# Package 'stops'

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Title Structure Optimized Proximity Scaling

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**Description** Methods that use flexible variants of multidimensional scaling (MDS) which incorporate parametric nonlinear distance transformations and trade-off the goodness-of-fit fit with structure considerations to find optimal hyperparameters, also known as structure optimized proximity scaling (STOPS) (Rusch, Mair & Hornik, 2023, <doi:10.1007/s11222-022-10197w>). The package contains various functions, wrappers, methods and classes for fitting, plotting and displaying different 1-way MDS models with ratio, interval, ordinal optimal scaling in a STOPS framework. These cover essentially the functionality of the package smacofx, including Torgerson (classical) scaling with power transformations of dissimilarities, SMA-COF MDS with powers of dissimilarities, Sammon mapping with powers of dissimilarities, elastic scaling with powers of dissimilarities, spherical SMACOF with powers of dissimilarities, (ALSCAL) s-stress MDS with powers of dissimilarities, r-stress MDS, MDS with powers of dissimilarities and configuration distances, elastic scaling powers of dissimilarities and configuration distances, Sammon mapping powers of dissimilarities and configuration distances, power stress MDS (POST-MDS), approximate power stress, Box-Cox MDS, local MDS, Isomap, curvilinear component analysis (CLCA), curvilinear distance analysis (CLDA) and sparsified (power) multidimensional scaling and (power) multidimensional distance analysis (experimental models from smacofx influenced by CLCA). All of these models can also be fit by optimizing over hyperparameters based on goodness-offit fit only (i.e., no structure considerations). The package further contains functions for optimization, specifically the adaptive Luus-Jaakola algorithm and a wrapper for Bayesian optimization with treed Gaussian process with jumps to linear models, and functions for various cstructuredness indices.

**Depends** R (>= 3.5.0), smacofx

**Imports** acepack, clue, cmaes, cordillera, dfoptim, DiceOptim, DiceKriging, energy, minerva, nloptr, pomp, pso, registry, scagnostics, smacof, tgp, vegan

Enhances stats
Suggests R.rsp

License GPL-2 | GPL-3

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2 Contents

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 ${\tt BankingCrisesDistances}$ 

Banking Crises Distances

# Description

Matrix of Jaccard distances between 70 countries (Hungary and Greece were combined to be the same observation) based on their binary time series of having had a banking crises in a year from 1800 to 2010 or not. See data(bankingCrises) in package Ecdat for more info. The last column is Reinhart & Rogoffs classification as a low (3), middle- (2) or high-income country (1).

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#### **Format**

A 69 x 70 matrix.

#### Source

data(bankingCrises) in library(Ecdat)

biplotmds.stops

S3 method for stops objects

### **Description**

S3 method for stops objects

#### Usage

```
## S3 method for class 'stops'
biplotmds(object, extvar, scale = TRUE)
```

#### **Arguments**

object An object of class stops

extvar Data frame with external variables.

scale if 'TRUE' external variables are standardized internally.

#### **Details**

If a model for individual differences is provided, the external variables are regressed on the group stimulus space configurations. For objects returned from 'biplotmds' we use the plot method in biplotmds. In the biplot called with plot() only the relative length of the vectors and their direction matters. Using the vecscale argument in plot() the user can control for the relative length of the vectors. If 'vecscale = NULL', the 'vecscale()' function from the 'candisc' package is used which tries to automatically calculate the scale factor so that the vectors approximately fill the same space as the configuration. In this method vecscale should usually be smaller than the one used in smacof by a factor of 0.1.

#### Value

Returns an object belonging to classes 'mlm' and 'mdsbi'. See 'lm' for details. R2vec: Vector containing the R2 values. See also biplotmds for the plot method.

bootmds.stops 5

bootmds.stops MDS Bootstrap for stops objects

### **Description**

Performs a bootstrap on an MDS solution. It works for derived dissimilarities only, i.e. generated by the call dist(data). The original data matrix needs to be provided, as well as the type of dissimilarity measure used to compute the input dissimilarities (note we cannot as of yet have any dissimilarity matrix).

### Usage

```
## S3 method for class 'stops'
bootmds(
   object,
   data,
   method.dat = "pearson",
   nrep = 100,
   alpha = 0.05,
   verbose = FALSE,
   ...
)
```

# **Arguments**

object Object of class stops or pcops.

data Initial data (before dissimilarity computation).

method.dat Dissimilarity computation used as MDS input. This must be one of "pearson", "spearman", "kendall", "euclidean", "maximum", "manhattan", "canberra", "binary".

nrep Number of bootstrap replications.

alpha Alpha level for condfidence ellipsoids.

verbose If 'TRUE', bootstrap index is printed out.

Additional arguments needed for dissimilarity computation as specified in sim2diss.

#### **Details**

In order to examine the stability solution of an MDS, a bootstrap on the raw data can be performed. This results in confidence ellipses in the configuration plot. The ellipses are returned as list which allows users to produce (and further customize) the plot by hand. See bootmds for more.

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#### Value

An object of class 'smacofboot', see bootmds. With values

- cov: Covariances for ellipse computation
- bootconf: Configurations bootstrap samples
- stressvec: Bootstrap stress values
- bootci: Stress bootstrap percentile confidence interval
- spp: Stress per point (based on stress.en)
- stab: Stability coefficient

#### **Examples**

```
dats <- na.omit(PVQ40[,1:5])
diss <- dist(t(dats))  ## Euclidean distances
fit <- stops(diss,loss="rstress",itmax=5,lower=0.2,upper=3)
set.seed(123)
resboot <- bootmds(fit, dats, method.dat = "euclidean", nrep = 2)
resboot</pre>
```

coef.stops

S3 coef method for stops objects

### **Description**

S3 coef method for stops objects

### Usage

```
## S3 method for class 'stops'
coef(object, ...)
```

# **Arguments**

```
object object of class stops
... addditional arguments
```

# Value

```
a vector of hyperparmeters theta
```

c\_association 7

c_association	c-association calculates the c-association based on the maximal information coefficient We define c-association as the aggregated association between any two columns in confe
	tion between any two columns in confs

# Description

c-association calculates the c-association based on the maximal information coefficient We define c-association as the aggregated association between any two columns in confs

# Usage

```
c_association(
  confs,
  aggr = NULL,
  alpha = 0.6,
  C = 15,
  var.thr = 1e-05,
  zeta = NULL
)
```

# Arguments

confs	a numeric matrix or data frame
aggr	the aggregation function for configurations of more than two dimensions. Defaults to max.
alpha	an optional number of cells allowed in the X-by-Y search-grid. Default value is $0.6$
С	an optional number determining the starting point of the X-by-Y search-grid. When trying to partition the x-axis into X columns, the algorithm will start with at most C X clumps. Default value is 15.
var.thr	minimum value allowed for the variance of the input variables, since mine can not be computed in case of variance close to 0. Default value is 1e-5.
zeta	integer in [0,1] (?). If NULL (default) it is set to 1-MIC. It can be set to zero for noiseless functions, but the default choice is the most appropriate parametrization for general cases (as stated in Reshef et al). It provides robustness.

### Value

a numeric value; association (aggregated maximal information coefficient MIC, see mine)

# **Examples**

```
x<-seq(-3,3,length.out=200)
y<-sqrt(3^2-x^2)
z<- sin(y-x)</pre>
```

8 *c\_clusteredness* 

```
confs<-cbind(x,y,z)
c_association(confs)</pre>
```

c\_clumpiness

c-clumpiness

# Description

Measures the c-clumpiness structure

# Usage

```
c_clumpiness(conf, aggr = NULL)
```

# Arguments

conf A numeric matrix.

aggr the aggregation function for configurations of more than two dimensions. De-

faults to max.

#### Value

```
a numeric value; clumpiness (see scagnostics)
```

# **Examples**

```
delts<-smacof::kinshipdelta
conf<-smacof::smacofSym(delts)$conf
plot(conf,pch=19,asp=1)
c_clumpiness(conf)</pre>
```

c\_clusteredness

c-clusteredness calculates c-clusteredness as the OPTICS cordillera.

The higher the more clustered.

# Description

c-clusteredness calculates c-clusteredness as the OPTICS cordillera. The higher the more clustered.

c\_clusteredness 9

#### Usage

```
c_clusteredness(
  confs,
  voidarg = NULL,
  minpts = 2,
  q = 2,
  epsilon = 2 * max(dist(confs)),
  distmeth = "euclidean",
  dmax = NULL,
  digits = 10,
  scale = 0,
  ...
)
```

#### Arguments

confs a numeric matrix or a dist object

voidarg a placeholder to allow to pass NULL as strucpar and not interfere with the other

arguments

minpts The minimum number of points that must make up a cluster in OPTICS (cor-

responds to k in the paper). It is passed to optics where it is called minPts.

Defaults to 2.

The norm used for the Cordillera. Defaults to 2.

epsilon The epsilon parameter for OPTICS (called epsilon\_max in the paper). Defaults

to 2 times the maximum distance between any two points.

distmeth The distance to be computed if X is not a symmetric matrix or a dist object

(otherwise ignored). Defaults to Euclidean distance.

dmax The winsorization value for the highest allowed reachability. If used for com-

parisons between different configurations this should be supplied. If no value is supplied, it is NULL (default); then dmax is taken from the data as the either

epsilon or the largest reachability, whatever is smaller.

digits The precision to round the raw Cordillera and the norm factor. Defaults to 10.

scale Should X be scaled if it is an asymmetric matrix or data frame? Can take values

TRUE or FALSE or a numeric value. If TRUE or 1, standardisation is to mean=0 and sd=1. If 2, no centering is applied and scaling of each column is done with the root mean square of each column. If 3, no centering is applied and scaling of all columns is done as X/max(standard deviation(allcolumns)). If 4, no centering is applied and scaling of all columns is done as X/max(rmsq(allcolumns)). If FALSE, 0 or any other numeric value, no standardisation is applied. Defaults to

0.

.. Additional arguments to be passed to cordillera::cordillera

#### Value

a numeric value; clusteredness (see cordillera)

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#### **Examples**

```
delts<-smacof::kinshipdelta
dis<-smacofSym(delts)$confdist
c_clusteredness(dis,minpts=3)</pre>
```

c\_complexity

c-complexity Calculates the c-complexity based on the minimum cell number. We define c-complexity as the aggregated minimum cell number between any two columns in confs. This is one of few c-structuredness indices not between 0 and 1, but can be between 0 and (theoretically) infinity

### **Description**

c-complexity Calculates the c-complexity based on the minimum cell number We define c-complexity as the aggregated minimum cell number between any two columns in confs This is one of few c-structuredness indices not between 0 and 1, but can be between 0 and (theoretically) infinity

### Usage

```
c_complexity(
  confs,
  aggr = NULL,
  alpha = 1,
  C = 15,
  var.thr = 1e-05,
  zeta = NULL
)
```

### **Arguments**

a numeric matrix or data frame
the aggregation function for configurations of more than two dimensions. Defaults to min.
an optional number of cells allowed in the X-by-Y search-grid. Default value is 1
an optional number determining the starting point of the X-by-Y search-grid. When trying to partition the x-axis into X columns, the algorithm will start with at most C X clumps. Default value is 15.
minimum value allowed for the variance of the input variables, since mine can not be computed in case of variance close to 0. Default value is 1e-5.
integer in $[0,1]$ (?). If NULL (default) it is set to 1-MIC. It can be set to zero for noiseless functions, but the default choice is the most appropriate parametrization for general cases (as stated in Reshef et al.). It provides robustness.

c\_convexity 11

### Value

a numeric value; complexity (aggregated minimum cell number MCN, see mine)

# **Examples**

```
x<-seq(-3,3,length.out=200)
y<-sqrt(3^2-x^2)
z<- sin(y-x)
confs<-cbind(x,y,z)
c_complexity(confs)</pre>
```

c\_convexity

c-convexity

# Description

Measures the c-convexity structure

### Usage

```
c_convexity(conf, aggr = NULL)
```

# Arguments

conf A numeric matrix.

aggr the aggregation function for configurations of more than two dimensions. De-

faults to max.

### Value

```
a numeric value; convexity (see scagnostics)
```

# **Examples**

```
delts<-smacof::kinshipdelta
conf<-smacof::smacofSym(delts)$conf
plot(conf,pch=19,asp=1)
c_convexity(conf)</pre>
```

12 c\_faithfulness

c_dependence	c-dependence calculates c-dependence as the aggregated distance correlation of each pair if nonidentical columns
	corretation of each pair if nontactifical columns

# **Description**

c-dependence calculates c-dependence as the aggregated distance correlation of each pair if non-identical columns

#### Usage

```
c_dependence(confs, aggr = NULL, index = 1)
```

### **Arguments**

confs a numeric matrix or data frame

aggr the aggregation function for configurations of more than two dimensions. De-

faults to max.

index exponent on Euclidean distance, in (0,2]

#### Value

a numeric value; dependence (aggregated distance correlation)

#### **Examples**

```
x<-1:10
y<-2+3*x+rnorm(10)
confs<-cbind(x,y)
c_dependence(confs,1.5)</pre>
```

c\_faithfulness

c-faithfulness calculates the c-faithfulness based on the index by Chen and Buja 2013 (M\_adj) with equal input neigbourhoods

# Description

c-faithfulness calculates the c-faithfulness based on the index by Chen and Buja 2013 ( $M_adj$ ) with equal input neigbourhoods

# Usage

```
c_faithfulness(confs, obsdiss, k = 3, ...)
```

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### **Arguments**

confs a numeric matrix or a dist object

obsdiss a symmetric numeric matrix or a dist object. Must be supplied.

k the number of nearest neighbours to be looked at

... additional arguments passed to dist()

#### Value

a numeric value; faithfulness

### **Examples**

```
delts<-smacof::kinshipdelta
dis<-smacofSym(delts)$confdist
c_faithfulness(dis,obsdiss=delts,k=3)</pre>
```

c\_functionality

c-functionality calculates the c-functionality based on the maximum edge value We define c-functionality as the aggregated functionality between any two columns of confs

# Description

c-functionality calculates the c-functionality based on the maximum edge value We define c-functionality as the aggregated functionality between any two columns of confs

### Usage

```
c_functionality(
  confs,
  aggr = NULL,
  alpha = 1,
  C = 15,
  var.thr = 1e-05,
  zeta = NULL
)
```

#### **Arguments**

confs a numeric matrix or data frame

aggr the aggregation function for configurations of more than two dimensions. De-

faults to mean

alpha an optional number of cells allowed in the X-by-Y search-grid. Default value is

1

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С	an optional number determining the starting point of the X-by-Y search-grid. When trying to partition the x-axis into X columns, the algorithm will start with at most C X clumps. Default value is 15.
var.thr	minimum value allowed for the variance of the input variables, since mine can not be computed in case of variance close to 0. Default value is 1e-5.
zeta	integer in [0,1] (?). If NULL (default) it is set to 1-MIC. It can be set to zero for noiseless functions, but the default choice is the most appropriate parametriza-

# tion for general cases (as stated in Reshef et al.). It provides robustness.

#### Value

a numeric value; functionality (aggregated maximaum edge value MEV, see mine)

#### **Examples**

```
x<-seq(-3,3,length.out=200)
y<-sqrt(3^2-x^2)
z<- sin(y-x)
confs<-cbind(x,y,z)
c_functionality(confs)</pre>
```

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C	H	1	ᆫ	ıa	1	L	ı	v	

c-hierarchy captures how well a partition/ultrametric (obtained by hclust) explains the configuration distances. Uses variance explained for euclidean distances and deviance explained for everything else.

### **Description**

c-hierarchy captures how well a partition/ultrametric (obtained by helust) explains the configuration distances. Uses variance explained for euclidean distances and deviance explained for everything else.

# Usage

```
c_hierarchy(confs, voidarg = NULL, p = 2, agglmethod = "complete")
```

#### **Arguments**

confs a numeric matrix

voidarg a placeholder to allow to pass NULL as strucpar and not interfere with the other

arguments

p the parameter of the Minokwski distances (p=2 euclidean and p=1 is manhattan)

agglmethod the method used for creating the clustering, see hclust.

#### Value

```
a numeric value; hierarchy (see cl_validity)
```

c\_inequality 15

#### **Examples**

```
delts<-smacof::kinshipdelta
conf<-smacofSym(delts)$conf
c_hierarchy(conf,p=2,agglmethod="single")</pre>
```

c\_inequality

c-inequality Calculates c-inequality (as in an economic measure of inequality) as Pearsons coefficient of variation of the fitted distance matrix. This can help with avoiding degenerate solutions. This is one of few c-structuredness indices not between 0 and 1, but 0 and infinity.

### **Description**

c-inequality Calculates c-inequality (as in an economic measure of inequality) as Pearsons coefficient of variation of the fitted distance matrix. This can help with avoiding degenerate solutions. This is one of few c-structuredness indices not between 0 and 1, but 0 and infinity.

#### Usage

```
c_inequality(confs, ...)
```

#### **Arguments**

confs a numeric matrix or data frame
... additional arguments (don't do anything)

#### Value

a numeric value; inequality (Pearsons coefficient of variation of the fitted distance matrix)

# Examples

```
x<-1:10
y<-2+3*x+rnorm(10)
z<- sin(y-x)
confs<-cbind(z,y,x)
c_inequality(confs)</pre>
```

16 c\_manifoldness

c_linearity	c-linearity calculates c-linearity as the aggregated multiple correla-
	tion of all columns of the configuration.

### **Description**

c-linearity calculates c-linearity as the aggregated multiple correlation of all columns of the configuration.

#### Usage

```
c_linearity(confs, aggr = NULL)
```

#### **Arguments**

confs a numeric matrix or data frame

aggr the aggregation function for configurations of more than two dimensions. De-

faults to max.

#### Value

a numeric value; linearity (aggregated multiple correlation of all columns of the configuration)

#### **Examples**

```
x<-1:10
y<-2+3*x+rnorm(10)
z<- sin(y-x)
confs<-cbind(z,y,x)
c_linearity(confs)</pre>
```

### c\_manifoldness

c-manifoldness calculates c-manifoldness as the aggregated maximal correlation coefficient (i.e., Pearson correlation of the ACE transformed variables) of all pairwise combinations of two different columns in confs. If there is an NA (happens usually when the optimal transformation of any variable is a constant and therefore the covariance is 0 but also one of the sds in the denominator), it gets skipped.

# Description

c-manifoldness calculates c-manifoldness as the aggregated maximal correlation coefficient (i.e., Pearson correlation of the ACE transformed variables) of all pairwise combinations of two different columns in confs. If there is an NA (happens usually when the optimal transformation of any variable is a constant and therefore the covariance is 0 but also one of the sds in the denominator), it gets skipped.

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### Usage

```
c_manifoldness(confs, aggr = NULL)
```

### **Arguments**

confs a numeric matrix or data frame

aggr the aggregation function for configurations of more than two dimensions. De-

faults to max.

# Value

a numeric value; manifoldness (aggregated maximal correlation, correlation of ACE tranformed x and y, see ace)

# **Examples**

```
x<--100:100
y<-sqrt(100^2-x^2)
confs<-cbind(x,y)
c_manifoldness(confs)</pre>
```

c\_mine

wrapper for getting the mine coefficients

# **Description**

wrapper for getting the mine coefficients

### Usage

```
c_mine(confs, master = NULL, alpha = 0.6, C = 15, var.thr = 1e-05, zeta = NULL)
```

# Arguments

confs	a numeric matrix or data frame with two columns
master	the master column
alpha	an optional number of cells allowed in the X-by-Y search-grid. Default value is 0.6
С	an optional number determining the starting point of the X-by-Y search-grid. When trying to partition the x-axis into X columns, the algorithm will start with at most C X clumps. Default value is 15.
var.thr	minimum value allowed for the variance of the input variables, since mine can not be computed in case of variance close to 0. Default value is 1e-5.
zeta	integer in [0,1] (?). If NULL (default) it is set to 1-MIC. It can be set to zero for noiseless functions, but the default choice is the most appropriate parametrization for general cases (as stated in Reshef et al. SOM; they call it epsilon in the paper). It provides robustness.

18 c\_nonmonotonicity

c_nonmonotonicity	c-nonmonotonicity calculates the c-nonmonotonicity based on the maximum asymmetric score We define c-nonmonotonicity as the aggregated nonmonotonicity between any two columns in confs this is one of few c-structuredness indices not between 0 and 1
	one of few c-structureaness indices not between 0 and 1

# Description

c-nonmonotonicity calculates the c-nonmonotonicity based on the maximum asymmetric score We define c-nonmonotonicity as the aggregated nonmonotonicity between any two columns in confs this is one of few c-structuredness indices not between 0 and 1

# Usage

```
c_nonmonotonicity(
  confs,
  aggr = NULL,
  alpha = 1,
  C = 15,
  var.thr = 1e-05,
  zeta = NULL
)
```

# Arguments

confs	a numeric matrix or data frame
aggr	the aggregation function for configurations of more than two dimensions. Defaults to $\max$ .
alpha	an optional number of cells allowed in the X-by-Y search-grid. Default value is $\boldsymbol{1}$
С	an optional number determining the starting point of the $X$ -by- $Y$ search-grid. When trying to partition the $x$ -axis into $X$ columns, the algorithm will start with at most $C$ $X$ clumps. Default value is 15.
var.thr	minimum value allowed for the variance of the input variables, since mine can not be computed in case of variance close to 0. Default value is 1e-5.
zeta	integer in [0,1] (?). If NULL (default) it is set to 1-MIC. It can be set to zero for noiseless functions, but the default choice is the most appropriate parametrization for general cases (as stated in Reshef et al. SOM). It provides robustness.

# Value

a numeric value; nonmonotonicity (aggregated maximal asymmetric score MAS, see mine)

c\_outlying 19

### **Examples**

```
x<-seq(-3,3,length.out=200)
y<-sqrt(3^2-x^2)
z<- sin(y-x)
confs<-cbind(x,y,z)
c_nonmonotonicity(confs)</pre>
```

c\_outlying

c-outlying

### **Description**

Measures the c-outlying structure

#### Usage

```
c_outlying(conf, aggr = NULL)
```

# Arguments

conf A numeric matrix.

aggr the aggregation function for configurations of more than two dimensions. De-

faults to max.

### Value

```
a numeric value; outlying (see scagnostics)
```

# **Examples**

```
delts<-smacof::kinshipdelta
conf3<-smacof::smacofSym(delts,ndim=3)$conf
c_outlying(conf3)</pre>
```

c\_regularity

c-regularity calculates c-regularity as 1 - OPTICS cordillera for k=2. The higher the more regular.

### **Description**

c-regularity calculates c-regularity as 1 - OPTICS cordillera for k=2. The higher the more regular.

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# Usage

```
c_regularity(
  confs,
  voidarg = NULL,
  q = 1,
  epsilon = 2 * max(dist(confs)),
  distmeth = "euclidean",
  dmax = NULL,
  digits = 10,
  scale = 0,
  ...
)
```

# Arguments

confs	a numeric matrix or a dist object
voidarg	a placeholder to allow to pass NULL as strucpar and not interfere with the other arguments
q	The norm used for the Cordillera. Defaults to 1 (and should always be 1 imo).
epsilon	The epsilon parameter for OPTICS (called epsilon_max in the paper). Defaults to 2 times the maximum distance between any two points.
distmeth	The distance to be computed if X is not a symmetric matrix or a dist object (otherwise ignored). Defaults to Euclidean distance.
dmax	The winsorization value for the highest allowed reachability. If used for comparisons this should be supplied. If no value is supplied, it is NULL (default), then dmax is taken from the data as minimum of epsilon or the largest reachability.
digits	The precision to round the raw Cordillera and the norm factor. Defaults to 10.
scale	Should X be scaled if it is an asymmetric matrix or data frame? Can take values TRUE or FALSE or a numeric value. If TRUE or 1, standardisation is to mean=0 and sd=1. If 2, no centering is applied and scaling of each column is done with the root mean square of each column. If 3, no centering is applied and scaling of all columns is done as X/max(standard deviation(allcolumns)). If 4, no centering is applied and scaling of all columns is done as X/max(rmsq(allcolumns)). If FALSE, 0 or any other numeric value, no standardisation is applied. Defaults to 0.
	Additional arguments to be passed to cordillera

### Value

```
a numeric value; regularity
```

# **Examples**

```
hpts<-expand.grid(seq(-5,5),seq(-5,5))
c_regularity(hpts)
hpts2<-cbind(jitter(hpts[,1]),jitter(hpts[,2]))
c_regularity(hpts2)</pre>
```

c\_shepardness 21

c_shepardness	c-shepardness calculates the c-shepardness as the correlation between		
	a loess smoother of the transformed distances and the transformed		
	dissimilarities		

# Description

c-shepardness calculates the c-shepardness as the correlation between a loess smoother of the transformed distances and the transformed dissimilarities

### Usage

```
c_shepardness(object, voidarg = NULL)
```

# Arguments

object an object of class smacofP

voidarg empty argument to allow passing NULL as strucpar

#### Value

a numeric value

# **Examples**

```
delts<-smacof::kinshipdelta
res<-smacofx::postmds(delts)</pre>
```

 ${\tt c\_shepardness(res)}$ 

c\_skinniness c-skinniness

# **Description**

Measures the c-skinniness structure

# Usage

```
c_skinniness(conf, aggr = NULL)
```

### **Arguments**

conf A numeric matrix.

aggr the aggregation function for configurations of more than two dimensions. De-

faults to max.

c\_sparsity

# Value

```
a numeric value; skinniness (see scagnostics)
```

# **Examples**

```
delts<-smacof::kinshipdelta
conf<-smacof::smacofSym(delts)$conf
plot(conf,pch=19,asp=1)
c_skinniness(conf)</pre>
```

c\_sparsity

c-sparsity

# Description

Measures the c-sparsity structure

#### Usage

```
c_sparsity(conf, aggr = NULL)
```

### **Arguments**

conf A numeric matrix.

aggr the aggregation function for configurations of more than two dimensions. De-

faults to max.

### Value

```
a numeric value; sparsity (see scagnostics)
```

# **Examples**

```
delts<-smacof::kinshipdelta
conf<-smacof::smacofSym(delts)$conf
plot(conf,pch=19,asp=1)
c_sparsity(conf)</pre>
```

c\_striatedness 23

 $c\_striatedness$   $c\_striatedness$ 

# Description

Measures the c-striatedness structure

# Usage

```
c_striatedness(conf, aggr = NULL)
```

### **Arguments**

conf A numeric matrix.

aggr the aggregation function for configurations of more than two dimensions. De-

faults to max.

#### Value

```
a numeric value; striatedness (see scagnostics)
```

### **Examples**

```
delts<-smacof::kinshipdelta
conf<-smacof::smacofSym(delts)$conf
plot(conf,pch=19,asp=1)
c_striatedness(conf)</pre>
```

c\_stringiness

c-stringiness

# Description

Measures the c-stringiness structure

# Usage

```
c_stringiness(conf, aggr = NULL)
```

# Arguments

conf A numeric matrix.

aggr the aggregation function for configurations of more than two dimensions. De-

faults to max.

24 jackmds.stops

#### Value

```
a numeric value; stringiness (see scagnostics)
```

# Examples

```
delts<-smacof::kinshipdelta
conf<-smacof::smacofSym(delts)$conf
plot(conf,pch=19,asp=1)
c_stringiness(conf)</pre>
```

jackmds.stops

MDS Jackknife for stops objects

#### **Description**

These functions perform an MDS Jackknife and plot the corresponding solution.

### Usage

```
## S3 method for class 'stops'
jackmds(object, eps = 1e-06, itmax = 5000, verbose = FALSE)
```

### **Arguments**

object Object of class peops.
eps Convergence criterion

itmax Maximum number of iterations

verbose If 'TRUE', intermediate stress is printed out.

#### **Details**

In order to examine the stability solution of an MDS, a Jackknife on the configurations can be performed (see de Leeuw & Meulman, 1986) and plotted. The plot shows the jackknife configurations which are connected to their centroid. In addition, the original configuration (transformed through Procrustes) is plotted. The Jackknife function itself returns also a stability measure (as ratio of between and total variance), a measure for cross validity, and the dispersion around the original smacof solution.

Note that this jackknife only resamples the configuration given the selected hyperparameters, so uncertainty with respect to the hyperparameter selection is not incorporated.

knn\_dist 25

### Value

An object of class 'smacofJK', see jackmds. With values

- smacof.conf: Original configuration
- jackknife.confboot: An array of n-1 configuration matrices for each Jackknife MDS solution
- comparison.conf: Centroid Jackknife configurations (comparison matrix)
- · cross: Cross validity
- stab: Stability coefficient
- disp: Dispersion
- loss: Value of the loss function (just used internally)
- ndim: Number of dimensions
- call: Model call
- niter: Number of iterations
- nobj: Number of objects

### **Examples**

```
diso<-kinshipdelta
fit <- stops(diso,loss="stress",lower=1,upper=5)
res.jk <- jackmds(fit)
plot(res.jk)</pre>
```

knn\_dist

calculate k nearest neighbours from a distance matrix

### Description

calculate k nearest neighbours from a distance matrix

#### Usage

```
knn_dist(dis, k)
```

#### **Arguments**

k

dis distance matrix

number of nearest neighbours (Note that with a tie, the function returns the alphanumerically first one!)

26 ljoptim

 ${\tt ljoptim} \qquad \qquad (A daptive) \ \textit{Version of Luus-Jaakola Optimization}$ 

# Description

Adaptive means that the search space reduction factors in the number of iterations; makes convergence faster at about 100 iterations

# Usage

```
ljoptim(
    x,
    fun,
    ...,
    red = ifelse(adaptive, 0.99, 0.95),
    lower,
    upper,
    acc = 1e-06,
    accd = 1e-04,
    itmax = 1000,
    verbose = 0,
    adaptive = TRUE
)
```

### **Arguments**

x	optional starting values
fun	function to minimize
	additional arguments to be passed to the function to be optimized
red	value of the reduction of the search region
lower	The lower contraints of the search region
upper	The upper contraints of the search region
acc	if the numerical accuracy of two successive target function values is below this, stop the optimization; defaults to $1\text{e-}6$
accd	if the width of the search space is below this, stop the optimization; defaults to 1e-4
itmax	maximum number of iterations
verbose	numeric value hat prints information on the fitting process; $>2$ is extremely verbose
adaptive	should the adaptive version be used? defaults to TRUE.

#### Value

A list with the components (optim)

- par The position of the optimimum in the search space (parameters that minimize the function; argmin fun)
- value The value of the objective function at the optimum (min fun)
- counts The number of iterations performed at convergence with entries faction for the number of iterations and gradient which is always NA at the moment
- convergence 0 successful completion by the accd or acc criterion, 1 indicate iteration limit was reached, 99 is a problem
- message is NULL (only for compatibility or future use)

#### **Examples**

```
fbana <- function(x) {
x1 <- x[1]
x2 <- x[2]
100 * (x2 - x1 * x1)^2 + (1 - x1)^2
}
res1<-ljoptim(c(-1.2,1),fbana,lower=-5,upper=5,accd=1e-16,acc=1e-16)
res1

set.seed(210485)
fwild <- function (x) 10*sin(0.3*x)*sin(1.3*x^2) + 0.00001*x^4 + 0.2*x+80
plot(fwild, -50, 50, n = 1000, main = "ljoptim() minimising 'wild function'")
res2<-ljoptim(50, fwild,lower=-50,upper=50,adaptive=FALSE,accd=1e-16,acc=1e-16)
points(res2$par,res2$value,col="red",pch=19)
res2</pre>
```

```
match_partial_ignorecase_nopunct
```

function for lookup that partially matched and ignores cases and punctuation

#### **Description**

function for lookup that partially matched and ignores cases and punctuation

#### Usage

```
match_partial_ignorecase_nopunct(lookup, entry, ...)
```

# **Arguments**

```
lookup the lookup string entry the registry entry
```

... additional arguments to pmatch

28 plot.stops

Pendigits500

Pen digits

#### Description

These data are a random sample of 500 of the 10992 pendigits data from Alimoglu (1996). The original data were from 44 writers who handwrote 250 times the digits 0,...,9. The digits were written inside a rectangular box with a resolution of 500 x 500 pixels and the first 10 per writer were ignored for further analysis. This led to 10992 digits. They were recorded in small time intervals by following the trajectory of the pen on the 500 x 500 grid and then normalized. From the normalized trajectory 8 points (x and y axis position) were randomly selected for each handwritten digit, leading to 16 predictors variables. We extarcted a random sample of 500 of them.

#### Usage

```
data(Pendigits500)
```

#### **Format**

A data frame with 500 rows and 17 variables

#### **Details**

The variables are

- The rownames of Pendigits500 refer to the data point of the 10992 original data
- V1-V16: trajectory points (x, y coordinate) of the grid
- digits: The digit actually written (the label)

#### Source

From A. Izenman (2010) Modern multivariate statistical techniques. Springer.

plot.stops

S3 plot method for stops objects

### **Description**

S3 plot method for stops objects

#### Usage

```
## S3 method for class 'stops'
plot(x, plot.type = "confplot", main, asp = 1, ...)
```

print.stops 29

# Arguments

×	an object of class stops
olot.type	String indicating which type of plot to be produced: "confplot", "resplot", "Shep ard", "stressplot", "bubbleplot" (see details)
main	the main title of the plot
asp	aspect ratio of x/y axis; defaults to 1; setting to 1 will lead to an accurate representation of the fitted distances.
	Further plot arguments passed: see 'plot.smacof' and 'plot' for detailed information.
	Details: See plot.smacofP
asp	the main title of the plot aspect ratio of x/y axis; defaults to 1; setting to 1 will lead to an accurate repsenation of the fitted distances.  Further plot arguments passed: see 'plot.smacof' and 'plot' for detailed infimation.

# Value

no return value, just plots

print.stops	S3 print method for stops objects

# Description

S3 print method for stops objects

# Usage

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

# Arguments

x stops object... additional arguments

# Value

no return value, just prints

30 residuals.stops

```
print.summary.stops
```

S3 print method for summary.stops

# Description

S3 print method for summary.stops

# Usage

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

### Arguments

x object of class summary.stops

... additional arguments

#### Value

no return value, just prints

residuals.stops

S3 residuals method for stops

# Description

S3 residuals method for stops

# Usage

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

### **Arguments**

```
object object of class stops
... addditional arguments
```

# Value

a vector of residuals (observed minus fitted distances)

stoploss 31

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Calculate the weighted multiobjective loss function used in STOPS

# Description

Calculate the weighted multiobjective loss function used in STOPS

# Usage

```
stoploss(
  obj,
  stressweight = 1,
  structures,
  strucweight = rep(-1/length(structures), length(structures)),
  strucpars,
  stoptype = c("additive", "multiplicative"),
  verbose = 0,
  registry = struc_reg
)
```

### **Arguments**

obj	object returned inside a stop_* function. Uses the stress.m slot for getting the stress.
stressweight	weight to be used for the fit measure; defaults to 1
structures	which c-structuredness indices to be included in the loss
strucweight	the weights of the structuredness indices; defaults to -1/#number of structures
strucpars	a list of parameters to be passed to the c-structuredness indices in the same order as the values in structures. If the index has no parameters or you want to use the defaults, supply NULL. (alternatively a named list that has the structure name as the element name).
stoptype	what type of weighted combination should be used? Can be 'additive' or 'multiplicative'.
verbose	verbose output
registry	an object of class registry. This can be used to add additional c-structuredness indices. Defaults of the registry created via .onLoad in zzz.R

# Value

a list with calculated stoploss (\$stoploss), structuredness indices (\$strucinidices) and hyperparameters (\$parameters and \$theta)

32 stops

stops

High Level STOPS Function

#### **Description**

This allows to fit STOPS models as described in Rusch, Mair, Hornik (2023).

# Usage

```
stops(
  dis,
  loss = "stress",
  theta = 1,
  type = "ratio",
  structures,
  ndim = 2,
 weightmat = NULL,
  init = NULL,
  stressweight = 1,
  strucweight,
  strucpars,
 optimmethod = c("SANN", "ALJ", "pso", "Kriging", "tgp", "direct", "stogo", "cobyla",
    "crs2lm", "isres", "mlsl", "neldermead", "sbplx", "hjk", "cmaes"),
  lower,
  upper,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  initpoints = 10,
  itmax = 50,
  itmaxps = 10000,
 model,
 control,
 registry = struc_reg,
)
```

### **Arguments**

theta

dis numeric matrix or dist object of a matrix of proximities

loss which loss function to be used for fitting, defaults to stress.

which ioss function to be used for fitting, defaults to stress.

hyperparameter vector starting values for the transformation functions. If the length is smaller than the number of hyperparameters for the MDS version the vector gets recycled (see the corresponding stop\_XXX function or the vignette for how theta must look like exactly for each loss). If larger than the number of hyperparameters for the MDS method, an error is thrown. If completely missing theta is set to 1 and recycled.

33 stops

type of MDS optimal scaling (implicit transformation). One of "ratio", "interval" type

or "ordinal". Default is "ratio". Not every type can be used with every loss, only

ratio works with all.

structures character vector of which c-structuredness indices should be considered; if miss-

ing no structure is considered.

ndim number of dimensions of the target space

weightmat (optional) a matrix of nonnegative weights; defaults to 1 for all off diagonals

init (optional) initial configuration

stressweight weight to be used for the fit measure; defaults to 1

strucweight vector of weights to be used for the c-structuredness indices (in the same order

as in structures); defaults to -1/length(structures) for each index

strucpars (possibly named with the structure). Metaparameters for the structuredness indices (gamma in the article). It's safest for it be a list of lists with the named

arguments for the structuredness indices and the order of the lists must be like the

order of structures. So something like this list(list(par1Struc1=par1Struc1,par2Struc1=p where parYStrucX are the named arguments for the metaparameter Y of the structure X the list elements corresponds to. For a structure without parameters, set NULL. Parameters in different list elements parYStrucX can have the same name. For example, say we want to use cclusteredness with metaparam-

eters epsilon=10 and k=4 (and the default for the other parameters), cdependence with no metaparameters and cfaithfulness with metaparameter k=7 one would list(list(epsilon=10,k=4),list(NULL),list(dis=obdiss,k=6)) for structures vector ("cclusteredness", "cdependence", "cfaithfulness"). The pa-

rameter lists must be in the same ordering as the indices in structures. If missing it is set to NULL and defaults are used. It is also possible to supply a structure's metaparameters as a list of vectors with named elements if the metaparameters

are scalars, so like list(c(par1Struc1=parStruc1, par2Struc1=par1Struc1,...),c(par1Struc2=p That can have unintended consequences if the metaparameter is a vector or ma-

trix.

optimmethod What solver to use. Currently supported are Bayesian optimization with Gaus-

sian Process priors and Kriging ("Kriging", see EGO.nsteps), Bayesian optimization with treed Gaussian processes with jump to linear models ("tgp", see dopt.gp), Adaptive LJ Search ("ALJ"), Particle Swarm optimization ("pso", see psoptim), simulated annealing ("SANN", optim), "direct (direct)", Stochastic Global Optimization ("stogo", stogo), COBYLA ("cobyla", cobyla), Controlled Random Search 2 with local mutation ("crs2lm", crs2lm), Improved Stochastic Ranking Evolution Strategy ("isres", isres), Multi-Level Single-Linkage ("mlsl", mlsl), Nelder-Mead ("neldermead", neldermead), Subplex ("sbplx", sbplx), Hooke-Jeeves Pattern Search ("hjk", hjk), CMA-ES ("cmaes",

cma\_es). Defaults to "ALJ" version. "tgp", "ALJ", "Kriging" and "pso" usually work well for relatively low values of 'itmax'.

lower The lower contraints of the search region. Needs to be a numeric vector of the

same length as the parameter vector theta.

The upper contraints of the search region. Needs to be a numeric vector of the upper

same length as the parameter vector theta.

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verbose numeric value hat prints information on the fitting process; >2 is very verbose.

stoptype which aggregation for the multi objective target function? Either 'additive' (de-

fault) or 'multiplicative'

initpoints number of initial points to fit the surrogate model for Bayesian optimization;

default is 10.

itmax maximum number of iterations of the outer optimization (for theta) or number of

steps of Bayesian optimization; default is 50. We recommend a higher number for ALJ (around 150). Note that due to the inner workings of some solvers, this may or may not correspond to the actual number of function evaluations performed (or PS models fitted). E.g., with tgp the actual number of function evaluation of the PS method is between itmax and 6\*itmax as tgp samples 1-6 candidates from the posterior and uses the best candidate. For pso it is the number of particles s times itmax. For cmaes it is usually a bit higher than itmax. This currently may get overruled by a control argument if it is used (and then set to either ewhat is supplie dby control or to the default of the method).

itmaxps maximum number of iterations of the inner optimization (to obtain the PS con-

figuration)

model a character specifying the surrogate model to use. For Kriging it specifies the

covariance kernel for the GP prior; see covTensorProduct-class defaults to "powerexp". For tgp it specifies the non stationary process used see bgp, defaults

to "btgpllm"

control a control argument passed to the outer optimization procedure. Will override

any other control arguents passed, especially verbose and itmax. For the effect of control, see the functions pomp::sannbox for SANN and pso::psoptim for pso, cmaes::cma\_es for cmaes, dfoptim::hjkb for hjk and the nloptr docs for the

algorithms direct, stogo, cobyla, crs2lm, isres, mlsl, neldermead, sbplx.

registry an object of class registry containing the c-structuredness indices. Defaults to

the what is created .onLoad.

... additional arguments passed to the outer optimization procedures (not fully tested).

#### Details

The combination of c-structurednes indices and stress uses the stress.m values, which are the explictly normalized stresses. Reported however is the stress-1 value which is sqrt(stress.m).

#### Value

A list with the components

• stoploss: the stoploss value

• optim: the object returned from the optimization procedure

• stressweight: the stressweight

• strucweight: the vector of structure weights

• call: the call

• optimmethod: The solver selected

stop\_apstress 35

- loss: The PS badness-of-fit function
- nobj: the number of objects in the configuration
- type: The type of stoploss scalacrisation (additive or multiplicative)
- fit: The fitted PS object (most importantly \$fit\$conf the fitted configuration)
- stoptype: Type of stoploss combinatio

#### **Examples**

```
data(kinshipdelta,package="smacof")
strucpar<-list(NULL,NULL) #parameters for indices</pre>
res1<-stops(kinshipdelta,loss="stress",
structures=c("cclumpiness","cassociation"),strucpars=strucpar,
lower=0,upper=10,itmax=10)
res1
#use higher itmax in general, we use 5 just to shorten the tests
data(BankingCrisesDistances)
strucpar<-list(c(epsilon=10,minpts=2),NULL) #parameters for indices</pre>
res1<-stops(BankingCrisesDistances[,1:69],loss="stress",verbose=0,</pre>
structures=c("cclusteredness","clinearity"),strucpars=strucpar,
lower=0,upper=10,itmax=5)
res1
strucpar<-list(list(alpha=0.6,C=15,var.thr=1e-5,zeta=NULL),</pre>
list(alpha=0.6,C=15,var.thr=1e-5,zeta=NULL))
res1<-stops(BankingCrisesDistances[,1:69],loss="stress",verbose=0,</pre>
structures=c("cfunctionality", "ccomplexity"), strucpars=strucpar,
lower=0,upper=10,itmax=5)
res1
```

stop\_apstress

STOPS version of approximated power stress models.

#### **Description**

This uses an approximation to power stress that can make use of smacof as workhorse. Free parameters are kappa, lambda and nu.

### Usage

```
stop_apstress(
    dis,
    theta = c(1, 1, 1),
    type = "ratio",
    ndim = 2,
```

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```
weightmat = 1 - diag(nrow(dis)),
init = NULL,
itmaxi = 1000,
...,
stressweight = 1,
structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
    "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
    strucweight = rep(1/length(structures), length(structures)),
    strucpars,
    verbose = 0,
    stoptype = c("additive", "multiplicative"),
    registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of parameters to optimize over. Must be of length three, with

the first the kappa argument, the second the lambda argument and the third the nu argument. One cannot supply upsilon and tau as of yet. Defaults to 1 1 1.

type MDS type.

ndim number of dimensions of the target space

weightmat (optional) a binary matrix of nonnegative weights

init (optional) initial configuration

itmaxi number of iterations. default is 1000.

... additional arguments to be passed to the fitting procedure

stressweight weight to be used for the fit measure; defaults to 1

structures a character vector listing the structure indices to use. They always are called

"cfoo" with foo being the structure.

strucweight weight to be used for the structures; defaults to 1/number of structures

strucpars a list of list of parameters for the structuredness indices; each list element cor-

responds to one index in the order of the appearance in structures vector. See

examples.

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype which weighting to be used in the multi-objective optimization? Either 'addi-

tive' (default) or 'multiplicative'.

registry registry object with c-structuredness indices.

#### Value

A list with the components

stop\_bcmds 37

- stress: the stress-1 value (sqrt stress.m)
- stress.m: default normalized stress
- stoploss: the weighted loss value
- struc: the structuredness indices
- parameters: the parameters used for fitting (kappa, lambda, nu)
- fit: the returned object of the fitting procedure
- stopobj: the stopobj object

stop\_bcmds

STOPS version of Box Cox Stress

## **Description**

STOPS version of Box Cox Stress

## Usage

```
stop_bcmds(
  dis,
  theta = c(1, 1, 0),
  type = "ratio",
  weightmat = NULL,
  init = NULL,
  ndim = 2,
  itmaxi = 5000,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

the ta the ta vector of powers; the first is mu (for the fitted distances), the second lambda (for the proximities), the third nu (for the weights). If a scalar is given it is recycled. Defaults to 1 1 0.

type MDS type. Is ignored here.

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weightmat (not used)

init (optional) initial configuration

ndim number of dimensions of the target space

itmaxi number of iterations

... additional arguments to be passed to the fitting procedure

stressweight weight to be used for the fit measure; defaults to 1

structures which structures to look for

strucweight weight to be used for the structures; defaults to 0.5

strucpars a list of parameters for the structuredness indices; each list element corresponds

to one index in the order of the appearance in structures

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype which weighting to be used in the multi-objective optimization? Either 'addi-

tive' (default) or 'multiplicative'.

registry registry object with c-structuredness indices.

#### Value

A list with the components

• stress: the stress-1

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (kappa, lambda)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

stop\_clca STOPS version of CLCA.

## **Description**

CLCA with free lambda0 and 20 epochs. Should we add alpha0?

stop\_clca 39

#### Usage

```
stop_clca(
  dis,
  theta = 3 * max(sd(dis)),
  type = "ratio",
  weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of explicit parameters; lambda0 for the maximal neighbourhood.

Defaults to 100.

type MDS type.

weightmat (optional) a matrix of nonnegative weights

init (optional) initial configuration

ndim number of dimensions of the target space

itmaxi number of iterations

... additional arguments to be passed to the fitting procedure

stressweight weight to be used for the fit measure; defaults to 1

structures a character vector listing the structure indices to use. They always are called

"cfoo" with foo being the structure.

strucweight weight to be used for the structures; defaults to 1/number of structures

strucpars a list of parameters for the structuredness indices; each list element corresponds

to one index in the order of the appearance in structures

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype which weighting to be used in the multi-objective optimization? Either 'addi-

tive' (default) or 'multiplicative'.

registry registry object with c-structuredness indices.

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#### Value

A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (tau)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

stop\_cldae

STOPS version of CLDA with free epsilon.

#### **Description**

CLDA with free lambda0 and epsilon and 20 epochs. Should we add alpha0?

```
stop_cldae(
  dis,
  theta = rep(3 * max(sd(dis)), 2),
  type = "ratio",
  weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

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## **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of explicit parameters; first is lambda0 for the maximal neigh-

bourhood and second is k for the number of neighbours for the geodesic dis-

tance.

type MDS type.

weightmat (optional) a matrix of nonnegative weights

init (optional) initial configuration

ndim number of dimensions of the target space

itmaxi number of iterations

. . . additional arguments to be passed to the fitting procedure

stressweight weight to be used for the fit measure; defaults to 1

structures a character vector listing the structure indices to use. They always are called

"cfoo" with foo being the structure.

strucweight weight to be used for the structures; defaults to 1/number of structures

strucpars a list of parameters for the structuredness indices; each list element corresponds

to one index in the order of the appearance in structures

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype which weighting to be used in the multi-objective optimization? Either 'addi-

tive' (default) or 'multiplicative'.

registry object with c-structuredness indices.

## Value

A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (tau)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

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stop\_cldak

STOPS version of CLDA with free k.

#### **Description**

CLDA with free lambda0 and k and 20 epochs. Should we add alpha0?

#### Usage

```
stop_cldak(
  dis,
  theta = c(3 * max(sd(dis)), nrow(dis)/4),
  type = "ratio",
  weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

#### **Arguments**

dis	numeric matrix or dist object of a matrix of proximities
theta	the theta vector of explicit parameters; first is lambda0 for the maximal neighbourhood and second is k for the number of neighbours for the geodesic distance.
type	MDS type.
weightmat	(optional) a matrix of nonnegative weights
init	(optional) initial configuration
ndim	number of dimensions of the target space
itmaxi	number of iterations
	additional arguments to be passed to the fitting procedure
stressweight	weight to be used for the fit measure; defaults to 1
structures	a character vector listing the structure indices to use. They always are called "cfoo" with foo being the structure.

stop\_cmdscale 43

strucweight	weight to be used for the structures; defaults to 1/number of structures
strucpars	a list of parameters for the structuredness indices; each list element corresponds to one index in the order of the appearance in structures
verbose	numeric value hat prints information on the fitting process; >2 is extremely verbose
stoptype	which weighting to be used in the multi-objective optimization? Either 'additive' (default) or 'multiplicative'.
registry	registry object with c-structuredness indices.

#### Value

A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (tau)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

stop\_cmdscale

STOPS version of strain

## **Description**

The free parameter is lambda for power transformations of the observed proximities.

```
stop_cmdscale(
    dis,
    theta = 1,
    type = "ratio",
    weightmat = NULL,
    ndim = 2,
    init = NULL,
    ...,
    stressweight = 1,
    structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
        "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
        "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
        "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
    strucweight = rep(1/length(structures), length(structures)),
```

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```
strucpars,
verbose = 0,
stoptype = c("additive", "multiplicative"),
itmaxi = 1000,
add = TRUE,
registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of powers; this must be a scalar of the lambda transformation

for the observed proximities.

type MDS type. Ignored here.

weightmat (optional) a matrix of nonnegative weights. Not used.

ndim number of dimensions of the target space

init (optional) initial configuration

... additional arguments to be passed to the fitting procedure

stressweight weight to be used for the fit measure; defaults to 1 structures which structuredness indices to be included in the loss

strucweight weight to be used for the structuredness indices; ; defaults to 1/#number of

structures

strucpars the parameters for the structuredness indices

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype How to construct the target function for the multi objective optimization? Either

'additive' (default) or 'multiplicative'

itmaxi number of iterations. No effect here.

add if TRUE dis is made to Euclidean distances registry registry object with c-structuredness indices.

#### Value

A list with the components

- stress: the badness-of-fit value (this isn't stress here but 1-(sum\_ndim(max(eigenvalues,0))/sum\_n(max(eigenvalues,0)). 1-GOF[2])
- stress.m: explictly normalized stress (manually calculated)
- stoploss: the weighted loss value
- indices: the values of the structuredness indices
- parameters: the parameters used for fitting (lambda)
- fit: the returned object of the fitting procedure, which is cmdscalex object with some extra slots for the parameters and stresses
- stopobj: the stopobj object

stop\_elastic 45

stop\_elastic

STOPS versions of elastic scaling models (via smacofSym)

## **Description**

The free parameter is lambda for power transformations the observed proximities. The fitted distances power is internally fixed to 1 and the power for the weights=delta is -2. Allows for a weight matrix because of smacof.

## Usage

```
stop_elastic(
  dis,
  theta = 1,
  type = "ratio",
  ndim = 2,
  weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  itmaxi = 1000,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

## **Arguments**

dis	numeric matrix or dist object of a matrix of proximities
theta	the theta vector of powers; this must be a scalar of the lambda transformation for the observed proximities. Defaults to 1.
type	MDS type. Defaults ot 'ratio'.
ndim	number of dimensions of the target space
weightmat	(optional) a matrix of nonnegative weights (NOT the elscal weights)
init	(optional) initial configuration
itmaxi	number of iterations
	additional arguments to be passed to the fitting procedure
stressweight	weight to be used for the fit measure; defaults to 1

stop\_isomap1

structures	which structuredness indices to be included in the loss
strucweight	weight to be used for the structuredness indices; ; defaults to $1/\#$ number of structures
strucpars	the parameters for the structuredness indices
verbose	numeric value hat prints information on the fitting process; >2 is extremely verbose
stoptype	How to construct the target function for the multi objective optimization? Either 'additive' (default) or 'multiplicative'
registry	registry object with c-structuredness indices.

## Value

A list with the components

- stress: the stress-1 (sqrt(stress.m))
- stress.m: default normalized stress (used for STOPS)
- stoploss: the weighted loss value
- indices: the values of the structuredness indices
- parameters: the parameters used for fitting (lambda)
- fit: the returned object of the fitting procedure
- stopobj: the stopobj objects

stop\_isomap1

STOPS version of isomap to optimize over integer k.

## **Description**

Free parameter is k.

```
stop_isomap1(
    dis,
    theta = 3,
    type = "ratio",
    weightmat = NULL,
    ndim = 2,
    init = NULL,
    stressweight = 1,
    structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
        "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
        "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
        "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
    strucweight = rep(1/length(structures), length(structures)),
```

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```
strucpars,
verbose = 0,
stoptype = c("additive", "multiplicative"),
itmaxi = NULL,
registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the number of shortest dissimilarities retained for a point (nearest neighbours),

the isomap parameter. Must be a numeric scalar. Defaults to 3.

type MDS type. Is "ratio".

weightmat (optional) a matrix of nonnegative weights ndim number of dimensions of the target space

init (optional) initial configuration

stressweight weight to be used for the fit measure; defaults to 1
structures which structuredness indices to be included in the loss

strucweight weight to be used for the structuredness indices; ; defaults to 1/#number of

structures

strucpars the parameters for the structuredness indices

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype How to construct the target function for the multi objective optimization? Either

'additive' (default) or 'multiplicative'

itmaxi placeholder for compatibility in stops call; not used

registry object with c-structuredness indices.

#### **Details**

Currently this version is a bit less flexible than the vegan one, as the only allowed parameter for isomap is the theta (k in isomap, no epsilon) and the shortest path is always estimated with argument "shortest". Also note that fragmentedOK is always set to TRUE which means that for theta that is too small only the largest conected group will be analyzed. If that's not wanted just set the theta higher.

#### Value

A list with the components

- stress: Not really stress but 1-GOF[2] where GOF is the second element returned from smacofx::cmdscale (the sum of the first ndim eigenvalues divided by the sum of all absolute eigenvalues).
- stress.m: default normalized stress (sqrt explicitly normalized stress; really the stress this time)

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- stoploss: the weighted loss value
- indices: the values of the structuredness indices
- parameters: the parameters used for fitting
- fit: the returned object of the fitting procedure
- stopobj: the stopobj object

stop\_isomap2

STOPS version of isomap over real epsilon.

## **Description**

Free parameter is eps.

#### Usage

```
stop_isomap2(
  dis,
  theta = stats::quantile(dis, 0.1),
  type = "ratio",
  weightmat = NULL,
  ndim = 2,
  init = NULL,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  itmaxi = NULL,
  registry = struc_reg
)
```

#### **Arguments**

ndim

dis numeric matrix or dist object of a matrix of proximities theta the number of shortest dissimilarities retained for a point (neighbourhood region), the isomap parameter. Defaults to the 0.1 quantile of the empirical distribution of dis. MDS type. Is "ratio". type weightmat (optional) a matrix of nonnegative weights number of dimensions of the target space

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(optional) initial configuration init weight to be used for the fit measure; defaults to 1 stressweight which structuredness indices to be included in the loss structures strucweight weight to be used for the structuredness indices; ; defaults to 1/#number of structures the parameters for the structuredness indices strucpars verbose numeric value hat prints information on the fitting process; >2 is extremely verbose How to construct the target function for the multi objective optimization? Either stoptype 'additive' (default) or 'multiplicative' itmaxi placeholder for compatibility in stops call; not used registry object with c-structuredness indices.

#### **Details**

registry

Currently this version is a bit less flexible than the vegan one, as the only allowed parameter for isomap is the theta (epsilon in isomap) and the shortest path is always estimated with argument "shortest". Also note that fragmentedOK is always set to TRUE which means that for theta that is too small only the largest conected group will be analyzed. If that's not wanted just set the theta higher.

#### Value

A list with the components

- stress: Not really stress but 1-GOF[2] where GOF is the second element returned from cmdscale (the sum of the first ndim absolute eigenvalues divided by the sum of all absolute eigenvalues).
- stress.m: default normalized stress (sqrt explicitly normalized stress; really the stress this
- stoploss: the weighted loss value
- indices: the values of the structuredness indices
- parameters: the parameters used for fitting
- fit: the returned object of the fitting procedure
- stopobj: the stopobj object

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stop\_lmds

STOPS version of lMDS

#### Description

STOPS version of IMDS

#### Usage

```
stop_lmds(
  dis,
  theta = c(2, 0.5),
  type = "ratio",
  weightmat = NULL,
  init = NULL,
  ndim = 2,
  itmaxi = 5000,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of powers; the first is k (for the neighbourhood), the second tau

(for the penalty). If a scalar is given it is recycled. Defaults to 2 and 0.5.

type MDS type. Ignored.

weightmat (not used)

init (optional) initial configuration

ndim number of dimensions of the target space

itmaxi number of iterations

.. additional arguments to be passed to the fitting procedure

stressweight weight to be used for the fit measure; defaults to 1

structures which structures to look for

strucweight weight to be used for the structures; defaults to 0.5

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strucpars	a list of parameters for the structuredness indices; each list element corresponds to one index in the order of the appearance in structure
verbose	numeric value hat prints information on the fitting process; >2 is extremely verbose
stoptype	which weighting to be used in the multi-objective optimization? Either 'additive' (default) or 'multiplicative'.
registry	registry object with c-structuredness indices.

#### Value

A list with the components

• stress: the stress-1

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (kappa, lambda)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

stop\_powerelastic STOPS version of elastic scaling with powers for proximities and distances

## **Description**

This is power stress with free kappa and lambda but rho is fixed to -2 and the weights are delta.

```
stop_powerelastic(
    dis,
    theta = c(1, 1),
    type = "ratio",
    weightmat = 1 - diag(nrow(dis)),
    init = NULL,
    ndim = 2,
    itmaxi = 1e+05,
    ...,
    stressweight = 1,
    structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
    "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
    strucweight = rep(1/length(structures), length(structures)),
```

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```
strucpars,
verbose = 0,
stoptype = c("additive", "multiplicative"),
registry = struc_reg
)
```

## **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of powers; a vector of length two where the first element is kappa

(for the fitted distances), the second lambda (for the observed proximities). If a

scalar for the free parameters is given it is recycled. Defaults to 1 1.

type MDS type. Defaults to "ratio".

weightmat (optional) a matrix of nonnegative weights

init (optional) initial configuration

ndim number of dimensions of the target space

itmaxi number of iterations

additional arguments to be passed to the fitting procedure

stressweight weight to be used for the fit measure; defaults to 1

structures which structures to look for

strucweight weight to be used for the structures; defaults to 0.5

strucpars a list of parameters for the structuredness indices; each list element corresponds

to one index in the order of the appearance in structures

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype which weighting to be used in the multi-objective optimization? Either 'addi-

tive' (default) or 'multiplicative'.

registry registry object with c-structuredness indices.

#### Value

A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (kappa, lambda)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

stop\_powermds 53

stop\_powermds STOPS version of powermds

## **Description**

This is power stress with free kappa and lambda but rho is fixed to 1, so no weight transformation.

## Usage

```
stop_powermds(
  dis,
  theta = c(1, 1),
  type = "ratio",
  weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  . . . ,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

## Arguments

dis	numeric matrix or dist object of a matrix of proximities
theta	the theta vector of powers; a vector of length 2 where the first element is kappa (for the fitted distances), the second lambda (for the observed proximities). If a scalar is given it is recycled. Defaults to 1,1.
type	MDS type. Defaults to "ratio".
weightmat	(optional) a matrix of nonnegative weights
init	(optional) initial configuration
ndim	number of dimensions of the target space
itmaxi	number of iterations
	additional arguments to be passed to the fitting procedure
stressweight	weight to be used for the fit measure; defaults to 1
structures	which structures to look for

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strucweight	weight to be used for the structures; defaults to 0.5
strucpars	a list of parameters for the structuredness indices; each list element corresponds to one index in the order of the appearance in structures
verbose	numeric value hat prints information on the fitting process; >2 is extremely verbose
stoptype	which weighting to be used in the multi-objective optimization? Either 'additive' (default) or 'multiplicative'.
registry	registry object with c-structuredness indices.

#### Value

A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (kappa, lambda)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

stop\_powersammon

STOPS version of sammon with powers

## **Description**

This is power stress with free kappa and lambda but rho is fixed to -1 and the weights are delta.

```
stop_powersammon(
    dis,
    theta = c(1, 1),
    type = "ratio",
    weightmat = NULL,
    init = NULL,
    ndim = 2,
    itmaxi = 10000,
    ...,
    stressweight = 1,
    structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
    "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
```

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```
strucweight = rep(1/length(structures), length(structures)),
strucpars,
verbose = 0,
stoptype = c("additive", "multiplicative"),
registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of powers; a vector of length two where the first element is kappa

(for the fitted distances), the second lambda (for the observed proximities). If a

scalar is given it is recycled for the free parameters. Defaults to 1 1.

type MDS type. Defaults to "ratio".

weightmat (optional) a matrix of nonnegative weights

init (optional) initial configuration

ndim number of dimensions of the target space

itmaxi number of iterations

... additional arguments to be passed to the fitting procedure

stressweight weight to be used for the fit measure; defaults to 1

structures which structures to look for

strucweight weight to be used for the structures; defaults to 0.5

strucpars a list of parameters for the structuredness indices; each list element corresponds

to one index in the order of the appearance in structures

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype which weighting to be used in the multi-objective optimization? Either 'addi-

tive' (default) or 'multiplicative'.

registry object with c-structuredness indices.

#### Value

A list with the components

• stress: the stress

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (kappa, lambda)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

56 stop\_powerstress

stop\_powerstress

STOPS version of powerstress

#### Description

Power stress with free kappa and lambda and rho.

## Usage

```
stop_powerstress(
  dis,
  theta = c(1, 1, 1),
  type = "ratio",
 weightmat = NULL,
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

#### **Arguments**

dis	numeric matrix or dist object of a matrix of proximities
theta	the theta vector of powers; the first is kappa (for the fitted distances), the second lambda (for the observed proximities), the third nu (for the weights). If a scalar is given it is recycled. Defaults to 1 1 1.
type	MDS type.
weightmat	(optional) a matrix of nonnegative weights
init	(optional) initial configuration
ndim	number of dimensions of the target space
itmaxi	number of iterations
	additional arguments to be passed to the fitting procedure
stressweight	weight to be used for the fit measure; defaults to 1
structures	a character vector listing the structure indices to use. They always are called "cfoo" with foo being the structure.

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strucweight	weight to be used for the structures; defaults to 1/number of structures
strucpars	a list of parameters for the structuredness indices; each list element corresponds to one index in the order of the appearance in structures
verbose	numeric value hat prints information on the fitting process; >2 is extremely verbose
stoptype	which weighting to be used in the multi-objective optimization? Either 'additive' (default) or 'multiplicative'.
registry	registry object with c-structuredness indices.

#### Value

A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (kappa, lambda, nu)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

stop\_rpowerstress

STOPS version of restricted powerstress

## **Description**

STOPS version of restricted powerstress

```
stop_rpowerstress(
    dis,
    theta = c(1, 1, 1),
    type = "ratio",
    weightmat = NULL,
    init = NULL,
    ndim = 2,
    itmaxi = 10000,
    ...,
    stressweight = 1,
    structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
    "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
```

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```
strucweight = rep(1/length(structures), length(structures)),
strucpars,
verbose = 0,
stoptype = c("additive", "multiplicative"),
registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of powers; the first two arguments are for kappa and lambda and

should be equal (for the fitted distances and observed proximities), the third nu (for the weights). Internally the kappa and lambda are equated. If a scalar is given it is recycled (so all elements of theta are equal); if a vector of length 2 is

given, it gets expanded to c(theta[1],theta[1],theta[2]). Defaults to 1 1 1.

type MDS type. Defaults to "ratio".

weightmat (optional) a matrix of nonnegative weights

init (optional) initial configuration

ndim number of dimensions of the target space itmaxi number of iterations, default is 10000.

... additional arguments to be passed to the fitting procedure powerStressMin

stressweight weight to be used for the fit measure; defaults to 1

structures a character vector listing the structure indices to use. They always are called

"cfoo" with foo being the structure.

strucweight weight to be used for the structures; defaults to 1/number of structures

strucpars a list of list of parameters for the structuredness indices; each list element cor-

responds to one index in the order of the appearance in structures vector. See

examples.

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype which weighting to be used in the multi-objective optimization? Either 'addi-

tive' (default) or 'multiplicative'.

registry object with c-structuredness indices.

#### Value

A list with the components

• stress: the stress-1 value

· stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (kappa=lambda, nu)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

stop\_rstress 59

stop\_rstress

STOPS version of rstress

## **Description**

Free parameter is kappa=2r for the fitted distances.

## Usage

```
stop_rstress(
  dis,
  theta = 1,
  type = "ratio",
  weightmat = NULL,
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  . . . ,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

## Arguments

structures

dis	numeric matrix or dist object of a matrix of proximities
theta	the theta vector of powers; this must be a scalar of the kappa=2*r transformation for the fitted distances proximities. Defaults to 1. Note that what is returned is r, not kappa.
type	MDS type. Default is "ratio"
weightmat	(optional) a matrix of nonnegative weights
init	(optional) initial configuration
ndim	number of dimensions of the target space
itmaxi	number of iterations.
	additional arguments to be passed to the fitting procedure
stressweight	weight to be used for the fit measure; defaults to 1

which structuredness indices to be included in the loss

stop\_sammon

strucweight	weight to be used for the structuredness indices; ; defaults to 1/#number of structures
strucpars	the parameters for the structuredness indices
verbose	numeric value hat prints information on the fitting process; >2 is extremely verbose
stoptype	How to construct the target function for the multi objective optimization? Either 'additive' (default) or 'multiplicative'
registry	registry object with c-structuredness indices.

#### Value

A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• indices: the values of the structuredness indices

• parameters: the parameters used for fitting

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

stop\_sammon

STOPS version of Sammon mapping

## **Description**

Uses smacofx::sammon. The free parameter is lambda for power transformations of the observed proximities.

```
stop_sammon(
    dis,
    theta = 1,
    type = "ratio",
    ndim = 2,
    init = NULL,
    weightmat = NULL,
    itmaxi = 1000,
    ...,
    stressweight = 1,
    structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
        "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
        "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity",
```

stop\_sammon 61

```
"cstringiness", "cclumpiness", "cinequality"),
strucweight = rep(1/length(structures), length(structures)),
strucpars,
verbose = 0,
stoptype = c("additive", "multiplicative"),
registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities theta the theta vector of powers; this must be a scalar of the lambda transformation for the observed proximities. Defaults to 1. MDS type. Ignored here. type number of dimensions of the target space ndim init (optional) initial configuration weightmat a matrix of nonnegative weights. Has no effect here. itmaxi number of iterations additional arguments to be passed to the fitting procedure stressweight weight to be used for the fit measure; defaults to 1 which structuredness indices to be included in the loss structures weight to be used for the structuredness indices; ; defaults to 1/#number of strucweight structures strucpars the parameters for the structuredness indices verbose numeric value hat prints information on the fitting process; >2 is extremely verstoptype How to construct the target function for the multi objective optimization? Either 'additive' (default) or 'multiplicative' registry registry object with c-structuredness indices.

#### Value

A list with the components

- stress: the stress/1 \*sqrt stress(
- stress.m: default normalized stress
- stoploss: the weighted loss value
- indices: the values of the structuredness indices
- parameters: the parameters used for fitting
- fit: the returned object of the fitting procedure smacofx::sammon
- stopobj: the stopobj object

stop\_sammon2

stop\_sammon2

Another STOPS version of Sammon mapping models (via smacofSym)

## **Description**

Uses Smacof, so it can deal with a weight matrix too. The free parameter is lambda for power transformations of the observed proximities. The fitted distances power is internally fixed to 1 and the power for the weights=delta is -1.

## Usage

```
stop_sammon2(
  dis,
  theta = 1,
  type = "ratio",
  ndim = 2,
  weightmat = NULL,
  init = NULL,
  itmaxi = 1000,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

#### **Arguments**

dis	numeric matrix or dist object of a matrix of proximities
theta	the theta vector of powers; this must be a scalar of the lambda transformation for the observed proximities. Defaults to 1.
type	MDS type
ndim	number of dimensions of the target space
weightmat	(optional) a matrix of nonnegative weights
init	(optional) initial configuration
itmaxi	number of iterations
	additional arguments to be passed to the fitting procedure
stressweight	weight to be used for the fit measure; defaults to 1

stop\_smacofSphere 63

structures	which structuredness indices to be included in the loss
strucweight	weight to be used for the structuredness indices; ; defaults to $1/\#$ number of structures
strucpars	the parameters for the structuredness indices
verbose	numeric value hat prints information on the fitting process; $>$ 2 is extremely verbose
stoptype	How to construct the target function for the multi objective optimization? Either 'additive' (default) or 'multiplicative'.
registry	registry object with c-structuredness indices.

## Value

A list with the components

- stress: the stress-1 (sqrt(stress.m))
- stress.m: default normalized stress (used for STOPS)
- stoploss: the weighted loss value
- indices: the values of the structuredness indices
- parameters: the parameters used for fitting (lambda)
- fit: the returned object of the fitting procedure
- stopobj: the stopobj object

stop\_smacofSphere

STOPS versions of smacofSphere models

## **Description**

The free parameter is lambda for power transformations the observed proximities. The fitted distances power is internally fixed to 1 and the power for the weights is 1.

```
stop_smacofSphere(
    dis,
    theta = 1,
    type = "ratio",
    ndim = 2,
    weightmat = NULL,
    init = NULL,
    itmaxi = 1000,
    ...,
    stressweight = 1,
    structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
```

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```
"cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
    "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
    strucweight = rep(1/length(structures), length(structures)),
    strucpars,
    verbose = 0,
    stoptype = c("additive", "multiplicative"),
    registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of powers; this must be a scalar of the lambda transformation

for the observed proximities. Defaults to 1.

type MDS type.

ndim number of dimensions of the target space weightmat (optional) a matrix of nonnegative weights

init (optional) initial configuration

itmaxi number of iterations

. . . additional arguments to be passed to the fitting procedure

stressweight weight to be used for the fit measure; defaults to 1
structures which structuredness indices to be included in the loss

strucweight weight to be used for the structuredness indices; ; defaults to 1/#number of

structures

strucpars the parameters for the structuredness indices

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype How to construct the target function for the multi objective optimization? Either

'additive' (default) or 'multiplicative'

registry object with c-structuredness indices.

## Value

#### A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• indices: the values of the structuredness indices

• parameters: the parameters used for fitting

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

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stop\_smacofSym

STOPS version of smacofSym models

## **Description**

The free parameter is lambda for power transformations the observed proximities. The fitted distances power is internally fixed to 1 and the power for the weights is 1.

## Usage

```
stop_smacofSym(
 dis,
  theta = 1,
  type = "ratio",
  ndim = 2,
 weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  itmaxi = 1000,
  . . . ,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
  "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
  "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity",
    "cstringiness", "cclumpiness", "cinequality"),
  stressweight = 1,
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

## **Arguments**

dis	numeric matrix or dist object of a matrix of proximities	
theta	the theta vector; must be a scalar for the lambda (proximity) transformation. Defaults to 1.	
type	MDS type. Defaults ot 'ratio'.	
ndim	number of dimensions of the target space	
weightmat	(optional) a matrix of nonnegative weights	
init	(optional) initial configuration	
itmaxi	number of iterations	
	additional arguments to be passed to the fitting	
structures	which structuredness indices to be included in the loss	
stressweight	weight to be used for the fit measure; defaults to 1	

stop\_smddae

strucweight	weight to be used for the structuredness indices; ; defaults to 1/#number of structures
strucpars	the parameters for the structuredness indices
verbose	numeric value hat prints information on the fitting process; >2 is extremely verbose
stoptype	How to construct the target function for the multi objective optimization? Either 'additive' (default) or 'multiplicative'
registry	registry object with c-structuredness indices.

#### Value

A list with the components

- stress: the stress-1 (sqrt(stress.m))
- stress.m: default normalized stress (used for STOPS)
- stoploss: the weighted loss value
- indices: the values of the structuredness indices
- parameters: the parameters used for fitting (lambda)
- fit: the returned object of the fitting procedure
- stopobj: the stops object

stop\_smddae STOPS version of sparsified multidimensional distance analysis for fixed eps and tau

## **Description**

smdda with free parameters tau and epsilon.

```
stop_smddae(
    dis,
    theta = c(100, 100),
    type = "ratio",
    weightmat = 1 - diag(nrow(dis)),
    init = NULL,
    ndim = 2,
    itmaxi = 10000,
    ...,
    stressweight = 1,
    structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
```

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```
"cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
strucweight = rep(1/length(structures), length(structures)),
strucpars,
verbose = 0,
stoptype = c("additive", "multiplicative"),
registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of explicit parameters; first is tau for the neighboourhood, sec-

ond is epsilon for isomapdist. Defaults to 100, 100.

type MDS type.

weightmat (optional) a matrix of nonnegative weights

init (optional) initial configuration

ndim number of dimensions of the target space

itmaxi number of iterations

... additional arguments to be passed to the fitting procedure

stressweight weight to be used for the fit measure; defaults to 1

structures a character vector listing the structure indices to use. They always are called

"cfoo" with foo being the structure.

strucweight weight to be used for the structures; defaults to 1/number of structures

strucpars a list of parameters for the structuredness indices; each list element corresponds

to one index in the order of the appearance in structures

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype which weighting to be used in the multi-objective optimization? Either 'addi-

tive' (default) or 'multiplicative'.

registry registry object with c-structuredness indices.

## Value

A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (tau)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

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stop\_smddak STOPS version of sparsified multidimensional distance analysis for

fixed k and tau

Description

smdda with free parameters tau and k.

## Usage

```
stop_smddak(
  dis,
  theta = c(100, 10),
  type = "ratio",
  weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

#### **Arguments**

dis	numeric matrix or dist object of a matrix of proximities	
theta	the theta vector of explicit parameters; first is tau for the neighbourhood, second is k. Defaults to 100, 10.	
type	MDS type.	
weightmat	(optional) a matrix of nonnegative weights	
init	(optional) initial configuration	
ndim	number of dimensions of the target space	
itmaxi	number of iterations	
	additional arguments to be passed to the fitting procedure	
stressweight	weight to be used for the fit measure; defaults to 1	
structures	a character vector listing the structure indices to use. They always are called "cfoo" with foo being the structure.	

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strucweight weight to be used for the structures; defaults to 1/number of structures

a list of parameters for the structuredness indices; each list element corresponds to one index in the order of the appearance in structures

verbose numeric value hat prints information on the fitting process; >2 is extremely verbose

stoptype which weighting to be used in the multi-objective optimization? Either 'additive' (default) or 'multiplicative'.

registry registry object with c-structuredness indices.

#### Value

A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (tau)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

stop\_smds

STOPS version of sparsified MDS.

## **Description**

smds with free tau.

```
stop_smds(
    dis,
    theta = c(100),
    type = "ratio",
    weightmat = 1 - diag(nrow(dis)),
    init = NULL,
    ndim = 2,
    itmaxi = 10000,
    ...,
    stressweight = 1,
    structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
    "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
```

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```
strucweight = rep(1/length(structures), length(structures)),
strucpars,
verbose = 0,
stoptype = c("additive", "multiplicative"),
registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of explicit parameters; tau for the neighbourhood. Defaults to

100.

type MDS type.

weightmat (optional) a matrix of nonnegative weights

init (optional) initial configuration

ndim number of dimensions of the target space

itmaxi number of iterations

.. additional arguments to be passed to the fitting procedure

stressweight weight to be used for the fit measure; defaults to 1

structures a character vector listing the structure indices to use. They always are called

"cfoo" with foo being the structure.

strucweight weight to be used for the structures; defaults to 1/number of structures

strucpars a list of parameters for the structuredness indices; each list element corresponds

to one index in the order of the appearance in structures

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype which weighting to be used in the multi-objective optimization? Either 'addi-

tive' (default) or 'multiplicative'.

registry object with c-structuredness indices.

#### Value

A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (tau)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

stop\_spmddae 71

stop_spmddae	STOPS version of sparsified post multidimensional distance analysis	
	for fixed tau and epsilon.	

## **Description**

Sparsified POST MDDA with free kappa, lambda, rho, tau and epsilon. Phew.

#### Usage

```
stop_spmddae(
  dis,
  theta = c(1, 1, 1, 100, 100),
  type = "ratio",
  weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  . . . ,
  stressweight = 1,
  structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness", "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

# Arguments

dis	numeric matrix or dist object of a matrix of proximities
theta	the theta vector of explicit parameters; the first is kappa (for the fitted distances), the second lambda (for the observed proximities), the third nu (for the weights), the fourth tau (for the neighbourhood), the fifth the epsilon for the geodesic distances. If a scalar or vector shorter than 5 is given it is recycled. Defaults to 1 1 1 100 10.
type	MDS type.
weightmat	(optional) a matrix of nonnegative weights
init	(optional) initial configuration
ndim	number of dimensions of the target space
itmaxi	number of iterations
	additional arguments to be passed to the fitting procedure

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stressweight	weight to be used for the fit measure; defaults to 1
structures	a character vector listing the structure indices to use. They always are called "cfoo" with foo being the structure.
strucweight	weight to be used for the structures; defaults to 1/number of structures
strucpars	a list of parameters for the structuredness indices; each list element corresponds to one index in the order of the appearance in structures
verbose	numeric value hat prints information on the fitting process; >2 is extremely verbose
stoptype	which weighting to be used in the multi-objective optimization? Either 'additive' (default) or 'multiplicative'.
registry	registry object with c-structuredness indices.

#### Value

A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (kappa, lambda, nu, tau)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

 $stop\_spmddak \qquad STOPS \ version \ of \ sparsified \ post \ multidimensional \ distance \ analysis \\ for \ fixed \ tau \ and \ k.$ 

## Description

Sparsified Post MDDA with free kappa, lambda, rho, tau and k. Phew.

```
stop_spmddak(
    dis,
    theta = c(1, 1, 1, 100, 10),
    type = "ratio",
    weightmat = 1 - diag(nrow(dis)),
    init = NULL,
    ndim = 2,
    itmaxi = 10000,
    ...,
    stressweight = 1,
```

stop\_spmddak 73

```
structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
    "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
    strucweight = rep(1/length(structures), length(structures)),
    strucpars,
    verbose = 0,
    stoptype = c("additive", "multiplicative"),
    registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of explicit parameters; the first is kappa (for the fitted distances),

the second lambda (for the observed proximities), the third nu (for the weights), the fourth tau (for the neighbourhood), the fifth the k for the geodesic distances. If a scalar or vector shorter than 5 is given it is recycled. Defaults to 1 1 1 100

10.

type MDS type.

weightmat (optional) a matrix of nonnegative weights

init (optional) initial configuration

ndim number of dimensions of the target space

itmaxi number of iterations

additional arguments to be passed to the fitting procedure

stressweight weight to be used for the fit measure; defaults to 1

structures a character vector listing the structure indices to use. They always are called

"cfoo" with foo being the structure.

strucweight weight to be used for the structures; defaults to 1/number of structures

strucpars a list of parameters for the structuredness indices; each list element corresponds

to one index in the order of the appearance in structures

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype which weighting to be used in the multi-objective optimization? Either 'addi-

tive' (default) or 'multiplicative'.

registry registry object with c-structuredness indices.

#### Value

A list with the components

• stress: the stress-1 value

· stress.m: default normalized stress

• stoploss: the weighted loss value

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- struc: the structuredness indices
- parameters: the parameters used for fitting (kappa, lambda, nu, tau)
- fit: the returned object of the fitting procedure
- stopobj: the stopobj object

stop\_spmds

STOPS version of sparsified POST-MDS for fixed tau

## **Description**

Sparsified power stress with free kappa, lambda, rho and tau.

#### Usage

```
stop_spmds(
  dis,
  theta = c(1, 1, 1, 100),
  type = "ratio",
  weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

#### Arguments

dis	numeric matrix or dist object of a matrix of proximities	
the the theta vector of explicit parameters; the first is kappa (for the fitted distances the second lambda (for the observed proximities), the third nu (for the weights the fourth tau (for the neighbourhood). If a scalar or vector shorter than 4 given it is recycled. Defaults to 1 1 1 100.		
type	MDS type.	
weightmat	(optional) a matrix of nonnegative weights	
init	(optional) initial configuration	

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number of dimensions of the target space ndim number of iterations itmaxi additional arguments to be passed to the fitting procedure stressweight weight to be used for the fit measure; defaults to 1 structures a character vector listing the structure indices to use. They always are called "cfoo" with foo being the structure. strucweight weight to be used for the structures; defaults to 1/number of structures a list of parameters for the structuredness indices; each list element corresponds strucpars to one index in the order of the appearance in structures verbose numeric value hat prints information on the fitting process; >2 is extremely verbose which weighting to be used in the multi-objective optimization? Either 'addistoptype tive' (default) or 'multiplicative'.

#### Value

registry

A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• struc: the structuredness indices

• parameters: the parameters used for fitting (kappa, lambda, nu, tau)

registry object with c-structuredness indices.

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

stop\_sstress STOPS version of sstress

## **Description**

Free parameter is lambda for the observed proximities. Fitted distances are transformed with power 2, weights have exponent of 1. Note that the lambda here works as a multiplicator of 2 (as sstress has f(delta^2)).

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#### Usage

```
stop_sstress(
  dis,
  theta = 1,
  type = type,
  weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 1e+05,
  stressweight = 1,
 structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
   "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  stoptype = c("additive", "multiplicative"),
  registry = struc_reg
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of powers; this must be a scalar of the lambda transformation

for the observed proximities. Defaults to 1. Note that the lambda here works as

a multiplicator of 2 (as sstress has f(delta^2)).

type MDS type.

weightmat (optional) a matrix of nonnegative weights

init (optional) initial configuration

ndim the number of dimensions of the target space

itmaxi number of iterations

... additional arguments to be passed to the fitting procedure

stressweight weight to be used for the fit measure; defaults to 1
structures which structuredness indices to be included in the loss

strucweight weight to be used for the structuredness indices; ; defaults to 1/#number of

structures

strucpars the parameters for the structuredness indices

verbose numeric value hat prints information on the fitting process; >2 is extremely ver-

bose

stoptype How to construct the target function for the multi objective optimization? Either

'additive' (default) or 'multiplicative'

registry registry object with c-structuredness indices.

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## Value

A list with the components

• stress: the stress-1 value

• stress.m: default normalized stress

• stoploss: the weighted loss value

• indices: the values of the structuredness indices

• parameters: the parameters used for fitting (lambda)

• fit: the returned object of the fitting procedure

• stopobj: the stopobj object

summary.stops

S3 summary method for stops

# Description

S3 summary method for stops

## Usage

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

## Arguments

```
object object of class stops
... addditional arguments
```

## Value

```
object of class 'summary.stops'
```

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Swissroll	Swiss roll
JW1331 011	DW iss Tou

## Description

A swiss roll data example where 150 data points are arranged on a swiss roll embedded in a 3D space.

## Usage

```
data(Swissroll)
```

#### **Format**

A data frame with 150 rows and 4 columns

## **Details**

A data frame with the variables (columns)

- x The x axis coordinate for each point
- y The y axis coordinate for each point
- z The z axis coordinate for each point
- col a color code for each point with points along the y axis having the same color (based on the viridis palette)

tgpoptim	Bayesian Optimization by a (treed) Bayesian Gaussian Process Prior
G	(with jumps to linear models) surrogate model Essentially a wrapper for the functionality in tgp that has the same slots as optim with defaults for STOPS models.

## Description

Bayesian Optimization by a (treed) Bayesian Gaussian Process Prior (with jumps to linear models) surrogate model Essentially a wrapper for the functionality in tgp that has the same slots as optim with defaults for STOPS models.

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#### Usage

```
tgpoptim(
    x,
    fun,
    ...,
    initpoints = 10,
    lower,
    upper,
    acc = 1e-08,
    itmax = 10,
    verbose = 0,
    model = "bgp"
)
```

## Arguments

X	optional starting values
fun	function to minimize
• • •	additional arguments to be passed to the function to be optimized
initpoints	the number of points to sample initially to fit the surrogate model
lower	The lower contraints of the search region
upper	The upper contraints of the search region
acc	if the numerical accuracy of two successive target function values is below this, stop the optimization; defaults to 1e-8
itmax	maximum number of iterations
verbose	numeric value hat prints information on the fitting process; >2 is extremely verbose
model	which surrogate model class to use (currently uses defaults only, will extend this

#### Value

A list with the components (for compatibility with optim)

to tweak the model)

- par The position of the optimum in the search space (parameters that minimize the function; argmin fun).
- value The value of the objective function at the optimum (min fun). Note we do not use the last value in the candidate list but the best candidate (which can but need not coincide).
- svalue The value of the surrogate objective function at the optimal parameters
- counts The number of iterations performed at convergence with entries faction for the number of iterations and gradient which is always NA at the moment
- convergence 0 successful completion by the accd or acc criterion, 1 indicate iteration limit was reached, 99 is a problem
- message is NULL (only for compatibility or future use)
- history the improvement history
- tgpout the output of the tgp model

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## **Examples**

```
fbana <- function(x) {
x1 <- x[1]
x2 <- x[2]
100 * (x2 - x1 * x1)^2 + (1 - x1)^2
}
res1<-tgpoptim(c(-1.2,1),fbana,lower=c(-5,-5),upper=c(5,5),acc=1e-16,itmax=20)
res1

fwild <- function (x) 10*sin(0.3*x)*sin(1.3*x^2) + 0.00001*x^4 + 0.2*x+80
plot(fwild, -50, 50, n = 1000, main = "Bayesian GP Optimization minimizing 'wild function'")
set.seed(210485)
res2<-tgpoptim(50, fwild,lower=-50,upper=50,acc=1e-16,itmax=20,model="btgpllm")
points(res2$par,res2$value,col="red",pch=19)</pre>
```

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