Package 'CluMix'

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Type Package

Title Clustering and Visualization of Mixed-Type Data

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Description Provides utilities for clustering subjects and variables of mixed data types. Similarities between subjects are measured by Gower's general similarity coefficient with an extension of Podani for ordinal variables. Similarities between variables can be assessed i) by combination of appropriate measures of association for different pairs of data types or ii) based on distance correlation. Alternatively, variables can also be clustered by the 'ClustOfVar' approach. The main feature of the package is the generation of a mixed-data heatmap. For visualizing similarities between either subjects or variables, a heatmap of the corresponding distance matrix can be drawn. Associations between variables can be explored by a 'confounder plot', which allows visual detection of possible confounding, collinear, or surrogate factors for some variables of primary interest. Distance matrices and dendrograms for subjects and variables can be derived and used for further visualizations and applications. This work was supported by BMBF grant 01ZX1609B, Germany.
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Description

Provides utilities for clustering subjects and variables of mixed data types. Similarities between subjects are measured by Gower's general similarity coefficient with an extension of Podani for ordinal variables. Similarities between variables can be assessed i) by combination of appropriate measures of association for different pairs of data types or ii) based on distance correlation. Alternatively, variables can also be clustered by the 'ClustOfVar' approach. The main feature of the package is the generation of a mixed-data heatmap. For visualizing similarities between either subjects or variables, a heatmap of the corresponding distance matrix can be drawn. Associations between variables can be explored by a 'confounder plot', which allows visual detection of possible confounding, collinear, or surrogate factors for some variables of primary interest. Distance matrices and dendrograms for subjects and variables can be derived and used for further visualizations and applications. This work was supported by BMBF grant 01ZX1609B, Germany.

Details

The DESCRIPTION file: This package was not yet installed at build time.

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	different types

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```
similarity.subjects Similarity matrix for subjects similarity.variables Similarity matrix for variables
```

The main function mix.heatmap of the package generates a mixed-data heatmap. For visualizing similarities between either subjects or variables, a heatmap of the corresponding distance matrix can be drawn (distmap). Associations between variables can be explored by the confounderPlot, which allows visual detection of possible confounding, collinear, or surrogate factors for some variables of primary interest. Distance matrices and dendrograms for subjects and variables can be derived by functions dist.subjects, dist.variables, dendro.subjects, and dendro.variables. Clustering subjects is based on Gower's general similarity coefficient. Variables can be clustered by i) combination of association measures, ii) distance correlation, iii) the ClustOfVar approach.

Author(s)

M. Hummel, D. Edelmann, A. Kopp-Schneider

Maintainer: Manuela Hummel <m.hummel@dkfz.de>

References

Hummel M, Edelmann D, Kopp-Schneider A. Clustering of samples and variables with mixed-type data. Submitted.

Gower J (1971). A general coefficient of similarity and some of its properties. Biometrics, 27:857-871.

Chavent M, Kuentz-Simonet V, Liquet B, Saracco J (2012). ClustOfVar: An R Package for the Clustering of Variables. Journal of Statistical Software, 50:1-16.

Szekely GJ, Rizzo ML, Bakirov NK (2007). Measuring and testing dependence by correlation of distances. The Annals of Statistics, 35.6:2769-2794.

Lyons R (2013). Distance covariance in metric spaces. The Annals of Probability, 41.5:3284-3305.

See Also

```
mix.heatmap
```

```
data(mixdata)
mix.heatmap(mixdata, rowmar=7)
```

4 association

association	Function to calculate a measure for association between two variables on arbitrary scales

Description

Similarities between variables used for clustering are calculated by this function. For each combination of different data types, an appropriate measure for association is chosen, see details.

Usage

```
association(x, y)
```

Arguments

```
x vector of class numeric, factor, ordered, or logical vector of class numeric, factor, ordered, or logical
```

Details

The following association measures for respective types of variables are chosen:

- quantitative vs quantitative/ordinal: absolute Spearman correlation coefficient
- ordinal vs ordinal: absolute Goodman and Kruskal's gamma coefficient (Goodman and Kruskal, 1954)
- quantitative/ordinal vs binary: absolute Goodman and Kruskal's gamma coefficient
- quantitative vs categorical (>2 categories): The categories of the categorical variable are reordered with respect to average ranks of the quantitative variable within those categories. Then absolute Spearman correlation coefficient is calculated as if it was an ordered factor. To avoid over-optimism, the reordering is only applied if a Kruskal-Wallis pre-test of association yields a significant result (p<0.05).
- ordinal vs categorical (>2 categories): as for 'quantitative vs categorical', but instead of Spearman correlation the absolute Goodman and Kruskal's gamma coefficient is calculated
- categorical vs categorical: Also in this case the reordering strategy is applied by "diagonalizing" the cross-table between the two factors (see optile from the extracat package). Association is then measured by absolute Goodman and Kruskal's gamma coefficient. To avoid over-optimism, the reordering is only applied if a chi-square pre-test of association yields a significant result (p<0.05).

Value

Estimated value of association between x and y

Author(s)

Manuela Hummel

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References

Goodman LA and Kruskal WH (1954). Measures of association for cross classifications. Journal of the American Statistical Association, 49:732-764.

See Also

```
similarity.variables, dist.variables,
```

Examples

```
x <- rnorm(100)
y <- as.factor(sample(1:3, 100, replace=TRUE))
association(x, y)</pre>
```

 ${\tt confounderPlot}$

Confounder Plot

Description

Plots similarities of all variables to an outcome variable against similarities of all variables to a predictor of interest

Usage

```
confounderPlot(data, S, x, y, labels, method = c("associationMeasures", "distcor"),
returnS = FALSE, plotLegend = TRUE, col, pch, font, cex.text, xlim, ylim, ...)
```

Arguments

data	data frame with variables of interest
S	similarity matrix; if missing it will be calculated from data by similarity.variables
X	name of the predictor variable (as used in data and S) of main interest, for which confounders / collinearities shall be detected
у	name of the outcome variable (as used in data and S)
labels	variable names used for plotting; have to be in corresponding order with columns of data; if missing, names of data are used
method	method to calculate similarities: combination of association measures ('associationMeasures') or distance correlation ('distcor')
returnS	shall similarity matrix be returned?
plotLegend	shall (default) legend be shown, indicating categorical and continuous variables
col	symbol and label color; by default categorical variables are shown in purple, continuous variables in black
pch	plotting symbol, default 16
font	font of plotted labels; by default names of variables x and y are shown in bold

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```
cex.text size of plotted labels

xlim, ylim axis limits

... graphical parameters passed to plot
```

Details

The similarities of all variables in a dataset with two variables of special interest (i.e. predictor and outcome of a regression model) are simultaneously visualized in a scatter plot, where the x-axis shows similarities to the predictor and the y-axis similarities to the outcome. The height of the predictor variable's point indicates its association with the outcome and hence its predicting ability. Variables in the upper right part are potential confounders for which prediction model should be adjusted, or collinear variables that should be removed. Variables in the lower right part are strongly related to the predictor, but not associated with the outcome. Variables very close to the outcome variable's point are potential surrogate outcomes.

Value

Scatterplot of variable similarities. Chosen predictor and outcome variables are highlighted in bold. Categorical/quantitative variables are shown in purple/black by default.

Author(s)

Manuela Hummel

See Also

```
similarity.variables
```

Examples

```
data(mixdata)
confounderPlot(mixdata, x="X2.quant", y="X1.cat")
```

dendro.subjects

Subjects dendrogram

Description

Get dendrogram for subjects (observations) based on variables of mixed data types

Usage

```
dendro.subjects(data, weights, linkage="ward.D2")
```

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Arguments

data data frame

weights optional vector of weights for variables in data

linkage agglomeration method used for hierarchical clustering; corresponds to parame-

ter method of hclust

Details

Distances between subjects are based on Gower's general similarity coefficient with an extension of Podani for ordinal variables, see gowdis. In the case that all variables are quantitative, Euclidean distances are used. Then a dendrogram is derived by standard hierarchical clustering (hclust with agglomeration method = "ward.D2" by default).

Value

An object of class dendrogram

Author(s)

Manuela Hummel

References

Gower J (1971). A general coefficient of similarity and some of its properties. Biometrics, 27:857-871.

Podani J (1999). Extending Gower's general coefficient of similarity to ordinal characters. Taxon, 48(2):331-340.

See Also

```
dendro.variables, dist.subjects, mix.heatmap
```

```
data(mixdata)

dend <- dendro.subjects(mixdata)
plot(dend)

## example with weights
w <- rep(1:2, each=5)
dend <- dendro.subjects(mixdata, weights=w)
plot(dend)</pre>
```

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Description

Get dendrogram for variables of mixed types

Usage

```
dendro.variables(data, method = c("associationMeasures", "distcor", "ClustOfVar"),
   linkage="ward.D2", associationFun = association, check.psd = TRUE)
```

Arguments

data data frame with variables of interest

method If "associationMeasures", similarities between variables are assessed by com-

bination of appropriate measures of association for different pairs of data types. If "distcor", distances between variables are calculated based on distance correlation. In both cases, then a dendrogram is derived by standard hierarchical clustering (hclust). If "ClustOfVar", variables are clustered by hclustvar

from the ClustOfVar package.

linkage agglomeration method used for hierarchical clustering when dist.variables.method = "association"

corresponds to parameter method of hclust

associationFun By default, appropriate association measures are chosen for each pair of vari-

ables, see association for details. But the user can also define a function that

for any two variables calculates a similarity measure. Ignored if dist.variables.method = "ClustOfVa

check.psd If TRUE, it is checked if the variable's similarity matrix S is positive semi-

definite (p.s.d.), and if not it is transformed to a p.s.d. one by nearPD, see dist.variables for details. Ignored if dist.variables.method = "ClustOfVar"

Details

Clustering of variables can either be done i) similarity-based using measures of association, ii) similarity-based using distance correlation, or iii) by the ClustOfVar approach, which uses principal components analysis for mixed data.

Value

An object of class dendrogram

Author(s)

Manuela Hummel

dist.subjects 9

References

Hummel M, Edelmann D, Kopp-Schneider A. Clustering of samples and variables with mixed-type data. Submitted.

Chavent M, Kuentz-Simonet V, Liquet B, Saracco J (2012). ClustOfVar: An R Package for the Clustering of Variables. Journal of Statistical Software, 50:1-16.

See Also

association, similarity.variables, dist.variables, dendro.subjects, mix.heatmap, hclustvar

Examples

```
data(mixdata)

dend1 <- dendro.variables(mixdata, method="associationMeasures")
plot(dend1)

dend2 <- dendro.variables(mixdata, method="distcor")
plot(dend2)

dend3 <- dendro.variables(mixdata, method="ClustOfVar")
plot(dend3)</pre>
```

dist.subjects

Distance matrix for subjects

Description

Get distance matrix for subjects (observations) based on variables of mixed data types

Usage

```
dist.subjects(data, weights, alwaysGower = FALSE)
```

Arguments

data data frame

weights optional vector of weights for variables in data

alwaysGower controls the way distances are calculated in case of exclusively continuous data;

if FALSE (default), Euclidean distances, if TRUE Gower's distances

Details

Distances between subjects are based on Gower's general similarity coefficient with an extension of Podani for ordinal variables, see gowdis. In the case that all variables are quantitative, either Euclidean distances or still Gower's distances can be used.

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Value

An object of class dist

Author(s)

Manuela Hummel

References

Gower J (1971). A general coefficient of similarity and some of its properties. Biometrics, 27:857-871.

Podani J (1999). Extending Gower's general coefficient of similarity to ordinal characters. Taxon, 48(2):331-340.

See Also

```
dendro.subjects, similarity.subjects, dist.variables, mix.heatmap
```

Examples

```
data(mixdata)

D <- dist.subjects(mixdata)

## example with weights
w <- rep(1:2, each=5)
D <- dist.subjects(mixdata, weights=w)</pre>
```

dist.variables

Distance matrix for variables

Description

Get distance matrix for variables of mixed types

Usage

```
dist.variables(data, method = c("associationMeasures", "distcor"),
associationFun = association, check.psd = TRUE)
```

Arguments

data data frame with variables of interest

 $method \qquad method \ to \ calculate \ distances: \ combination \ of \ association \ measures \ ('association Measures')$

or distance correlation ('distcor')

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associationFun only applies if method = 'associationMeasures': by default, appropriate association measures are chosen for each pair of variables, see association for details. But the user can also define a function that for any two variables

calculates a similarity measure.

check.psd only applies if method = 'associationMeasures': if TRUE, it is checked if

the variable's similarity matrix S is positive semi-definite (p.s.d.), and if not it is transformed to a p.s.d. one by nearPD.

Details

A distance matrix for variables can be derived by combining different measures of association or by a distance correlation approach. For the association measure approach, for each pair of variables, similarity coefficients s_ij are calculated, see association for details. Distances are then calculated as d_ij = sqrt(1 - s_ij). If the similarity matrix is (made) positive semi-definite, those distances have metric properties (Gower, 1971), which means for instance that the triangular inequality holds. The distance correlation approach uses generalized distance correlation based on Gower's similarity coefficient between sample elements. The distance is then defined by 1 minus the square root of the distance correlation matrix.

Value

An object of class dist

Author(s)

Manuela Hummel, Dominic Edelmann

References

Hummel M, Edelmann D, Kopp-Schneider A. Clustering of samples and variables with mixed-type data. Submitted.

Gower J (1971). A general coefficient of similarity and some of its properties. Biometrics, 27:857-871.

Szekely GJ, Rizzo ML, Bakirov NK (2007). Measuring and testing dependence by correlation of distances. The Annals of Statistics, 35.6:2769-2794.

Lyons R (2013). Distance covariance in metric spaces. The Annals of Probability, 41.5:3284-3305.

See Also

association, similarity.variables, dendro.variables, dist.subjects, mix.heatmap

```
data(mixdata)

D1 <- dist.variables(mixdata, method="association")

D2 <- dist.variables(mixdata, method="distcor")</pre>
```

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distmap	Display similarity matrix	

Description

Calculates and visualizes a similarity matrix for subjects or variables in an image plot

Usage

```
distmap(data, what = c("subjects", "variables"), variables.method =
c("associationMeasures", "distcor"), varweights, linkage = "ward.D2",
reorderdend, col, ...)
```

Arguments

data	data.frame with original data or similarity matrix
what	Shall similarity matrix of subjects or variables be visualized?; ignored if data is a similarity matrix
variables.metho	od
	method to calculate similarities if what = "variables": combination of association measures ("associationMeasures") or distance correlation ("distcor")
varweights	optional vector of variable weights, used for calculating Gower's distances between subjects; ignored if what = "associationMeasures"
linkage	agglomeration method used for hierarchical clustering; corresponds to parameter method of $hclust$
reorderdend	optional numeric values for reordering the dendrogram (maintaining the constraints on the dendrogram), see wts option of reorder.dendrogram
col	Color palette; defaults to blue-scale palette, where darker blue indicates higher similarity
	graphical parameters passed to heatmap. 2

Details

If data is a data.frame, the similarity matrix is calculated for subjects (if what = "subjects") or variables (if what = "variables"). Similarities for subjects are calculated by similarity.subjects. \ Similarities for variables are derived by similarity.variables. Alternatively, data can also be a previously calculated similarity matrix.

Value

Image plots and dendrograms

Author(s)

Manuela Hummel

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See Also

similarity.variables, dist.variables, similarity.subjects, dist.subjects, mix.heatmap

Examples

```
data(mixdata)
## subjects
distmap(mixdata, what="subjects")
# example with variable weights
w <- rep(1:2, each=5)
distmap(mixdata, what="subjects", varweights=w)
## variables
distmap(mixdata, what="variables", method="association")
distmap(mixdata, what="variables", method="distcor")</pre>
```

mix.heatmap

Heatmap for data with variables of mixed types

Description

Produces a heatmap visualizing all samples and variables of a dataset. Both samples and variables are clustered using methods suitable for mixed-type data. Different types of variables are indicated by different color schemes.

Usage

Arguments

data frame where columns are variables (of different data types) and rows are observations (subjects, samples)

D. subjects A previously calculated distance matrix (class dissimilarity) for subjects can

be given. If missing, it is calculated by dist. subjects. If set to NULL, no

clustering is done and original order in data will be preserved.

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D. variables A previously calculated distance matrix (of class dissimilarity) for variables

can be given. If missing, it is calculated by dist.variables. If set to NULL, no

clustering is done and original order in data will be preserved.

dend.subjects A dendrogram for subjects can be given; then no distances between subjects

will be calculated and D. subjects will be ignored.

dend.variables A dendrogram for variables can be given; then no distances between variables

will be calculated and D. variables will be ignored.

varweights optional vector of variable weights, used for calculating Gower's distances be-

tween subjects

dist.variables.method

If "associationMeasures", similarities between variables are assessed by combination of appropriate measures of association for different pairs of data types. If "distcor", distances between variables are calculated based on distance correlation. In both cases, then a dendrogram is derived by standard hierarchical clustering (hclust). If "ClustOfVar", variables are clustered by hclustvar

from the ClustOfVar package.

linkage agglomeration method used for hierarchical clustering; corresponds to parame-

ter method of hclust

associationFun By default, appropriate association measures are chosen for each pair of vari-

ables, see association for details. But the user can also define a function that

for any two variables calculates a similarity measure. Ignored if dist.variables.method = "ClustOfVa

or "distcor"

row (variable) labels; if missing, column names of data are used

rowmar margin for row (variable) labels
lab.cex size of row (variable) labels

ColSideColors vector of length nrow(data) specifying colors for a color bar added on top of

the heatmap

RowSideColors vector of length ncol(data) specifying colors for a color bar added to the left

of the heatmap

col.cont color palette for continuous variables; defaults to red-blue color palette

cont.fixed.range

If FALSE, color range of each continuous variable is defined by respective individual variable's range. If TRUE, all continuous variables are assumed to have similar range and hence shall have the same color range; "extreme colors" then correspond to extreme values over all continuous variables and are applied to all of them equally. In any case, in order to prevent outlier values to dominate the color scale, "extreme colors" are restricted to 2.5% and 97.5% quantiles.

Defaults to FALSE

cont.range if cont.fixed.range=TRUE, extreme value limits for coloring continuous vari-

ables can be specified; if missing, extreme values are taken from the data; ig-

nored if cont.fixed.range=FALSE

col.ord List with names of colors for the lowest and highest categories of ordinal vari-

ables. A color palette will be created correspondingly based on the number of

categories. Defaults to a green color palette

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col.cat vector of colors for categorical variables

legend.colbar class labels for subject groups defined by ColSideColors legend.rowbar class labels for variable groups defined by RowSideColors

legend.mat shall legend matrix for heatmap be shown?

legend.cex size of legend text

legend.srt legend matrix label string rotation in degrees; i.e. legend.srt = 90 produces

vertical labels

Details

If no dendrograms or distance matrices are given, subjects and/or samples are clustered with methods for mixed-type data. Similarities between subjects are measured by Gower's general similarity coefficient with an extension of Podani for ordinal variables, see gowdis. Similarities between variables can be assessed by combination of appropriate measures of association for different pairs of data types, see association, or based on distance correlation. Then standard hierarchical clustering with by default Ward's minimum variance method is applied. Alternatively, variables can also be clustered by the ClustOfVar approach.

Variables are shown as rows of the heatmap, samples as columns.

Value

A mixed-data heatmap with dendrograms and annotation

Note

The heatmap is currently limited to 200 variables = columns of data = heatmap rows.

Author(s)

Manuela Hummel, m.hummel@dkfz.de

References

Hummel M, Edelmann D, Kopp-Schneider A. Clustering of samples and variables with mixed-type data. Submitted.

Gower J (1971). A general coefficient of similarity and some of its properties. Biometrics, 27:857-871.

Chavent M, Kuentz-Simonet V, Liquet B, Saracco J (2012). ClustOfVar: An R Package for the Clustering of Variables. Journal of Statistical Software, 50:1-16.

Szekely GJ, Rizzo ML, Bakirov NK (2007). Measuring and testing dependence by correlation of distances. The Annals of Statistics, 35.6:2769-2794.

Lyons R (2013). Distance covariance in metric spaces. The Annals of Probability, 41.5:3284-3305.

See Also

dist.variables, dist.subjects, dendro.variables, dendro.subjects, distmap

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Examples

```
data(mixdata)
mix.heatmap(mixdata, rowmar=7, legend.mat=TRUE)

## with distance correlation
mix.heatmap(mixdata, dist.variables.method="distcor", rowmar=7, legend.mat=TRUE)

## with (random) color bars
colbar <- rep(5:7, nrow(mixdata))
rowbar <- rep(c("darkorange","grey"), ncol(mixdata))
mix.heatmap(mixdata, ColSideColors=colbar, RowSideColors=rowbar,
legend.colbar=c("1","2","3"), legend.rowbar=c("a","b"), rowmar=7)

## example with variable weights
w <- rep(1:2, each=5)
mix.heatmap(mixdata, varweights=w, rowmar=7)</pre>
```

mixdata

Small example dataset with variables of different types

Description

Simulated dataset with quantitative, ordinal and categorical variables. Some variables are correlated and some are associated to sample groups.

Usage

```
data(mixdata)
```

Format

mixdata is a data frame with 40 samples (rows) and 10 variables (columns). The variable names indicate their type, i.e. '.quant' (quantitative), '.ord' (ordinal), '.cat' (categorical).

```
data(mixdata)
str(mixdata)
```

similarity.subjects 17

similarity.subjects Similarity matrix for subjects

Description

Get similarity matrix for subjects (observations) based on variables of mixed data types

Usage

```
similarity.subjects(data, weights)
```

Arguments

data data frame

weights optional vector of weights for variables in data

Details

Distances d.ij between subjects are calculated based on Gower's general similarity coefficient with an extension of Podani for ordinal variables, see gowdis. In the case that all variables are quantitative, Euclidean distances are used. Similarities s.ij are calculated as s.ij = 1 - d.ij.

Value

Matrix of similarity values for each pair of subjects

Author(s)

Manuela Hummel

References

Gower J (1971). A general coefficient of similarity and some of its properties. Biometrics, 27:857-871.

Podani J (1999). Extending Gower's general coefficient of similarity to ordinal characters. Taxon, 48(2):331-340.

See Also

```
dendro.subjects, dist.subjects, mix.heatmap
```

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Examples

```
data(mixdata)

S <- similarity.subjects(mixdata)

## example with weights
w <- rep(1:2, each=5)
S <- similarity.subjects(mixdata, weights=w)</pre>
```

similarity.variables Similarity matrix for variables

Description

Get similarity matrix for variables of mixed types

Usage

```
similarity.variables(data, method = c("associationMeasures", "distcor"),
associationFun = association, check.psd = TRUE, make.psd = TRUE)
```

Arguments

data data frame with variables of interest $method\ to\ calculate\ distances:\ combination\ of\ association\ measures\ (\ 'association\ Measures\ ')$ method or distance correlation ('distcor') associationFun only applies if method = 'associationMeasures': appropriate association measures are chosen for each pair of variables, see association for details. But the user can also define a function that for any two variables calculates a similarity measure. check.psd only applies if method = 'associationMeasures': if TRUE, it is checked if the variable's similarity matrix S is positive semi-definite (p.s.d.), and if not it is transformed to a p.s.d. one by nearPD. make.psd only applies if method = 'associationMeasures': if TRUE, and if the similarity matrix is not positive semi-definite, it is transformed to a p.s.d. one by nearPD. Ignored if check.psd = FALSE

Details

A similarity matrix for variables can be derived by combining different measures of association or by a distance correlation approach. For the association measure approach, for each pair of variables, similarity coefficients s_ij are calculated, see association for details. If the similarity matrix is (made) positive semi-definite, distances d_ij = sqrt(1 - s_ij) have metric properties (Gower, 1971), which means for instance that the triangular inequality holds. The distance correlation approach uses generalized distance correlation based on Gower's similarity coefficient between sample elements.

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Value

Matrix of similarity values for each pair of variables

Author(s)

Manuela Hummel, Dominic Edelmann

References

Hummel M, Edelmann D, Kopp-Schneider A. Clustering of samples and variables with mixed-type data. Submitted.

Gower J (1971). A general coefficient of similarity and some of its properties. Biometrics, 27:857-871.

Szekely GJ, Rizzo ML, Bakirov NK (2007). Measuring and testing dependence by correlation of distances. The Annals of Statistics, 35.6:2769-2794.

Lyons R (2013). Distance covariance in metric spaces. The Annals of Probability, 41.5:3284-3305.

See Also

association, dist.variables, dendro.variables, dist.subjects, mix.heatmap

```
data(mixdata)
S1 <- similarity.variables(mixdata)
S2 <- similarity.variables(mixdata, method="distcor")</pre>
```

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