

# Package ‘stops’

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**Title** Structure Optimized Proximity Scaling

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**Description** A collection of methods that fit nonlinear distance transformations in multidimensional scaling (MDS) and trade-off the fit with structure considerations to find optimal parameters also known as structure optimized proximity scaling (STOPS) (Rusch, Mair & Hornik, 2023, <doi:10.1007/s11222-022-10197-w>). The package contains various functions, wrappers, methods and classes for fitting, plotting and displaying different MDS models in a STOPS framework like Torgerson (classical) scaling, scaling by majorizing a complex function (SMACOF), Sammon mapping, elastic scaling, symmetric SMACOF, spherical SMACOF, s-stress, r-stress, power MDS, power elastic scaling, power Sammon mapping, power stress MDS (POST-MDS), approximate power stress, Box-Cox MDS, local MDS and Isomap. All of these models can also be fit individually with given hyperparameters or by optimizing over hyperparameters based on 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 c-structuredness indices.

**Depends** R (>= 3.5.0), smacof, rgl

**Imports** cordillera, MASS, pso, scatterplot3d, acepack, minerva,  
energy, DiceOptim, DiceKriging, tgp, pomp, vegan, scagnostics,  
clue, cmaes, dfoptim, nloptr

**Enhances** stats

**Suggests** sp, R.rsp

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## R topics documented:

apStressMin . . . . .	4
BankingCrisesDistances . . . . .	5
bcStressMin . . . . .	6
cmds . . . . .	8
cmdscale . . . . .	8
coef.stops . . . . .	9
conf_adjust . . . . .	9
c_association . . . . .	10
c_clumpiness . . . . .	11
c_clusteredness . . . . .	11
c_complexity . . . . .	13
c_convexity . . . . .	14
c_dependence . . . . .	14
c_faithfulness . . . . .	15
c_functionality . . . . .	16
c_hierarchy . . . . .	17
c_inequality . . . . .	17
c_linearity . . . . .	18
c_manifoldness . . . . .	19
c_mine . . . . .	20
c_nonmonotonicity . . . . .	20
c_outlying . . . . .	21
c_regularity . . . . .	22
c_skinniness . . . . .	23
c_sparsity . . . . .	24
c_striatedness . . . . .	24
c_stringiness . . . . .	25
doubleCenter . . . . .	26
enorm . . . . .	26
knn_dist . . . . .	27
ljoptim . . . . .	27
lmds . . . . .	29
mkBmat . . . . .	30
mkPower . . . . .	31
mkPower2 . . . . .	31
Pendigits500 . . . . .	32
plot.cmdscaleE . . . . .	32

plot.smacofP . . . . .	34
plot.stops . . . . .	36
plot3d.cmdscaleE . . . . .	37
plot3d.stops . . . . .	38
plot3dstatic . . . . .	38
plot3dstatic.cmdscaleE . . . . .	39
plot3dstatic.stops . . . . .	40
powerStressMin . . . . .	40
print.cmdscale . . . . .	42
print.sammon . . . . .	43
print.stops . . . . .	43
print.summary.smacofP . . . . .	44
print.summary.stops . . . . .	44
procruster . . . . .	45
residuals.stops . . . . .	45
sammon . . . . .	46
secularEq . . . . .	46
sqdist . . . . .	47
stoploss . . . . .	47
stops . . . . .	48
stop_apstress . . . . .	54
stop_bcstress . . . . .	55
stop_cmdscale . . . . .	57
stop_elastic . . . . .	58
stop_isomap1 . . . . .	59
stop_isomap2 . . . . .	61
stop_lmids . . . . .	63
stop_powerelastic . . . . .	64
stop_powermids . . . . .	65
stop_powersammon . . . . .	67
stop_powerstress . . . . .	68
stop_rpowerstress . . . . .	70
stop_rstress . . . . .	71
stop_sammon . . . . .	73
stop_sammon2 . . . . .	74
stop_smacofSphere . . . . .	75
stop_smacofSym . . . . .	77
stop_sstress . . . . .	78
summary.cmdscale . . . . .	80
summary.sammon . . . . .	80
summary.smacofP . . . . .	81
summary.stops . . . . .	81
Swissroll . . . . .	82
tgoptim . . . . .	82
torgerson . . . . .	84

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apStressMin

*Approximate Power Stress SMACOF*


---

### Description

Minimize approximate power stress by minimization-majorization.

### Usage

```
apStressMin(
  delta,
  tau = 1,
  ups = 1,
  weightmat = 1 - diag(nrow(delta)),
  init = NULL,
  ndim = 2,
  eps = 1e-06,
  itmax = 1000,
  verbose = FALSE
)
```

### Arguments

delta	dist object or a symmetric, numeric data.frame or matrix of distances
tau	the power of the transformation of the proximities; defaults to 1
ups	the power of the transformation for weightmat; defaults to 1
weightmat	a square, symmetric matrix of finite weights (same dimensions as delta)
init	starting configuration
ndim	dimension of the configuration; defaults to 2
eps	numeric accuracy of the iteration
itmax	maximum number of iterations
verbose	should iteration output be printed; if TRUE then yes

### Value

an object of class 'smacofP' (inheriting from 'smacofB', see [smacofSym](#)). It is a list with the components

- delta: Observed dissimilarities, not normalized
- obsdiss: Observed transformed dissimilarities
- dhats: Observed transformed dissimilarities, normalized
- confdist: Configuration dissimilarities, NOT normalized
- conf: Matrix of fitted configuration, NOT normalized

- stress: Default stress (stress 1; sqrt of explicitly normalized stress)
- spp: Stress per point (based on stress.en)
- ndim: Number of dimensions
- model: Name of MDS model
- niter: Number of iterations
- nobj: Number of objects
- type: Type of MDS model
- weightmat: weighting matrix
- pars: hyperparameter vector theta

and some additional components

- stress.m: default stress for the COPS and STOP defaults to the explicitly normalized stress on the normalized, transformed dissimilarities. The square of stress-1 in stress.
- deltaorig: observed, untransformed dissimilarities
- tau: tau parameter
- ups: epsilon parameter

### Author(s)

Thomas Rusch

### See Also

[smacofSym](#)

### Examples

```
dis<-smacof::kinshipdelta
res<-apStressMin(as.matrix(dis),tau=2,ups=0.7)
res
summary(res)
plot(res)
```

---

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).

**Format**

A 69 x 70 matrix.

**Source**

data(bankingCrises) in library(Ecdat)

---

bcStressMin

*An MDS version for minimizing BoxCox Stress (Chen & Buja 2013)*

---

**Description**

An MDS version for minimizing BoxCox Stress (Chen & Buja 2013)

**Usage**

```
bcStressMin(
  delta,
  init = NULL,
  verbose = 0,
  ndim = 2,
  mu = 1,
  lambda = 1,
  rho = 0,
  itmax = 2000,
  addD0 = 1e-04
)
```

**Arguments**

delta	dissimilarity or distance matrix
init	initial configuration. If NULL a classical scaling solution is used.
verbose	prints progress if > 3.
ndim	the dimension of the configuration
mu	mu parameter. Should be 0 or larger for everything working ok. If mu<0 it works but the model is strange and normalized stress tends towards 0 regardless of fit. Use normalized stress at your own risk in that case.
lambda	lambda parameter. Must be larger than 0.
rho	the rho parameter.
itmax	number of optimizing iterations, defaults to 2000.
addD0	a small number that's added for D(X)=0 for numerical evaluation of worst fit (numerical reasons, see details). If addD0=0 the normalized stress for mu!=0 and mu+lambda!=0 is correct, but will give useless normalized stress for mu=0 or mu+lambda!=0.

## Details

For numerical reasons with certain parameter combinations, the normalized stress uses a configuration as worst result where every  $d(X)$  is  $0 + \text{addD0}$ . The same number is not added to the delta so there is a small inaccuracy of the normalized stress (but negligible if  $\min(\text{delta}) \gg \text{addD0}$ ). Also, for  $\mu < 0$  or  $\mu + \lambda < 0$  the normalization cannot generally be trusted (in the worst case of  $D(X) = 0$  one would have an  $0^{(-a)}$ ).

## Value

an object of class 'bcmnds' (also inherits from 'smacofP'). It is a list with the components

- delta: Observed dissimilarities, not normalized
- obsdiss: Observed transformed dissimilarities, not normalized
- confdist: Configuration dissimilarities, NOT normalized
- conf: Matrix of fitted configuration, NOT normalized
- stress: Default stress (stress 1; sqrt of explicitly normalized stress)
- ndim: Number of dimensions
- model: Name of MDS model
- niter: Number of iterations
- nobj: Number of objects
- pars: hyperparameter vector theta

and some additional components

- stress.m: default stress is the explicitly normalized stress on the normalized, transformed dissimilarities
- deltaorig: observed, untransformed dissimilarities
- mu: mu parameter (for attraction)
- lambda: lambda parameter (for repulsion)
- rho: rho parameter (for weights)

## Author(s)

Lisha Chen & Thomas Rusch

## Examples

```
dis<-smacof::kinshipdelta
res<-bcStressMin(as.matrix(dis),mu=2,lambda=1.5,rho=0)
res
summary(res)
plot(res)
```

---

cmds	<i>normalization function Classical Scaling</i>
------	---

---

**Description**

normalization function Classical Scaling

**Usage**

cmds(Do)

**Arguments**

Do                   dissimilarity matrix

---

cmdscale	<i>Wrapper to cmdscale for S3 class</i>
----------	---

---

**Description**

Wrapper to cmdscale for S3 class

**Usage**

cmdscale(d, k = 2, eig = TRUE, ...)

**Arguments**

d                    a distance structure such as that returned by 'dist' or a full symmetric matrix containing the dissimilarities

k                    the maximum dimension of the space which the data are to be represented in

eig                  indicates whether eigenvalues should be returned.

...                  additional parameters passed to cmdscale. See [cmdscale](#)

**Details**

overloads base::cmdscale and adds class attributes for which there are methods. The functionality is duplicated in the cops package.

**Value**

An object of class 'cmdscaleE' and inheriting from [cmdscale](#). This function just adds an extra slot to the list with the call, adds column labels to the \$points.



---

coef.stops	<i>S3 coef method for stops objects</i>
------------	---

---

**Description**

S3 coef method for stops objects

**Usage**

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

**Arguments**

object	object of class stops
...	additional arguments

**Value**

a vector of hyperparameters theta

---

conf_adjust	<i>conf_adjust: a function to procrustes adjust two matrices</i>
-------------	--

---

**Description**

conf\_adjust: a function to procrustes adjust two matrices

**Usage**

```
conf_adjust(conf1, conf2, verbose = FALSE, eps = 1e-12, itmax = 100)
```

**Arguments**

conf1	reference configuration, a numeric matrix
conf2	another configuration to be adjusted, a numeric matrix
verbose	should adjustment be output; default to FALSE
eps	numerical accuracy
itmax	maximum number of iterations

**Value**

A list of configuration matrices. The 'ref.conf' is the reference configuration, the 'other.conf' is the Procrustes adjusted configuration and the 'comparison.conf' is the one that was adjusted.

---

c_association	<i>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</i>
---------------	---

---

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

### Value

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

### Examples

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

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

---

c_clumpiness	<i>c-clumpiness</i>
--------------	---------------------

---

### 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. Defaults 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)
```

---

c_clusteredness	<i>c-clusteredness calculates c-clusteredness as the OPTICS cordillera. The higher the more clustered.</i>
-----------------	--

---

### Description

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

**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 (corresponds to $k$ in the paper). It is passed to <code>optics</code> where it is called <code>minPts</code> . Defaults to 2.
q	The norm used for the Cordillera. Defaults to 2.
epsilon	The epsilon parameter for OPTICS (called <code>epsilon_max</code> in the paper). Defaults to 2 times the maximum distance between any two points.
distmeth	The distance to be computed if $X$ is not a symmetric matrix or a dist object (otherwise ignored). Defaults to Euclidean distance.
dmax	The winsorization value for the highest allowed reachability. If used for comparisons between different configurations this should be supplied. If no value is supplied, it is NULL (default); then <code>dmax</code> 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 $X/\max(\text{standard deviation}(\text{allcolumns}))$ . If 4, no centering is applied and scaling of all columns is done as $X/\max(\text{rmsq}(\text{allcolumns}))$ . If FALSE, 0 or any other numeric value, no standardisation is applied. Defaults to 0.
...	Additional arguments to be passed to <code>cordillera::cordillera</code>

**Value**

a numeric value; clusteredness (see `cordillera`)

**Examples**

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

```
dis<-smacofSym(delts)$confdist
c_clusteredness(dis,minpts=3)
```

---

c_complexity	<i>c-complexity</i> 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
C	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](#))

**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)
```

---

c_convexity	<i>c-convexity</i>
-------------	--------------------

---

**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. Defaults 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)
```

---

c_dependence	<i>c-dependence calculates c-dependence as the aggregated distance correlation of each pair if nonidentical columns</i>
--------------	---

---

**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)
```

**Arguments**

confs	a numeric matrix or data frame
aggr	the aggregation function for configurations of more than two dimensions. Defaults 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)
```

---

c_faithfulness	<i>c-faithfulness calculates the c-faithfulness based on the index by Chen and Buja 2013 (M_adj) with equal input neighbourhoods</i>
----------------	--

---

**Description**

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

**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

**Examples**

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

---

c_functionality	<i>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</i>
-----------------	--

---

### 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
C	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 maximum edge value MEV, see [mine](#))

### Examples

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



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

---

c_hierarchy	<i>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.</i>
-------------	---

---

### Description

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.

### 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 <a href="#">hclust</a> .

### Value

a numeric value; hierarchy (see [cl\\_validity](#))

### Examples

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

---

c_inequality	<i>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.</i>
--------------	--

---

### Description

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

**Usage**

```
c_inequality(confs)
```

**Arguments**

confs            a numeric matrix or data frame

**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)
```

---

c_linearity	<i>c-linearity calculates c-linearity as the aggregated multiple correlation of all columns of the configuration.</i>
-------------	---

---

**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. Defaults to max.

**Value**

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

**Examples**

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

---

c_manifoldness	<i>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.</i>
----------------	---

---

### 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. Defaults to max.

### Value

a numeric value; manifoldness (aggregated maximal correlation, correlation of ACE transformed x and y, see [ace](#))

### Examples

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

---

c_mine	<i>wrapper for getting the mine coefficients</i>
--------	--

---

### Description

wrapper for getting the mine coefficients

### Usage

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

### Arguments

conf	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
C	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	<i>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</i>
-------------------	--

---

### Description

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

**Usage**

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

---

c\_outlying

*c-outlying*


---

**Description**

Measures the c-outlying structure

**Usage**

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

**Arguments**

conf	A numeric matrix.
aggr	the aggregation function for configurations of more than two dimensions. Defaults to max.

**Value**

a numeric value; outlying (see [scagnostics](#))

**Examples**

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

---

c_regularity	<i>c-regularity calculates c-regularity as 1 - OPTICS cordillera for k=2. The higher the more regular.</i>
--------------	--

---

**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.

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

**Value**

a numeric value; regularity

**Examples**

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

---

c\_skininess

*c-skininess*


---

**Description**

Measures the c-skininess structure

**Usage**

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

**Arguments**

conf	A numeric matrix.
aggr	the aggregation function for configurations of more than two dimensions. Defaults to max.

**Value**

a numeric value; skininess (see [scagnostics](#))

**Examples**

```
delts<-smacof::kinshipdelta
conf<-smacof::smacofSym(delts)$conf
plot(conf,pch=19,asp=1)
c_skininness(conf)
```

---

c_sparsity	<i>c-sparsity</i>
------------	-------------------

---

**Description**

Measures the c-sparsity structure

**Usage**

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

**Arguments**

conf	A numeric matrix.
aggr	the aggregation function for configurations of more than two dimensions. Defaults 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)
```

---

c_striatedness	<i>c-striatedness</i>
----------------	-----------------------

---

**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. Defaults to max.

**Value**

a numeric value; striatedness (see [scagnostics](#))

**Examples**

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

---

c_stringiness	<i>c-stringiness</i>
---------------	----------------------

---

**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. Defaults 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)
```

---

doubleCenter	<i>double centering</i>
--------------	-------------------------

---

**Description**

double centering

**Usage**

doubleCenter(x)

**Arguments**

x                    numeric matrix

---

enorm	<i>Explicit Norm</i>
-------	----------------------

---

**Description**

Explicit Norm

**Usage**

enorm(x, w = 1)

**Arguments**

x                    numeric matrix  
w                    weight

**Value**

a numeric scalar; the sum( $w*x^2$ )

---

knn_dist	<i>calculate k nearest neighbours from a distance matrix</i>
----------	--

---

**Description**

calculate k nearest neighbours from a distance matrix

**Usage**

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

**Arguments**

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

---

ljoptim	<i>(Adaptive) Version of Luus-Jaakola Optimization</i>
---------	--

---

**Description**

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

**Usage**

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

**Arguments**

x	optional starting values
fun	function to minimize
...	additional arguments to be passed to the function to be optimized
red	value of the reduction of the search region
lower	The lower constraints of the search region
upper	The upper constraints 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 that prints information on the fitting process; >2 is extremely verbose
adaptive	should the adaptive version be used? defaults to TRUE.

**Value**

A list with the components ([optim](#))

- par The position of the optimum 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 fcn 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
```

---

lmds

*An function for local MDS (Chen & Buja 2006)*


---

### Description

An function for local MDS (Chen & Buja 2006)

### Usage

```
lmds(delta, init = NULL, ndim = 3, k = 2, tau = 1, itmax = 5000, verbose = 0)
```

### Arguments

delta	dissimilarity or distance matrix
init	initial configuration. If NULL a classical scaling solution is used.
ndim	the dimension of the configuration
k	the k neighbourhood parameter
tau	the penalty parameter (suggested to be in [0,1])
itmax	number of optimizing iterations, defaults to 5000.
verbose	prints progress if > 4.

### Details

Note that k and tau are not independent. It is possible for normalized stress to become negative if the tau and k combination is so that the absolute repulsion for the found configuration dominates the local stress substantially less than the repulsion term does for the solution of  $D(X)=\Delta$ , so that the local stress difference between the found solution and perfect solution is nullified. This can typically be avoided if tau is between 0 and 1. If not, set k and or tau to a smaller value.

### Value

an object of class 'lmds' (also inherits from 'smacofP'). See [powerStressMin](#). It is a list with the components as in power stress

- delta: Observed dissimilarities, not normalized
- obsdiss: Observed transformed dissimilarities, not normalized
- confdist: Configuration dissimilarities, NOT normalized
- conf: Matrix of fitted configuration, NOT normalized
- stress: Default stress (stress 1; sqrt of explicitly normalized stress)
- ndim: Number of dimensions
- model: Name of MDS model
- niter: Number of iterations
- nobj: Number of objects

- pars: hyperparameter vector theta

and some additional components

- stress.m: default stress is the explicitly normalized stress on the normalized, transformed dissimilarities
- deltaorig: observed, untransformed dissimilarities
- tau: tau parameter
- k: k parameter

### Author(s)

Lisha Chen & Thomas Rusch

### Examples

```
dis<-smacof::kinshipdelta
res<- lmds(as.matrix(dis),k=2,tau=0.1)
res
summary(res)
plot(res)
```

---

mkBmat

*MkBmat function (internal)*

---

### Description

MkBmat function (internal)

### Usage

```
mkBmat(x)
```

### Arguments

x                    matrix

---

mkPower	<i>MakePower Old</i>
---------	----------------------

---

**Description**

MakePower Old

**Usage**

mkPower(x, r)

**Arguments**

x	matrix
r	numeric (power)

**Value**

the matrix to a power

---

mkPower2	<i>MakePower</i>
----------	------------------

---

**Description**

MakePower

**Usage**

mkPower2(x, theta)

**Arguments**

x	matrix
theta	numeric (power)

Pendigits500

*Pen digits*

---

**Description**

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

**Usage**

```
data(Pendigits500)
```

**Format**

A data frame with 500 rows and 17 variables

**Details**

The variables are

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

**Source**

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

---

plot.cmdscaleE*S3 plot method for cmdscaleE*

---

**Description**

S3 plot method for cmdscaleE



**Usage**

```
## S3 method for class 'cmdscaleE'
plot(
  x,
  plot.type = c("confplot"),
  plot.dim = c(1, 2),
  col,
  label.conf = list(label = TRUE, pos = 3, col = 1, cex = 0.8),
  identify = FALSE,
  type = "p",
  pch = 20,
  asp = 1,
  main,
  xlab,
  ylab,
  xlim,
  ylim,
  legpos,
  ...
)
```

**Arguments**

x	cmdscaleE object
plot.type	type of plot
plot.dim	dimensions used for plotting
col	color
label.conf	list of label options
identify	boolean flag for interactively identify points
type	type of plot
pch	plotting character
asp	aspect ratio (defaults to 1)
main	main title
xlab	label of x axis
ylab	label of y axis
xlim	limits of x axis
ylim	limits of y axis
legpos	position of legend
...	additional arguments passed to plot

**Details**

This function duplicates the plot method for smacof so it can be used with cmdscaleE objects. See [plot.smacof](#) for the arguments.

**Value**

No return value, just plots a 'cmdscaleE' object.

---

plot.smacofP	<i>S3 plot method for smacofP objects</i>
--------------	---

---

**Description**

S3 plot method for smacofP objects

**Usage**

```
## S3 method for class 'smacofP'
plot(
  x,
  plot.type = "confplot",
  plot.dim = c(1, 2),
  bubscale = 5,
  col,
  label.conf = list(label = TRUE, pos = 3, col = 1, cex = 0.8),
  identify = FALSE,
  type = "p",
  pch = 20,
  asp = 1,
  main,
  xlab,
  ylab,
  xlim,
  ylim,
  legend = TRUE,
  legpos,
  loess = TRUE,
  ...
)
```

**Arguments**

x	an object of class smacofP
plot.type	String indicating which type of plot to be produced: "confplot", "resplot", "Shepard", "stressplot", "transplot", "bubbleplot" (see details)
plot.dim	dimensions to be plotted in confplot; defaults to c(1, 2)
bubscale	Scaling factor (size) for the bubble plot
col	vector of colors for the points
label.conf	List with arguments for plotting the labels of the configurations in a configuration plot (logical value whether to plot labels or not, label position, label color)

identify	If 'TRUE', the 'identify()' function is called internally that allows to add configuration labels by mouse click
type	What type of plot should be drawn (see also 'plot')
pch	Plot symbol
asp	Aspect ratio; defaults to 1 so distances between x and y are represented accurately; can lead to slightly weird looking plots if the variance on one axis is much smaller than on the other axis; use NA if the standard type of R plot is wanted where the ylim and xlim arguments define the aspect ratio - but then the distances seen are no longer accurate
main	plot title
xlab	label of x axis
ylab	label of y axis
xlim	scale of x axis
ylim	scale of y axis
legend	Flag whether legends should be drawn for plots that have legends
legpos	Position of legend in plots with legends
loess	should loess fit be added to Shepard plot
...	Further plot arguments passed: see 'plot.smacof' and 'plot' for detailed information.

## Details

- Configuration plot (plot.type = "confplot"): Plots the MDS configurations.
- Residual plot (plot.type = "resplot"): Plots the dissimilarities against the fitted distances with a linear regression line (without an intercept as in ratio MDS).
- Linearized Shepard diagram (plot.type = "Shepard"): Diagram with the transformed observed dissimilarities against the transformed fitted distance as well as loess curve and a least squares line. The fitted lines do not have an intercept.
- Transformation Plot (plot.type = "transplot"): Diagram with the observed dissimilarities (lighter) and the transformed observed dissimilarities (darker) against the fitted distances together with the nonlinear regression curve (no intercept). Works for lmds or bcStress models too, but is somewhat nonsensical due to them being energy models.
- Stress decomposition plot (plot.type = "stressplot"): Plots the stress contribution in of each observation. Note that it rescales the stress-per-point (SPP) from the corresponding smacof function to percentages (sum is 100). The higher the contribution, the worse the fit. Only implemented for models from the classical stress world, not for bcmds or lmds (throws an error).
- Bubble plot (plot.type = "bubbleplot"): Combines the configuration plot with the point stress contribution. The larger the bubbles, the better the fit. Only implemented for models from the classical stress world, bcmds or lmds (throws an error).

## Value

no return value; just plot for class 'smacofP' (see details)

---

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 = c("confplot"), main, asp = NA, ...)
```

**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 NA; setting to 1 will lead to an accurate representation of the fitted distances.
...	Further plot arguments passed: see 'plot.smacof' and 'plot' for detailed information. Details: <ul style="list-style-type: none"> <li>• Configuration plot (plot.type = "confplot"): Plots the MDS configurations.</li> <li>• Residual plot (plot.type = "resplot"): Plots the dissimilarities against the fitted distances.</li> <li>• Linearized Shepard diagram (plot.type = "Shepard"): Diagram with the transformed observed dissimilarities against the transformed fitted distance as well as loess smooth and a least squares line.</li> <li>• Stress decomposition plot (plot.type = "stressplot", only for SMACOF objects in \$fit): Plots the stress contribution in of each observation. Note that it rescales the stress-per-point (SPP) from the corresponding smacof function to percentages (sum is 100). The higher the contribution, the worse the fit.</li> <li>• Bubble plot (plot.type = "bubbleplot", only available for SMACOF objects \$fit): Combines the configuration plot with the point stress contribution. The larger the bubbles, the better the fit.</li> </ul>

**Value**

no return value, just plots

---

plot3d.cmdscaleE      *S3 plot3d method for class cmdscaleE*

---

### Description

This methods produces a dynamic 3D configuration plot.

### Usage

```
## S3 method for class 'cmdscaleE'  
plot3d(  
  x,  
  plot.dim = c(1, 2, 3),  
  xlab,  
  ylab,  
  zlab,  
  col,  
  main,  
  bgpng = NULL,  
  ax.grid = TRUE,  
  sphere.rgl = FALSE,  
  ...  
)
```

### Arguments

x	object of class cmdscaleE
plot.dim	vector of length 3 with dimensions to be plotted
xlab	label of x axis
ylab	label of y axis
zlab	label of z axis
col	color of the text labels
main	plot title
bgpng	Background image from rgl library; 'NULL' for white background
ax.grid	If 'TRUE', axes grid is plotted.
sphere.rgl	If 'TRUE', rgl sphere (background) is plotted.
...	Further plot arguments passed: see 'plot3d' in package 'rgl' for detailed information.

### Value

No return value, just plots a 'cmdscale' object.

---

plot3d.stops	<i>S3 plot3d method for class stops</i>
--------------	---

---

**Description**

This methods produces a dynamic 3D configuration plot.

**Usage**

```
## S3 method for class 'stops'
plot3d(x, ...)
```

**Arguments**

x	object of class stops
...	Further plot arguments to the method of the class of slot \$fit, see <a href="#">plot.smacof</a> or <a href="#">plot3d.cmdscaleE</a> . Also see 'rgl' in package 'rgl'

**Value**

no return value, just plots

---

plot3dstatic	<i>plot3dstatic: static 3D plots</i>
--------------	--------------------------------------

---

**Description**

A static 3d plot S3 generic

**Usage**

```
plot3dstatic(x, plot.dim = c(1, 2, 3), main, xlab, ylab, zlab, col, ...)
```

**Arguments**

x	object
plot.dim	dimensions to plot
main	main title
xlab	label for x axis
ylab	label for y axis
zlab	label for z axis
col	color
...	other arguments

**Details**

A static 3d plot

**Value**

No return value, just plots.

---

plot3dstatic.cmdscaleE

*3D plots: plot3dstatic method for class cmdscaleE*

---

**Description**

This methods produces a static 3D configuration plot.

**Usage**

```
## S3 method for class 'cmdscaleE'  
plot3dstatic(x, plot.dim = c(1, 2, 3), main, xlab, ylab, zlab, col, ...)
```

**Arguments**

x	object of class cmdscaleE
plot.dim	vector of length 3 with dimensions to be plotted
main	plot title
xlab	label of x axis
ylab	label of y axis
zlab	label of z axis
col	color of the text labels
...	Further plot arguments passed: see 'scatterplot3d' in package 'scatterplot3d' for detailed information.

**Value**

No return value, just plots a 'cmdscaleE' object.

---

`plot3dstatic.stops`      *S3 plot3dstatic method for class stops*

---

### Description

This methods produces a static 3D configuration plot.

### Usage

```
## S3 method for class 'stops'
plot3dstatic(x, ...)
```

### Arguments

`x`                    object of class stops  
`...`                Further plot arguments to the method of the class of slot fit, see [plot3dstatic](#) or [plot3dstatic.cmdscaleE](#). Also see 'scatterplot3d' in package 'scatterplot3d'.

### Value

no return value, just plots

---

`powerStressMin`      *Power Stress SMACOF*

---

### Description

An implementation to minimize power stress by minimization-majorization. Usually more accurate but slower than `powerStressFast`.

### Usage

```
powerStressMin(
  delta,
  kappa = 1,
  lambda = 1,
  nu = 1,
  weightmat = 1 - diag(nrow(delta)),
  init = NULL,
  ndim = 2,
  acc = 1e-10,
  itmax = 50000,
  verbose = FALSE
)
```



**Arguments**

delta	dist object or a symmetric, numeric data.frame or matrix of distances
kappa	power of the transformation of the fitted distances; defaults to 1
lambda	the power of the transformation of the proximities; defaults to 1
nu	the power of the transformation for weightmat; defaults to 1
weightmat	a matrix of finite weights
init	starting configuration
ndim	dimension of the configuration; defaults to 2
acc	numeric accuracy of the iteration
itmax	maximum number of iterations. Defaults to 50000.
verbose	should iteration output be printed; if > 1 then yes

**Value**

an object of class 'smacofP' (inheriting from 'smacofB', see [smacofSym](#)). It is a list with the components

- delta: Observed dissimilarities, not normalized
- obsdiss: Observed transformed dissimilarities, not normalized
- confdist: Configuration dissimilarities, NOT normalized
- conf: Matrix of fitted configuration, NOT normalized
- stress: Default stress (stress 1; sqrt of explicitly normalized stress)
- spp: Stress per point (based on stress.en)
- ndim: Number of dimensions
- model: Name of smacof model
- niter: Number of iterations
- nobj: Number of objects
- type: Type of MDS model
- weightmat: weighting matrix
- pars: hyperparameter vector theta

and some additional components

- stress.m: default stress is the explicitly normalized stress on the normalized, transformed dissimilarities
- deltaorig: observed, untransformed dissimilarities
- kappa: kappa parameter
- lambda: lambda parameter
- nu: nu parameter (aka rho)

**Note**

The functionality related to power stress and the 'smacofP' class is also available in the 'cops' package. Expect masking when both are loaded.

**Author(s)**

Jan de Leeuw & Thomas Rusch

**See Also**

[smacofSym](#)

**Examples**

```
dis<-smacof::kinshipdelta
res<-powerStressMin(as.matrix(dis),kappa=2,lambda=1.5,nu=2,
                    weightmat=as.matrix(dis/2),itmax=1000)
res
summary(res)
plot(res)
```

---

print.cmdscale	<i>S3 print method for cmdscale</i>
----------------	-------------------------------------

---

**Description**

S3 print method for cmdscale

**Usage**

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

**Arguments**

x	cmdscale object
...	additional arguments

**Value**

No return value, just prints.

---

print.sammon	<i>S3 print method for sammon objects</i>
--------------	---

---

**Description**

S3 print method for sammon objects

**Usage**

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

**Arguments**

x	cmdscale object
...	additional arguments

**Value**

No return value, just prints.

---

print.stops	<i>S3 print method for stops objects</i>
-------------	--

---

**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.smacofP` *S3 print method for summary.smacofP*

---

**Description**

S3 print method for `summary.smacofP`

**Usage**

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

**Arguments**

`x` object of class `summary.smacofP`  
`...` additional arguments

**Value**

No return value, just prints a `'summary.smacofP'`

---

`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

---

procruster	<i>procruster: a procrustes function</i>
------------	--

---

**Description**

procruster: a procrustes function

**Usage**

```
procruster(x)
```

**Arguments**

x                    numeric matrix

**Value**

A double or complex matrix.

---

residuals.stops	<i>S3 residuals method for stops</i>
-----------------	--------------------------------------

---

**Description**

S3 residuals method for stops

**Usage**

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

**Arguments**

object                object of class stops  
...                    additional arguments

**Value**

a vector of residuals (observed minus fitted distances)

---

sammon	<i>Wrapper to sammon for S3 class</i>
--------	---------------------------------------

---

**Description**

Wrapper to sammon for S3 class

**Usage**

```
sammon(d, y = NULL, k = 2, ...)
```

**Arguments**

d	a distance structure such as that returned by 'dist' or a full symmetric matrix. Data are assumed to be dissimilarities or relative distances, but must be positive except for self-distance. This can contain missing values.
y	An initial configuration. If NULL, 'cmdscale' is used to provide the classical solution. (If there are missing values in 'd', an initial configuration must be provided.) This must not have duplicates.
k	The dimension of the configuration
...	Additional parameters passed to sammon, see <a href="#">sammon</a>

**Details**

overloads MASS::sammon and adds class attributes for which there are methods. The functionality is duplicated in the cops package.

**Value**

An object of class 'sammonE' that inherits from [sammon](#). This function only adds an extra slot to the list with the call, adds column labels to the \$points and assigns S3 classes 'sammonE', 'cmdscale'. It also adds a slot obsdiss with normalized dissimilarities.

---

secularEq	<i>Secular Equation</i>
-----------	-------------------------

---

**Description**

Secular Equation

**Usage**

```
secularEq(a, b)
```

**Arguments**

a	matrix
b	matrix

---

sqdist	<i>Squared distances</i>
--------	--------------------------

---

**Description**

Squared distances

**Usage**

```
sqdist(x)
```

**Arguments**

x	numeric matrix
---	----------------

**Value**

a matrix of squared distances

---

stoploss	<i>Calculate the weighted multiobjective loss function used in STOPS</i>
----------	--

---

**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,
  type = 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).
type	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	<i>stops: structure optimized proximity scaling</i>
-------	---

---

**Description**

A package for "structure optimized proximity scaling" (STOPS), a collection of methods that fit nonlinear distance transformations in multidimensional scaling (MDS) and trade-off the fit with structure considerations to find optimal parameters or optimal configurations. The package contains various functions, wrappers, methods and classes for fitting, plotting and displaying different MDS models in a STOPS framework like Torgerson scaling, SMACOF, Sammon mapping, elastic scaling, symmetric SMACOF, spherical SMACOF, sstress, rstress, powermds, power elastic scaling, power sammon mapping, power stress, Isomap, approximate power stress, restricted power stress. All of these models can also be fit as MDS variants (i.e., no structuredness). The package further contains functions for optimization (Adaptive Luus-Jaakola and for Bayesian optimization with treed Gaussian process with jump to linear models) and functions for various structuredness indices. This allows to fit STOPS models as described in Rusch, Mair, Hornik (2023).

**Usage**

```
stops(
  dis,
  loss = c("strain", "stress", "smacofSym", "powerstress", "powermds", "powerelastic",
    "powerstrain", "elastic", "sammon", "sammon2", "smacofSphere", "powersammon",
    "rstress", "sstress", "isomap", "isomapeps", "bcstress", "lmds", "apstress",
    "rpowerstress"),
```



```

theta = 1,
structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
  "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
  "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
  "cskinniness", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
ndim = 2,
weightmat = NULL,
init = NULL,
stressweight = 1,
strucweight,
strucpars,
optimmethod = c("SANN", "ALJ", "pso", "Kriging", "tgp", "DIRECT", "stogo", "cobyla",
  "crs2lm", "isres", "mlsl", "neldermead", "sbplx", "hjk", "cmaes"),
lower,
upper,
verbose = 0,
type = c("additive", "multiplicative"),
initpoints = 10,
itmax = 50,
itmaxps = 10000,
model,
control,
...
)

```

### Arguments

<code>dis</code>	numeric matrix or dist object of a matrix of proximities
<code>loss</code>	which loss function to be used for fitting, defaults to stress.
<code>theta</code>	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 <code>stop_XXX</code> 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.
<code>structures</code>	character vector of which c-structuredness indices should be considered; if missing no structure is considered.
<code>ndim</code>	number of dimensions of the target space
<code>weightmat</code>	(optional) a matrix of nonnegative weights; defaults to 1 for all off diagonals
<code>init</code>	(optional) initial configuration
<code>stressweight</code>	weight to be used for the fit measure; defaults to 1
<code>strucweight</code>	vector of weights to be used for the c-structuredness indices (in the same order as in structures); defaults to $-1/\text{length}(\text{structures})$ for each index
<code>strucpars</code>	(possibly named with the structure). Metaparameters for the structuredness indices (gamma in the article). It's safest for it be a list of lists with the named arguments for the structuredness indices and the order of the lists must be like the

order of structures. So something like this `list(list(par1Struc1=par1Struc1,par2Struc1=par2Struc1,par3Struc1=par3Struc1),parYStrucX)` 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=par2Struc2,par2Struc2=par1Struc2,...))`. That can have unintended consequences if the metaparameter is a vector or matrix.

<code>optimmethod</code>	What solver to use. Currently supported are Bayesian optimization with Gaussian Process priors and Kriging ("Kriging"), Bayesian optimization with treed Gaussian processes with jump to linear models ("tgp"), Adaptive LJ Search ("ALJ"), Particle Swarm optimization ("pso"), simulated annealing ("SANN"), "DIRECT", Stochastic Global Optimization ("stogo"), COBYLA ("cobyla"), Controlled Random Search 2 with local mutation ("crs2lm"), Improved Stochastic Ranking Evolution Strategy ("isres"), Multi-Level Single-Linkage ("mlsl"), Nelder-Mead ("neldermead"), Subplex ("sbplx"), Hooke-Jeeves Pattern Search ("hjk"), CMA-ES ("cmaes"). Defaults to "ALJ" version. tgp, ALJ, Kriging and pso usually work well for relatively low values of <code>itmax</code> .
<code>lower</code>	The lower constraints of the search region. Needs to be a numeric vector of the same length as the parameter vector <code>theta</code> .
<code>upper</code>	The upper constraints of the search region. Needs to be a numeric vector of the same length as the parameter vector <code>theta</code> .
<code>verbose</code>	numeric value that prints information on the fitting process; <code>&gt;2</code> is very verbose.
<code>type</code>	which aggregation for the multi objective target function? Either 'additive' (default) or 'multiplicative'
<code>initpoints</code>	number of initial points to fit the surrogate model for Bayesian optimization; default is 10.
<code>itmax</code>	maximum number of iterations of the outer optimization (for <code>theta</code> ) 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 <code>itmax</code> and <code>6*itmax</code> as tgp samples 1-6 candidates from the posterior and uses the best candidate. For pso it is the number of particles <code>s</code> times <code>itmax</code> . For cmaes it is usually a bit higher than <code>itmax</code> . This currently may get overruled by a control argument if it is used (and then set to either <code>ewhat</code> is supplied by control or to the default of the method).
<code>itmaxps</code>	maximum number of iterations of the inner optimization (to obtain the PS configuration)

model	a character specifying the surrogate model to use. For Kriging it specifies the covariance kernel for the GP prior; see <code>covTensorProduct-class</code> defaults to "powerexp". For tgp it specifies the non stationary process used see <code>bgp</code> , defaults to "btgpllm"
control	a control argument passed to the outer optimization procedure. Will override any other control arguments passed, especially verbose and itmax. For the effect of control, see the functions <code>pomp::sannbox</code> for SANN and <code>pso::psoptim</code> for pso, <code>cmaes::cma_es</code> for cmaes, <code>dfoptim::hjk</code> for hjk and the <code>nloptr</code> docs for the algorithms DIRECT, stogo, cobyla, crs2lm, isres, mlsl, neldermead, sbplx.
...	additional arguments passed to the outer optimization procedures (not fully tested).

## Details

The stops package provides five categories of important functions:

Models & Algorithms:

- `stops()` ... which fits STOPS models as described in Rusch et al. (2023). By setting `cordweight` or `strucweight` to zero they can also be used to fit metric MDS for many different models, see below.
- `powerStressMin()`... a workhorse for fitting many stresses, including s-stress, r-stress (De Leeuw, 2014), Sammon mapping with power transformations (`powersammon`), elastic scaling with power transformation (`powerelastic`), power stress. They can most conveniently be accessed via the stops functions and setting `stressweight=1` and `cordweight` or `strucweight=0` or by the dedicated functions starting with `stop_foo` where `foo` is the method and setting `stressweight=1` and `strucweight=0`. It uses the nested majorization algorithm for r-stress of De Leeuw(2014).
- `bcStressMin()`... a workhorse for fitting Box-Cox stress (Chen & Buja, 2013).
- `lmds()`... a workhorse for the local MDS of Chen & Buja (2008).

Structuredness Indices: Various c-structuredness as `c_foo()`, where `foo` is the name of the structuredness. See Rusch et al. (2023).

Optimization functions:

- `ljoptim()` ... An (adaptive) version of the Luus-Jakola random search

Wrappers and convenience functions:

- `conf_adjust()`: procrustes adjustment of configurations
- `cmdscale()`, `sammon()`: wrappers that return S3 objects
- `stop_smacofSym()`, `stop_sammon()`, `stop_cmdscale()`, `stop_rstress()`, `stop_powerstress()`, `stop_smacofSphere()`, `stop_sammon2()`, `stop_elastic()`, `stop_sstress()`, `stop_powerelastic()`, `stop_powersammon()`, `stop_powersmnds()`, `stop_isomap()`, `stop_isomapeps()`, `stop_bcstress()`, `stop_lmds()`, `stop_apstress()`, `stops_rpowerstress()`: stop versions of these MDS models.
- `stoploss()` ... a function to calculate stoploss (Rusch et al., 2023)

Methods: For most of the objects returned by the high-level functions S3 classes and methods for standard generics were implemented, including `print`, `summary`, `plot`, `plot3d`, `plot3dstatic`.

References:

- Rusch, T., Mair, P., & Hornik, K. (2023). Structure-based hyperparameter selection with Bayesian optimization in multidimensional scaling. *Statistics & Computing*, 33, [28]. <https://doi.org/10.1007/s11222-022-10197-w>

Authors: Thomas Rusch, Lisha Chen, Jan de Leeuw, Patrick Mair, Kurt Hornik

Maintainer: Thomas Rusch

The combination of c-structurednes indices and stress uses the stress.m values, which are the explicitly normalized stresses. Reported however is the stress-1 value which is  $\sqrt{\text{stress.m}}$ .

## 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
- losstype: 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)

## Examples

```
data(kinshipdelta, package="smacof")
```

```
strucpars<-list(list(epsilon=10, minpts=2, scale=3), list(NULL))
dissm<-as.matrix(kinshipdelta)
```

```
#STOPS with strain
resstrain<-stops(dissm, loss="strain", theta=1, structures=c("cclusteredness", "cdependence"),
strucpars=strucpars, optimmethod="ALJ", lower=0, upper=10, itmax=10)
resstrain
summary(resstrain)
plot(resstrain)
```

```
#STOPS with stress
strucpars<-list(list(epsilon=10, minpts=2, scale=3), NULL)
resstress<-stops(dissm, loss="stress",
structures=c("cclusteredness", "cdependence"),
strucpars=strucpars, optimmethod="ALJ", lower=0, upper=10)
resstress
summary(resstress)
plot(resstress)
plot(resstress, "Shepard")
```

```

#STOPS with powerstress
respstress<-stops(dissm,loss="powerstress",
structures=c("cclusteredness","cdependence"),
strucpars=strucpars,weightmat=dissm,
itmaxps=1000,optimmethod="ALJ",lower=c(0,0,1),upper=c(10,10,10))
respstress
summary(respstress)
plot(respstress)

#STOPS with bcstress
resbcstress<-stops(dissm,loss="bcstress",
structures=c("cclusteredness","cdependence"),
strucpars=strucpars,optimmethod="ALJ",lower=c(0,1,0),upper=c(10,10,10))
resbcstress
summary(resbcstress)
plot(resbcstress)

#STOPS with lmds
reslmds<-stops(dissm,loss="lmds",
structures=c("cclusteredness","clinearity"),
strucpars=strucpars,optimmethod="ALJ",lower=c(2,0),upper=c(10,2))
reslmds
summary(reslmds)
plot(reslmds)

#STOPS with Isomap (the epsilon version)
resiso<-stops(dissm,loss="isomapeps",
structures=c("cclusteredness","clinearity"),
strucpars=strucpars,optimmethod="ALJ",lower=70,upper=120)
resiso
summary(resiso)
plot(resiso)

data(kinshipdelta,package="smacof")
strucpar<-list(NULL,NULL) #parameters for indices
res1<-stops(kinshipdelta,loss="stress",
structures=c("cclumpiness","cassociation"),strucpar=
strucpar,lower=0,upper=10,itmax=10)
res1

data(BankingCrisesDistances)
strucpar<-list(c(epsilon=10,minpts=2),NULL) #parameters for indices
res1<-stops(BankingCrisesDistances[,1:69],loss="stress",verbose=0,
structures=c("cclusteredness","clinearity"),strucpar=
strucpar,lower=0,upper=10)
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)
res1
```

---

stop\_apstress

*STOPS version of approximated power stress models.*


---

### Description

This uses an approximation to power stress that can make use of smacof as workhorse. Free parameters are tau and upsilon.

### Usage

```
stop_apstress(
  dis,
  theta = c(1, 1),
  ndim = 2,
  weightmat = NULL,
  init = NULL,
  itmax = 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,
  type = 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 two, with the first the tau argument and the second the upsilon argument. It can also be a scalar of the tau and upsilon transformation for the observed proximities and gets recycled for both ups and tau (so they are equal). Defaults to 1 1.
ndim	number of dimensions of the target space
weightmat	(optional) a binary matrix of nonnegative weights
init	(optional) initial configuration
itmax	number of iterations. default is 1000.

...	additional arguments to be passed to the fitting procedure
stressweight	weight to be used for the fit measure; defaults to 1
structures	a character vector listing the structure indices to use. They always are called "cfoo" with foo being the structure.
strucweight	weight to be used for the structures; defaults to 1/number of structures
strucpars	a list of list of parameters for the structuredness indices; each list element corresponds to one index in the order of the appearance in structures vector. See examples.
verbose	numeric value that prints information on the fitting process; >2 is extremely verbose
type	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 (sqrt stress.m)
- stress.m: default normalized stress
- stoploss: the weighted loss value
- struc: the structuredness indices
- parameters: the parameters used for fitting (kappa=1, tau, ups)
- fit: the returned object of the fitting procedure
- stopobj: the stopobj object

---

stop_bcstress	<i>STOPS version of Box Cox Stress</i>
---------------	--

---

### Description

STOPS version of Box Cox Stress

### Usage

```
stop_bcstress(
  dis,
  theta = c(1, 1, 0),
  weightmat = NULL,
  init = NULL,
  ndim = 2,
  itmax = 5000,
  ...,
  stressweight = 1,
  structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
```

```

"association", "nonmonotonicity", "functionality", "complexity", "faithfulness",
"regularity", "hierarchy", "convexity", "striatedness", "outlying",
"skinniness", "sparsity", "stringiness", "clumpiness", "inequality"),
strucweight = rep(1/length(structures), length(structures)),
strucpars,
verbose = 0,
type = c("additive", "multiplicative")
)

```

### Arguments

<code>dis</code>	numeric matrix or dist object of a matrix of proximities
<code>theta</code>	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.
<code>weightmat</code>	(not used)
<code>init</code>	(optional) initial configuration
<code>ndim</code>	number of dimensions of the target space
<code>itmax</code>	number of iterations
<code>...</code>	additional arguments to be passed to the fitting procedure
<code>stressweight</code>	weight to be used for the fit measure; defaults to 1
<code>structures</code>	which structures to look for
<code>strucweight</code>	weight to be used for the structures; defaults to 0.5
<code>strucpars</code>	a list of parameters for the structuredness indices; each list element corresponds to one index in the order of the appearance in structures
<code>verbose</code>	numeric value that prints information on the fitting process; >2 is extremely verbose
<code>type</code>	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\_cmdscale                      *STOPS version of strain*

---

### Description

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

### Usage

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

### 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.
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 verbose

type	How to construct the target function for the multi objective optimization? Either 'additive' (default) or 'multiplicative'
itmax	placeholder for compatibility in stops call; not used

### Value

A list with the components

- stress: Sqrt of explicitly normalized stress.
- stress.m: explicitly 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_elastic	<i>STOPS versions of elastic scaling models (via smacofSym)</i>
--------------	---

---

### 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,
  ndim = 2,
  weightmat = NULL,
  init = NULL,
  itmax = 1000,
  ...,
  stressweight = 1,
  structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
    "cskininess", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  type = 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.
ndim	number of dimensions of the target space
weightmat	(optional) a matrix of nonnegative weights (NOT the elscal weights)
init	(optional) initial configuration
itmax	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 that prints information on the fitting process; >2 is extremely verbose
type	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 ( $\sqrt{\text{stress.m}}$ )
- 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
- 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.

**Usage**

```

stop_isomap1(
  dis,
  theta = 3,
  weightmat = NULL,
  ndim = 2,
  init = NULL,
  stressweight = 1,
  structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
    "cskininess", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  type = c("additive", "multiplicative"),
  itmax = NULL
)

```

**Arguments**

<code>dis</code>	numeric matrix or dist object of a matrix of proximities
<code>theta</code>	the number of shortest dissimilarities retained for a point (nearest neighbours), the isomap parameter. Must be a numeric scalar. Defaults to 3.
<code>weightmat</code>	(optional) a matrix of nonnegative weights
<code>ndim</code>	number of dimensions of the target space
<code>init</code>	(optional) initial configuration
<code>stressweight</code>	weight to be used for the fit measure; defaults to 1
<code>structures</code>	which structuredness indices to be included in the loss
<code>strucweight</code>	weight to be used for the structuredness indices; ; defaults to 1/#number of structures
<code>strucpars</code>	the parameters for the structuredness indices
<code>verbose</code>	numeric value that prints information on the fitting process; >2 is extremely verbose
<code>type</code>	How to construct the target function for the multi objective optimization? Either 'additive' (default) or 'multiplicative'
<code>itmax</code>	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 connected 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 where GOF is the first element returned from cmdscale (the sum of the first ndim absolute eigenvalues divided by the sum of all absolute eigenvalues).
- stress.m: default normalized stress (sqrt explicitly normalized stress; really the stress this 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

*STOPS version of isomap over real epsilon.*


---

**Description**

Free parameter is eps.

**Usage**

```
stop_isomap2(
  dis,
  theta = stats::quantile(dis, 0.1),
  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,
  type = c("additive", "multiplicative"),
  itmax = NULL
)
```

**Arguments**

<code>dis</code>	numeric matrix or dist object of a matrix of proximities
<code>theta</code>	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 <code>dis</code> .
<code>weightmat</code>	(optional) a matrix of nonnegative weights
<code>ndim</code>	number of dimensions of the target space
<code>init</code>	(optional) initial configuration
<code>stressweight</code>	weight to be used for the fit measure; defaults to 1
<code>structures</code>	which structuredness indices to be included in the loss
<code>strucweight</code>	weight to be used for the structuredness indices; ; defaults to 1/#number of structures
<code>strucpars</code>	the parameters for the structuredness indices
<code>verbose</code>	numeric value that prints information on the fitting process; >2 is extremely verbose
<code>type</code>	How to construct the target function for the multi objective optimization? Either 'additive' (default) or 'multiplicative'
<code>itmax</code>	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 connected 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 where GOF is the first element returned from `cmdscale` (the sum of the first `ndim` absolute eigenvalues divided by the sum of all absolute eigenvalues).
- `stress.m`: default normalized stress (sqrt explicitly normalized stress; really the stress this 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\_lmids

*STOPS version of LMDS*


---

## Description

STOPS version of LMDS

## Usage

```
stop_lmids(
  dis,
  theta = c(2, 0.5),
  weightmat = NULL,
  init = NULL,
  ndim = 2,
  itmax = 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,
  type = 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.
weightmat	(not used)
init	(optional) initial configuration
ndim	number of dimensions of the target space
itmax	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 that prints information on the fitting process; >2 is extremely verbose
type	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_powerelastic	<i>STOPS version of elastic scaling with powers for proximities and distances</i>
-------------------	---

---

### 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, -2),
  weightmat = NULL,
  init = NULL,
  ndim = 2,
  itmax = 1e+05,
  ...,
  stressweight = 1,
  structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
    "cskininess", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  type = 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.
weightmat	(optional) a matrix of nonnegative weights
init	(optional) initial configuration
ndim	number of dimensions of the target space
itmax	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 that prints information on the fitting process; >2 is extremely verbose
type	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\_powermds

*STOPS version of powermds*

---

**Description**

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

**Usage**

```

stop_powermds(
  dis,
  theta = c(1, 1),
  weightmat = NULL,
  init = NULL,
  ndim = 2,
  itmax = 1e+05,
  ...,
  stressweight = 1,
  structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
    "cskininess", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  type = c("additive", "multiplicative")
)

```

**Arguments**

<code>dis</code>	numeric matrix or dist object of a matrix of proximities
<code>theta</code>	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.
<code>weightmat</code>	(optional) a matrix of nonnegative weights
<code>init</code>	(optional) initial configuration
<code>ndim</code>	number of dimensions of the target space
<code>itmax</code>	number of iterations
<code>...</code>	additional arguments to be passed to the fitting procedure
<code>stressweight</code>	weight to be used for the fit measure; defaults to 1
<code>structures</code>	which structures to look for
<code>strucweight</code>	weight to be used for the structures; defaults to 0.5
<code>strucpars</code>	a list of parameters for the structuredness indices; each list element corresponds to one index in the order of the appearance in structures
<code>verbose</code>	numeric value that prints information on the fitting process; >2 is extremely verbose
<code>type</code>	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\_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),
  weightmat = NULL,
  init = NULL,
  ndim = 2,
  itmax = 1e+05,
  ...,
  stressweight = 1,
  structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "cregularity", "chierarchy", "cconvexity", "cstriatedness", "coutlying",
    "cskininess", "csparsity", "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  type = 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.
weightmat	(optional) a matrix of nonnegative weights
init	(optional) initial configuration

ndim	number of dimensions of the target space
itmax	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 that prints information on the fitting process; >2 is extremely verbose
type	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	<i>STOPS version of powerstress</i>
------------------	-------------------------------------

---

### Description

Power stress with free kappa and lambda and rho.

### Usage

```
stop_powerstress(
  dis,
  theta = c(1, 1, 1),
  weightmat = NULL,
  init = NULL,
  ndim = 2,
  itmax = 10000,
  ...,
  stressweight = 1,
```

```

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

```

### Arguments

<code>dis</code>	numeric matrix or dist object of a matrix of proximities
<code>theta</code>	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.
<code>weightmat</code>	(optional) a matrix of nonnegative weights
<code>init</code>	(optional) initial configuration
<code>ndim</code>	number of dimensions of the target space
<code>itmax</code>	number of iterations
<code>...</code>	additional arguments to be passed to the fitting procedure
<code>stressweight</code>	weight to be used for the fit measure; defaults to 1
<code>structures</code>	a character vector listing the structure indices to use. They always are called "cfoo" with foo being the structure.
<code>strucweight</code>	weight to be used for the structures; defaults to 1/number of structures
<code>strucpars</code>	a list of parameters for the structuredness indices; each list element corresponds to one index in the order of the appearance in structures
<code>verbose</code>	numeric value that prints information on the fitting process; >2 is extremely verbose
<code>type</code>	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, nu)
- `fit`: the returned object of the fitting procedure
- `stopobj`: the stopobj object

---

stop\_rpowerstress      *STOPS version of restricted powerstress*

---

## Description

STOPS version of restricted powerstress

## Usage

```
stop_rpowerstress(
  dis,
  theta = c(1, 1, 1),
  weightmat = NULL,
  init = NULL,
  ndim = 2,
  itmax = 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,
  type = c("additive", "multiplicative")
)
```

## Arguments

<code>dis</code>	numeric matrix or dist object of a matrix of proximities
<code>theta</code>	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 <code>c(theta[1],theta[1],theta[2])</code> . Defaults to 1 1 1.
<code>weightmat</code>	(optional) a matrix of nonnegative weights
<code>init</code>	(optional) initial configuration
<code>ndim</code>	number of dimensions of the target space
<code>itmax</code>	number of iterations. default is 10000.
<code>...</code>	additional arguments to be passed to the fitting procedure <code>powerStressMin</code>
<code>stressweight</code>	weight to be used for the fit measure; defaults to 1
<code>structures</code>	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 that prints information on the fitting process; >2 is extremely verbose
type	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 ( $\kappa=\lambda$ ,  $\nu$ )
- fit: the returned object of the fitting procedure
- stopobj: the stopobj object

---

stop_rstress	<i>STOPS</i> version of <i>rstress</i>
--------------	--

---

### Description

Free parameter is  $\kappa$  for the fitted distances.

### Usage

```
stop_rstress(
  dis,
  theta = 1,
  weightmat = NULL,
  init = NULL,
  ndim = 2,
  itmax = 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,
  type = c("additive", "multiplicative")
)

```

### Arguments

<code>dis</code>	numeric matrix or dist object of a matrix of proximities
<code>theta</code>	the theta vector of powers; this must be a scalar of the kappa transformation for the fitted distances proximities. Defaults to 1. Note the kappa here differs from Jan's version where the parameter was called r and the relationship is $r = \text{kappa}/2$ or $\text{kappa} = 2r$ .
<code>weightmat</code>	(optional) a matrix of nonnegative weights
<code>init</code>	(optional) initial configuration
<code>ndim</code>	number of dimensions of the target space
<code>itmax</code>	number of iterations
<code>...</code>	additional arguments to be passed to the fitting procedure
<code>stressweight</code>	weight to be used for the fit measure; defaults to 1
<code>structures</code>	which structuredness indices to be included in the loss
<code>strucweight</code>	weight to be used for the structuredness indices; ; defaults to $1/\text{\#number of structures}$
<code>strucpars</code>	the parameters for the structuredness indices
<code>verbose</code>	numeric value hat prints information on the fitting process; $>2$ is extremely verbose
<code>type</code>	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
- `stress.m`: default normalized stress
- `stoploss`: the weighted loss value
- `indices`: the values of the structuredness indices
- `parameters`: the parameters used for fitting
- `fit`: the returned object of the fitting procedure
- `stopobj`: the stopobj object



---

 stop\_sammon

*STOPS version of Sammon mapping*


---

### Description

Uses MASS::sammon. The free parameter is lambda for power transformations of the observed proximities. The fitted distances power is internally fixed to 1 and the power for the weights=delta is -1.

### Usage

```
stop_sammon(
  dis,
  theta = 1,
  ndim = 2,
  init = NULL,
  weightmat = NULL,
  itmax = 1000,
  ...,
  stressweight = 1,
  structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskininess", "csparsity",
    "cstringiness", "cclumpiness", "cinequality"),
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  type = 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.
ndim	number of dimensions of the target space
init	(optional) initial configuration
weightmat	a matrix of nonnegative weights. Has no effect here.
itmax	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 that prints information on the fitting process; >2 is extremely verbose
type	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
- 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\_sammon2

*Another STOPS version of Sammon mapping models (via smacofSym)*

---

### Description

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

### Usage

```
stop_sammon2(
  dis,
  theta = 1,
  ndim = 2,
  weightmat = NULL,
  init = NULL,
  itmax = 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,
  type = 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.
ndim	number of dimensions of the target space
weightmat	(optional) a matrix of nonnegative weights
init	(optional) initial configuration
itmax	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 verbose
type	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 ( $\sqrt{\text{stress.m}}$ )
- 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
- fit: the returned object of the fitting procedure
- stopobj: the stopobj object

---

stop\_smacofSphere

*STOPS versions of smacofSphere models*

---

**Description**

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

**Usage**

```

stop_smacofSphere(
  dis,
  theta = 1,
  ndim = 2,
  weightmat = NULL,
  init = NULL,
  itmax = 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,
  type = 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.
ndim	number of dimensions of the target space
weightmat	(optional) a matrix of nonnegative weights
init	(optional) initial configuration
itmax	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 verbose
type	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

- 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.

### Usage

```
stop_smacofSym(
  dis,
  theta = 1,
  ndim = 2,
  weightmat = NULL,
  init = NULL,
  itmax = 1000,
  ...,
  structures = c("cclusteredness", "clinearity", "cdependence", "cmanifoldness",
    "cassociation", "cnonmonotonicity", "cfunctionality", "ccomplexity", "cfaithfulness",
    "chierarchy", "cconvexity", "cstriatedness", "coutlying", "cskinniness", "csparsity",
    "cstringiness", "cclumpiness", "cinequality"),
  stressweight = 1,
  strucweight = rep(1/length(structures), length(structures)),
  strucpars,
  verbose = 0,
  type = 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.
ndim	number of dimensions of the target space
weightmat	(optional) a matrix of nonnegative weights
init	(optional) initial configuration

itmax	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 verbose
type	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 ( $\sqrt{\text{stress.m}}$ )
- 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
- fit: the returned object of the fitting procedure
- stopobj: the stops object

---

stop_sstress	<i>STOPS version of sstress</i>
--------------	---------------------------------

---

### 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 multiplier of 2 (as sstress has  $f(\delta^2)$ ).

### Usage

```
stop_sstress(
  dis,
  theta = 1,
  weightmat = NULL,
  init = NULL,
  ndim = 2,
  itmax = 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,
type = c("additive", "multiplicative")
)

```

### Arguments

<code>dis</code>	numeric matrix or dist object of a matrix of proximities
<code>theta</code>	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 multiplier of 2 (as sstress has $f(\delta^2)$ ).
<code>weightmat</code>	(optional) a matrix of nonnegative weights
<code>init</code>	(optional) initial configuration
<code>ndim</code>	the number of dimensions of the target space
<code>itmax</code>	number of iterations
<code>...</code>	additional arguments to be passed to the fitting procedure
<code>stressweight</code>	weight to be used for the fit measure; defaults to 1
<code>structures</code>	which structuredness indices to be included in the loss
<code>strucweight</code>	weight to be used for the structuredness indices; ; defaults to $1/\text{number of structures}$
<code>strucpars</code>	the parameters for the structuredness indices
<code>verbose</code>	numeric value that prints information on the fitting process; $>2$ is extremely verbose
<code>type</code>	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
- `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

---

summary.cmdscale	<i>S3 summary method for cmdscale</i>
------------------	---------------------------------------

---

**Description**

S3 summary method for cmdscale

**Usage**

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

**Arguments**

object	object of class cmdscale
...	additional arguments

**Value**

No return value, just prints.

---

summary.sammon	<i>S3 summary method for sammon</i>
----------------	-------------------------------------

---

**Description**

S3 summary method for sammon

**Usage**

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

**Arguments**

object	object of class sammon
...	additional arguments

**Value**

No return value, just prints.



---

summary.smacofP	<i>S3 summary method for smacofP</i>
-----------------	--------------------------------------

---

**Description**

S3 summary method for smacofP

**Usage**

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

**Arguments**

object	object of class smacofP
...	additional arguments

**Value**

an object of class summary.smacofP

---

summary.stops	<i>S3 summary method for stops</i>
---------------	------------------------------------

---

**Description**

S3 summary method for stops

**Usage**

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

**Arguments**

object	object of class stops
...	additional arguments

**Value**

object of class 'summary.stops'

---

 Swissroll

*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.

**Usage**

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

**Arguments**

x	optional starting values
fun	function to minimize
...	additional arguments to be passed to the function to be optimized
initpoints	the number of points to sample initially to fit the surrogate model
lower	The lower constraints of the search region
upper	The upper constraints 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 that 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 `fnction` 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

**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="btgpplm")
points(res2$par,res2$value,col="red",pch=19)
res2

```

---

torgerson

*Torgerson scaling*


---

**Description**

Torgerson scaling

**Usage**

```
torgerson(delta, p = 2)
```

**Arguments**

delta	symmetric, numeric matrix of distances
p	target space dimensions

**Value**

a matrix (a Torgerson scaling configuration)

# Index

- \* **clustering**
  - stops, [48](#)
- \* **multivariate**
  - stop\_apstress, [54](#)
  - stop\_bcstress, [55](#)
  - stop\_cmdscale, [57](#)
  - stop\_elastic, [58](#)
  - stop\_isomap1, [59](#)
  - stop\_isomap2, [61](#)
  - stop\_lmids, [63](#)
  - stop\_powerelastic, [64](#)
  - stop\_powersmids, [65](#)
  - stop\_powersammon, [67](#)
  - stop\_powerstress, [68](#)
  - stop\_rpowerstress, [70](#)
  - stop\_rstress, [71](#)
  - stop\_sammon, [73](#)
  - stop\_sammon2, [74](#)
  - stop\_smacofSphere, [75](#)
  - stop\_smacofSym, [77](#)
  - stop\_sstress, [78](#)
  - stops, [48](#)
- ace, [19](#)
- apStressMin, [4](#)
- BankingCrisesDistances, [5](#)
- bcStressMin, [6](#)
- bgp, [51](#)
- c\_association, [10](#)
- c\_clumpiness, [11](#)
- c\_clusteredness, [11](#)
- c\_complexity, [13](#)
- c\_convexity, [14](#)
- c\_dependence, [14](#)
- c\_faithfulness, [15](#)
- c\_functionality, [16](#)
- c\_hierarchy, [17](#)
- c\_inequality, [17](#)
- c\_linearity, [18](#)
- c\_manifoldness, [19](#)
- c\_mine, [20](#)
- c\_nonmonotonicity, [20](#)
- c\_outlying, [21](#)
- c\_regularity, [22](#)
- c\_skininess, [23](#)
- c\_sparsity, [24](#)
- c\_striatedness, [24](#)
- c\_stringiness, [25](#)
- cl\_validity, [17](#)
- cmds, [8](#)
- cmdscale, [8](#), [8](#)
- coef.stops, [9](#)
- conf\_adjust, [9](#)
- cordillera, [12](#), [23](#)
- doubleCenter, [26](#)
- enorm, [26](#)
- hclust, [17](#)
- knn\_dist, [27](#)
- ljoptim, [27](#)
- lmids, [29](#)
- mine, [10](#), [13](#), [16](#), [21](#)
- mkBmat, [30](#)
- mkPower, [31](#)
- mkPower2, [31](#)
- optics, [12](#)
- optim, [28](#), [83](#)
- Pendigits500, [32](#)
- plot.cmdscaleE, [32](#)
- plot.smacof, [33](#), [38](#)
- plot.smacofP, [34](#)
- plot.stops, [36](#)

plot3d.cmdscaleE, 37, 38  
plot3d.stops, 38  
plot3dstatic, 38, 40  
plot3dstatic.cmdscaleE, 39, 40  
plot3dstatic.stops, 40  
powerStressMin, 29, 40  
print.cmdscale, 42  
print.sammon, 43  
print.stops, 43  
print.summary.smacofP, 44  
print.summary.stops, 44  
procruster, 45

residuals.stops, 45

sammon, 46, 46  
scagnostics, 11, 14, 22–25  
secularEq, 46  
smacofSym, 4, 5, 41, 42  
sqdist, 47  
stop\_apstress, 54  
stop\_bcstress, 55  
stop\_cmdscale, 57  
stop\_elastic, 58  
stop\_isomap1, 59  
stop\_isomap2, 61  
stop\_lmids, 63  
stop\_powerelastic, 64  
stop\_powermds, 65  
stop\_powersammon, 67  
stop\_powerstress, 68  
stop\_rpowerstress, 70  
stop\_rstress, 71  
stop\_sammon, 73  
stop\_sammon2, 74  
stop\_smacofSphere, 75  
stop\_smacofSym, 77  
stop\_sstress, 78  
stoploss, 47  
stops, 48  
summary.cmdscale, 80  
summary.sammon, 80  
summary.smacofP, 81  
summary.stops, 81  
Swissroll, 82

tgoptim, 82  
torgerson, 84