Package 'GMD'

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Title Generalized Minimum Distance of distributions
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Description GMD is a package for non-parametric distance measurement between two discrete frequency distributions.
Depends R (>= 2.9.0), stats, grDevices, gplots
Suggests datasets, MASS, cluster
Enhances stats, cluster, gplots
License GPL (>=2)
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Collate 'zzz.R' 'GMD-package.R' 'GMD-internal.R' 'GMD-data.R' 'ghist.R' 'gdist.R' 'css.R' 'heatmap3.R' 'gmdp.R' 'gmdm.R' R topics documented:
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cage
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Description

Computate Generalized Minimum Distance (GMD) between discrete distributions and clustering tools

Details

Package: GMD
Type: Package
License: GPL (>= 2)

This package contains:

- 1) modules and functions for GMD computation, with GMD algorithm implemented in C to interface with R.
- 2) related clustering and visualization tools for distributions.

An overview of functions

Function	Description
ghist	Generalized Histogram Computation and Visualization
gdist	Generalized Distance Matrix Computation
CSS	Computing Clustering Sum-of-Squares and
	evaluating the clustering by the "elbow" method
heatmap.3	Enhanced Heatmap Representation with Dendrogram and Partition
gmdp	Computation of GMD on a pair of histograms
gmdm	Computation of GMD Matrix on a set of histograms

To install from online repositories (e.g. CRAN) install.packages(pkgs="GMD", repos="http://cran.r-project.org")

Sometimes the offical repository might not be up to date, then ## you may install it from a down-

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loaded source file; please replace ## '<current-version>' with actual version numbers: Note that as ## new versions are release, the '<current-version>' changes. install.packages(pkgs="GMD_<current-version>.tar.gz", repos=NULL)

Load the package and get a complete list of functions, use library(GMD) ls("package:GMD") ## help documantation of the package help(GMD) # this page

Author(s)

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```
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```

References

```
Zhao et al (2011), "Systematic Clustering of Transcription Start Site Landscapes", PLoS ONE 6(8): e23409.
```

```
http://dx.plos.org/10.1371/journal.pone.0023409
```

See citation ("GMD") for BibTeX entries for LaTeX users.

See Also

```
gmdp, gmdm, cage, chipseq, ghist, gdist, css, elbow, heatmap.3
```

Examples

```
require(GMD)  # load GMD
help(GMD)  # a help document of GMD
data(package="GMD") # a list of datasets available in GMD
ls("package:GMD") # a list of functions available in GMD
help(package="GMD") # help documentation on GMD
citation("GMD") # citation for publications
demo("GMD-demo") # run the demo

## view GMD vignette
vignette("GMD-vignette",package="GMD")
```

CAGE Data: Transcription Start Site Distributions (TSSDs) by CAGE tags

Description

cage

Transcription Start Site Distributions (TSSDs) by CAGE tags.

Usage

```
cage
cagel
```

Details

cage is a list of 20 named TSSDs. cage1 is a longer version of cage, with 50 named TSSDs.

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References

Zhao et al (2011), "Systematic Clustering of Transcription Start Site Landscapes", *PLoS ONE* **6**(8): e23409.

```
http://dx.plos.org/10.1371/journal.pone.0023409
```

See Also

gmdp and gmdm, with examples using cage. chipseq for histone marks by ChIP-seq reads.

Examples

```
help(cage)
data(cage)
class(cage)
length(cage)
names(cage)
## Not run: cage

data(cagel)
names(cagel)
## Not run: cagel
```

chipseq

ChIP-seq data: ChIP-seq Enrichment around TSSs

Description

The Distributions of Histone Modification Enrichment (and Others) by ChIP-seq reads that are binned, aligned and averaged around +/-5000nt of Transcription Start Sites (TSSs) of scattered-type TSSDs (see References).

Usage

```
chipseq_mES
chipseq_hCD4T
```

Details

chipseq_mES is a list of 6 named ChIP-seq read distributions from mouse ES cells. chipseq_hCD4T is a list of 40 named ChIP-seq read distributions from human CD4+ T cells.

References

Zhao et al (2011), "Systematic Clustering of Transcription Start Site Landscapes", *PLoS ONE* **6**(8): e23409.

```
http://dx.plos.org/10.1371/journal.pone.0023409
```

See Also

gmdp and gmdm, with examples using chipseq. cage for data of Transcription Start Sites (TSSs) by CAGE tags.

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Examples

```
require(GMD)
help(chipseq)
data(chipseq_mES)
class(chipseq_mES)
length(chipseq_mES)
names(chipseq_mES)
## Not run: chipseq_mES
data(chipseq_hCD4T)
names(chipseq_hCD4T)
```

css

Clustering Sum-of-Squares for clustering evaluation

Description

Evaluation on the varaince of a clustering model using squared Euclidean distances, based on distance matrix and cluster membership.

Usage

```
css(dist.obj,clusters)

## Computing Sum-of-Squares given Hierarchical Clustering
css.hclust(dist.obj, hclust.obj=NULL,hclust.FUN=hclust,
hclust.FUN.MoreArgs=list(method="ward"),k=NULL)
```

Arguments

```
dist.obj a 'dist' object as produced by dist or gdist.

clusters a vector with cluster memberships.

k numeric, the upper bound of the number of clusters to compute. DEFAULT: 20 or the number of observations (if less than 20).

hclust.obj a 'hclust' object, generated by hclust

hclust.FUN a function, to generate a hierarchical clustering. Ignored with hclust.obj specified. DEFAULT: hclust

hclust.FUN.MoreArgs

a list, containing arguments that are passed to hclust.FUN.
```

Details

Clustering Sum-of-Squares for clustering evaluation.

6 elbow

Value

css returns a 'css' object, which is a list containing the following components

k number of clusters

wss k within-cluster sum-of-squares totwss total within-cluster sum-of-square totbss total between-cluster sum-of-square tss total sum of squares of the data

, and with an attribute 'meta' that contains the input components

dist.obj (the input) distance matrix clusters (the input) cluster membership

css.hclust returns a 'css.multi' object, which is a data.frame containing the following columns

k number of clusters

ev explained variance given k

totbss total between-cluster sum-of-square tss total sum of squares of the data

, and with an attribute 'meta' that contains

cmethod the clustering methoddist.obj (the input) distance matrixk (the input) number of clusters

clusters the 'hclust' object that is either by input or computed by default

See Also

elbow for "elbow" plot using 'css.multi' object

elbow

The "Elbow" Method for Clustering Evaluation

Description

Determining the number of clusters in a data set by the "elbow" rule.

Usage

```
## find a "good" k given thresholds of EV and its increment.
elbow(x,inc.thres,ev.thres,precision=3,print.warning=TRUE)
## a wrapper of `elbow' testing multiple threshold to find a "good" k.
elbow.batch(x,inc.thres=c(0.01,0.05,0.1),
```

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```
ev.thres=c(0.95,0.9,0.8,0.75,0.67,0.5,0.33),precision=3)
## S3 mathod for class `elbow'
plot.elbow(x,elbow.obj,main,xlab="k",
ylab="Explained Variance",type="b",pch=20,col.abline="red",
lty.abline=3,if.plot.new=TRUE,print.info=TRUE,
mar=c(4,5,3,3),omi=c(0.75,0,0,0),...)
```

Arguments

Х	a 'css.multi' object, generated by css.hclust
inc.thres	numeric with value(s) from 0 to 1, the threshold of the increment of EV. A single value is used in elbow while a vector of values in elbow.batch.
ev.thres	numeric with value(s) from 0 to 1 , the threshold of EV. A single value is used in elbow while a vector of values in elbow.batch.
precision	integer, the number of digits to round for numerical comparison.
print.warnin	ng
	logical, whether to print warning messages.
elbow.obj	a 'elbow' object, generated by elbow or elbow.batch
main	an overall title for the plot.
ylab	a title for the y axis.
xlab	a title for the x axis.
type	<pre>what type of plot should be drawn. See help("plot", package="graphics").</pre>
pch	Either an integer specifying a symbol or a single character to be used as the default in plotting points (see par).
col.abline	color for straight lines through the current plot (see option col in par).
lty.abline	line type for straight lines through the current plot (see option lty in par).
if.plot.new	logical, whether to start a new plot device or not.
print.info	logical, whether to print the information of 'elbow.obj'.
mar	A numerical vector of the form 'c(bottom, left, top, right)' which gives the number of lines of margin to be specified on the four sides of the plot (see option mar in par). The default is 'c(4, 5, 3, 3) + 0.1'.
omi	A vector of the form 'c(bottom, left, top, right)' giving the size of the outer margins in inches (see option omi in par).
• • •	arguments to be passed to method plot.elbow, such as graphical parameters (see par).

Details

Determining the number of clusters in a data set by the "elbow" rule and thresholds in the explained variance (EV) and its increment.

Value

Both elbow and elbow.btach return a 'elbow' object (if a "good" k exists), which is a list containing the following components

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```
k number of clusters
ev explained variance given k
inc.thres the threshold of the increment in EV
ev.thres the threshold of the EV
```

, and with an attribute 'meta' that contains

description A description about the "good" k

See Also

css and css.hclust for computing Clustering Sum-of-Squares.

Examples

```
## load library
require("GMD")
## simulate data around 12 points in Euclidean space
pointv <- data.frame(x=c(1,2,2,4,4,5,5,6,7,8,9,9),
y=c(1,2,8,2,4,4,5,9,9,8,1,9))
set.seed(2012)
mydata <- c()
for (i in 1:nrow(pointv)){
mydata <- rbind(mydata,cbind(rnorm(10,pointv[i,1],0.1),</pre>
rnorm(10,pointv[i,2],0.1)))
\label{eq:mydata} \mbox{ \ensuremath{\texttt{mydata}}$ \ensuremath{\texttt{colnames}}$ (mydata) \ensuremath{\texttt{c}}$ - c("x","y") }
plot(mydata,type="p",pch=21, main="Simulated data")
## determine a "good" k using elbow
dist.obj <- dist(mydata[,1:2])</pre>
hclust.obj <- hclust(dist.obj)</pre>
css.obj <- css.hclust(dist.obj,hclust.obj)</pre>
elbow.obj <- elbow.batch(css.obj)</pre>
print(elbow.obj)
\#\# make partition given the "good" k
k \leftarrow elbow.obj$k; cutree.obj \leftarrow cutree(hclust.obj, k=k)
mydata$cluster <- cutree.obj</pre>
## draw a elbow plot and label the data
dev.new(width=12, height=6)
par(mfcol=c(1,2), mar=c(4,5,3,3), omi=c(0.75,0,0,0))
plot (mydata$x, mydata$y, pch=as.character (mydata$cluster),
col=mydata$cluster,cex=0.75,main="Clusters of simulated data")
plot.elbow(css.obj,elbow.obj,if.plot.new=FALSE)
## clustering with more relaxed thresholds (, resulting a smaller "good" k)
elbow.obj2 <- elbow.batch(css.obj,ev.thres=0.90,inc.thres=0.05)</pre>
mydata$cluster2 <- cutree(hclust.obj,k=elbow.obj2$k)</pre>
dev.new(width=12, height=6)
par(mfcol=c(1,2), mar=c(4,5,3,3), omi=c(0.75,0,0,0))
```

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```
plot (mydata$x, mydata$y, pch=as.character(mydata$cluster2),
col=mydata$cluster2,cex=0.75,main="Clusters of simulated data")
plot.elbow(css.obj,elbow.obj2,if.plot.new=FALSE)
```

equalize.list

Make members of a list equal size

Description

Make member bins of a hist object equal size

Usage

```
equalize.list(x)
```

Arguments

Х

a list of numeric vectors

Details

Make members of a list equal size

gdist

Generalized Distance Matrix Computation

Description

gdist computes and returns the distance matrix computed by using user-defined distance measure.

Usage

```
gdist(x,method="euclidean",MoreArgs=NULL,diag=FALSE,upper=FALSE)
is.dist(d)
```

Arguments

х	a numeric matrix, data frame or 'dist' object.
method	the distance measure to be used. This can either be one of the methods used in dist (see help("dist", package="stats")) or "correlation", "correlation.of.observations" and "correlation.of.variables". In addition, user-defined distance measure are also allowed, which returns a <i>dist</i> object and should at least have attributes "Size" and "Labels".
	object and should at least have attributes Size and Labers.
MoreArgs	a list of other arguments to be passed to gdist.
diag	logical value indicating whether the diagonal of the distance matrix should be

printed by print.dist. logical value indicating whether the upper triangle of the distance matrix should upper

be printed by print.dist.

an R object. d

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Details

is.dist tests if its argument is a 'dist' object.

The distance (or dissimilarity) function (FUN) can be any distance measure applied to x. For instance, "euclidean", "maximum", "manhattan", "canberra", "binary", "minkowski", "correlation.of.variables", "correlation.of.observations" or gmdm. "correlation.of.variables" computes the correlation distance of the variables (the columns); all the other compute the distances between the observations (the rows) of a data matrix.

Value

gdist returns an object of 'dist'.

Examples

```
## load library
require("GMD")
require(cluster)
## compute distance using Euclidean metric (default)
data(ruspini)
x <- gdist(ruspini)
## see a dendrogram result by hierarchical clustering
dev.new(width=12, height=6)
plot(hclust(x),
main="Cluster Dendrogram of Ruspini data",
xlab="Observations")
## convert to a distance matrix
m <- as.matrix(x)</pre>
## convert from a distance matrix
d <- as.dist(m)</pre>
stopifnot(d == x)
## Use correlations between variables "as distance"
data(USJudgeRatings)
dd <- gdist(x=USJudgeRatings,method="correlation.of.variables")</pre>
dev.new(width=12, height=6)
plot(hclust(dd),
main="Cluster Dendrogram of USJudgeRatings data",
xlab="Variables")
```

get.sep

Get row or column lines of separation for heatmap.3

Description

Get row or column lines of separation for heatmap. 3 according to clusters

Usage

```
get.sep(clusters, type=c("row", "column", "both"))
```

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Arguments

```
clusters a numerical vector, indicating the cluster labels of observations.

type string, one of the following: c("row", "column", "both")
```

Details

Get row or column lines of separation for heatmap. 3 according to clusters

ghist

Generalized Histogram Computation

Description

Generalized Histogram Computation with classes to contain a single histogram or multiple histograms

Usage

```
ghist(data,n,breaks=if (!invalid(n)) NULL else "Sturges",
bins=NULL,digits=1)

gbreaks(data, n)

is.ghist(x)

as.ghist(x,bins)

is.mhist(x)

as.mhist(x,bins)
```

Arguments

data	a vector of values for which the histogram is desired.
n	a single number giving the number of bins for the histogram.
breaks	a vector giving the breakpoints between histogram bins, or a character string naming an algorithm to compute the number of bins, or a function to compute the number of bins (see help("dist", package="graphics")).
bins	character vecter, the bin labels.
digits	integer, the number of digits to round for breaks.
х	an R object.
h	an object of class mhist

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Details

```
ghist generates a single histogram.
```

gbreaks generate bin boundaries for a histogram.

is.ghist returns TRUE if x is an object of codeghist and FALSE otherwise.

as . ghist is a generic function. The method for numeric vectors will return a ghist object.

is.mhist returns TRUE if x is an object of codemhist and FALSE otherwise.

as.mhist is a generic function. The method is for numeric list, matrices or data frames and will return a mhist object.

mhist2matrix convert a mhist object into a numeric matrix, filling observations by row.

See Also

```
plot.mhist mhist.summary plot.mhist.summary
```

gmdm

Generalized Minimum Distance Matrix

Description

Computing Generalized Minimum Distance Matrix

Usage

```
gmdm(data,labels,pseudocount=0,sliding=TRUE,resolution=1)
## S3 method for class `gmdm'
print.gmdm(x, ...)
## convert a `gmdm' object into a `dist' object
as.dist.gmdm(m, diag=FALSE, upper=FALSE)
## compute GMDM and convert into a `dist' object
dist.gmdm(data, diag=FALSE, upper=FALSE, ...)
```

Arguments

data a list of numeric vectors, a numeric matrix or data.frame

x a gmdm object.m a gmdm object.

labels a character vector of the same length of x, giving the names of the numeric

vectors.

pseudocount a numeric value to be allocated for each position to reduce bias; by default

pseudocount = 0.

sliding logical, indicating whether sliding is allowed or not for an optimal solution; by

default sliding = TRUE.

resolution relative resolution, numeric (>=1), changing the size of the bin by multiplying

the value. A larger value (lower resolution) is more computational efficiet but

missing details.

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diag	logical value indicating whether the diagonal of the distance matrix should be printed by print.dist.
upper	logical value indicating whether the upper triangle of the distance matrix should be printed by print.dist.
	arguments to be passed to method

Details

Computing Generalized Minimum Distance Matrix

Value

gmdm returns an object of class gmdm, a list with components

labels: a string vector, giving the names of distributions

data.ori: a list of numeric vectors, giving the original input

data: a list of numeric vectors, giving the normalized version of the original input

dm: a numeric numeric, the pairwise distance matrix of GM-Distances

gap.pair: a numeric matrix, giving the gap pair of each alignment per row: i.e. relative shifts between distributions of the optimal hit

sliding: logical, indicating whether sliding is performed

pseudocount: a numeric value that is allocated at each position in addition to original values

References

```
See citation ("GMD")
```

See Also

```
plot.gmdm, gmdp
```

gmdp

Generalized Minimum Distance between a pair of distributions

Description

Generalized Minimum Distance between a pair of distributions

Usage

```
gmdp(v1, v2, labels=c("v1","v2"), pseudocount=0, sliding=TRUE,
resolution=1)

## S3 method for class `gmdp'
print.gmdp(x, print.mode=c("brief","detailed","full"),
digits=3, ...)
```

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Arguments

v1 a numeric vector, giving positional counts as a discrete distribution. v2 a numeric vector, giving positional counts as a discrete distribution. labels a string vector of length 2, giving the names of v1 and v2 respectively. a numeric value to be allocated for each position to reduce bias; by default pseudocount pseudocount = 0.logical, indicating whether sliding is allowed or not for an optimal solution; by sliding default sliding = TRUE. resolution relative resolution, numeric (>=1), changing the size of the bin by multiplying the value. A larger value (lower resolution) is more computational efficiet but missing details. an object of class gmdp. print.mode a string of the following: c ("brief", "detailed", "full"), indicating whether to print in full mode (default). integer, indicating the number of decimal places to be printed. digits arguments to be passed to method.

Details

Generalized Minimum Distance between a pair of distributions

Value

gmdp returns an object of class gmdp, a numeric with an attribute of *meta* in a list with components:

labels: a string vector, giving the names of distributions

v1.ori: a numeric vector, the first input distribution

v2.ori: a numeric vector, the second input distribution

v1: a numeric vector, the normalized version of the first input distribution

v2: a numeric vector, the normalized version of the second input distribution

distance: numeric, the GM-Distance (GMD)

sliding: logical, indicating whether sliding is performed

pseudocount: a numeric value that is allocated at each position in addition to original values

gap.pair: a numeric matrix, giving one gap pair per row: i.e. relative shifts between distributions of one optimal hit

n.hit: numeric, the number of (equally good) optimal hits

References

```
See citation ("GMD")
```

See Also

```
print.gmdp, summary.gmdp, plot.gmdp, gmdm
```

Examples

```
require(GMD)
gmdp(c(4,1,1,0,0,0,3,1),c(2,1,1,0,0,0,3,3),sliding=FALSE)
x <- gmdp(c(4,1,1,0,0,0,3,1), c(1,1,2,1,1,0,0,0,3,3,5,5),
pseudocount=1, sliding=TRUE)
print(x)
print(x, "full")</pre>
```

heatmap.3

Enhanced Heatmap Representation with Dendrogram and Partition

Description

Enhanced heatmap representation with dendrograms and partition given the *elbow criterion* or a desired number of clusters.

- 1) a dendrogram added to the left side and to the top, according to cluster analysis;
- 2) partitions in highlighted rectangles, according to the "elbow" rule or a desired number of clusters.

Usage

```
heatmap.3(x, diss=inherits(x, "dist"), Rowv=TRUE, Colv=TRUE,
    dendrogram=c("both", "row", "column", "none"), dist.row, dist.col,
    dist.FUN=qdist, dist.FUN.MoreArgs=list(method = "euclidean"),
    hclust.row, hclust.col, hclust.FUN=hclust,
    hclust.FUN.MoreArgs=list(method = "ward"), scale=c("none", "row",
    "column"), na.rm=TRUE, cluster.by.row=FALSE, cluster.by.col=FALSE,
    kr=NA, kc=NA, row.clusters=NA, col.clusters=NA, revR=FALSE,
    revC=FALSE, add.expr, breaks, x.center, color.FUN="bluered",
    sepList=list(NULL, NULL), sep.color=c("gray45", "gray45"),
    sep.lty=1, sep.lwd=2, cellnote, cex.note=1, notecol="cyan",
    na.color=par("bg"), trace=c("none", "column", "row", "both"),
    tracecol="cyan", hline, vline, linecol=tracecol, labRow=TRUE,
    labCol=TRUE, margin.for.labRow, margin.for.labCol,
    ColIndividualColors, RowIndividualColors, cexRow, cexCol,
    labRow.by.group=FALSE, labCol.by.group=FALSE, key=TRUE,
    keysize=1.5, mapsize=9, mapratio=4/3, sidesize=3,
    cex.key.main=0.75, cex.key.xlab=0.75, cex.key.ylab=0.75,
    density.info=c("histogram", "density", "none"), denscol=tracecol,
    densadj=0.25, main="Heatmap", sub="", xlab="", ylab="", cex.main=2,
    cex.sub=1.5, font.main=2, font.sub=3, adj.main=0.5, mgp.main=c(1.5,
    0.5, 0), mar.main=3, mar.sub=3, if.plot=TRUE,
    plot.row.partition=FALSE, plot.col.partition=FALSE,
    cex.partition=1.25, color.partition.box="gray45",
    color.partition.border="#FFFFFF", plot.row.individuals=FALSE,
    plot.col.individuals=FALSE, plot.row.clusters=FALSE,
    plot.col.clusters=FALSE, plot.row.clustering=FALSE,
    plot.col.clustering=FALSE, plot.row.individuals.list=FALSE,
    plot.col.individuals.list=FALSE, plot.row.clusters.list=FALSE,
    plot.col.clusters.list=FALSE, plot.row.clustering.list=FALSE,
    plot.col.clustering.list=FALSE, row.data=FALSE, col.data=FALSE,
    if.plot.info=FALSE, text.box, cex.text=1, ...)
```

Arguments

data matrix or data frame, or dissimilarity matrix or 'dist' object determined by the value of the 'diss' argument. ##diss logical flag: if TRUE (default for dist or dissimilarity objects), then x is assumed to be a dissimilarity matrix. If FALSE, then \times is treated as a matrix of observations by variables. logical, whether the x is a dissimilarity matrix diss one of the following: TRUE, a 'dend' object, a vector or NULL/FALSE; deter-Rowv mines if and how the row dendrogram should be reordered. one of the following: "Rowv", TRUE, a 'dend' object, a vector or NULL/FALSE; Colv determines if and how the column dendrogram should be reordered. character string indicating whether to draw 'none', 'row', 'column' or 'both' dendrogram dendrograms. Defaults to 'both'. a dist object for row observations. dist.row a dist object for column observations. dist.col function used to compute the distance (dissimilarity) between both rows and dist.FUN columns. Defaults to gdist. dist.FUN.MoreArgs a list of other arguments to be passed to gdist a helust object (as produced by helust) for row observations. hclust.row hclust.col a helust object (as produced by helust) for column observations. hclust.FUN function used to compute the hierarchical clustering when "Rowv" or "Colv" are not dendrograms. Defaults to hclust. hclust.FUN.MoreArgs a list of other arguments to be passed to hclust. Defaults to list (method="ward") scale character indicating if the values should be centered and scaled in either the row direction or the column direction, or none. The default is "none". logical, whether NA values will be removed when scaling. na.rm cluster.by.row logical, whether to cluster *row* observations and reorder the input accordingly. cluster.by.col logical, whether to cluster column observations and reorder the input accordingly. numeric, number of clusters in rows; suppressed when row.cluster is speckr ified. DEFAULT: NULL. numeric, number of clusters in columns; suppressed when col.cluster is kc specified. DEFAULT: NULL. row.clusters a numerical vector, indicating the cluster labels of row observations. col.clusters a numerical vector, indicating the cluster labels of *column* observations. logical indicating if the row order should be 'rev'ersed for plotting. revR logical indicating if the column order should be 'rev'ersed for plotting, such that revC e.g., for the symmetric case, the symmetry axis is as usual. expression that will be evaluated after the call to image. Can be used to add add.expr components to the plot.

breaks numeric, either a numeric vector indicating the splitting points for binning x into colors, or a integer number of break points to be used, in which case the break points will be spaced equally between range (x). DEFAULT: 16 when not specified. numeric, a value of x for centering colors to x.center function or function name in characters, for colors in the heatmap color.FUN sepList a list of length 2 giving the row and column lines of separation. sep.color color for lines of separation. line type for lines of separation. sep.lty line width for lines of separation. sep.lwd (optional) matrix of character strings which will be placed within each color cellnote cell, e.g. cell labels or p-value symbols. relative font size of cellnote. cex.note notecol color of cellnote. na.color Color to use for missing value (NA). Defaults to the plot background color. character string indicating whether a solid "trace" line should be drawn across trace "row"s or down "column"s, "both" or "none". The distance of the line from the center of each color-cell is proportional to the size of the measurement. Defaults to "none". character string giving the color for "trace" line. Defaults to "cyan"; tracecol Vector of values within cells where a horizontal dotted line should be drawn. hline only plotted if 'trace' is 'row' or 'both'. Default to the median of the breaks. vline Vector of values within cells where a vertical dotted line should be drawn; only drawn if 'trace' 'column' or 'both'. vline default to the median of the breaks. the color of hline and vline. Defaults to the value of 'tracecol'. linecol labRow character vectors with row labels to use; defaults to rownames (x). labCol character vectors with column labels to use; defaults to colnames (x). margin.for.labRow a numerical value gives the margin to plot labRow. margin.for.labCol a numerical value gives the margin to plot labCol. ColIndividualColors (optional) character vector of length ncol (x) containing the color names for a horizontal side bar that may be used to annotate the columns of x. RowIndividualColors (optional) character vector of length nrow (x) containing the color names for a vertical side bar that may be used to annotate the rows of x. positive numbers, used as 'cex.axis' in for column axis labeling. The default cexRow currently only uses number of columns. positive numbers, used as 'cex.axis' in for the row axis labeling. The default cexCol

labRow.by.group

logical, whether group unique labels for rows.

currently only uses number of rows.

labCol.by.group

logical, whether group unique labels for columns.

key	logical indicating whether a color-key should be shown.	
keysize	numeric value indicating the relative size of the key	
mapsize	numeric value indicating the relative size of the heatmap.	
mapratio	the width-to-height ratio of the heatmap.	
sidesize	numeric value indicating the relative size of the sidebars.	
cex.key.main	a numerical value giving the amount by which main-title of color-key should be magnified relative to the default.	
cex.key.xlab	a numerical value giving the amount by which xlab of color-key should be magnified relative to the default.	
cex.key.ylab	a numerical value giving the amount by which ${\tt ylab}$ of color-key should be magnified relative to the default.	
density.info	character string indicating whether to superimpose a 'histogram', a 'density' plot, or no plot ('none') on the color-key.	
denscol	character string giving the color for the density display specified by 'density.info', defaults to the same value as 'tracecol'.	
densadj	Numeric scaling value for tuning the kernel width when a density plot is drawn on the color key. (See the 'adjust' parameter for the 'density' function for details.) Defaults to 0.25 .	
main	an overall title for the plot. See $help("title", package="graphics")$.	
sub	a subtitle for the plot, describing the distance and/or alignment gap (the "shift").	
xlab	a title for the x axis. See help("title", package="graphics").	
ylab	a title for the y axis. See help("title", package="graphics").	
cex.main	a numerical value giving the amount by which main-title should be magnified relative to the default.	
cex.sub	a numerical value giving the amount by which sub-title should be magnified relative to the default.	
font.main	An integer which specifies which font to use for main-title.	
font.sub	An integer which specifies which font to use for sub-title.	
adj.main	The value of 'adj' determines the way in which main-title strings are justified.	
mgp.main	the margin line (in 'mex' units) for the main-title.	
mar.main	a numerical vector of the form c(bottom, left, top, right) which gives the number of lines of margin to be specified on the four sides of the main-title.	
mar.sub	a numerical vector of the form $c(bottom, left, top, right)$ which gives the number of lines of margin to be specified on the four sides of the subtitle.	
if.plot	logical, whether to plot. Reordered matrix is returned without graphical output if FALSE.	
plot.row.partition		
logical, whether to plot <i>row</i> partition.		
plot.col.partition logical, whether to plot <i>column</i> partition.		
cex.partition		
	a numerical value giving the amount by which partition should be magnified relative to the default.	

```
color.partition.box
                color for the partition box.
color.partition.border
                color for the partition border.
plot.row.individuals
                logical, whether to make a plot of row observations.
plot.col.individuals
                logical, whether to make a plot of column observations.
plot.row.clusters
                logical, whether to make a summary plot of row clusters.
plot.col.clusters
                logical, whether to make a summary plot of column clusters.
plot.row.clustering
                logical, whether to make a summary plot of overall row clustering.
plot.col.clustering
                logical, whether to make a summary plot of overall column clustering.
plot.row.individuals.list
                a list of expressions that is used to plot.row.individuals
plot.col.individuals.list
                a list of expressions that is used to plot.col.individuals
plot.row.clusters.list
                a list of expressions that is used to plot.row.clusters
plot.col.clusters.list
                a list of expressions that is used to plot.col.clusters
plot.row.clustering.list
                a list of expressions that is used to plot.row.clustering
plot.col.clustering.list
                a list of expressions that is used to plot.col.clustering
row.data
                (optional) data used to plot.row.individuals, plot.row.clusters
                or plot.row.clustering
col.data
                (optional) data used to plot.col.individuals, plot.col.clusters
                or plot.col.clustering
if.plot.info logical, whether to plot text.box.
                character plotted when if.plot.info is TRUE.
text.box
                a numerical value giving the amount by which text.box should be magnified
cex.text
                relative to the default.
                arguments to be passed to method heatmap.3.
                help("image", package="graphics").
```

Details

Enhanced heatmap representation with partition and summary statistics (optional). This is an enhanced version of 'heatmap.2' function in the Package **gplots**. The enhancement includes: 1) Improved performance with optional input of precomputed dist object and holust object. 2) Highlight of specific cells using rectangles. For instance, the cells of clusters of interests. (Examples should be included in future.) 3) Add-on plots in addition to the heatmap, such as cluster-wise summary plots and overall clustering summary plots, to the right of or under the heatmap.

Value

A reordered matrix according to row or/and col dendrogram(s) and indices that used for reordering.

Examples

```
## Example1: mtcars
## load library
require("GMD")
## load data
data(mtcars)
## heatmap on raw data
x <- as.matrix(mtcars)</pre>
dev.new(width=10,height=8)
heatmap.3(x)
                                      # default, with reordering and dendrogram
                                     # no reordering and no dendrogram
heatmap.3(x, Rowv=FALSE, Colv=FALSE)
heatmap.3(x, dendrogram="row", Colv=FALSE) # row dendrogram with only row reordering
heatmap.3(x, dendrogram="col")
                                      # col dendrogram
heatmap.3(x, dendrogram="col", Rowv=FALSE) # col dendrogram with only col reordering
heatmapOut <-
heatmap.3(x, scale="column")
                                     # sacled by column
                                      # view the list that is returned
names (heatmapOut)
heatmap.3(x, scale="column", x.center=0) \# colors centered around 0
heatmap.3(x, scale="column",trace="column")  # trun "trace" on
## coloring cars (row observations) by brand
brands <- sapply(rownames(x), function(e) strsplit(e, " ")[[1]][1])</pre>
names(brands) <- c()</pre>
brands.index <- as.numeric(as.factor(brands))</pre>
RowIndividualColors <- rainbow(max(brands.index))[brands.index]</pre>
heatmap.3(x, scale="column", RowIndividualColors=RowIndividualColors)
\#\# coloring attributes (column features) randomly (just for a test :)
heatmap.3(x, scale="column", ColIndividualColors=rainbow(ncol(x)))
## add a single plot for all row individuals
dev.new(width=12,height=8)
expr1 <- list(quote(plot(row.data[rowInd, "hp"], 1:nrow(row.data),</pre>
xlab="hp",ylab="",yaxt="n",main="Gross horsepower")),
quote(axis(2,1:nrow(row.data),rownames(row.data)[rowInd],las=2)))
heatmap.3(x, scale="column", plot.row.individuals=TRUE, row.data=x,
plot.row.individuals.list=list(expr1))
## -----
## Example2: ruspini
## load library
require("GMD")
require(cluster)
```

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```
## load data
data(ruspini)
## heatmap on a `dist' object
x <- gdist(ruspini)
main <- "Heatmap of Ruspini data"</pre>
dev.new(width=10,height=10)
heatmap.3(x, main=main, mapratio=1) # with a title and a map in square!
heatmap.3(x, main=main, revC=TRUE) # reverse column for a symmetric look
heatmap.3(x, main=main, kr=2, kc=2) # partition by predefined number of clusters
## show partition by elbow
css.multi.obj <- css.hclust(x,hclust(x))</pre>
elbow.obj <- elbow.batch(css.multi.obj,ev.thres=0.90,inc.thres=0.05)
heatmap.3(x, main=main, revC=TRUE, kr=elbow.obj$k, kc=elbow.obj$k)
## show elbow info as subtitle
heatmap.3(x, main=main, sub=sub("\n"," ",attr(elbow.obj,"description")),
cex.sub=1.25, revC=TRUE, kr=elbow.obj$k, kc=elbow.obj$k)
```

invalid

Test if a value is missing, empty, or contains only NA or NULL values

Description

A copy of gtools:::invalid

Usage

invalid(x)

Arguments

Х

value to be tested

Details

see invalid in package:gtools for details

legend

Add Legends to Plots

Description

This function can be used to add legends to plots. Note that a call to the function locator(1) can be used in place of the x and y arguments.

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Usage

```
legend(x, y, legend, fill, col=par("col"), border="black", lty, lwd,
    pch, angle=45, density, bty="o", bg=par("bg"), box.lwd=par("lwd"),
    box.lty=par("lty"), box.col=par("fg"), pt.bg=NA, cex=1, pt.cex=cex,
    pt.lwd=lwd, xjust=0, yjust=1, x.intersp=1, y.intersp=1, adj=c(0,
    0.5), text.width, text.col=par("col"), merge=do.lines && has.pch,
    trace=FALSE, plot=TRUE, ncol=1, horiz=FALSE, title, inset=0, xpd,
    title.col=text.col, title.adj=0.5, seg.len=2)
```

Arguments

8	
X	the x coordinates to be used to position the legend.
У	the y coordinates to be used to position the legend. x and y can be specified by keyword or in any way which is accepted by xy . coords: See 'Details'.
legend	a character or expression vector. of length ≥ 1 to appear in the legend. Other objects will be coerced by as .graphicsAnnot.
fill	if specified, this argument will cause boxes filled with the specified colors (or shaded in the specified colors) to appear beside the legend text.
col	the color of points or lines appearing in the legend.
border	the border color for the boxes (used only if fill is specified).
lty	the line types for lines appearing in the legend.
lwd	the line widths for lines appearing in the legend. One of lty and lwd <i>must</i> be specified for line drawing.
pch	the plotting symbols appearing in the legend, either as vector of 1-character strings, or one (multi character) string. <i>Must</i> be specified for symbol drawing.
angle	angle of shading lines.
density	the density of shading lines, if numeric and positive. If \mathtt{NULL} or negative or \mathtt{NA} color filling is assumed.
bty	the type of box to be drawn around the legend. The allowed values are " \circ " (the default) and "n".
bg	the background color for the legend box. (Note that this is only used if $bty != "n"$.)
box.lwd	the line type for the legend box.
box.lty	the line width for the legend box.
box.col	the color for the legend box.
pt.bg	the background color for the points, corresponding to its argument bg.
cex	character expansion factor relative to current par ("cex").
pt.cex	expansion factor(s) for the points.
pt.lwd	line width for the points, defaults to the one for lines, or if that is not set, to $par("lwd")$.
xjust	how the legend is to be justified relative to the legend x location. A value of 0 means left justified, 0.5 means centered and 1 means right justified.
yjust	the same as x just for the legend y location.
x.intersp	character interspacing factor for horizontal (x) spacing.
y.intersp	the same for vertical (y) line distances.

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adj	numeric of length 1 or 2; the string adjustment for legend text. Useful for y-adjustment when labels are plotmath expressions.
text.width	the width of the legend text in x ("user") coordinates. (Should be positive even for a reversed x axis.) Defaults to the proper value computed by strwidth (legend).
text.col	the color used for the legend text.
merge	logical; if TRUE, merge points and lines but not filled boxes. Defaults to TRUE if there are points and lines.
trace	logical; if TRUE, shows how legend does all its magical computations.
plot	logical. If FALSE, nothing is plotted but the sizes are returned.
ncol	the number of columns in which to set the legend items (default is 1, a vertical legend).
horiz	logical; if TRUE, set the legend horizontally rather than vertically (specifying horiz overrides the ncol specification).
title	a character string or length-one expression giving a title to be placed at the top of the legend. Other objects will be coerced by as.graphicsAnnot.
inset	inset distance(s) from the margins as a fraction of the plot region when legend is placed by keyword.
хрd	if supplied, a value of the graphical parameter 'xpd' to be used while the legend is being drawn.
title.col	color for title.
title.adj	horizontal adjustment for title: see the help for $par("adj")$.
seg.len	the length of lines drawn to illustrate lty and/or lwd (in units of character widths).

Details

see legend in package:graphics for details; Note: Old versions of graphics:::legend do not have 'border' option.

mhist.summary

Bin-wise summary of histograms

Description

Bin-wise summary of a mhist object of histograms

Usage

```
mhist.summary(h, ...)
plot.mhist.summary(x,bins,plot.ci=TRUE,col=NULL,
ci.color="orchid1",tcl=-0.25,omi=c(0.5,0.5,1.0,0.25),mar=c(3,3,3,1),
mgp=c(2,0.5,0),if.plot.new=TRUE,...)
```

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Arguments

h	a "mhist" object as produced by as.mhist
х	a mhist.summary object as produced by mhist.summary
bins	character vecter, the bin labels; if non-specific, bins are numbered/labeled starting with one.
plot.ci	logical, indicating whether plot error bars that represent the 0.50 confidence interval (CI)
col	color of the histogram
ci.color	color of the error bars
tcl	the length of tick marks as a fraction of the height of a line of text. See option tcl inhelp("par", package="graphics").
omi	a vector of the form 'c(bottom, left, top, right)' giving the size of the outer margins in inches. See option omi inhelp ("par", package="graphics").
mar	a numerical vector of the form c(bottom, left, top, right) which gives the number of lines of margin to be specified on the four sides of the plot. See option mar inhelp("par", package="graphics").
mgp	the margin line (in 'mex' units) for the axis title, axis labels and axis line.
if.plot.new	logical, whether starting a new device or not.
•••	arguments to be passed to method plot.mhist.summary. See help("barplot2", package="gplots").

Details

Bin-wise summary of a mhist object of histograms

Value

```
mhist.summary returns a mhist.summary object
```

See Also

```
mhist plot.mhist plot.gmdp plot.gmdm
```

plot.gmdm Plot Function for Class gmdm

Description

Plot Function for Class gmdm

Usage

```
plot.gmdm(x, labels, colors, main, ylab="Fraction", xlab="Position",
    label.length.max=8, label.line.max=3, cex.text=1,
    cex.tickmark=0.75, if.plot.new=TRUE, ...)
```

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Arguments

an object of class gmdm.
a string vector of the same length as $x\$data$, giving the names of the numeric vectors in $x\$data$.
the colors of the discrete distributions; the default is "Dark2" colors in Color-Brewer palettes if not specified.
an overall title for the plot. See $help("title", package="graphics")$ the default title is used if not specified.
a title for the y axis. See help("title", package="graphics").
a title for the x axis. See help("title", package="graphics").
.max
numeric, giving the maximum string width allowed in diagonal labels.
ax
numeric, giving the maximum number of lines allowed in diagonal labels.
a numerical value giving the amount by which plot text should be magnified relative to the default.
a numerical value giving the amount by which tickmarks should be magnified relative to the default.
logical, indicating whether to start a new plot device.
arguments to be passed to methods, see gmdp.

Details

Plot Function for Class gmdm

References

See help (GMD)

See Also

```
gmdm, gmdp
```

Examples

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```
data(chipseq_hCD4T) # load data

## pairwise distance and alignment based on GMD metric
plot(gmdm(chipseq_mES,sliding=FALSE))

## clustering on spatial distributions of histone modifications
x <- gmdm(chipseq_hCD4T,sliding=FALSE,resolution=10)
heatmap.3(x,revC=TRUE)</pre>
```

plot.gmdp

Plot function for class gmdp

Description

Plot Function for Class gmdp

Usage

Arguments

X	an object of class gmdp.
labels	a string vector of the same length of x -labels, giving the names of the numeric vectors in x .
colors	the colors of the discrete distributions. See $\texttt{help("plot.mhist", package="GMD")}$.
main	an overall title for the plot.
ylab	a title for the y axis. See help("plot.mhist", package="GMD").
xlab	a title for the x axis. See help("plot.mhist", package="GMD").
xlim	numeric vectors of length 2, giving the x coordinates ranges.
if.text.gmd	logical, indicating whether GM-Distance is reported in the subtitle.
if.text.gap	logical, indicating whether gap is reported in the subtitle.
	arguments to be passed to methods. See help("plot.mhist", package="GMD").

Details

Plot Function for Class gmdp

References

See help(GMD)

See Also

gmdp

plot.mhist 27

Examples

```
require("GMD") # load library
data(cage) # load data

## measure pairwise distance
x <- gmdp(cage[["Pfkfb3 (T02R00AEC2D8)"]], cage[["Csf1 (T03R0672174D)"]])
print(x) # print a brief version by default
print(x, print.mode="full") # print a full version by default

## show alignment
plot(x, labels=c("Pfkfb3", "Csf1"), beside=FALSE)

## show another alignment
plot(gmdp(cage[["Hig1 (T09R0743763C)"]], cage[["Cd72 (T04R028B8BC9)"]]),
labels=c("Hig1 (T09R0743763C)", "Cd72 (T04R028B8BC9)"),
beside=FALSE)</pre>
```

plot.mhist

Plot multiple histograms side-by-side or as subplots.

Description

Given a list, matrix or data.frame of histograms, plot multiple histograms side-by-side or as subplots.

Usage

```
plot.mhist(x, beside=TRUE, labels, colors, main, sub, ylab, xlab,
    xticks, x.las=1, xticks.type=c("pretty", "original"), xlim, ylim,
    font.type=1, font.family=c("sans", "serif", "mono"), cex.main=1.75,
    cex.sub=cex.main * 0.9, cex.lab=1.25, cex.tickmark=0.75,
    cex.legend=1.5, tcl=-0.25, omi=c(0.5, 0.5, 1, 0.25), mar=c(4, 1, 0,
    1), mgp=c(0, 0.5, 0), bin.unit=0.8, legend.lab=labels,
    legend.pos=c("topright", "top", "topleft"), ...)
```

Arguments

Х	a numeric matrix or data frame, representing distributions by rows (bins by columns); or a list of numeric vectors as distributions.	
beside	logical, whether plot histograms side-by-side.	
labels	a string vector of labels for the histograms in x; should have the same number as of the histograms. the colors for the histograms; by default they are set to colors generated from palette Dark2. Colors will be recycled if the size is smaller than the number of the histograms.	
colors		
main	an overall title for the plot. See help("title", package="graphics").	
sub	a subtitle for the plot, describing the distance and/or alignment gap (the "shift").	
ylab	a title for the y axis. See help("title", package="graphics").	
xlab	a title for the x axis. See help("title", package="graphics").	

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xticks	a string vector indicating the tickmark labels at x-axis. Defult: NULL.
x.las	numeric in 0,1,2,3; the style of axis labels. See option las inhelp ("par", package="graphics").
xticks.type	stinrg in "pretty", "original", whether plot the xticks in a pretty way or as is.
xlim	<pre>range of x values, as in help("plot", package="graphics").</pre>
ylim	<pre>range of y values, as in help("plot", package="graphics").</pre>
font.type	the name of a font type for drawing text. See font in par. DEFAULT: font.type = 1, corresponding to plain text.
font.family	the name of a font family for drawing text. See family in par; DEFAULT: font.family = "sans", corresponding to san serif typeface.
cex.main	a numerical value giving the amount by which ${\tt main}$ -title should be magnified relative to the default.
cex.sub	a numerical value giving the amount by which $\verb"sub-title"$ should be magnified relative to the default.
cex.lab	a numerical value giving the amount by which xlab and ylab should be magnified relative to the default.
cex.tickmark	a numerical value giving the amount by which tickmarks should be magnified relative to the default.
cex.legend	a numerical value giving the amount by which legends should be magnified relative to the default.
tcl	the length of tick marks as a fraction of the height of a line of text. See option tcl inhelp("par", package="graphics").
omi	a vector of the form 'c(bottom, left, top, right)' giving the size of the outer margins in inches. See option omi inhelp ("par", package="graphics").
mar	a numerical vector of the form c(bottom, left, top, right) which gives the number of lines of margin to be specified on the four sides of the plot. See option mar inhelp("par", package="graphics").
mgp	the margin line (in 'mex' units) for the axis title, axis labels and axis line. See option $mgp\ inhelp\ ("par", package="graphics")$.
bin.unit	numeric, indicating the width of a group of bar(s) in unit of x axis.
legend.lab	legend labels, a string vector of the same length of distributions in \mathbf{x} , using labels by default. No legend is displayed when it is NA.
legend.pos	string, a keyword to be used to position the legend. See $help("legend", package="graphics")$.
	arguments to be passed to method ${\tt plot.mhist},$ such as graphical parameters (see ${\tt par}).$

Details

Given a list, matrix or data.frame of histograms, plot multiple histograms side-by-side or as subplots.

References

See help(GMD)

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See Also

```
mhist mhist.summary plot.mhist.summary plot.gmdp plot.gmdm
```

Examples

```
## load library
require("GMD")
## create two normally-distributed samples
## with unequal means and unequal variances
set.seed(2012)
v1 <- rnorm(1000, mean=-5, sd=10)
v2 <- rnorm(1000, mean=10, sd=5)
## create common bins
n <- 20 # desired number of bins
breaks <- gbreaks(c(v1, v2), n) # bin boundaries</pre>
x <-
list(ghist(v1, breaks=breaks, digits=0),
ghist(v2,breaks=breaks,digits=0))
mhist.obj <- as.mhist(x)</pre>
## plot histograms side-by-side
plot(mhist.obj, mar=c(1.5, 1, 1, 0),
main="Histograms of simulated normal distributions")
## plot histograms as subplots,
## with corresponding bins aligned
plot(mhist.obj,beside=FALSE,mar=c(1.5,1,1,0),
main="Histograms of simulated normal distributions")
```

summary.gmdp

Summary Function for Class gmdp

Description

Summary Function for Class gmdp

Usage

```
summary.gmdp(object, ...)
```

Arguments

```
object an object of class gmdp.arguments to be passed to methods, see summary.
```

Details

Summary Function for Class gmdp

References

```
See help (GMD)
```

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See Also

gmdp

ts2df

Convert time series to data frame

Description

A copy of wq:::ts2df; see ts2df in package:wq for details

Usage

```
ts2df(x, mon1=1, addYr=FALSE, omit=FALSE)
```

Arguments

x monthly time series vector

mon1 starting month number, i.e., first column of the data frame

addYr rows are normally labelled with the year of the starting month, but addYr =

TRUE will add 1 to this year number

omit if TRUE, then rows with any NA will be removed.

Details

see ts2df in package:wq for details. Note: $wq_0.3-4$ asks for R (>= 2.12.0); but GMD supports R (>= 2.9.0).

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