Package 'nlnet'

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Type Package

Title Nonlinear Network, Clustering, and Variable Selection Based on DCOL

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Description It includes four methods: DCOL-based K-profiles clustering, non-linear network reconstruction, non-linear hierarchical clustering, and variable selection for generalized additive model. References: Tianwei Yu (2018)<DOI:10.1002/sam.11381>; Haodong Liu and others (2016)<DOI:10.1371/journal.pone.0158247>; Kai Wang and others (2015)<DOI:10.1155/2015/918954>; Tianwei Yu and others (2010)<DOI:10.1109/TCBB.2010.73>.

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Imports ROCR, TSP, igraph, fdrtool, coin, methods, graphics, stats, earth, randomForest, e1071

NeedsCompilation no

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Contents

data.gen *Simulated Data Generation*

Description

Generating gene matrix as a example of input.

Usage

```
data.gen(n.genes=100, n.samples=100, n.grps=10, aver.grp.size=10,
n.fun.types=6, epsilon=0.1, n.depend=0)
```

Arguments

n.genes	the number of rows of the matrix.
n.samples	the number of columns of the matrix.
n.grps	the number of hidden clusters.
aver.grp.size	averge number of genes in a cluster.
n.fun.types	number of function types to use.
epsilon	noise level.
n.depend	data generation dependence structure. can be 0, 1, 2.

Details

The data generation scheme is described in detail in IEEE ACM Trans. Comput. Biol. Bioinform. 10(4):1080-85.

Value

return the data including gene and clustering.

data	the gene matrix
grps	the predicted clustering

Author(s)

Tianwei Yu<tyu8@emory.edu>

Examples

```
##generating a gene matrix with 100 genes, some in 5 clusters, and 100 samples per gene.
output<-data.gen(n.genes=100, n.samples=10, n.grps=5)
##get the gene matrix from the source of data.
matrix<-output$data
##get the hiden clusters from the source of data.
grps<-output$grp
```

KPC *implementation of K-Profiles Clustering*

Description

implementation of K-Profiles Clustering

Usage

```
KPC(dataset, nCluster, maxIter = 100, p.max = 0.2, p.min = 0.05)
```

Arguments

dataset	the data matrix with genes in the row and samples in the column
nCluster	the number of clusters K
maxIter	the maximum number of iterations
p.max	the starting p-value cutoff to exclude noise genes
p.min	the final p-value cutoff to exclude noise genes

Value

Return a list about gene cluster and the list of value p

cluster	gene cluster
p.list	a list of value p

Author(s)

Tianwei Yu <tianwei.yu@emory.edu>

References

http://www.hindawi.com/journals/bmri/aa/918954/

See Also

data.gen

Examples

```
## generating the data matrix & hiden clusters as a sample
input<-data.gen(n.genes=40, n.grps=4)
## now input includes data matrix and hiden clusters, so get the matrix as input.
input<-input$data

## set nCluster value to 4
kpc<-KPC(input,nCluster=4)
```

```
##get the hiden cluster result from "KPC"
cluster<-kpc$cluster
##get the list of p
p<-kpc$p.list
```

---

nlhc *Non-Linear Hierarchical Clustering*

Description

The non-linear hierarchical clustering based on DCOL

Usage

```
nlhc(array, hamil.method = "nn", concorde.path = NA,
use.normal.approx = FALSE, normalization = "standardize", combine.linear = TRUE,
use.traditional.hclust = FALSE, method.traditional.hclust = "average")
```

Arguments

`array`	the data matrix with no missing values
`hamil.method`	the method to find the hamiltonian path.
`concorde.path`	If using the Concorde TSP Solver, the local directory of the solver
`use.normal.approx`	whether to use the normal approximation for the null hypothesis.
`normalization`	the normalization method for the array.
`combine.linear`	whether linear association should be found by correlation to combine with non-linear association found by DCOL.
`use.traditional.hclust`	whether traditional agglomerative clustering should be used.
`method.traditional.hclust`	the method to pass on to hclust() if traditional method is chosen.

Details

Hamil.method: It is passed onto the function tsp of library TSP. To use linkern method, the user needs to install concord as instructed in TSP.

use.normal.approx: If TRUE, normal approximation is used for every feature, AND all covariances are assumed to be zero. If FALSE, generates permutation based null distribution - mean vector and a variance-covariance matrix.

normalization: There are three choices - "standardize" means removing the mean of each row and make the standard deviation one; "normal_score" means normal score transformation; "none" means do nothing. In that case we still assume some normalization has been done by the user such that each row has approximately mean 0 and sd 1.

combine.linear: The two pieces of information is combined at the start to initiate the distance matrix.

Value

Returns a hclust object same as the output of hclust(). Reference: help(hclust)

`merge`	an n-1 by 2 matrix. Row i of merge describes the merging of clusters at step i of the clustering. If an element j in the row is negative, then observation -j was merged at this stage. If j is positive then the merge was with the cluster formed at the (earlier) stage j of the algorithm.
`height`	a set of n-1 real values, the value of the criterion associated with the clusterig method for the particular agglomeration
`order`	a vector giving the permutation of the original observations suitable for plotting, in the sense that a cluster plot using this ordering and matrix merge will not have crossings of the branches.
`labels`	labels for each of the objects being clustered
`call`	the call which produced the result
`dist.method`	the distance that has been used to create d
`height.0`	original calculation of merging height

Author(s)

Tianwei Yu <tianwei.yu@emory.edu>

References

http://www.ncbi.nlm.nih.gov/pubmed/24334400

See Also

`data.gen`

Examples

```
## generating the data matrix & hiden clusters as a sample
input<-data.gen(n.genes=40, n.grps=4)
## now input includes data matrix and hiden clusters, so get the matrix as input.
input<-input$data

nlhc.data<-nlhc(input)
plot(nlhc.data)
##get the merge from the input.
merge<-nlhc.data$merge
```

nlnet *Non-Linear Network reconstruction from expression matrix*

Description

Non-Linear Network reconstruction method

Usage

```
nlnet(input, min.fdr.cutoff=0.05,max.fdr.cutoff=0.2, conn.proportion=0.007,
gene.fdr.plot=FALSE, min.module.size=0, gene.community.method="multilevel",
use.normal.approx=FALSE, normalization="standardize", plot.method="communitygraph")
```

Arguments

input	the data matrix with no missing values.
min.fdr.cutoff	the minimun allowable value of the local false discovery cutoff in establishing links between genes.
max.fdr.cutoff	the maximun allowable value of the local false discovery cutoff in establishing links between genes.
conn.proportion	the target proportion of connections between all pairs of genes, if allowed by the fdr cutoff limits.
gene.fdr.plot	whether plot a figure with estimated densities, distribution functions, and (local) false discovery rates.
min.module.size	the min number of genes together as a module.
gene.community.method	the method for community detection.
use.normal.approx	whether to use the normal approximation for the null hypothesis.
normalization	the normalization method for the array.
plot.method	the method for graph and community ploting.

Details

gene.community.method: It provides three kinds of community detection method: "mutilevel", "label.propagation" and "leading.eigenvector".

use.normal.approx: If TRUE, normal approximation is used for every feature, AND all covariances are assumed to be zero. If FALSE, generates permutation based null distribution - mean vector and a variance-covariance matrix.

normalization: There are three choices: "standardize" means removing the mean of each row and make the standard deviation one; "normal_score" means normal score transformation; "none"

means do nothing. In that case we still assume some normalization has been done by the user such that each row has approximately mean 0 and sd 1.

plot.method: It provides three kinds of ploting method: "none" means ploting no graph, "communitygraph" means ploting community with graph, "graph" means ploting graph, "membership" means ploting membership of the community

Value

it returns a graph and the community membership of the graph.

`algorithm`	The algorithm name for community detection
`graph`	An igraph object including edges : Numeric vector defining the edges, the first edge points from the first element to the second, the second edge from the third to the fourth, etc.
`community`	Numeric vector, one value for each vertex, the membership vector of the community structure.

Author(s)

Haodong Liu <liuhaodong0828@gmail.com>

References

https://www.ncbi.nlm.nih.gov/pubmed/27380516

See Also

`data.gen`

Examples

```
 ## generating the data matrix & hiden clusters as a sample
  input<-data.gen(n.genes=40, n.grps=4)
## now input includes data matrix and hiden clusters, so get the matrix as input.
input<-input$data
##change the ploting method
 result<-nlnet(input,plot.method="graph")
  ## get the result and see it values
 graph<-result$graph ##a igraph object.
 comm<-result$community ##community of the graph

 ## use different community detection method
 #nlnet(input,gene.community.method="label.propagation")

 ## change the fdr pro to control connections of genes
 ## adjust the modularity size
 #nlnet(input,conn.proportion=0.005,min.module.size=10)
```

nvsd *Nonlinear Variable Selection based on DCOL*

Description

This is a nonlinear variable selection procedure for generalized additive models. It's based on DCOL, using forward stagewise selection. In addition, a cross-validation is conducted to tune the stopping alpha level and finalize the variable selection.

Usage

```
nvsd(X, y, fold = 10, step.size = 0.01, stop.alpha = 0.05, stop.var.count = 20,
max.model.var.count = 10, roughening.method = "DCOL", do.plot = F, pred.method = "MARS")
```

Arguments

X	The predictor matrix. Each row is a gene (predictor), each column is a sample. Notice the dimensionality is different than most other packages, where each column is a predictor. This is to conform to other functions in this package that handles gene expression type of data.
y	The numerical outcome vector.
fold	The fold of cross-validation.
step.size	The step size of the roughening process.
stop.alpha	The alpha level (significance of the current selected predictor) to stop the iterations.
stop.var.count	The maximum number of predictors to select in the forward stagewise selection. Once this number is reached, the iteration stops.
max.model.var.count	The maximum number of predictors to select. Notice this can be smaller than the stop.var.count. Stop.var.count can be set more liniently, and this parameter controls the final maximum model size.
roughening.method	The method for roughening. The choices are "DCOL" or "spline".
do.plot	Whether to plot the points change in each step.
pred.method	The prediction method for the cross validation variable selection. As forward stagewise procedure doesn't do prediction, a method has to be borrowed from existing packages. The choices include "MARS", "RF", and "SVM".

Details

Please refer to the reference for details.

Value

A list object is returned. The components include the following.

selected.pred	The selected predictors (row number).
all.pred	The selected predictors by the forward stagewise selection. The $selected.pred is a subset of this.

Author(s)

Tianwei Yu<tianwei.yu@emory.edu>

References

https://arxiv.org/abs/1601.05285

See Also

stage.forward

Examples

```
X<-matrix(rnorm(2000),ncol=20)
y<-sin(X[,1])+X[,2]^2+X[,3]
nvsd(t(X),y,stop.alpha=0.001,step.size=0.05)
```

---

stage.forward *Nonlinear Forward stagewise regression using DCOL*

Description

The subroutine conducts forward stagewise regression using DCOL. Either DCOL roughening or spline roughening is conducted.

Usage

```
stage.forward(X, y, step.size = 0.01, stop.alpha = 0.01,
stop.var.count = 20, roughening.method = "DCOL", tol = 1e-08,
spline.df = 5, dcol.sel.only = FALSE, do.plot = F)
```

Arguments

X	The predictor matrix. Each row is a gene (predictor), each column is a sample. Notice the dimensionality is different than most other packages, where each column is a predictor. This is to conform to other functions in this package that handles gene expression type of data.
y	The numerical outcome vector.
step.size	The step size of the roughening process.

stop.alpha	The alpha level (significance of the current selected predictor) to stop the iterations.
stop.var.count	The maximum number of predictors to select. Once this number is reached, the iteration stops.
roughening.method	The method for roughening. The choices are "DCOL" or "spline".
tol	The tolerance level of sum of squared changes in the residuals.
spline.df	The degree of freedom for the spline.
dcol.sel.only	TRUE or FALSE. If FALSE, the selection of predictors will consider both linear and nonlinear association significance.
do.plot	Whether to plot the points change in each step.

Details

Please refer to the reference manuscript for details.

Value

A list object is returned. The components include the following.

found.pred	The selected predictors (row number).
ssx.rec	The magnitude of variance explained using the current predictor at each step.
$sel.rec	The selected predictor at each step.
$p.rec	The p-value of the association between the current residual and the selected predictor at each step.

Author(s)

Tianwei Yu<tianwei.yu@emory.edu>

References

https://arxiv.org/abs/1601.05285

See Also

nvsd

Examples

```
X<-matrix(rnorm(2000),ncol=20)
y<-sin(X[,1])+X[,2]^2+X[,3]
stage.forward(t(X),y,stop.alpha=0.001,step.size=0.05)
```

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