) or over the whole eta range (FALSE). Set to TRUE.	

Details

The input increase_rho consists of a logical indicating if rho should be adjusted if algorithm did not converged within the given maximal number of iterations. Two integers specify the maximal rho that is allowed and the step size.

Value

Returns list with

PCA	object of type PCAloc.
PC	local loadings of PCA
gamma	optimal value for gamma.
eta	optimal value for eta.
eta_tpo	values of Trade-Off-Product for eta from optimization process.
auc	area under the curve for varying gamma values.

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sparsePCAloc

parsparameters and respective sparsity entrywise and mixed and explained variance.plotggplot object for optimal parameter selection.plot_infoadditional data for plotting functions.

Examples

sparsePCAloc

Calculate Sparse Principle Components

Description

Calculate Sparse Principle Components

Usage

```
sparsePCAloc(
 eta,
  gamma,
 COVS,
  cor = FALSE,
 rho = NULL,
 k = NULL,
  eps_threshold = NULL,
  eps_ADMM = 1e-04,
  n_{max} = 200,
 eps_root = 0.1,
 maxiter_root = 50,
  increase_rho = list(TRUE, 100, 1),
  convergence_plot = TRUE,
  starting_value = NULL,
  adjust_eta = TRUE,
  trace = TRUE
)
```

Arguments

eta	numeric, degree of sparsity.
gamma	numeric, distribution of sparsity.
COVS	list of covariance or correlation matrices.
cor	logical, if starting value for correlation or covariance matrices should be used.
rho	numeric bigger than zero, penalty for ADMM.
k	number of components to calculate.
eps_threshold	tolerance for thresholding.
eps_ADMM	tolerance for ADMM convergence.
n_max	number of maximal iterations.
eps_root	tolerance for root finder.
maxiter_root	maximal number of iterations for root finder.
increase_rho	list with entries for stable convergence. See Details.
convergence_plo	ot
	logical, if convergence plot should be displayed.
starting_value	optional given starting value.
adjust_eta	logical, if eta should be adjusted by the variance.
trace	logical, if messages should be displayed.

Details

The input increase_rho consists of a logical indicating if rho should be adjusted if algorithm did not converged within the given maximal number of iterations. Two integers specify the maximal rho that is allowed and the step size.

Value

An object of class "PCAloc" containing the following elements:

PC	Matrix of dimension Np x k of stacked loading vectors.
р	Number of variables.
Ν	Number of neighborhoods.
k	Number of components.
COVS	List of covariance matrices sorted by neighborhood.
gamma	Sparsity distribution.
eta	Amount of sparsity.

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converged	Logical, if ADMM converged with given specifications.
n_steps	Number of steps used.
summary	Description of result per component.
residuals	Primary and secondary residuals.

Examples

```
C1 = diag(c(1.1, 0.9, 0.6))

C2 = matrix(c(1.1, 0.1, -0.1,

0.1, 1.0, -0.2,

-0.1, -0.2, 0.7), ncol = 3)

C3 = (C1 + C2)/2

sparsePCAloc(eta = 1, gamma = 0.5, cor = FALSE, COVS = list(C1, C2, C3),

n_max = 100, increase_rho = list(FALSE, 100, 1))
```

sparsity_entries Entry-wise Sparsity in the Loadings

Description

Entry-wise Sparsity in the Loadings

Usage

```
sparsity_entries(PC, N, p, tolerance = 0, k = 1, scaled = TRUE)
```

Arguments

PC	matrix-like object of PCs.
Ν	integer, number of groups.
р	integer, number of variables.
tolerance	tolerance for sparsity.
k	integer or integer vector of which component should be used.
scaled	logical, if total number or percentage of possible sparse entries should be re- turned.

Value

Returns either a percentage (scaled = TRUE) or the amount of zero-values entries (scaled = FALSE).

Examples

```
PC = matrix(c(1,0,2,3,0,7,0,1,0,1,0.001,0), ncol = 2)
sparsity_entries(PC, N = 2, p = 3, tolerance = 0, k = 1, scaled = FALSE)
sparsity_entries(PC, N = 2, p = 3, tolerance = 0.001, k = 2, scaled = TRUE)
```

sparsity_group Group-wise Sparsity in the Loadings

Description

Group-wise Sparsity in the Loadings

Usage

sparsity_group(PC, N, p, tolerance = 0, k = 1, scaled = TRUE)

Arguments

PC	matrix-like object of PCs.
Ν	integer, number of groups.
р	integer, number of variables.
tolerance	tolerance for sparsity.
k	integer, which components should be used. Does not work for multiple PCs simultaneously.
scaled	logical, if total number or percentage of possible sparse entries should be re- turned.

Value

Returns either a matrix of percentages (scaled = TRUE) or the amounts of zero-values entries (scaled = FALSE) for each group/neighborhood.

Examples

```
PC = matrix(c(1,0,2,3,0,7,0,1,0,1,0.001,0), ncol = 2)
sparsity_group(PC, N = 2, p = 3, tolerance = 0, k = 1, scaled = FALSE)
sparsity_group(PC, N = 2, p = 3, tolerance = 0.001, k = 2, scaled = TRUE)
```

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sparsity_mixed Mixed Sparsity of the Loadings

Description

Mixed Sparsity of the Loadings

Usage

```
sparsity_mixed(PC, p, N, k = 1, tolerance = 0.001, mean = "arithmetic")
```

Arguments

PC	matrix-like object of PCs.
р	integer, number of variables.
Ν	integer, number of groups.
k	integer, which components should be used. Does not work for multiple PCs simultaneously.
tolerance	tolerance for sparsity.
mean	if "arithmetic" or "geometric" mean should be used.

Value

Returns the geometric mean of the percentage of entry-wise and group-wise sparsity.

Examples

```
PC = matrix(c(1,0,2,3,0,7,0,1,0,1,0.001,0), ncol = 2)
sparsity_mixed(PC, N = 2, p = 3, tolerance = 0, k = 1)
sparsity_mixed(PC, N = 2, p = 3, tolerance = 0.001, k = 2, mean = "geometric")
```

sparsity in the Boundary per e	sparsity_summary	<i>Entry-wise Sparsity in the Loadings per Group</i>
--------------------------------	------------------	--

Description

Entry-wise Sparsity in the Loadings per Group

Usage

```
sparsity_summary(PC, N, p, tolerance = 0, k = 1, scaled = FALSE)
```

Arguments

PC	matrix-like object of PCs.
Ν	integer, number of groups.
р	integer, number of variables.
tolerance	tolerance for sparsity.
k	integer or integer vector of which component should be used.
scaled	logical, if total number or percentage of possible sparse entries should be re- turned.

Value

Returns either a matrix of percentages (scaled = TRUE) or the amounts of zero-values entries (scaled = FALSE) for each group/neighborhood.

Examples

```
PC = matrix(c(1,0,2,3,0,7,0,1,0,1,0.001,0), ncol = 2)
sparsity_summary(PC, N = 2, p = 3, tolerance = 0, k = 1, scaled = FALSE)
sparsity_summary(PC, N = 2, p = 3, tolerance = 0.001, k = 2, scaled = TRUE)
```

ssMRCD

Spatially Smoothed MRCD Estimator

Description

The ssMRCD function calculates the spatially smoothed MRCD estimator from Puchhammer and Filzmoser (2023).

Usage

```
ssMRCD(
    x,
    groups = NULL,
    weights,
    lambda,
    TM = NULL,
    alpha = 0.75,
    maxcond = 50,
    maxcsteps = 200,
    n_initialhsets = NULL
)
```

ssMRCD

Arguments

x	a list of matrices containing the observations per neighborhood sorted which can be obtained by the function restructure_as_list, or matrix or data frame containing data. If matrix or data.frame, group vector has to be given.
groups	vector of neighborhood assignments
weights	weighting matrix, symmetrical, rows sum up to one and diagonals need to be zero (see also geo_weights or rescale_weights .
lambda	numeric between 0 and 1.
ТМ	target matrix (optional), default value is the covMcd from robustbase.
alpha	numeric, proportion of values included, between 0.5 and 1.
maxcond	optional, maximal condition number used for rho-estimation.
maxcsteps	maximal number of c-steps before algorithm stops.
n_initialhsets	number of initial h-sets, default is 6 times number of neighborhoods.

Value

An object of class "ssMRCD" containing the following elements:

MRCDcov	List of ssMRCD-covariance matrices sorted by neighborhood.
MRCDicov	List of inverse ssMRCD-covariance matrices sorted by neighborhood.
MRCDmu	List of ssMRCD-mean vectors sorted by neighborhood.
mX	List of data matrices sorted by neighborhood.
Ν	Number of neighborhoods.
mT	Target matrix.
rho	Vector of regularization values sorted by neighborhood.
alpha	Scalar what percentage of observations should be used.
h	Vector of how many observations are used per neighborhood, sorted.
numiter	The number of iterations for the best initial h-set combination.
c_alpha	Consistency factor for normality.
weights	The weighting matrix.
lambda	Smoothing factor.
obj_fun_values	A matrix with objective function values for all initial h-set combinations (rows) and iterations (columns).

best6pack	initial h-set combinations with best objective function value after c-step iterations
Ксоч	returns MRCD-estimates without smoothing.

References

Puchhammer P. and Filzmoser P. (2023): Spatially smoothed robust covariance estimation for local outlier detection. doi:10.48550/arXiv.2305.05371

See Also

plot.ssMRCD, summary.ssMRCD, restructure_as_list

Examples

```
# create data set
x1 = matrix(runif(200), ncol = 2)
x2 = matrix(rnorm(200), ncol = 2)
x = list(x1, x2)
# create weighting matrix
W = matrix(c(0, 1, 1, 0), ncol = 2)
# calculate ssMRCD
ssMRCD(x, weights = W, lambda = 0.5)
```

summary.locOuts Summary of Local Outlier Detection

Description

Prints a summary of the locOuts object obtained by the function local_outliers_ssMRCD.

Usage

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

Arguments

object	a locOuts object.
	further parameters passed on.

Value

Prints a summary of the locOuts object.

summary.PCAloc

See Also

plot.locOuts

Examples

summary method
summary(outs)

summary.PCAloc Summary method for PCAloc

Description

Summary method for PCAloc

Usage

S3 method for class 'PCAloc'
summary(object, ...)

Arguments

object	object of class PCAloc
	other input variables.

Value

Summary for PCAloc

See Also

sparsePCAloc

Examples

```
summary(pca)
```

summary.ssMRCD Summary Method for ssMRCD Object

Description

Summarises most important information of output ssMRCD.

Usage

S3 method for class 'ssMRCD'
summary(object, ...)

Arguments

object	object of class "ssMRCD", output of ssMRCD.
	further parameters.

Value

Prints a summary of the ssMRCD object.

See Also

See also ssMRCD, plot.ssMRCD.

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time_weights

Description

Band weight matrix for time series groupings

Usage

```
time_weights(N, off_diag)
```

Arguments

Ν	number of groups.
off_diag	vector for off-diagonal values unequal to zero.

Value

Returns weight matrix for time series groups appropriate for ssMRCD.

See Also

geo_weights, rescale_weights

Examples

time_weights(N = 10, off_diag = c(2,1))

weatherAUT2021 Austrian Weather Data 2021

Description

This data is a subset of the GeoSphere Austria monthly weather data of 2021 averaged using the median. Stations with missing values are removed.

Usage

weatherAUT2021

A data frame with 183 rows and 10 columns:

name Unique name of the weather station in German.

lon, lat Longitude and latitude of the weather station.

alt Altitude of the weather station (meter).

- **p** Average air pressure (hPa).
- s Monthly sum of sunshine duration (hours).
- vv Wind velocity (meter/second).

t Air temperature in 2 meters above the ground in (°C).

rsum Average daily sum of precipitation (mm).

rel Relative air humidity (percent).

Source

The original data was downloaded here (December 2022): https://data.hub.geosphere.at/ dataset/klima-v1-1m.

References

Data Source: GeoSphere Austria - https://data.hub.geosphere.at.

Examples

```
data(weatherAUT2021)
summary(weatherAUT2021)
```

weatherHoheWarte Vienna Weather Time Series (1960-2023)

Description

This data is a subset of the GeoSphere Austria daily weather data of the time 1960-2023 for the weather station Hohe Warte in Vienna.

Usage

weatherHoheWarte

Format

A data frame with 23372 rows and 18 columns including 13 weather measurements:

time Time of measurement in date format.

cloud_cover Daily mean of cloud coverage, values between 1 and 100.

global_radiation Daily sum of global radiation (J/cm^2).

vapor_pressure Daily mean of vapour pressuer (hPa).

max_wind_speed Maximal wind speed (m/s).

air_pressure Daily mean of air pressure (hPa).

relative_humidity Daily mean of relative humidity (percent).

precipitation Daily sum of precepitation (mm).

sight Sight distance at 1pm (m).

sunshine_duration Daily sum of sunshine duration (h).

temperature_max Daily maximum of temperature at 2m air height (°C).

temperature_min Daily minimum of temperature at 2m air height (°C).

temperature_mean Daily mean of temperature at 2m air height (°C).

wind_velocity Daily mean of wind speed (m/s).

year Year of measurement.

month Month of measurement.

day Day of the year of measurement.

season Season of measuremen (1 = winter, 2 = spring, 3 = summer, 4 = fall).

Source

The original data was downloaded here (April 2024): https://data.hub.geosphere.at/dataset/klima-v2-1d.

References

Data Source: GeoSphere Austria - https://data.hub.geosphere.at.

```
data(weatherHoheWarte)
summary(weatherHoheWarte)
```

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