# Package 'cops'

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```
Title Cluster Optimized Proximity Scaling
```

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**Description** Multidimensional scaling (MDS) methods that aim at pronouncing the clustered appearance of the configura-

tion (Rusch, Mair & Hornik, 2021, <doi:10.1080/10618600.2020.1869027>). They achieve this by transforming proximities/distances with power functions and augment the fitting criterion with a clusteredness index, the OP-

TICS Cordillera (Rusch, Hornik & Mair, 2018, <doi:10.1080/10618600.2017.1349664>). There are two variants: One for finding the configuration directly (COPS-C) for ratio, power, interval and nonmetric MDS (Borg & Groenen, 2005, ISBN:978-0-387-28981-6), and one for using the augmented fitting criterion to find optimal parameters (P-COPS). The package contains various functions, wrappers, methods and classes for fitting, plotting and displaying different MDS models in a COPS framework like ratio, interval and non-metric MDS for COPS-C and P-COPS with Torgerson scaling (Torgerson, 1958, ISBN:978-0471879459), scaling by majorizing a complex function (SMA-

COF; de Leeuw, 1977, <a href="https://escholarship.org/uc/item/4ps3b5mj">https://escholarship.org/uc/item/4ps3b5mj</a>), Sammon mapping (Sammon, 1969, <a href="https://escholarship.org/uc/item/4ps3b5mj">doi:10.1109/T-C.1969.222678</a>), elastic scaling (McGee, 1966, <a href="https://escholarship.org/uc/item/4ps3b5mj">doi:10.1109/T-C.1969.222678</a>), elastic scaling (McGee, 1966, <a href="https://escholarship.org/uc/item/4ps3b5mj">doi:10.1109/T-C.1969.222678</a>), elastic scaling (McGee, 1966, <a href="https://escholarship.org/uc/item/4ps3b5mj">doi:10.1109/T-C.1969.222678</a>), restress (de Leeuw, Groenen & Mair, 2016, <a href="https://escholarship.org/uc/item/4ps3b5mj">https://escholarship.org/uc/item/4ps3b5mj</a>), restress (de Leeuw, Groenen & Mair, 2016, <a href="https://escholarship.org/uc/item/4ps3b5mj">https://escholarship.org/uc/item/4ps3b5mj</a>), restress (de Leeuw, Groenen & Mair, 2016, <a href="https://escholarship.org/uc/item/4ps3b5mj">https://escholarship.org/uc/item/4ps3b5mj</a>), restress (de Leeuw, Groenen & Mair, 2016, <a href="https://escholarship.org/uc/item/4ps3b5mj">https://escholarship.org/uc/item/4ps3b5mj</a>), restress (de Leeuw, Groenen & Mair, 2016, <a href="https://escholarship.org/uc/item/4ps3b5mj">https://escholarship.org/uc/item/4ps3b5mj</a>), restress (de Leeuw, Groenen & Mair, 2016, <a href="https://escholarship.org/uc/item/4ps3b5mj">https://escholarship.org/uc/item/4ps3b5mj</a>), restress (de Leeuw, Groenen & Mair, 2016, <a href="https://escholarship.org/uc/item/4ps3b5mj">https://escholarship.org/uc/item/4ps3b5mj</a>), restress (de Leeuw, Groenen & Mair, 2016, <a href="https://escholarship.org/uc/item/4ps3b5mj">https://escholarship.org/uc/item/4ps3b5mj</a>)

//rpubs.com/deleeuw/142619>), power stress (Buja & Swayne, 2002 <doi:10.1007/s00357-001-0031-

0>), restricted power stress, approximate power stress, power elastic scaling, power Sammon mapping (for all Rusch, Mair & Hornik, 2021, <doi:10.1080/10618600.2020.1869027>). All of these models can also solely be fit as MDS with power transformations. The package further contains a function for pattern search optimization, the ``Adaptive Luus-Jaakola Algorithm" (Rusch, Mair & Hornik, 2021, <doi:10.1080/10618600.2020.1869027>).

**Depends** R (>= 3.1.2), cordillera (>= 0.7-2), smacof (>= 1.10-4)

**Imports** MASS, minqa, pso, scatterplot3d, NlcOptim, Rsolnp, dfoptim, subplex, cmaes, crs, nloptr, rgenoud, GenSA

Suggests R.rsp, rmarkdown

VignetteBuilder R.rsp

# **R** topics documented:

nkingCrisesDistances	3
dscale	3
nf_adjust	4
os	5
ostress	8
ostressMin	9
o_apstress	12
o_cmdscale	
o_elastic	
p_powerelastic	
p_powermds	18
powersammon	20
powerstress	22
o_rpowerstress	
o_rstress	25
o_sammon	26
o_sammon2	28
o_smacofSphere	30
o_smacofSym	31
o_sstress	33
ubleCenter	34
orm	35
ptim	35
Bmat	37
Power	37
pps	38
ist	41
ot.cops	41
ot.pcops	42
ot.smacofP	44
ot3dstatic	46

Bani	king	Crise.	sDist	ances

Index	54
	torgerson
	sqdist
	secularEq
	scale_adjust
	sammon
	procruster
	powerStressMin
	powerStressFast
	plot3dstatic.cmdscaleE

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)

cmdscale

Wrapper to cmdscale for S3 class

# **Description**

Wrapper to cmdscale for S3 class

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

4 conf\_adjust

# **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 stops package.

### Value

Object of class "cmdscaleE' and 'cmdscale' extending cmdscale. This wrapper only adds an extra slot to the list with the call, adds column labels to the \$points and assigns S3 class 'cmdscaleE' and 'cmdscale'.

## **Examples**

```
dis<-as.matrix(smacof::kinshipdelta)</pre>
res<-cmdscale(dis)</pre>
```

conf\_adjust

conf\_adjust: a function to procrustes adjust two matrices

# **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, a numeric matrix
verbose	should adjustment be output; default to FALSE
eps	numerical accuracy

maximum number of iterations itmax

### Value

a list with ref.conf being the reference configuration, other.conf the adjusted coniguration and comparison.conf the comparison configuration

cops 5

cops

cops: cluster optimized proximity scaling

# Description

About the package cops: Cluster optimized proximity scaling (COPS) refers to multidimensional scaling methods that aim at pronouncing the clustered appearance of the configuration. They achieve this by transforming proximities/distances with power functions and augment the fitting criterion with a clusteredness index, the OPTICS Cordillera (Rusch, Hornik & Mair 2018). There are two variants: One for finding the configuration directly for given parameters (COPS-C), and one for using the augmented fitting criterion to find optimal parameters for the power transformations (P-COPS). The package contains various functions, wrappers, methods and classes for fitting, plotting and displaying different MDS models in a COPS framework like Torgerson scaling, SMA-COF, Sammon mapping, elastic scaling, symmetric SMACOF, spherical SMACOF, sstress, rstress, powermds, power elastic scaling, power sammon mapping, powerstress. All of these models can also solely be fit as MDS with power transformations. The package further contains functions for optimization (Adaptive LJ Algorithmus).

About the function cops: The high level function allows for minimizing copstress for a clustered MDS configuration. Allows to choose COPS-C (finding a configuration from copstress with cordillera penalty) and profile COPS (finding hyperparameters for MDS models with power transformations). It is a wrapper for copstressMin and pcops.

#### Usage

```
cops(
    dis,
    variant = c("1", "2", "Variant1", "Variant2", "v1", "v2", "COPS-C", "P-COPS",
    "configuration-c", "profile", "copstress-c", "p-copstress", "COPS-P", "copstress-p",
        "cops-c", "p-cops", "copsc", "pcops"),
    ...
)
```

### Arguments

```
dis a dissimilarity matrix or a dist object

variant a character string specifying which variant of COPS to fit. Allowed is any of the following "1","2","Variant1","Variant2","v1","v2","COPS-C","P-COPS","configuration-c","profile","copstress-c","p-copstress". Defaults to "COPS-C".

... arguments to be passed to copstressMin (for Variant 1) or pcops (for Variant 2).
```

#### **Details**

The cops package provides five categories of important functions:

Models & Algorithms:

6 cops

• cops() ... high level interface to fit COPS models as described in Rusch et al. (2021). By setting cordweight to zero they can also be used to fit metric MDS for many different models, see below.

- copstressMin()... The workhorse for fitting a COPS-C model. Can also be called directly.
- pcops()... The workhorse for fitting a P-COPS model. Can also be called directly.
- powerStressMin()... a workhorse for fitting s-stress, r-stress (de Leeuw, 2014), p-stress (e.g., Rusch et al., 2021), Sammon mapping with power transformations (powersammon) and elastic scaling with power transformation (powerelastic). They can conveniently also be fitted via the cops functions and setting stressweight=1 and cordweight or by the dedicated functions starting with cops\_XXX where XXX is the method and setting stressweight=1 and cordweight=0. It uses the nested majorization algorithm for r-stress of De Leeuw (2014).

### 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 to be used with cops
- copstress() ... a function to calculate copstress (Rusch et al., 2021)
- cop\_smacofSym(), cop\_sammon(), cop\_cmdscale(), cop\_rstress(), cop\_powerstress(), cop\_smacofSphere(), cop\_sammon2(), cop\_elastic(), cop\_sstress(), cop\_powerelastic(), cop\_powersammon(): cop versions of these MDS models.

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, plot3dstatic.

#### References:

- Rusch, T., Hornik, K. & Mair, P. (2018) Assessing and quantifying clusteredness: The OP-TICS Cordillera. Journal of Computational and Graphical Statistics, 27 (1), 220-233. doi:10.1080/ 10618600.2017.1349664
- Rusch, T., Mair, P. & Hornik, K. (2021) Cluster optimized proximity scaling. Journal of Computational and Graphical Statistics. doi:10.1080/10618600.2020.1869027

Authors: Thomas Rusch, Jan de Leeuw, Patrick Mair

Maintainer: Thomas Rusch

#### Value

For COPS-C Variant 1 see copstressMin, for P-COPS Variant 2 see pcops

# Examples

data(BankingCrisesDistances)

# shorthand function for COPS-C (finding configuration with copstress)

cops 7

```
res<-cops(BankingCrisesDistances[,1:69],variant="COPS-C",
          stressweight=0.98,cordweight=0.02,itmax=1000)
# Note: itmax is very small here for illustration; will give a non-convergence
# warning of the optimizer which disappears at itmax=275000
res
summary(res)
plot(res)
plot(res,"reachplot")
plot(res,"transplot")
plot(res, "Shepard")
#shorthand function for P-COPS (hyperparameter search for powerstress)
res<-cops(BankingCrisesDistances[,1:69],variant="P-COPS")
res
summary(res)
plot(res)
plot(res,"reachplot")
plot(res,"transplot")
plot(res, "Shepard")
dis<-as.matrix(smacof::kinshipdelta)</pre>
#COPS-C with equal weight to stress and cordillera
res1<-cops(dis,variant="COPS-C",stressweight=0.5,cordweight=0.5,
          minpts=2,itmax=500) #use higher itmax in real
res1
summary(res1)
plot(res1)
plot(res1, "reachplot")
#s-stress type copstress (i.e. kappa=2, lambda=2)
res3<-cops(dis,variant="COPS-C",kappa=2,lambda=2,stressweight=0.5,cordweight=0.5)
summary(res3)
plot(res3)
# power-stress type profile copstress
# search for optimal kappa and lambda between
# kappa=0.5,lambda=0.5 and kappa=2,lambda=5
# nu is fixed on -1
ws<-1/dis
diag(ws) < -1
res5<-cops(dis, variant="P-COPS", loss="powerstress",
          theta=c(1.4,3,-1), lower=c(1,0.5,-1), upper=c(3,5,-1),
          weightmat=ws, stressweight=0.9,cordweight=0.1)
res5
summary(res5)
plot(res5)
```

8 copstress

copstress

Calculates copstress for given MDS object

# Description

Calculates copstress for given MDS object

# Usage

```
copstress(
  obj,
  stressweight = 1,
  cordweight = 5,
  q = 1,
  minpts = 2,
  epsilon = 10,
  rang = NULL,
  verbose = 0,
  normed = TRUE,
  scale = c("std", "sd", "proc", "none"),
  init,
  ...
)
```

# Arguments

obj	MDS object (supported are sammon, cmdscale, smacof, rstress, powermds)
stressweight	weight to be used for the fit measure; defaults to 1
cordweight	weight to be used for the cordillera; defaults to 0.5
q	the norm of the cordillera; defaults to 1
minpts	the minimum points to make up a cluster in OPTICS; defaults to 2
epsilon	the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults to $10$
rang	range of the distances (min distance minus max distance). If NULL (default) the cordillera will be normed to each configuration's maximum distance, so an absolute value of goodness-of-clusteredness.
verbose	numeric value hat prints information on the fitting process; >2 is very verbose (copstress level), >3 is extremely (up to MDS optimization level)
normed	should the cordillera be normed; defaults to TRUE
scale	should the configuration be scale adjusted.
init	a reference configuration when doing procrustes adjustment
	additional arguments to be passed to the cordillera function

copstressMin 9

### Value

A list with the components

- copstress: the weighted loss value
- OC: the Optics cordillera value
- parameters: the parameters used for fitting (kappa, lambda)
- cordillera: the cordillera object

copstressMin

Fitting a COPS-C Model (COPS Variant 1).

# **Description**

Minimizing Copstress to obtain a clustered MDS configuration with given hyperparameters theta.

```
copstressMin(
  delta,
  kappa = 1,
  lambda = 1,
  nu = 1,
  theta = c(kappa, lambda, nu),
  type = c("ratio", "interval", "ordinal"),
  ties = "primary"
  weightmat = 1 - diag(nrow(delta)),
  ndim = 2,
  init = NULL,
  stressweight = 0.975,
  cordweight = 0.025,
  q = 1,
 minpts = ndim + 1,
  epsilon = 10,
  dmax = NULL,
 optimmethod = c("NelderMead", "Newuoa", "BFGS", "SANN", "hjk", "solnl", "solnp",
  "subplex", "snomadr", "hjk-Newuoa", "hjk-BFGS", "BFGS-hjk", "Newuoa-hjk", "cmaes",
    "direct", "direct-Newuoa", "direct-BFGS", "genoud", "gensa"),
  verbose = 0,
  scale = c("sd", "rmsq", "std", "proc", "none"),
  normed = TRUE,
  accuracy = 1e-07,
  itmax = 5000,
  stresstype = c("stress-1", "stress"),
)
```

10 copstressMin

#### **Arguments**

delta numeric matrix or dist object of a matrix of proximities

kappa power transformation for fitted distances
lambda power transformation for proximities
nu power transformation for weights

theta the theta vector of powers; the first is kappa (for the fitted distances if it exists),

the second lambda (for the observed proximities if it exist), the third is nu (for the weights if it exists). If less than three elements are is given as argument, it will be recycled. Defaults to 1 1 1. Will override any kappa, Imabda, nu

parameters if they are given and do not match

type what type of MDS to fit. Currently one of "ratio", "interval" or "ordinal". Default

is "ratio".

ties the handling of ties for ordinal (nonmetric) MDS. Possible are "primary" (de-

fault), "secondary" or "tertiary".

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

ndim number of dimensions of the target space

init (optional) initial configuration

stressweight weight to be used for the fit measure; defaults to 0.975 cordweight weight to be used for the cordillera; defaults to 0.025

q the norm of the cordillera; defaults to 1

minpts the minimum points to make up a cluster in OPTICS; defaults to ndim+1

epsilon the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults

to 10

dmax The winsorization limit of reachability distances in the OPTICS Cordillera. If

supplied, it should be either a numeric value that matches max(rang) or NULL; if NULL it is found as 1.5 times (for kappa >1) or 1 times (for kappa <=1) the maximum reachbility value of the power torgerson model with the same lambda. If dmax and rang are supplied and dmax is not max(rang), a warning is given

and rang takes precedence.

range of the reachabilities to be considered. If missing it is found from the initial

configuration by taking 0 as the lower boundary and dmax (see above) as upper

boundary. See also cordillera

optimmethod What optimizer to use? Choose one string of 'Newuoa' (from package minqa),

'NelderMead', 'hjk' (Hooke-Jeeves algorithm from dfoptim), 'solnl' (from nl-cOptim), 'solnp' (from Rsolnp), 'subplex' (from subplex), 'SANN' (simulated annealing), 'BFGS', 'snomadr' (from crs), 'genoud' (from rgenoud), 'gensa' (from GenSA), 'cmaes' (from cmaes) and 'direct' (from nloptr). See the according R packages for details on these solvers. There are also combinations that proved to work well good, like 'hjk-Newuoa', 'hjk-BFGS', 'BFGS-hjk', 'Newuoa-hjk', 'direct-Newuoa' and 'direct-BFGS'. Usually hjk, BFGS, newuoa, subplex and solnl work rather well in an acceptable time frame (depending on

the smoothness of copstress). Default is 'hjk-Newuoa'.

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

copstressMin 11

scale Allows to scale the configuration for the OC (the scaled configuration is also

returned as \$conf). One of "none" (so no scaling), "sd" (configuration divided by the highest standard deviation of the columns), "std" (standardize all columns !NOTE: This does not preserve the relative distances of the optimal config), "proc" (procrustes adjustment to the initial fit) and "rmsq" (configuration divided

by the maximum root mean square of the columns). Default is "sd".

normed should the cordillera be normed; defaults to TRUE

accuracy numerical accuracy, defaults to 1e-7

itmax maximum number of iterations. Defaults to 5000. If itmax is (too) small, some

optimizers will print warnings. For example, for optimizers using NEWUOA, an iteration number of 10\*length(par)^2 is recommended. The number of parameters to optimize over for the COPS problem is number of objects \* target space dimensions and can grow large very quickly, so being able to live with

these warnings is probably a good idea.

stresstype which stress to use in the copstress. Defaults to stress-1. If anything else is set,

explicitly normed stress which is (stress-1)^2. Using stress-1 puts more weight

on MDS fit.

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

#### Value

A list with the components

· delta: the original transformed dissimilarities

- obsdiss: the explicitly normed transformed dissimilarities (which are approximated by the fit)
- · confdist: the fitted distances
- conf: the configuration to which the scaling of argument scale was applied
- confo: the unscaled but explicitly normed configuration returned from the fitting procedure. Scaling applied to confo gives conf.
- par, pars : the theta vector of powers tranformations (kappa,lambda,nu)
- niter: number of iterations of the optimizer.
- stress: the square root of explicitly normalized stress (calculated for confo).
- spp: stress per point
- · ndim: number of dimensions
- model: Fitted model name with optimizer
- · call: the call
- nobj: the number of objects
- type, loss, losstype: stresstype
- stress.m: The stress used for copstress. If stresstype="stress-1" this is like \$stress else it is stress^2
- stress.en: another ways to calculate the stress
- deltaorig: the original untransformed dissimilarities

12 cop\_apstress

- copstress: the copstress loss value
- resmat: the matrix of residuals
- weightmat: the matrix of untransformed weights
- OC: the (normed) OPTICS Cordillera object (calculated for scaled conf)
- OCv: the (normed) OPTICS Cordillera value alone (calculated for scaled conf)
- optim: the object returned from the optimization procedure
- stressweight, cordweight: the weights of the stress and OC respectively (v\_1 and v\_2)
- optimmethod: The solver used
- type: the type of MDS fitted

# **Examples**

cop\_apstress

PCOPS version of approximated power stress model.

# Description

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

```
cop_apstress(
  dis,
  theta = c(1, 1, 1),
  ndim = 2,
  weightmat = NULL,
  init = NULL,
  itmaxi = 1000,
    ...,
  stressweight = 1,
  cordweight = 0.5,
  q = 1,
  minpts = ndim + 1,
  epsilon = 10,
```

cop\_apstress 13

```
rang = NULL,
verbose = 0,
normed = TRUE,
scale = "sd",
stresstype = "default"
)
```

# **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

itmaxi number of iterations. default is 1000.

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

stressweight weight to be used for the fit measure; defaults to 1 cordweight weight to be used for the cordillera; defaults to 0.5

q the norm of the cordillera; defaults to 1

minpts the minimum points to make up a cluster in OPTICS; defaults to ndim+1

epsilon the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults

to 10

range of the distances (min distance minus max distance). If NULL (default)

the cordillera will be normed to each configuration's maximum distance, so an

absolute value of goodness-of-clusteredness.

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

bose

normed should the cordillera be normed; defaults to TRUE

scale should the configuration be scale adjusted

stresstype which stress to report. Only takes smacofs default stress currrently.

### Value

A list with the components

• stress: the stress

• stress.m: default normalized stress

• copstress: the weighted loss value

• OC: the Optics cordillera value

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

14 cop\_cmdscale

• fit: the returned object of the fitting procedure (which has all smacofB elements and some more

• cordillera: the cordillera object

cop\_cmdscale

PCOPS version of strain

# Description

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

# Usage

```
cop_cmdscale(
  dis,
  theta = c(1, 1, 1),
 weightmat = NULL,
 ndim = 2,
  init = NULL,
  itmaxi = 1000,
 stressweight = 1,
  cordweight = 0.5,
 q = 1,
 minpts = ndim + 1,
  epsilon = 10,
 rang = NULL,
  verbose = 0,
  scale = "sd",
 normed = TRUE,
  stresstype = "default"
)
```

# **Arguments**

مائا م	
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
ndim	number of dimensions of the target space
init	(optional) initial configuration
itmaxi	number of iterations. No effect here.
	additional arguments to be passed to the fitting procedure
stressweight	weight to be used for the fit measure; defaults to 1

cop\_elastic 15

cordweight	weight to be used for the cordillera; defaults to 0.5
q	the norm of the corrdillera; defaults to 1
minpts	the minimum points to make up a cluster in OPTICS; defaults to ndim+1
epsilon	the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults to $10$
rang	range of the distances (min distance minus max distance). If NULL (default) the cordillera will be normed to each configuration's maximum distance, so an absolute value of goodness-of-clusteredness.
verbose	numeric value hat prints information on the fitting process; >2 is extremely verbose
scale	should the configuration be scale adjusted
normed	should the cordillera be normed; defaults to TRUE
stresstype	which stress to report. Only takes cmdscales default stress currrently.

### Value

A list with the components

• stress: the stress

• stress.m: default normalized stress

• copstress: the weighted loss value

• OC: the Optics cordillera value

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

• fit: the returned object of the fitting procedure

• cordillera: the cordillera object

cop\_elastic

PCOPS versions of elastic scaling models (via smacofSym)

# Description

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

```
cop_elastic(
  dis,
  theta = 1,
  ndim = 2,
  weightmat = 1,
  init = NULL,
```

16 cop\_elastic

```
itmaxi = 1000,
...,
stressweight = 1,
cordweight = 0.5,
q = 1,
minpts = ndim + 1,
epsilon = 10,
rang = NULL,
verbose = 0,
normed = TRUE,
scale = "sd",
stresstype = "default"
)
```

# 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

itmaxi number of iterations. default is 1000.

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

stressweight weight to be used for the fit measure; defaults to 1 cordweight weight to be used for the cordillera; defaults to 0.5

q the norm of the corrdillera; defaults to 1

minpts the minimum points to make up a cluster in OPTICS; defaults to ndim+1

epsilon the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults

to 10

range of the distances (min distance minus max distance). If NULL (default)

the cordillera will be normed to each configuration's maximum distance, so an

absolute value of goodness-of-clusteredness.

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

bose

normed should the cordillera be normed; defaults to TRUE

scale should the configuration be scale adjusted

stresstype which stress to report. Only takes smacofs default stress currrently.

### Value

A list with the components

· stress: the stress

cop\_powerelastic 17

- · stress.m: default normalized stress
- copstress: the weighted loss value
- OC: the Optics cordillera value
- parameters: the parameters used for fitting (kappa, lambda)
- fit: the returned object of the fitting procedure
- cordillera: the cordillera object

cop\_powerelastic

PCOPS version of elastic scaling with powers

# Description

PCOPS version of elastic scaling with powers

# Usage

```
cop_powerelastic(
  dis,
  theta = c(1, 1),
 weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
 stressweight = 1,
 cordweight = 0.5,
  q = 1,
 minpts = ndim + 1,
  epsilon = 10,
  rang = NULL,
  verbose = 0,
  scale = "sd",
 normed = TRUE,
 stresstype = c("default", "stress1", "rawstress", "normstress", "enormstress",
    "enormstress1")
)
```

# **Arguments**

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

18 cop\_powermds

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

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

stressweight weight to be used for the fit measure; defaults to 1 cordweight weight to be used for the cordillera; defaults to 0.5

q the norm of the cordillera; defaults to 1

minpts the minimum points to make up a cluster in OPTICS; defaults to ndim+1

epsilon the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults

to 10

range of the distances (min distance minus max distance). If NULL (default)

the cordillera will be normed to each configuration's maximum distance, so an

absolute value of goodness-of-clusteredness.

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

bose

scale should the configuration be scale adjusted

normed should the cordillera be normed; defaults to TRUE

stresstype which stress to report? Defaults to explicitly normed stress

#### Value

A list with the components

• stress: the stress

· stress.m: default normalized stress

• copstress: the weighted loss value

• OC: the Optics cordillera value

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

• fit: the returned object of the fitting procedure

• cordillera: the cordillera object

cop\_powermds PCOPS version of powermds

### **Description**

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

cop\_powermds 19

### Usage

```
cop_powermds(
  dis,
  theta = c(1, 1, 1),
 weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = itmaxi,
  stressweight = 1,
  cordweight = 0.5,
  q = 1,
 minpts = ndim + 1,
  epsilon = 10,
  rang = NULL,
  verbose = 0,
  scale = "sd",
  normed = TRUE,
 stresstype = c("default", "stress1", "rawstress", "normstress", "enormstress",
    "enormstress1")
)
```

#### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

theta the theta vector of powers; a vector of length 2 where the first element is kappa

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

scalar is given it is recycled. Defaults to 1.

weightmat (optional) a matrix of nonnegative weights

init (optional) initial configuration

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

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

stressweight weight to be used for the fit measure; defaults to 1 cordweight weight to be used for the cordillera; defaults to 0.5

q the norm of the cordillera; defaults to 1

minpts the minimum points to make up a cluster in OPTICS; defaults to ndim+1

epsilon the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults

to 10

range of the distances (min distance minus max distance). If NULL (default)

the cordillera will be normed to each configuration's maximum distance, so an

absolute value of goodness-of-clusteredness.

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

bose

20 cop\_powersammon

scale should the configuration be scale adjusted

normed should the cordillera be normed; defaults to TRUE

stresstype which stress to report? Defaults to whatever whim is my default (currently explicitly normed stress)

#### Value

A list with the components

• stress: the stress

· stress.m: default normalized stress

• copstress: the weighted loss value

• OC: the Optics cordillera value

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

• fit: the returned object of the fitting procedure

• cordillera: the cordillera object

cop\_powersammon

PCOPS version of sammon with powers

# Description

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

```
cop_powersammon(
  dis,
  theta = c(1, 1),
  weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  stressweight = 1,
  cordweight = 0.5,
  q = 1,
  minpts = ndim + 1,
  epsilon = 10,
  rang = NULL,
  verbose = 0.
  scale = "sd",
  normed = TRUE,
 stresstype = c("default", "stress1", "rawstress", "normstress", "enormstress",
    "enormstress1")
)
```

cop\_powersammon 21

### **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 itmaxi number of iterations. default is 10000.

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

stressweight weight to be used for the fit measure; defaults to 1 cordweight weight to be used for the cordillera; defaults to 0.5

q the norm of the cordillera; defaults to 1

minpts the minimum points to make up a cluster in OPTICS; defaults to ndim+1

epsilon the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults

to 10

range of the distances (min distance minus max distance). If NULL (default)

the cordillera will be normed to each configuration's maximum distance, so an

absolute value of goodness-of-clusteredness.

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

bose

scale should the configuration be scale adjusted

normed should the cordillera be normed; defaults to TRUE

stresstype which stress to report? Defaults to explicitly normed stress

#### Value

A list with the components

• stress: the stress

• stress.m: default normalized stress

• copstress: the weighted loss value

• OC: the Optics cordillera value

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

• fit: the returned object of the fitting procedure

• cordillera: the cordillera object

22 cop\_powerstress

cop\_powerstress

COPS version of powerstress

# Description

Power stress with free kappa and lambda and rho (the theta argument).

# Usage

```
cop_powerstress(
  dis,
  theta = c(1, 1, 1),
 weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  stressweight = 1,
  cordweight = 0.5,
 q = 1,
 minpts = ndim + 1,
  epsilon = 10,
 rang = NULL,
 verbose = 0,
  scale = "sd",
 normed = TRUE,
 stresstype = c("default", "stress1", "rawstress", "normstress", "enormstress",
    "enormstress1")
)
```

# Arguments

dis	numeric matrix or dist object of a matrix of proximities
theta	the theta vector of powers; the first is kappa (for the fitted distances), the second lambda (for the observed proximities), the third nu (for the weights). If a scalar is given it is recycled. Defaults to 1 1 1.
weightmat	(optional) a matrix of nonnegative weights
init	(optional) initial configuration
ndim	number of dimensions of the target space
itmaxi	number of iterations. default is 10000.
	additional arguments to be passed to the fitting procedure
stressweight	weight to be used for the fit measure; defaults to 1
cordweight	weight to be used for the cordillera; defaults to 0.5
q	the norm of the cordillera; defaults to 1

cop\_rpowerstress 23

minpts	the minimum points to make up a cluster in OPTICS; defaults to ndim+1
epsilon	the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults to $10$
rang	range of the distances (min distance minus max distance). If NULL (default) the cordillera will be normed to each configuration's maximum distance, so an absolute value of goodness-of-clusteredness.
verbose	numeric value hat prints information on the fitting process; $>$ 2 is extremely verbose
scale	should the configuration be scale adjusted
normed	should the cordillera be normed; defaults to TRUE
stresstype	which stress to report? Defaults to explicitly normed stress

### Value

A list with the components

• stress: the stress

stress.m: default normalized stress copstress: the weighted loss value

• OC: the Optics cordillera value

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

• fit: the returned object of the fitting procedure

• cordillera: the cordillera object

cop\_rpowerstress

PCOPS version of restricted powerstress.

# Description

This is a power stress where kappa and lambda are free to vary but restricted to be equal, so the same exponent will be used for distances and dissimilarities. nu (for the weights) is also free.

```
cop_rpowerstress(
  dis,
  theta = c(1, 1, 1),
  weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  ...,
  stressweight = 1,
  cordweight = 0.5,
```

24 cop\_rpowerstress

### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

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

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

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

weightmat (optional) a matrix of nonnegative weights

init (optional) initial configuration

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

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

stressweight weight to be used for the fit measure; defaults to 1 cordweight weight to be used for the cordillera; defaults to 0.5

q the norm of the cordillera; defaults to 1

minpts the minimum points to make up a cluster in OPTICS; defaults to ndim+1

epsilon the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults

to 10

range of the distances (min distance minus max distance). If NULL (default)

the cordillera will be normed to each configuration's maximum distance, so an

absolute value of goodness-of-clusteredness.

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

bose

scale should the configuration be scale adjusted

normed should the cordillera be normed; defaults to TRUE

stresstype which stress to report? Defaults to explicitly normed stress

#### Value

A list with the components

• stress: the stress1 value (sqrt(stress.m))

cop\_rstress 25

- · stress.m: default normalized stress
- copstress: the weighted loss value
- OC: the Optics cordillera value
- parameters: the parameters used for fitting (kappa, lambda)
- fit: the returned object of the fitting procedure
- cordillera: the cordillera object

cop\_rstress

PCOPS version of rstress

# **Description**

Free parameter is kappa for the fitted distances.

# Usage

```
cop_rstress(
  dis,
  theta = c(1, 1, 1),
 weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  stressweight = 1,
  cordweight = 0.5,
 q = 1,
 minpts = ndim + 1,
 epsilon = 10,
  rang = NULL,
 verbose = 0,
  scale = "sd",
 normed = TRUE,
 stresstype = c("default", "stress1", "rawstress", "normstress", "enormstress",
    "enormstress1")
)
```

### **Arguments**

dis numeric matrix or dist object of a matrix of proximities

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=kappa/2 or kappa=2r.

weightmat (optional) a matrix of nonnegative weights

26 cop\_sammon

init (optional) initial configuration

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

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

stressweight weight to be used for the fit measure; defaults to 1 cordweight weight to be used for the cordillera; defaults to 0.5

q the norm of the cordillera; defaults to 1

minpts the minimum points to make up a cluster in OPTICS; defaults to ndim+1

epsilon the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults

to 10

range of the distances (min distance minus max distance). If NULL (default)

the cordillera will be normed to each configuration's maximum distance, so an

absolute value of goodness-of-clusteredness.

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

bose

scale should the configuration be scale adjusted

normed should the cordillera be normed; defaults to TRUE

stresstype which stress to report? Defaults to explicitly normed stress

### Value

A list with the components

• stress: the stress

stress.m: default normalized stress copstress: the weighted loss value

• OC: the Optics cordillera value

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

• fit: the returned object of the fitting procedure

• cordillera: the cordillera object

cop\_sammon PCOPS 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.

cop\_sammon 27

### Usage

```
cop_sammon(
  dis,
  theta = 1,
  ndim = 2,
  init = NULL,
 weightmat = NULL,
  itmaxi = 100,
  stressweight = 1,
  cordweight = 0.5,
  q = 1,
 minpts = ndim + 1,
  epsilon = 10,
  rang = NULL,
  verbose = 0,
  scale = "sd",
 normed = TRUE,
  stresstype = "default"
)
```

#### **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 (optional) a matrix of nonnegative weights itmaxi number of iterations. default is 1000.

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

stressweight weight to be used for the fit measure; defaults to 1 cordweight weight to be used for the cordillera; defaults to 0.5

q the norm of the corrdillera; defaults to 1

minpts the minimum points to make up a cluster in OPTICS; defaults to ndim+1

epsilon the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults

to 10

range of the distances (min distance minus max distance). If NULL (default)

the cordillera will be normed to each configuration's maximum distance, so an

absolute value of goodness-of-clusteredness.

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

bose

scale should the configuration be scale adjusted

normed should the cordillera be normed; defaults to TRUE

stresstype which stress to report. Only takes smacofs default stress currrently.

28 cop\_sammon2

### Value

A list with the components

• stress: the stress

• stress.m: default normalized stress

• copstress: the weighted loss value

• OC: the Optics cordillera value

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

• fit: the returned object of the fitting procedure

• cordillera: the cordillera object

cop\_sammon2

Another COPS versions 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.

```
cop_sammon2(
  dis,
  theta = 1,
  ndim = 2,
 weightmat = NULL,
  init = NULL,
  itmaxi = 1000,
  stressweight = 1,
  cordweight = 0.5,
  q = 1,
 minpts = ndim + 1,
  epsilon = 10,
  rang = NULL,
  verbose = 0,
  normed = TRUE,
  scale = "sd",
  stresstype = "default"
)
```

cop\_sammon2 29

### **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 transforma-

tion for the observed proximities. Defaults to 1.

ndim number of dimensions of the target space

weightmat (optional) a matrix of nonnegative weights (NOT the sammon weights)

init (optional) initial configuration

itmaxi number of iterations. default is 1000.

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

stressweight weight to be used for the fit measure; defaults to 1 cordweight weight to be used for the cordillera; defaults to 0.5

q the norm of the corrdillera; defaults to 1

minpts the minimum points to make up a cluster in OPTICS; defaults to ndim+1

epsilon the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults

to 10

range of the distances (min distance minus max distance). If NULL (default)

the cordillera will be normed to each configuration's maximum distance, so an

absolute value of goodness-of-clusteredness.

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

bose

normed should the cordillera be normed; defaults to TRUE

scale should the configuration be scale adjusted

stresstype which stress to report. Only takes smacofs default stress currrently.

#### Value

A list with the components

• stress: the stress

· stress.m: default normalized stress

• copstress: the weighted loss value

• OC: the Optics cordillera value

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

• fit: the returned object of the fitting procedure

• cordillera: the cordillera object

30 cop\_smacofSphere

cop\_smacofSphere

PCOPS 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

```
cop_smacofSphere(
 dis,
  theta = 1,
 ndim = 2,
 weightmat = NULL,
  init = NULL,
  itmaxi = 1000,
  stressweight = 1,
 cordweight = 0.5,
 q = 1,
 minpts = ndim + 1,
 epsilon = 10,
 rang = NULL,
 verbose = 0,
 normed = TRUE,
 scale = "sd",
 stresstype = "default"
)
```

# 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
itmaxi	number of iterations. default is 1000.
	additional arguments to be passed to the fitting procedure
stressweight	weight to be used for the fit measure; defaults to 1
cordweight	weight to be used for the cordillera; defaults to 0.5
q	the norm of the corrdillera; defaults to 1
minpts	the minimum points to make up a cluster in OPTICS; defaults to ndim+1

cop\_smacofSym 31

epsilon	the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults to 10
rang	range of the distances (min distance minus max distance). If NULL (default) the cordillera will be normed to each configuration's maximum distance, so an absolute value of goodness-of-clusteredness.
verbose	numeric value hat prints information on the fitting process; >2 is extremely verbose
normed	should the cordillera be normed; defaults to TRUE
scale	should the configuration be scale adjusted
stresstype	which stress to report. Only takes smacofs default stress currrently.

# Value

A list with the components

• stress: the stress

• stress.m: default normalized stress

• copstress: the weighted loss value

• OC: the Optics cordillera value

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

• fit: the returned object of the fitting procedure

• cordillera: the cordillera object

cop\_smacofSym

PCOPS versions 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.

```
cop_smacofSym(
  dis,
  theta = 1,
  ndim = 2,
  weightmat = NULL,
  init = NULL,
  itmaxi = 1000,
   ...,
  stressweight = 1,
  cordweight = 0.5,
  q = 1,
```

32 cop\_smacofSym

```
minpts = ndim + 1,
epsilon = 10,
rang = NULL,
verbose = 0,
normed = TRUE,
scale = "sd",
stresstype = "default"
)
```

#### **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

itmaxi number of iterations. default is 1000

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

stressweight weight to be used for the fit measure; defaults to 1 cordweight weight to be used for the cordillera; defaults to 0.5

q the norm of the cordillera; defaults to 1

minpts the minimum points to make up a cluster in OPTICS; defaults to ndim+1

epsilon the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults

to 10

range of the distances (min distance minus max distance). If NULL (default)

the cordillera will be normed to each configuration's maximum distance, so an

absolute value of goodness-of-clusteredness.

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

bose

normed should the cordillera be normed; defaults to TRUE

scale should the configuration be scale adjusted

stresstype which stress to report. Only takes smacofs default stress currrently.

### Value

A list with the components

• stress: the stress

stress.m: default normalized stress copstress: the weighted loss value

• OC: the Optics cordillera value

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

cop\_sstress 33

• fit: the returned object of the fitting procedure (which has all smacofB elements and some more)

• cordillera: the cordillera object

cop\_sstress

PCOPS version of sstress

# Description

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

# Usage

```
cop_sstress(
  dis,
  theta = c(2, 1, 1),
 weightmat = 1 - diag(nrow(dis)),
  init = NULL,
  ndim = 2,
  itmaxi = 10000,
  stressweight = 1,
  cordweight = 0.5,
  q = 1,
 minpts = ndim + 1,
  epsilon = 10,
  rang = NULL,
  verbose = 0,
  scale = "sd",
  normed = TRUE,
 stresstype = c("default", "stress1", "rawstress", "normstress", "enormstress",
    "enormstress1")
)
```

#### **Arguments**

dis	numeric matrix or dist object of a matrix of proximities
theta	the theta vector of powers; this must be a scalar of the lambda transformation for the observed proximities. Defaults to 1. Note that the lambda here works as a multiplicator of 2 (as sstress has f(delta^2)).
weightmat	(optional) a matrix of nonnegative weights
init	(optional) initial configuration
ndim	number of dimensions of the target space

34 doubleCenter

itmaxi number of iterations. default is 10000.

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

stressweight weight to be used for the fit measure; defaults to 1 cordweight weight to be used for the cordillera; defaults to 0.5

q the norm of the cordillera; defaults to 1

minpts the minimum points to make up a cluster in OPTICS; defaults to ndim+1

epsilon the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults

to 10

range of the distances (min distance minus max distance). If NULL (default)

the cordillera will be normed to each configuration's maximum distance, so an

absolute value of goodness-of-clusteredness.

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

bose

scale should the configuration be scale adjusted

normed should the cordillera be normed; defaults to TRUE

stresstype which stress to report? Defaults to explicitly normed stress

#### Value

A list with the components

• stress: the stress

• stress.m: default normalized stress

• copstress: the weighted loss value

• OC: the Optics cordillera value

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

• fit: the returned object of the fitting procedure

• cordillera: the cordillera object

doubleCenter Double centering of a matrix

# Description

Double centering of a matrix

# Usage

doubleCenter(x)

### **Arguments**

x numeric matrix

enorm 35

# Value

the double centered matrix

enorm

Explicit Normalization Normalizes distances

# Description

Explicit Normalization Normalizes distances

# Usage

```
enorm(x, w = 1)
```

# Arguments

x numeric matrix w weight

### Value

a constant

ljoptim

(Adaptive) Version of Luus-Jakola Optimization

# **Description**

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

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

36 ljoptim

### **Arguments**

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

#### Value

A list with the components (see also optim)

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

#### **Examples**

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

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

mkBmat 37

mkBmat

Auxfunction1

# Description

only used internally

# Usage

```
mkBmat(x)
```

# Arguments

Х

matrix

## Value

a matrix

mkPower

Take matrix to a power

# Description

Take matrix to a power

# Usage

```
mkPower(x, r)
```

## Arguments

x matrix

r numeric (power)

## Value

a matrix

38 pcops

pcops

Profile COPS Function (aka COPS Variant 2)

#### **Description**

Metaparameter selection for MDS models baseed on the Profile COPS approach (COPS Variant 2). It uses copstress for hyperparameter selection. It is a special case of a STOPS model.

#### Usage

```
pcops(
  dis,
 loss = c("stress", "smacofSym", "smacofSphere", "strain", "sammon", "rstress",
  "powermds", "sstress", "elastic", "powersammon", "powerelastic", "powerstress",
    "sammon2", "powerstrain", "apstress", "rpowerstress"),
 weightmat = NULL,
 ndim = 2,
  init = NULL,
  theta = 1,
  stressweight = 1,
  cordweight,
 q = 2,
 minpts = ndim + 1,
 epsilon = 100,
 optimmethod = c("ALJ", "pso", "SANN", "DIRECT", "DIRECTL", "stogo", "MADS", "hjk"),
  lower = 0.5,
  upper = 5,
  verbose = 0,
  scale = c("proc", "sd", "none", "std"),
  normed = TRUE,
  s = 4,
  stresstype = "default",
  acc = 1e-07,
  itmaxo = 200,
 itmaxi = 10000,
)
```

#### Arguments

dis

numeric matrix or dist object of a matrix of proximities

loss

which loss function to be used for fitting, defaults to strain. Currently allows for the following models:

Power transformations of observed proximities only (theta must be scalar):
 Strain loss or classical scaling (strain, workhorse is cmdscale), Kruskall's

pcops 39

stress for symmetric matrices (smacofSym or stress and smacofSphere for scaling onto a sphere; workhorse is smacof), Sammon mapping (sammon or sammon2; for the earlier the workhorse is sammon from MASS for the latter it is smacof), elastic scaling (elastic, the workhorse is smacof), Takane et al's s-Stress sstress (workhorse is powerstressMin)

- Power transformations of fitted distances only (theta must be scalar): De Leeuw's r-stress rstress (workhorse is powerstressMin)
- Power transformations of fitted distances and observed proximities (theta must be scalar or of length 2): Power MDS (powermds), Sammon mapping/elastic scaling with powers (powersammon, powerelastic)
- Power transformations of fitted distances, observed proximities and weights (theta must be of length 3 at most): powerstress (POST-MDS, powerstress), restricted powerstress with equal transformations for distances and proximities (rpowerstress); workhorse is powerstressMin)
- Approximation to power stress (theta must be of length 2): Approximated power stress (apstress; workhorse is smacof)

weightmat

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

ndim

number of dimensions of the target space

init

(optional) initial configuration. If not supplied, the Torgerson scaling result of the dissimilarity matrix dis^theta[2]/enorm(dis^theta[2],weightmat) is used.

theta

the theta vector of powers; see the corresponding cop\_XXX function for which theta are allowed. If a scalar is given as argument, it will be recycled. Defaults to 1

stressweight

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

cordweight

weight to be used for the cordillera; if missing gets estimated from the initial configuration so that copstress = 0 for theta=c(1,1)

α

the norm of the cordillera; defaults to 1

minpts

the minimum points to make up a cluster in OPTICS; defaults to ndim+1

epsilon

the epsilon parameter of OPTICS, the neighbourhood that is checked; defaults to 10

rang

range of the minimum reachabilities to be considered. If missing it is found from the initial configuration by taking 1.5 times the maximal minimum reachability of the model with theta=c(1,1). If NULL it will be normed to each configuration's minimum and maximum distance, so an absolute value of goodness-of-clusteredness. Note that the latter is not necessarily desirable when comparing configurations for their relative clusteredness. See also cordillera.

optimmethod

What general purpose optimizer to use? Defaults to our adaptive LJ version (ALJ). Also allows particle swarm optimization with s particles ("pso") and simulated annealing ("SANN"), "DIRECT" and "DIRECTL", Hooke-Jeeves ("hjk"), StoGo ("stogo"), and "MADS". We recommend not using SANN and pso with the rstress, sstress and the power stress models. We made good experiences with ALJ, stogo, DIRECT and DIRECTL and also MADS.

lower

A vector of the lower box contraints of the search region. Its length must match the length of theta.

40 pcops

upper A vector of the upper box contraints of the search region. Its length must match

the length of theta.

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

bose. Note that for models with some parameters fixed, the iteration progress of the optimizer shows different values also for the fixed parameters because due to the modular setup we always optimize over a three parameter vector. These

values are inconsequential however as internally they will be fixed.

scale should the configuration be scaled and/or centered for calculating the cordillera?

"std" standardizes each column of the configurations to mean=0 and sd=1 (typically not a good idea), "sd" scales the configuration by the maximum standard devation of any column (default), "proc" adjusts the fitted configuration to the init configuration (or the Togerson scaling solution if init=NULL). This parameter only has an effect for calculating the cordillera, the fitted and returned con-

figuration is NOT scaled.

normed should the cordillera be normed; defaults to TRUE

s number of particles if pso is used

stresstype what stress to be used for comparisons between solutions. Currently not imple-

mented and pcops uses explicitly normalized stress for copstress (not stress-1).

Stress-1 is reported by the print function though.

acc termination threshold difference of two successive outer minimization steps.

itmaxo iterations of the outer step (optimization over the hyperparmeters; if solver al-

lows it). Defaults to 200.

itmaxi iterations of the inner step (optimization of the MDS). Defaults to 10000 (whichis

huge).

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

#### Value

A list with the components

• copstress: the weighted loss value

• OC: the OPTICS cordillera for the scaled configuration (as defined by scale)

• optim: the object returned from the optimization procedure

• stress: the stress (square root of stress.m)

· stress.m: default normalized stress

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

• fit: the returned object of the fitting procedure

• cordillera: the cordillera object

```
dis<-as.matrix(smacof::kinshipdelta)
set.seed(210485)
#configuration is scaled with highest column sd for calculating cordilera
res1<-pcops(dis,loss="strain",lower=0.1,upper=5,minpts=2)</pre>
```

pdist 41

```
res1
summary(res1)
plot(res1)
```

pdist

Squared p-distances

# Description

Squared p-distances

## Usage

```
pdist(x, p)
```

## **Arguments**

x numeric matrix

p p>0 the Minkoswki distance

#### Value

squared Minkowski distance matrix

plot.cops

S3 plot method for cops objects

# Description

S3 plot method for cops objects

#### Usage

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

42 plot.pcops

#### **Arguments**

x an object of class cops

plot.type String indicating which type of plot to be produced: "confplot", "reachplot",

"resplot", "transplot", "Shepard", "stressplot" (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

represenation of the fitted distances.

... Further plot arguments passed: see 'plot.smacof' and 'plot' for detailed infor-

mation.
Details:

• Configuration plot (plot.type = "confplot"): Plots the MDS configurations.

• Reachability plot (plot.type = "confplot"): Plots the OPTICS reachability plot and the OPTICS cordillera

• Residual plot (plot.type = "resplot"): Plots the dissimilarities against the fitted distances.

- 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.
- Transformation Plot (plot.type = "transplot"): Diagram with the observed dissimilarities (lighter) and the transformed observed dissimilarities (darker) against the fitted distances together with loess smoothing lines
- 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.
- 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.

#### **Examples**

dis<-as.matrix(smacof::kinshipdelta)
resl<-copstressMin(dis,itmax=20)
plot(resl)</pre>

plot.pcops

S3 plot method for p-cops objects

#### Description

S3 plot method for p-cops objects

plot.pcops 43

#### Usage

```
## S3 method for class 'pcops'
plot(x, plot.type = c("confplot"), main, asp = NA, ...)
```

#### **Arguments**

X	an object of class cops
plot.type	String indicating which type of plot to be produced: "confplot", "reachplot", "resplot", "transplot", "Shepard", "stressplot" (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 represenation of the fitted distances.
• • •	Further plot arguments passed: see 'plot.smacof' and 'plot' for detailed information.
	Details

- Configuration plot (plot.type = "confplot"): Plots the MDS configurations.
- Reachability plot (plot.type = "confplot"): Plots the OPTICS reachability plot and the OPTICS cordillera
- Residual plot (plot.type = "resplot"): Plots the dissimilarities against the fitted distances.
- 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.
- Transformation Plot (plot.type = "transplot"): Diagram with the observed dissimilarities (lighter) and the transformed observed dissimilarities (darker) against the fitted distances together with loess smoothing lines
- 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
- 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.

```
dis<-as.matrix(smacof::kinshipdelta)
resl<-pcops(dis,loss="strain",lower=0.1,upper=5,minpts=2)
plot(resl)
plot(resl,plot.type="Shepard")</pre>
```

plot.smacofP

plot.smacofP

S3 plot method for smacofP objects

## Description

S3 plot method for smacofP objects

## Usage

```
## S3 method for class 'smacofP'
plot(
 Х,
 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')

plot.smacofP 45

pch Plot symbol

asp Aspect ratio; defaults to 1 so distances between x and y are represented accu-

rately; can lead to slighlty 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.

Datailar

#### Details:

- Configuration plot (plot.type = "confplot"): Plots the MDS configurations.
- Residual plot (plot.type = "resplot"): Plots the dissimilarities against the fitted distances.
- 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.
- 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
- 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.
- Bubble plot (plot.type = "bubbleplot"): Combines the configuration plot with the point stress contribution. The larger the bubbles, the better the fit.

#### **Examples**

. . .

```
dis<-as.matrix(smacof::kinshipdelta)
res<-powerStressMin(dis)
plot(res)
plot(res,"reachplot")
plot(res,"Shepard")
plot(res,"resplot")
plot(res,"transplot")
plot(res,"stressplot")
plot(res,"bubbleplot")</pre>
```

plot3dstatic plot3dstatic: static 3D plots

## 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

```
plot3dstatic.cmdscaleE
```

3D plots: plot3dstatic method for class cmdscale

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

powerStressFast 47

#### **Arguments**

X	object of class cmdscale
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.

powerStressFast

Power stress minimization by NEWUOA

#### **Description**

An implementation to minimize power stress by a derivative-free trust region optimization algorithm (NEWUOA). Much faster than majorizing as used in powerStressMin but perhaps less accurate.

#### Usage

```
powerStressFast(
  delta,
  kappa = 1,
  lambda = 1,
  nu = 1,
  weightmat = 1 - diag(nrow(delta)),
  init = NULL,
  ndim = 2,
  acc = 1e-12,
  itmax = 50000,
  verbose = FALSE
)
```

# Arguments

delta dist object or a symmetric, numeric data.frame or matrix of distances power of the transformation of the fitted distances; defaults to 1 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 starting configuration

48 powerStressFast

ndim dimension of the configuration; defaults to 2

acc The smallest value of the trust region radius that is allowed. If not defined, then

1e-10 will be used.

itmax maximum number of iterations. Default is 50000. verbose should iteration output be printed; if > 1 then yes

#### Value

a smacofP object (inheriting form smacofB, see smacofSym). It is a list with the components

- delta: Observed dissimilarities, not normalized
- obsdiss: Observed dissimilarities, normalized
- confdist: Configuration dissimilarities, NOT normalized
- conf: Matrix of fitted configuration, NOT normalized
- stress: Default stress (stress 1, square root of the explicitly normalized stress on the normalized, transformed dissimilarities)
- 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

#### and some additional components

- gamma: Empty
- stress.m: default stress for the COPS and STOP. Defaults to the explicitly normalized stress on the normalized transformed dissimilarities
- stress.en: explicitly stress on the normalized, transformed dissimilarities and normalized transformed distances
- deltaorig: observed, untransformed dissimilarities
- weightmat: weighting matrix

#### See Also

```
smacofSym
```

```
dis<-smacof::kinshipdelta
res<-powerStressFast(as.matrix(dis),kappa=2,lambda=1.5)
res
summary(res)
plot(res)</pre>
```

powerStressMin 49

powerStressMin

Power Stress SMACOF

#### **Description**

An implementation to minimize power stress by minimization-majorization. Usually more accurate but slower than powerStressFast. Uses a repeat loop.

#### 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. Default is 50000.
verbose	should iteration output be printed; if $> 1$ then yes

#### Value

a smacofP object (inheriting form smacofB, see smacofSym). It is a list with the components

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

50 procruster

- 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

and some additional components

- stress.m: default stress for the COPS and STOP defaults to the explicitly normalized stress on the normalized, transformed dissimilarities
- stress.en: a manually calculated stress on the normalized, transformed dissimilarities and normalized transformed distances which is not correct
- deltaorig: observed, untransformed dissimilarities
- weightmat: weighting matrix

#### See Also

```
smacofSym
```

## **Examples**

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

procruster

procruster: a procrustes function

#### **Description**

```
procruster: a procrustes function
```

#### Usage

```
procruster(x)
```

#### **Arguments**

Х

numeric matrix

#### Value

a matrix

sammon 51

sa	mm	n	n

Wrapper to sammon for S3 class

## 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.
У	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 sammon

#### **Details**

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

#### Value

Object of class sammonE' inheriting from sammon. This wrapper only adds an extra slot to the list with the call, adds column labels to the \$points and assigns S3 classes 'sammonE', 'sammon' and 'cmdscale'. It also adds a slot obsdiss with normalized dissimilarities.

```
dis<-as.matrix(smacof::kinshipdelta)
res<-sammon(dis)</pre>
```

52 secularEq

scale\_adjust

Adjusts a configuration

## Description

Adjusts a configuration

## Usage

```
scale_adjust(conf, ref, scale = c("sd", "std", "proc", "none"))
```

#### **Arguments**

conf a configuration

ref a reference configuration (only for scale="proc")

scale Scale adjustment. "std" standardizes each column of the configurations to mean=0

and sd=1, "sd" scales the configuration by the maximum standard devation of

any column, "proc" adjusts the fitted configuration to the reference

#### Value

The scale adjusted configuration.

secularEq

Secular Equation

## Description

Secular Equation

#### Usage

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

#### **Arguments**

a matrix b matrix

#### Value

a matrix

sqdist 53

sqdist

Squared distances

## Description

Squared distances

## Usage

```
sqdist(x)
```

## Arguments

Х

numeric matrix

## Value

squared distance matrix

torgerson

Torgerson scaling

## Description

Torgerson scaling

## Usage

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

# Arguments

delta symmetric, numeric matrix of distances

p target space dimensions

## Value

```
a n x p matrix (the configuration)
```

```
dis<-as.matrix(smacof::kinshipdelta)
res<-torgerson(dis)</pre>
```

# **Index**

alvatorina	con amonafoum 21
* clustering cops, 5	<pre>cop_smacofSym, 31 cop_sstress, 33</pre>
cops, 3 copstressMin, 9	cops, 5
pcops, 38	copstress, 8
* multivariate	copstressMin, 5, 6, 9
	cordillera, 10, 39
cop_apstress, 12	Cordiffera, 10, 39
cop_cmdscale, 14	doubleCenter, 34
cop_elastic, 15	doddicechter, 54
cop_powerelastic, 17	enorm, 35
cop_powermds, 18	,,
cop_powersammon, 20	ljoptim, 35
cop_powerstress, 22	
cop_rpowerstress, 23	mkBmat, 37
cop_rstress, 25	mkPower, 37
cop_sammon, 26	
cop_sammon2, 28	optim, <i>36</i>
cop_smacofSphere, 30	5 6 20
cop_smacofSym, 31	pcops, 5, 6, 38
cop_sstress, 33	pdist, 41
cops, 5	plot.cops, 41
copstress, 8	plot.pcops, 42
copstressMin, 9	plot.smacofP, 44
pcops, 38	plot3dstatic, 46
	plot3dstatic.cmdscaleE, 46
BankingCrisesDistances, 3	powerStressFast, 47
emdecale 2 4	powerStressMin, 49
cmdscale, 3, 4	procruster, 50
conf_adjust, 4	sammon, <i>51</i> , <i>5</i> 1
cop_apstress, 12	
cop_cmdscale, 14	scale_adjust, 52 secularEq, 52
cop_elastic, 15	**
cop_powerelastic, 17	smacofSym, 48–50
cop_powermds, 18	sqdist, 53
cop_powersammon, 20	torgerson, 53
cop_powerstress, 22	tor ger 3011, <i>33</i>
cop_rpowerstress, 23	
cop_rstress, 25	
cop_sammon, 26	
cop_sammon2, 28	
cop_smacofSphere, 30	