Package 'DiffCorr'

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Type Package

Title Analyzing and Visualizing Differential Correlation Networks in Biological Data

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Description A method for identifying pattern changes between 2 experimental conditions in correlation networks (e.g., gene co-expression networks), which builds on a commonly used association measure, such as Pearson's correlation coefficient. This package includes functions to calculate correlation matrices for high-dimensional dataset and to test differential correlation, which means the changes in the correlation relationship among variables (e.g., genes and metabolites) between 2 experimental conditions.

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Depends fdrtool, igraph, multtest, pcaMethods

Imports graphics, grDevices, stats, utils

Suggests knitr, prettydoc, rmarkdown, testthat (>= 3.0.0)

VignetteBuilder knitr

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Contents

`AraMetLeaves` *A metabolite data set from Arabidopsis leaves by GC-TOF/MS*

Description

A metabolite data set. The Arabidopsis metabolome of the aerial regions of individual WT plants and the mto1 and tt4 mutants were analyzed by GC-TOF/MS.

Details

50 samples (WT, n = 17; mto1, n = 13; and tt4, n = 20, biological replicates).

A matrix containing 59 metabolites (rows) and 50 observations (columns).

MetaboLights accession no.: MTBLS40

For comparisons with data from roots (Fukushima et al. 2011) we selected 59 commonly-detected metabolites in both datasets using MetMask http://metmask.sourceforge.net.

Author(s)

Atsushi Fukushima

References

Miyako Kusano, Atsushi Fukushima et al. BMC Syst Biol 2007 1:53

AraMetRoots *A metabolite data set from Arabidopsis roots by GC-TOF/MS*

Description

A metabolite data set. The Arabidopsis metabolome of the roots of individual WT plants and the mto1 and tt4 mutants were analyzed by GC-TOF/MS.

Details

53 root samples (WT, n = 17; mto1 n = 16; and tt4, n = 20, biological replicates).

A matrix containing 59 metabolites (rows) and 53 observations (columns).

MetaboLights accession no.: MTBLS45

For comparisons with data from aerial parts (Kusano, Fukushima et al. 2007) we selected 59 commonly-detected metabolites in both datasets using MetMask http://metmask.sourceforge.net.

Author(s)

Atsushi Fukushima

References

Atsushi Fukushima et al. BMC Syst Biol 2011 5:1.

cluster.molecule *Hierarchical clustering of molecules*

Description

Cluster molecules

Usage

```
cluster.molecule(
  data,
  method = "pearson",
  linkage = "average",
  absolute = FALSE
)
```

Arguments

data	matrix or data frame
method	c("pearson", "spearman", "kendall", "euclidean", "maximum", "manhattan", "canberra", "binary", or "minkowski")
linkage	c("average", "ward", "single", "complete", "mcquitty", "median", "centroid")
absolute	if TRUE, then 1-|COR| else 1-COR, default is FALSE

Value

an object of class 'hclust'

Author(s)

Atsushi Fukushima

Examples

```
cluster.molecule(as.matrix(t(iris[,1:4])), "pearson", "average")
```

---

comp.2.cc.fdr *Export differential correlations between two conditions*

Description

Export differential correlations of comparison of two correlation matrices

Usage

```
comp.2.cc.fdr(
  output.file = "res.txt",
  data1,
  data2,
  method = "pearson",
  p.adjust.methods = "local",
  threshold = 0.05,
  save = FALSE
)
```

Arguments

output.file	can specify file name of the results exported
data1	data matrix under condition 1
data2	data matrix under condition 2
method	c("pearson", "spearman", "kendall")
p.adjust.methods	c("local", holm", "hochberg", "hommel", "bonferroni", "BH", "BY", "fdr", "none")

threshold	a threshold of significance levels of differential correlation
save	exports the results as a text if TRUE (default: FALSE)

Value

data.frame

Author(s)

Atsushi Fukushima

References

Fukushima, A. Gene (2013) 518, 209-214

Examples

```
## Not run:
data(AraMetRoots)
AraMetRoots[AraMetRoots==0] <- NA
AraMetRootsImp <- completeObs(pca(log2(AraMetRoots), nPcs=3, method="ppca"))
comp.2.cc.fdr(output.file="res.txt", AraMetRootsImp[,1:17], method="spearman",
              AraMetRootsImp[,18:37], threshold=0.05)

## End(Not run)
```

---

compcorr *Compare two correlation coefficients*

Description

Compare two correlation coefficients using Fisher's Z-transformation

Usage

```
compcorr(n1, r1, n2, r2)
```

Arguments

n1	sample size under condition 1
r1	correlation coefficient under condition 1
n2	sample size under condition 2
r2	correlation coefficient under condition 1

Value

list of result (diff and p-value)

Author(s)

Atsushi Fukushima

References

http://www.fon.hum.uva.nl/Service/Statistics/Two_Correlations.html http://support.sas.com/ctx/samples/index.jsp?sid=494 http://support.sas.com/ctx/samples/index.jsp?sid=494

Examples

```
compcorr(10, 0.1, 10, 0.9)
```

---

cor.dist *Additional distance functions correlation distance (1-r)*

Description

Additional distance functions Correlation distance (1-r)

Usage

```
cor.dist(data, methods = "pearson", absolute = FALSE)
```

Arguments

data	a data matrix ([data.frame object] row: metabolites, col: samples or replicates)
methods	a character string indicating which correlation coefficient is to be calculated. One of "pearson" (default), "spearman", or "kendall" can be abbreviated.
absolute	TRUE means that absolute value of the correlation coefficient is used (Default: FALSE).

Details

These functions were originally from 'hybridHclust' package. We modified the functions slightly. See also the reference manual in detail.

Value

the resulting correlation matrix

Author(s)

Atsushi Fukushima

Examples

```
cor.dist(as.matrix(t(iris[,1:4])))
```

cor2.test *Correlation Test*

Description

Correlation Test

Usage

```
cor2.test(n, r, method = c("pearson", "kendall", "spearman"))
```

Arguments

n	the number of samples
r	the correlation coefficient
method	"pearson" and "spearman" can be used.

Value

p-value

Author(s)

Atsushi Fukushima

References

http://aoki2.si.gunma-u.ac.jp/R/cor2.html

Examples

```
cor2.test(30, 0.6)
```

generate_g *Generating graph from data matrix*

Description

Generating graph from data matrix

Usage

```
generate_g(
  data,
  method = "pearson",
  cor.thr = 0.6,
  neg.flag = 1,
  node.col = "red",
  node.size = 7,
  edge.col = "blue",
  edge.width = 3
)
```

Arguments

data	data matrix or data frame
method	c("Pearson", "Spearman", "Kendall")
cor.thr	a threshold of correlation coefficient (default: r >= 0.6)
neg.flag	flag where uses or not negative correlations
node.col	specifies color of nodes in a graph (default: red)
node.size	specifies size of nodes in a graph (default: 7)
edge.col	specifies color of edges in a graph (default: blue)
edge.width	specifies width of edges in a graph (default: 3)

Value

igraph object

Author(s)

Atsushi Fukushima

Examples

```
library(igraph)
mat <- matrix(runif(100), nr=10)
rownames(mat) <- as.character(1:10)
generate_g(mat)
```

`get.eigen.molecule` *Get eigen molecule*

Description

Get eigen molecule

Usage

```
get.eigen.molecule(data, groups, whichgroups = NULL, methods = "svd", n = 10)
```

Arguments

`data`	a data matrix ([data.frame object] row: molecules, col: samples or replicates)
`groups`	a vector of group memberships as returned by cutree
`whichgroups`	a vector of group numbers to examine
`methods`	c("svd", "nipals", "rnipals", "bpca", "ppca"). See also pca() function in pcaMethods package
`n`	top n principal components

Value

the resulting vector.

Author(s)

Atsushi Fukushima

Examples

```
library(pcaMethods)
data(golub, package = "multtest")
hc.mol1 <- cluster.molecule(golub[1:100, 1:27], "pearson", "average")
g1 <- cutree(hc.mol1, h=0.6)
res1 <- get.eigen.molecule(golub[1:100,], g1)
```

get.eigen.molecule.graph *Getting graph from eigengene module list*

Description

Getting graph from eigengene module list

Usage

```
get.eigen.molecule.graph(eigen.list, label = "Module")
```

Arguments

eigen.list	the resulting vector from get.eigen.molecule
label	a label of module extracted (default: "Module")

Value

igraph object

Author(s)

Atsushi Fukushima

Examples

```
library(pcaMethods)
library(igraph)
data(golub, package = "multtest")
hc.mol1 <- cluster.molecule(golub[, 1:27], "pearson", "average")
g1 <- cutree(hc.mol1, h=0.4)
res1 <- get.eigen.molecule(golub, g1)
g1.eigen <- get.eigen.molecule.graph(res1)
```

get.lfdr *Getting local false discovery rate (lfdr)*

Description

Getting local false discovery rate (lfdr) using 'fdrtool' package

Usage

```
get.lfdr(r)
```

Arguments

r	a vector of correlation coefficient under condition

Value

list of lfdr

Author(s)

Atsushi Fukushima

References

Strimmer, K. Bioinformatics (2008) 24, 1461-1462

Examples

```
library("fdrtool")
data(pvalues)
get.lfdr(pvalues)
```

---

get.min.max *Get minimum and maximum*

Description

Get minimum and maximum

Usage

```
get.min.max(d)
```

Arguments

d	data matrix or data frame

Value

list object of minimum value or maximum value in a data

Author(s)

Atsushi Fukushima

Examples

```
get.min.max(iris[,1:2])
```

`plotClusterMolecules` *Plot cluster molecules*

Description

Plot cluster molecules

Usage

```
plotClusterMolecules(
  data,
  groups = NULL,
  group.no = NULL,
  title = NULL,
  ylim = NULL,
  order = NULL,
  scale.center = FALSE,
  scale.scale = FALSE,
  frame = "white",
  col = NULL,
  bottom.mar = 5,
  xlab = "Samples",
  ylab = "Relative abundance"
)
```

Arguments

`data`	data matrix or data frame
`groups`	a vector of group memberships as returned by cutree
`group.no`	the group number to be plotted
`title`	a title for the graph
`ylim`	a vector indicating the upper and lower limit for the y-axis
`order`	whether or not to order the columns of the data matrix
`scale.center`	unless NULL, each row is scaled using scale
`scale.scale`	unless NULL, each row is scaled using scale.
`frame`	the color of the frame that is drawn as the background of the plot
`col`	If NULL, all genes will be drawn in the default color (blue). If the text "random" is given, then a set of colors will be generated by
`bottom.mar`	The size of the bottom margin of the plots as sent in par(mar=c(...))
`xlab`	a lalel of x axis (defalt: "Samples")
`ylab`	a lalel of y axis (defalt: "Relative abundance")

Value

a graph

Author(s)

Atsushi Fukushima

References

this function was originally from Watson M (2005) BMC Bioinformatics 7:509

Examples

```
library(pcaMethods)
data(golub, package = "multtest")
hc.mol1 <- cluster.molecule(golub[, 1:27], "pearson", "average")
g1 <- cutree(hc.mol1, h=0.4)
plotClusterMolecules(golub[,1:27], g1, 3)
```

---

plotDiffCorrGroup *Plot DiffCorr group*

Description

Plot DiffCorr group

Usage

```
plotDiffCorrGroup(
  data,
  groups1 = NULL,
  groups2 = NULL,
  group1.no = NULL,
  group2.no = NULL,
  g1,
  g2,
  g1.order = NULL,
  g2.order = NULL,
  title1 = NULL,
  title2 = NULL,
  ...
)
```

Arguments

data	a data matrix or data frame
groups1	a vector of row group membership as produced by cutree under condition 1
groups2	a vector of row group membership as produced by cutree under condition 2
group1.no	the group number to be plotted (condition 1)
group2.no	the group number to be plotted (condition 2)
g1	a vector describing the columns of the data belonging to condition 1
g2	a vector describing the columns of the data belonging to condition 2
g1.order	whether or not to order the columns of the data matrix for condition 1. If "average", then the columns are ordered by the average expression value. If the name of a gene (row), then the columns are orderd according to the expression levels of that gene. If NULL, columns remain in their original order.
g2.order	See g1.order
title1	A title for the left hand graph
title2	A title for the right hand graph
...	other parameters to be passed to this function

Value

a graph

Author(s)

Atsushi Fukushima

Examples

```
library(pcaMethods)
data(golub, package = "multtest")
hc.mol1 <- cluster.molecule(golub[, 1:27], "pearson", "average")
hc.mol2 <- cluster.molecule(golub[, 28:38], "pearson", "average")
g1 <- cutree(hc.mol1, h=0.4)
g2 <- cutree(hc.mol2, h=0.4)
##
plotDiffCorrGroup(golub, g1, g2, 21, 24, 1:27, 28:38,
                  scale.center=TRUE, scale.scale=TRUE,
                  ylim=c(-5,5))
```

scalingMethods *scalingMethods*

Description

The pre-treatment methods

Usage

```
scalingMethods(
  data,
  methods = c("auto", "range", "pareto", "vast", "level", "power")
)
```

Arguments

data	a data matrix ([data.frame object] row: molecules, col: samples or replicates)
methods	the chosen methods.

Value

the resulting data frame (or scaled data matrix)

Author(s)

Atsushi Fukushima

Examples

```
scalingMethods(iris[,1:4], "level")
```

uncent.cor2dist *Additional distance functions correlation distance (uncentered)*

Description

Additional distance functions correlation distance (uncentered)

Usage

```
uncent.cor2dist(data, i, absolute = FALSE)
```

Arguments

data	a data matrix ([data.frame object] row: metabolites, col: samples or replicates)
i	i-th row of data
absolute	TRUE means that absolute value of the correlation coefficient is used (Default: FALSE).

Details

These functions were originally from 'hybridHclust' package. We modified the functions slightly. See also the reference manual in detail.

Value

the resulting correlation matrix

Author(s)

Atsushi Fukushima

Examples

```
uncent.cor2dist(as.matrix(t(iris[,1:4])), 1) ## NOT RUN!
```

---

uncent.cordist *Calculating all pairwise distances using correlation distance*

Description

Calculating all pairwise distances using correlation distance

Usage

```
uncent.cordist(data, absolute = FALSE)
```

Arguments

data	a data matrix ([data.frame object] row: metabolites, col: samples or replicates)
absolute	TRUE means that absolute value of the correlation coefficient is used (Default: FALSE).

Details

These functions were originally from 'hybridHclust' package. We modified the functions slightly. See also the reference manual in detail.

Value

the resulting correlation matrix

Author(s)

Atsushi Fukushima

Examples

```
uncent.cordist(as.matrix(t(iris[,1:4]))) ## NOT RUN!
```

---

write.modules *Writing modules into a text file*

Description

Writing modules into a text file

Usage

```
write.modules(cutree.res, mod.list, outfile = "module_list.txt")
```

Arguments

cutree.res	the result of cutree function
mod.list	the result of get.eigen.molecule
outfile	file name of output

Value

a text file

Author(s)

Atsushi Fukushima

Examples

```
## Not run:
data(golub, package = "multtest")
hc.mol1 <- cluster.molecule(golub[, 1:27], "pearson", "average")
g1 <- cutree(hc.mol1, h=0.4)
res1 <- get.eigen.molecule(golub, g1)
write.modules(g1, res1)

## End(Not run)
```

Index