Package 'stops'

June 28, 2024

Title Structure Optimized Proximity Scaling

Version 1.6-2

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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, scagnostics, smacof, tgp, vegan

Enhances stats Suggests R.rsp

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LazyData true

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<pre>URL https://r-forge.r-project.org/projects/stops/</pre>
VignetteBuilder R.rsp
Encoding UTF-8
RoxygenNote 7.3.1
NeedsCompilation no
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Repository CRAN
Date/Publication 2024-06-28 07:30:02 UTC

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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).

4 bootmds.stops

Format

A 69 x 70 matrix.

Source

data(bankingCrises) in library(Ecdat)

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", "bi-

nary".

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

c_association	c-association calculates the c-association based on the maximal infor-
_	mation coefficient We define c-association as the aggregated associa-
	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 = max,
  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)

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

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

 $c_clumpiness$

c-clumpiness

Description

Measures the c-clumpiness structure

Usage

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

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.

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Usage

```
c_clusteredness(
  confs,
  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

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)
```

```
delts<-smacof::kinshipdelta
```

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```
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 = min,
  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 min.
alpha	an optional number of cells allowed in the X-by-Y search-grid. Default value is 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.). It provides robustness.

Value

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

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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 = max)
```

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>
```

c_dependence

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

Description

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

Usage

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

c_faithfulness

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, ...)
```

Arguments

confs a numeric matrix or a dist object

obsdiss a symmetric numeric matrix or a dist object k the number of nearest neighbours to be looked at

... additional arguments passed to dist()

Value

```
a numeric value; faithfulness
```

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

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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 = max,
  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 mean
alpha	an optional number of cells allowed in the X-by-Y search-grid. Default value is 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.). It provides robustness.

Value

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

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

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

c_hierarchy

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, p = 2, agglmethod = "complete")
```

Arguments

confs a numeric matrix

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)
```

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.

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Usage

```
c_inequality(confs)
```

Arguments

confs

a numeric matrix or data frame

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>
```

c_linearity

c-linearity calculates c-linearity as the aggregated multiple correlation 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 = max)
```

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)

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

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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.

Usage

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

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)

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

16 c_nonmonotonicity

c_mine	wrapper for getting the mine coefficients	
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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.

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

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

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Usage

```
c_nonmonotonicity(
  confs,
  aggr = max,
  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 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)

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

18 c_regularity

Usage

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

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.

Usage

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

Arguments

confs a numeric matrix or a dist object

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.

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The distance to be computed if X is not a symmetric matrix or a dist object (otherwise ignored). Defaults to Euclidean distance.

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

dmax

```
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

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)
```

Arguments

object an object of class smacofP

Value

a numeric value

c_sparsity

Examples

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

c_skinniness

c-skinniness

Description

Measures the c-skinniness structure

Usage

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

Arguments

conf A numeric matrix.

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

faults to max.

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 = max)
```

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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

c-striatedness

Description

Measures the c-striatedness structure

Usage

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

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)
```

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

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c_stringiness	c-stringiness
C_Stringiness	c bii iii ciicob

Description

Measures the c-stringiness structure

Usage

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

Arguments

conf A numeric matrix.

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

faults to max.

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 = 100, verbose = FALSE)
```

Arguments

object Object of class peops. eps Convergence criterion

itmax Maximum number of iterations

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

knn_dist 23

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.

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="powermds",lower=c(1,1),upper=c(5,5),itmaxps=100)
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)
```

24 ljoptim

Arguments

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

ljoptim

(Adaptive) 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

Х	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 1e-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.

Pendigits500 25

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>
```

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 500×500 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 500×500 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)
```

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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, ...)
```

Arguments

x	an object of class stops
plot.type	String indicating which type of plot to be produced: "confplot", "resplot", "Shepard", "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 represenation of the fitted distances.
• • •	Further plot arguments passed: see 'plot.smacof' and 'plot' for detailed information.
	Details: See plot.smacofP

Value

no return value, just plots

print.stops 27

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

```
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

28 stoploss

residuals.stops

S3 residuals method for stops

Description

S3 residuals method for stops

Usage

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

Arguments

object of class stops
... addditional arguments

Value

a vector of residuals (observed minus fitted distances)

stoploss

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

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

Value

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

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", "mls1", "neldermead", "sbplx", "hjk", "cmaes"),
  lower,
  upper,
  verbose = 0,
```

```
stoptype = c("additive", "multiplicative"),
initpoints = 10,
itmax = 50,
itmaxps = 10000,
model,
control,
...
)
```

Arguments

dis numeric matrix or dist object of a matrix of proximities

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

theta 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.

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

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 in-

dices (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 metaparameters 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 parameter 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=par1Struc1,...)

That can have unintended consequences if the metaparameter is a vector or matrix.

optimmethod

What solver to use. Currently supported are Bayesian optimization with Gaussian 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 ("mls1", mls1), 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'.

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 same length as the parameter vector theta.

numeric value hat prints information on the fitting process; >2 is very verbose. which aggregation for the multi objective target function? Either 'additive' (de-

fault) or 'multiplicative'

number of initial points to fit the surrogate model for Bayesian optimization; default is 10.

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).

maximum number of iterations of the inner optimization (to obtain the PS configuration)

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"

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.

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

lower

upper

verbose

stoptype

initpoints

itmax

itmaxps

model

control

• • •

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
- 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

```
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,
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),
list(alpha=0.6,C=15,var.thr=1e-5,zeta=NULL))
res1<-stops(BankingCrisesDistances[,1:69],loss="stress",verbose=0,
structures=c("cfunctionality", "ccomplexity"), strucpars=strucpar,
lower=0,upper=10,itmax=5)
res1
```

stop_apstress 33

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,
 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")
)
```

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.

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

Value

A list with the components

• 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", "cstriatedness", "coutlying",
        "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
    strucweight = rep(1/length(structures), length(structures)),
```

stop_bcmds 35

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

Arguments

dis numeric matrix or dist object of a matrix of proximities

theta the theta 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.

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'.

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

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stop_clca

STOPS version of CLCA.

Description

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

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")
)
```

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

stop_cldae 37

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'.

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")
)
```

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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'.

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")
)
```

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.

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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'.

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)),
        strucpars,
        verbose = 0,
```

stop_cmdscale 41

```
stoptype = c("additive", "multiplicative"),
itmaxi = 1000,
add = TRUE
)
```

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 disatnces

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

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")
)
```

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
structures	which structuredness indices to be included in the loss

stop_isomap1 43

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'

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

44 stop_isomap1

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

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

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)
- 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 45

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
)
```

Arguments

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.
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

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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

Details

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 cmd-scale (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 time)
- 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_1mds

STOPS version of lMDS

Description

STOPS version of IMDS

```
stop_lmds(
   dis,
   theta = c(2, 0.5),
   type = "ratio",
   weightmat = NULL,
   init = NULL,
   ndim = 2,
```

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```
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")
)
```

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

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 ver-

bose

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

tive' (default) or 'multiplicative'.

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

48 stop_powerelastic

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.

Usage

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

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 streutures 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'.

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

STOPS version of powermds

Description

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

```
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,
```

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

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

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'.

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

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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.

Usage

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

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

stop_powerstress

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'.

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

stop_powerstress

STOPS version of powerstress

Description

Power stress with free kappa and lambda and rho.

```
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")
)
```

stop_powerstress 53

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.

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'.

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

54 stop_rpowerstress

stop_rpowerstress

STOPS version of restricted powerstress

Description

STOPS version of restricted powerstress

Usage

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

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]). 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

stop_rstress 55

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

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

STOPS version of rstress

Description

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

```
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",
```

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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")
)
```

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 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
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'

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_sammon

STOPS version of Sammon mapping

Description

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

Usage

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

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. Ignored here.
ndim	number of dimensions of the target space
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
structures	which structuredness indices to be included in the loss

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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'

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

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.

```
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"),
```

stop_sammon2 59

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

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'.

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

 $stop_smacofSphere$

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.

Usage

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

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

stop_smacofSym 61

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'

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_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.

```
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)),
```

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

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

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'

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 63

stop_smddae STOPS version of sparsified multidimensional distance analysis for fixed eps and tau

Description

smdda with free parameters tau and epsilon.

Usage

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

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, second 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.	

stop_smddak

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'.

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_smddak

STOPS version of sparsified multidimensional distance analysis for fixed k and tau

Description

smdda with free parameters tau and k.

```
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)),
```

stop_smddak 65

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

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.

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'.

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_smds

STOPS version of sparsified MDS.

Description

smds with free tau.

Usage

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

Arguments dis

	J I
theta	the theta vector of explicit parameters; tau for the neighbourhood. Defaults to
	100.
type	MDS type.

numeric matrix or dist object of a matrix of proximities

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

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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'.

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

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.

```
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")
)
```

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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

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'.

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 69

stop_spmddak	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.

Usage

```
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,
 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")
)
```

Arguments

stressweight

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

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

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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'.

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_spmds

STOPS version of sparsified POST-MDS for fixed tau

Description

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

```
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",
```

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

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). If a scalar or vector shorter than 4 is

given it is recycled. Defaults to 1 1 1 100.

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'.

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

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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)).

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")
)
```

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

summary.stops 73

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'

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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CIA/ T	ssr	7 I I
	331 V	

Swiss roll

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 (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

Х	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 to tweak the model)

Value

A list with the components (for compatibility with optim)

- 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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