# Package 'ssMRCD'

July 23, 2025

Type Package

Title Spatially Smoothed MRCD Estimator

Version 1.1.0

Maintainer Patricia Puchhammer <patricia.puchhammer@tuwien.ac.at>

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.

License GPL-3

**Encoding UTF-8** 

LazyData true

Imports stats, grDevices, graphics, robustbase, scales, car, dbscan, plot3D, dplyr, ggplot2, expm, foreach, doParallel, rrcov, DescTools, rootSolve, parallel, Matrix, reshape2

RoxygenNote 7.2.3

**Suggests** knitr, rmarkdown, testthat (>= 3.0.0)

Config/testthat/edition 3

**Depends** R (>= 4.0.0)

VignetteBuilder knitr

NeedsCompilation no

**Author** Patricia Puchhammer [aut, cre, cph], Peter Filzmoser [aut]

Repository CRAN

**Date/Publication** 2024-08-23 11:10:02 UTC

2 Contents

# **Contents**

Index

align_PC	3
biplot.PCAloc	4
contamination_random	5
eval_objective	6
explained_var	6
geo_weights	7
groups_gridbased	8
local_outliers_ssMRCD	9
3 —	11
- E	12
<u>.</u>	13
plot.PCAloc	15
plot.ssMRCD	16
plot_loadings	18
plot_scores	19
plot_score_distances	20
rescale_weights	22
	22
restructure_as_list	24
<del>-</del>	24
scores	25
scores.OD	26
scores.SD	27
screeplot.PCAloc	28
select_smoothing	30
select_sparsity	31
	33
	35
sparsity_group	36
sparsity_mixed	37
sparsity_summary	37
ssMRCD	38
summary.locOuts	40
summary.PCAloc	41
summary.ssMRCD	42
time_weights	43
weatherAUT2021	43
weatherHoheWarte	44

**46** 

align\_PC 3

align_PC	Align Loadings of Principal Components	

## 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
N	integer, number of groups/neighborhoods
p	integer, number of variables
type	character indicating how loadings are aligned (see details), options are "largest", "maxvar", "nonzero", "mean", "scalar", "none".
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

biplot.PCAloc

Biplot for PCAloc

## Description

Biplot for PCAloc

## Usage

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

## **Arguments**

x 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 5

## **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 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])
```

6 explained\_var

eval\_objective

Objective function value for local sparse PCA

## **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

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

geo\_weights 7

## **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

Inverse Geographic Weight Matrix

## Description

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

```
geo_weights(coordinates, groups)
```

8 groups\_gridbased

## **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**

vector of first coordinate of data set.
 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**

## **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 distances. 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. vector of next distances for all observations. next\_distance 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. coordinates of centers of neighborhoods. centersN matneighbor matrix storing information which observations where used to calculate next distance for each observation ( object of class "ssMRCD" and output of ssMRCD covariance estimation. ssMRCD

### 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 11

k = 10)

outs

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)
```

12 parameter\_tuning

parameter\_tuning

Optimal Smoothing Parameter for ssMRCD based on Local Outliers

## 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 13

#### **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)
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.

```
## 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,
    ...
)
```

14 plot.locOuts

#### Arguments

X	a locOuts object obtained by the function local_outliers_ssMRCD.	
type	vector containing the types of plots that should be plotted, possible values $c("hist", "spatial", "lines", "3D")$ .	
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 15

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

```
x object of class PCAloctype 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)
```

16 plot.ssMRCD

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**

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

plot.ssMRCD 17

for plot type "ellipses" a matrix specifying the positions of the centers of the centersN covariance estimation centers, see also geo\_weights. coloring scheme used for plot type "ellipses", either "trace" or "regularity" colour\_scheme or "none". xlim\_upper numeric giving the upper x limit for plot type "convergence". manual\_rescale for plot type "ellipses" numeric used to re-scale ellipse sizes. legend logical, if color legend should be included. xlim vector of xlim (see par). vlim 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 variabilty 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,
```

18 plot\_loadings

plot\_loadings

Plots of loadings of PCAloc object

## Description

Plots of loadings of PCAloc object

#### Usage

```
plot_loadings(object, ...)
```

## **Arguments**

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 19

## 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

X data matrix.

PC loadings from PCA.

groups vector containing group assignments.

ssMRCD object.

... other input arguments, see details.

## **Details**

Additional parameters that can be given to the function are:

20 plot\_score\_distances

```
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)
```

## Description

Distance-distance plot of scores of PCA

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

plot\_score\_distances 21

## **Arguments**

Χ	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)
```

22 residuals.ssMRCD

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

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

residuals.ssMRCD 23

#### **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

X 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)
```

24 scale\_ssMRCD

#### **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 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

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

scores 25

#### **Arguments**

ssMRCD object, see ssMRCD

X 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

26 scores.OD

#### Usage

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

## **Arguments**

X 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 per-

formed.

#### 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 27

## Usage

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

## **Arguments**

X 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, scores.SD, sparsePCAloc, scale_ssMRCD
```

## **Examples**

scores.SD

Score Distances for PCAloc

## **Description**

Score Distances for PCAloc

28 screeplot.PCAloc

#### Usage

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

## **Arguments**

X data matrix of observations.

PC loadings of sparse local PCA.

groups grouping vector for locality.

ssMRCD object used for PCA calculation.

#### Value

Returns vector of score distances of observations.

#### See Also

```
scores, scores.OD, sparsePCAloc, scale_ssMRCD
```

## **Examples**

screeplot.PCAloc

Screeplot for PCAloc

## **Description**

Screeplot for PCAloc

screeplot.PCAloc 29

## Usage

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

### **Arguments**

x 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.

30 select\_smoothing

select\_smoothing

Optimal Smoothing Parameter for ssMRCD based on Residuals

### 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**

Χ data matrix containing observations. grouping vector corresponding to X. groups weights weight matrix for groups, see rescale\_weights, and geo\_weights. lambda vector of parameter values for smoothing, between 0 and 1. target matrix, if not given MCD (or MRCD if non regular) is used with default TM 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. integer, number of cores used for parallel computing. cores

#### 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.

select\_sparsity 31

## **Examples**

select\_sparsity

Optimal Sparsity Parameter Selection for PCA

## **Description**

Optimal Sparsity Parameter Selection for PCA

```
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
)
```

32 select\_sparsity

#### **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.

sparsePCAloc 33

```
pars parameters and respective sparsity entrywise and mixed and explained variance.

plot ggplot object for optimal parameter selection.

plot_info additional data for plotting functions.
```

## **Examples**

sparsePCAloc

Calculate Sparse Principle Components

## Description

Calculate Sparse Principle Components

```
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
)
```

34 sparsePCAloc

#### **Arguments**

n\_max

eta numeric, degree of sparsity. numeric, distribution of sparsity. gamma

COVS list of covariance or correlation matrices.

cor logical, if starting value for correlation or covariance matrices should be used.

numeric bigger than zero, penalty for ADMM. rho

number of components to calculate.

tolerance for thresholding. eps\_threshold

eps\_ADMM tolerance for ADMM convergence. number of maximal iterations.

tolerance for root finder. eps\_root

maximal number of iterations for root finder. maxiter\_root

increase\_rho list with entries for stable convergence. See Details.

convergence\_plot

logical, if convergence plot should be displayed.

starting\_value optional given starting value.

logical, if eta should be adjusted by the variance. adjust\_eta

logical, if messages should be displayed. trace

#### **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.

Number of variables. р

Number of neighborhoods. Ν

Number of components. k

COVS List of covariance matrices sorted by neighborhood.

Sparsity distribution. gamma

Amount of sparsity. eta

sparsity\_entries 35

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**

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.

N integer, number of groups.

p 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).

36 sparsity\_group

### **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.

N integer, number of groups.

p 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 returned.

#### Value

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

```
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)
```

sparsity\_mixed 37

sparsity_mixed	Mixed S

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.

p integer, number of variables.

N integer, number of groups.

k integer, which components should be used. Does not work for multiple PCs

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\_summary

Entry-wise Sparsity in the Loadings per Group

## **Description**

Entry-wise Sparsity in the Loadings per Group

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

38 ssMRCD

## Arguments

PC matrix-like object of PCs.

N integer, number of groups.

p 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).

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

ssMRCD 39

#### **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.

TM 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.

N 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).

40 summary.locOuts

best6pack Kcov initial h-set combinations with best objective function value after c-step iterations. 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 41

#### See Also

```
plot.locOuts
```

## **Examples**

summary.PCAloc

Summary method for PCAloc

## Description

Summary method for PCAloc

## Usage

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

## **Arguments**

```
object of class PCAloc other input variables.
```

## Value

Summary for PCAloc

## See Also

```
sparsePCAloc
```

42 summary.ssMRCD

#### **Examples**

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

### Value

Prints a summary of the ssMRCD object.

## See Also

```
See also ssMRCD, plot.ssMRCD.
```

time\_weights 43

time\_weights

Band weight matrix for time series groupings

## Description

Band weight matrix for time series groupings

## Usage

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

## Arguments

N 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

44 weatherHoheWarte

#### **Format**

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

weatherHoheWarte 45

#### **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<sup>2</sup>).
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)
```

# **Index**

```
* datasets
                                                  sparsePCAloc, 27, 28, 33, 41
    weatherAUT2021, 43
                                                  sparsity_entries, 35
    weatherHoheWarte, 44
                                                  sparsity_group, 36
                                                  sparsity_mixed, 37
adjbox, 10
                                                  sparsity_summary, 37
align_PC, 3
                                                  ssMRCD, 7-12, 16, 17, 22-26, 38, 42, 43
                                                  summary.locOuts, 10, 40
biplot.PCAloc, 4
                                                  summary.PCAloc, 41
                                                  summary.ssMRCD, 17, 40, 42
contamination_random, 5
                                                  time_weights, 43
eval_objective, 6
explained_var, 6
                                                  weatherAUT2021, 43
                                                  weatherHoheWarte, 44
geo_weights, 7, 17, 22, 30, 39, 43
groups_gridbased, 8
local_outliers_ssMRCD, 9, 13, 14, 17, 22, 40
objective_matrix, 11
par, 14, 17
parameter_tuning, 5, 12
plot.loc0uts, 10, 13, 17, 41
plot.PCAloc, 15
plot.ssMRCD, 16, 40, 42
plot_loadings, 18
plot_score_distances, 20
plot_scores, 19
rescale_weights, 8, 22, 30, 39, 43
residuals.ssMRCD, 22
restructure_as_list, 24, 39, 40
scale_ssMRCD, 24, 26-28
scores, 25, 27, 28
scores.OD, 26, 28
scores. SD, 27, 27
screeplot.PCAloc, 28
select_smoothing, 30
select_sparsity, 31
```