Package ‘predictionet’
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Description This package contains a set of functions related to network inference combining genomic data and prior information extracted from biomedical literature and structured biological databases. The main function is able to generate networks using Bayesian or regression-based inference methods; while the former is limited to < 100 of variables, the latter may infer networks with hundreds of variables. Several statistics at the edge and node levels have been implemented (edge stability, predictive ability of each node, ...) in order to help the user to focus on high quality subnetworks. Ultimately, this package is used in the 'Predictive Networks' web application developed by the Dana-Farber Cancer Institute in collaboration with Entagen.
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Inference for predictive networks designed for (but not limited to) genomic data

This package contains a set of functions related to network inference combining genomic data and prior information extracted from biomedical literature and structured biological databases. The main function is able to generate networks using bayesian or regression-based inference methods; while the former is limited to < 100 of variables, the latter may infer network with hundreds of variables. Several statistics at the edge and node levels have been implemented (edge stability, predictive ability of each node,...) in order to help the user to focus on high quality subnetworks. Ultimately, this package is used in the ‘Predictive Networks’ web application developed by the Dana-Farber Cancer Institute in collaboration with

Details

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Author(s)

Benjamin Haibe-Kains, Catharina Olsen, Gianluca Bontempi, John Quackenbush
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http://compbio.dfci.harvard.edu/
adj.get.hops

Function to identify all children of a parent

Description

This function uses a depth-first search algorithm to identify all the children (and their corresponding depth) of a node.

Usage

adj.get.hops(adjmat)

Arguments

adjmat
adjacency matrix; parents in rows, children in columns

Details

The algorithm is based on the depth-first search.

Value

two-column matrix containing the names of the children in the first column and their corresponding depth in the descent in the second column

Author(s)

Benjamin Haibe-Kains

Examples

```r
## check whether a list of two nodes are children of another node
set.seed(54321)
mytopo <- matrix(sample(0:1, 100, replace=TRUE, prob=c(0.7,0.3)), nrow=10, dimnames=list(LETTERS[1:10], LETTERS[1:10]))
adj.get.hops(adjmat=mytopo)
```
Function to remove cycles that may be present in a directed graph represented by an adjacency matrix

Description
This function removes cycles that may be present in a directed graph represented by an adjacency matrix,

Usage
adj.remove.cycles(adjmat, from, maxlength)

Arguments
adjmat adjacency matrix with positive entries represent evidence for the presence of an edge and entries less or equal than zero represent absence of an edge; parents in row, children in columns.
from indices or names of nodes for which the cycles present in the childhood should be removed; if missing, all cycles will be removed.
maxlength maximum length of path, once this length is reached no longer paths will be searched for.

Details
This function may be useful when it comes to generate a bayesian network using a topology identified from an source of information where cycles are allowed. When cycles are removed, the function tries to keep the most positive entries.

Value
A list of two items
adjmat.acyclic an adjacency matrix without cycles
adjmat.removed a matrix of booleans representing the edges that have been removed from the original adjacency matrix to make it acyclic

Author(s)
Benjamin Haibe-Kains

Examples
set.seed(54321)
xx <- matrix(sample(c(0,1), 100, replace=TRUE), nrow=10, ncol=10)
adj.remove.cycles(adjmat=xx, from=1, maxlength=3)
Function to discretize data based on user specified cutoffs

Description
This function enable discretization of data based on cutoffs specified by the users

Usage
data.discretize(data, cuts)

Arguments
data matrix of continuous or categorical values (gene expressions for example); observations in rows, features in columns.
cuts list of cutoffs for each variable.

Details
This function is discretizing the continuous value in data using the cutoffs specified in cuts to create categories represented by increasing integers in 1,2,...n where n is the maximum number of categories in the dataset.

Value
a matrix of categorical values where categories are {1,2,...n} depending on the list of cutoffs specified in cuts; observations in rows, features in columns.

Author(s)
Benjamin Haibe-Kains

See Also
discretize

Examples
## load gene expression data for colon cancer data, list of genes related to RAS signaling pathway and the corresponding priors
data(exp0.colon.ras)
## discretize the data in 3 categories
categories <- rep(3, ncol(data.ras))
## estimate the cutoffs (tertiles) for each gene
cuts.discrim <- lapply(apply(rbind("nbcat"=categories, data.ras), 2, function(x) { y <- x[1]; x <- x[-1]; return(quantile(x=x, probs=seq(0, 1, length.out=y+1), na.rm=TRUE)[-c(1, y+1)] })), function(x) { return(x[[1]]})
data.ras.bin <- data.discretize(data=data.ras, cuts=cuts.discrim)
**eval.network**  
*Function computing the f1-score, comparing an inferred topology with a given topology*

**Description**
This function computes the f1-score for an inferred topology using a topology provided by the user.

**Usage**
```
eval.network(topo, true.topo)
```

**Arguments**
- `topo`  
  Inferred topology, an edge between variables X and Y corresponds to net[X,Y]=1.
- `true.topo`  
  Topology the user wants to compare the inferred topology with, e.g. the true network using generated datasets. An edge between variables X and Y corresponds to net[X,Y]=1.

**Value**
The computed f1-score, defined as $2*TP/(2*TP+FN+FP)$

**Author(s)**
Benjamin Haibe-Kains, Catharina Olsen

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**expO.colon.ras**  
*Gene expression, annotations, clinical data and priors for the colon cancer tumors collected by the expression project for oncology (expO).*

**Description**
This dataset contains (part of) the gene expression, annotations and clinical data as published by the expO project ([http://www.intgen.org/expo/](http://www.intgen.org/expo/)). Genes related to KRAS mutations were retrieved from Bild et al, Nature, 2006. Only genes with known gene symbols were selected resulting in a dataset of 292 human colon tumors and 259 RAS-related genes.

**Usage**
```
data(expO.colon.ras)
```

**Format**
- **exp0.colon.ras** is a dataset containing four matrices:
  - **demo.ras**  
    Clinical information of the colon cancer patients whose tumors were hybridized.
  - **data.ras**  
    Matrix containing expression of genes related to RAS.
  - **annot.ras**  
    Matrix containing annotations of the genes related to RAS.
  - **priors.ras**  
    Matrix of priors counts for all the genes related to RAS. Each value represents the number of times an interaction was observed for a specific pair of genes (parents in rows, children in columns).
Details

The microarray platform used in the expO project is the Affymetrix HG-U133PLUS2 GeneChip.

Source

https://expo.intgen.org/geo/

References

http://www.intgen.org/expo/


Examples

data(expO.colon.ras)

---

**jorissen.colon.ras**  
*Gene expression, annotations, clinical data and priors for the colon cancer tumors collected by Jorissen and colleagues in 2009.*

Description

This dataset contains (part of) the gene expression, annotations and clinical data as published by Jorissen and colleagues in 2009. Genes related to KRAS mutations were retrieved from Bild et al, Nature, 2006. Only genes with known gene symbols were selected resulting in a dataset of 290 human colon tumors and 259 RAS-related genes.

Usage

data(jorissen.colon.ras)

Format

**jorissen.colon.ras** is a dataset containing four matrices:

- **demo2.ras** clinical information of the colon cancer patients whose tumors were hybridized.
- **data2.ras** matrix containing expression of genes related to RAS.
- **annot2.ras** matrix containing annotations of the genes related to RAS.
- **priors2.ras** matrix of priors counts for all the genes related to RAS. Each value represents the number of times an interaction was observed for a specific pair of genes (parents in rows, children in columns).

Details

The microarray platform used in Jorissen’s dataset is the Affymetrix HG-U133PLUS2 GeneChip.
mcc

Source


References


Examples

data(jorissen.colon.ras)

mcc

Function to compute the Matthews Correlation Coefficient (MCC) in a classification framework

Description

This function computes the Matthews Correlation Coefficient (MCC) in a classification framework.

Usage

mcc(ct, nbcat = nrow(ct))

Arguments

c t: contingency table

nbcat: number of categories

Value

MCC estimate

Author(s)

Benjamin Haibe-Kains
net2pred

Function fitting a regression model for each gene in the data

Description

Function to fit a regression model for each variable in the dataset or alternatively each variable of interest.

Usage

net2pred(net, data, categories, predn, perturbations, method = c("linear", "linear.penalized", "cpt"), seed)

Arguments

net
    network object.

data
    matrix of continuous or categorical values (gene expressions for example); observations in rows, features in columns.

categories
    if this parameter missing, 'data' should be already discretized; otherwise either a single integer or a vector of integers specifying the number of categories used to discretize each variable (data are then discretized using equal-frequency bins) or a list of cutoffs to use to discretize each of the variables in 'data' matrix. If method='bayesnet' and categories is missing, data should contain categorical values and the number of categories will determine from the data.

predn
    indices or names of variables to fit during network inference. If missing, all the variables will be used for network inference.

perturbations
    matrix of 0,1 specifying whether a gene has been perturbed (e.g., knockdown, overexpression) in some experiments. Dimensions should be the same than data.

method
    type of predictive model to fit; linear for linear regression model, linear.penalized for regularized linear regression model, cpt for conditional probability tables estimated after discretization of the data.

seed
    set the seed to make the cross-validation and network inference deterministic.

Value

a new network object with the predictive models

Author(s)

Benjamin Haibe-Kains, Catharina Olsen

Examples

## load gene expression data for colon cancer data, list of genes related to RAS signaling pathway and the corresponding priors
data(expO.colon.ras)
## create matrix of perturbations (no perturbations in this dataset)
pert <- matrix(0, nrow=nrow(data.ras), ncol=ncol(data.ras), dimnames=dimnames(data.ras))
## number of genes to select for the analysis
genen <- 10
## select only the top genes

go.i <- dimnames(annot.ras)[[1]][order(abs(log2(annot.ras[, "fold.change"])), decreasing=TRUE)[1:genen]]
mydata <- data.ras[, go.i, drop=FALSE]
myannot <- annot.ras[go.i, , drop=FALSE]
mydemo <- demo.ras
mypert <- pert[, go.i, drop=FALSE]

### regression-based network inference

### infer global network from data and priors

mynet <- netinf(data=mydata, perturbations=mypert, priors=mypriors, priors.count=TRUE, priors.weight=0.5, maxparents=3, method="regrnet", seed)
net2pred(net=mynet, data=mydata, method="linear")

---

**netinf**

*Function performing network inference by combining priors and genomic data*

**Description**

Main function of the `predictionet` package, `netinf` infers a gene network by combining priors and genomic data. The two main network inference methodologies implemented so far are the bayesian and regression-based inferences.

**Usage**

```r
netinf(data, categories, perturbations, priors, predn, priors.count = TRUE, priors.weight = 0.5, maxparents = 3, ensemble.maxnsol = 3, causal=TRUE, seed, bayesnet.maxcomplexity=0, bayesnet.maxiter=100, verbose = FALSE)
```

**Arguments**

- **data**
  - matrix of continuous or categorical values (gene expressions for example); observations in rows, features in columns.

- **categories**
  - if this parameter missing, 'data' should be already discretized; otherwise either a single integer or a vector of integers specifying the number of categories used to discretize each variable (data are then discretized using equal-frequency bins) or a list of cutoffs to use to discretize each of the variables in 'data' matrix. If method='bayesnet' and categories is missing, data should contain categorical values and the number of categories will determine from the data.

- **perturbations**
  - matrix of 0,1 specifying whether a gene has been perturbed (e.g., knockdown, overexpression) in some experiments. Dimensions should be the same than data.

- **priors**
  - matrix of prior information available for gene-gene interaction (parents in rows, children in columns). Values may be probabilities or any other weights (citations count for instance). If priors counts are used the parameter priors.count should be TRUE so the priors are scaled accordingly.

- **predn**
  - indices or names of variables to fit during network inference. If missing, all the variables will be used for network inference. Note that for bayesian network inference (method="bayesnet") this parameter is ignored and a network will be generated using all the variables.
priors.count  TRUE if priors specified by the user are number of citations (count) for each interaction. FALSE if probabilities or any other weight in [0,1] are reported instead.
priors.weight  real value in [0,1] specifying the weight to put on the priors (0=only the data are used, 1=only the priors are used to infer the topology of the network).
maxparents  maximum number of parents allowed for each gene.
subset  vector of indices to select only subset of the observations.
method  regrnet for regression-based network inference, bayesnet for bayesian network inference with the catnet package.
ensemble  TRUE if the ensemble approach should be used, FALSE otherwise.
ensemble.model  Could be either full or best depending how the equivalent networks are selected to be included in the ensemble network: for full bootstrapping is used to identify all the statistically equivalent networks, it best only the top ensemble.maxnsol are considered at each step of the feature selection.
ensemble.maxnsol  maximum number of solutions to consider at each step of the feature selection for the method=ensemble.regrnet, default is 3.
causal  'TRUE' if the causality should be inferred from the data, 'FALSE' otherwise
seed  set the seed to make the network inference deterministic.
bayesnet.maxcomplexity  maximum complexity for bayesian network inference, see Details.
bayesnet.maxiter  maximum number of iterations for bayesian network inference, see Details.
verbose  TRUE if messages should be printed, FALSE otherwise.

**Details**

bayesnet.maxcomplexity and bayesnet.maxiter are parameters to be passed to the network inference method (see cnSearchOrder and cnSearchSA from the catnet package for more details).

Relevance score is either MRMR scores if causal=FALSE or causality score if causal=FALSE.

**Value**

method  name of the method used for network inference.
ensemble  is the network build using the ensemble approach?
topology  adjacency matrix representing the topology of the inferred network; parents in rows, children in columns.
topology.coeff  if method='regrnet' topology.coeff contains an adjacency matrix with the coefficients used in the local regression model; parents in rows, children in columns. Additionally the beta_0 values for each model in the first row of the matrix
edge.relevance  relevance score for each edge (see Details).

**Author(s)**

Benjamin Haibe-Kains, Catharina Olsen
Examples

```r
## load gene expression data for colon cancer data, list of genes related to RAS signaling pathway and the corresponding priors
data(expO.colon.ras)
## create matrix of perturbations (no perturbations in this dataset)
pert <- matrix(0, nrow=nrow(data.ras), ncol=ncol(data.ras), dimnames=dimnames(data.ras))

## number of genes to select for the analysis
ngen <- 10
## select only the top genes
goi <- dimnames(annot.ras)[[1]][order(abs(log2(annot.ras[,"fold.change"])), decreasing=TRUE)[1:ngen]]
mydata <- data.ras[, goi, drop=FALSE]
myannot <- annot.ras[goi, , drop=FALSE]
mydemo <- demo.ras
mypert <- pert[, goi, drop=FALSE]

########################
## regression-based network inference
########################
## infer global network from data and priors
mynet <- netinf(data=mydata, perturbations=mypert, priors=mypriors, priors.count=TRUE, priors.weight=0.5, maxparents=3, method="regrnet", seed=54321)

## plot network topology
mytopo <- mynet$topology
library(network)
xnet <- network(x=mytopo, matrix.type="adjacency", directed=TRUE, loops=FALSE, vertex.attrnames=dimnames(mytopo)[[1]])
plot.network(x=xnet, displayisolates=TRUE, displaylabels=TRUE, boxed.labels=FALSE, label.pos=0, arrowhead.cex=2, vertex.cex=4, vertex.col="royalblue", jitter=FALSE, pad=0.5)

## export network as a 'gml' file that you can import into Cytoscape
## Not run: rr <- netinf2gml(object=mynet, file="/predictionet_regrnet")

########################
## bayesian network inference
########################
## discretize gene expression values in three categories
categories <- rep(3, ncol(mydata))
## estimate the cutoffs (tertiles) for each gene
cuts.discr <- lapply(apply(rbind("nbcat"=categories, mydata), 2, function(x) { y <- x[1]; x <- x[-1]; return(list(quantile(x=x, probs=seq(0, 1, length.out=y+1), na.rm=TRUE)[-c(1, y+1)])) }), function(x) { return(x[[1]])
mydata <- data.discretize(data=mydata, cuts=cuts.discr)

## infer a bayesian network network from data and priors
## Not run: mynet <- netinf(data=mydata, perturbations=mypert, priors=mypriors, priors.count=TRUE, priors.weight=0.5, maxparents=3, method="bayesnet", seed=54321)

## plot network topology
## Not run: mytopo <- mynet$topology
## Not run: library(network)
## Not run: xnet <- network(x=mytopo, matrix.type="adjacency", directed=TRUE, loops=FALSE, vertex.attrnames=dimnames(mytopo)[[1]])
## Not run: plot.network(x=xnet, displayisolates=TRUE, displaylabels=TRUE, boxed.labels=FALSE, label.pos=0, arrowhead.cex=2, vertex.cex=4, vertex.col="royalblue", jitter=FALSE, pad=0.5)

## export network as a 'gml' file that you can import into Cytoscape
## Not run: rr <- netinf2gml(object=mynet, file="/predictionet_bayesnet")
```
Description

The function netinf.cv perform a cross-validation loop and infers a gene network by combining priors and genomic data in each fold. This allows to estimate the predictive ability of the inferred network as well as edge stability.

Usage

netinf.cv(data, categories, perturbations, priors, predn, priors.count = TRUE, priors.weight = 0.5, ... "cpt"), nfold = 10, causal = TRUE, seed, bayesnet.maxcomplexity = 0, bayesnet.maxiter = 100, verbose = FALSE)

Arguments

data matrix of continuous or categorical values (gene expressions for example); observations in rows, features in columns.
categories if this parameter missing, 'data' should be already discretized; otherwise either a single integer or a vector of integers specifying the number of categories used to discretize each variable (data are then discretized using equal-frequency bins) or a list of cutoffs to use to discretize each of the variables in 'data' matrix. If method='bayesnet', this parameter should be specified by the user.
perturbations matrix of 0, 1 specifying whether a gene has been perturbed (e.g., knockdown, overexpression) in some experiments. Dimensions should be the same than data.
priors matrix of prior information available for gene-gene interaction (parents in rows, children in columns). Values may be probabilities or any other weights (citations count for instance). If priors counts are used the parameter priors.count should be TRUE so the priors are scaled accordingly.
predn indices or names of variables to fit during network inference. If missing, all the variables will be used for network inference.
priors.count TRUE if priors specified by the user are number of citations (count) for each interaction, FALSE if probabilities or any other weight in [0,1] are reported instead.
priors.weight real value in [0,1] specifying the weight to put on the priors (0=only the data are used, 1=only the priors are used to infer the topology of the network).
maxparents maximum number of parents allowed for each gene.
subset vector of indices to select only subset of the observations.
method regrnet for regression-based network inference, bayesnet for bayesian network inference with the catnet package.
ensemble TRUE if the ensemble approach should be used, FALSE otherwise.
ensemble.maxnsol Number of equivalent solutions chosen at each step.
predmodel type of predictive model to fit; linear for linear regression model, linear.penalized for regularized linear regression model, cpt for conditional probability tables estimated after discretization of the data.
nfold number of folds for the cross-validation.
causal 'TRUE' if the causality should be inferred from the data, 'FALSE' otherwise
seed set the seed to make the cross-validation and network inference deterministic.
bayesnet.maxcomplexity maximum complexity for bayesian network inference, see Details.
bayesnet.maxiter maximum number of iterations for bayesian network inference, see Details.
verbose TRUE if messages should be printed, FALSE otherwise.
Details

bayesnet.maxcomplexity and bayesnet.maxiter are parameters to be passed to the network inference method (see cnSearchOrder and cnSearchSA from the catnet package for more details).

Value

method name of the method used for network inference.

topology topology of the model inferred using the entire dataset.

topology.coeff if method='regrnet' topology.coeff contains an adjacency matrix with the coefficients used in the local regression model; parents in rows, children in columns. Additionally the beta_0 values for each model in the first row of the matrix

topology.cv topology of the networks inferred at each fold of the cross-validation.

topology.coeff.cv if method='regrnet' topology.coeff contains an adjacency matrix with the coefficients used in the local regression model; parents in rows, children in columns. Additionally the beta_0 values for each model in the first row of the matrix. Inferred at each fold of the cross-validation

prediction.score.cv list of prediction scores (R2, NRMSE, MCC) computed at each fold of the cross-validation.

topology.cv

topology.coeff.cv

topology.coeff.cv

topology.coeff.cv

edge.stability stability of the edges inferred during cross-validation; only the stability of the edges present in the network inferred using the entire dataset is reported.

edge.stability.cv stability of the edges inferred during cross-validation.

edge.relevance mean relevance score for each across folds in cross-validation.

edge.relevance.cv relevance score for each across computed during cross-validation.

Author(s)

Benjamin Haibe-Kains, Catharina Olsen

Examples

```r
## load gene expression data for colon cancer data, list of genes related to RAS signaling pathway and the corresponding priors
data(expO.colon.ras)
## create matrix of perturbations (no perturbations in this dataset)
pert <- matrix(0, nrow=nrow(data.ras), ncol=ncol(data.ras), dimnames=dimnames(data.ras))

## number of genes to select for the analysis
genen <- 10
## select only the top genes

goi <- dimnames(annot.ras)[[1]][order(abs(log2(annot.ras[, "fold.change"])), decreasing=TRUE)[1:genen]]

mydata <- data.ras[, goi, drop=FALSE]
myannot <- annot.ras[goi, , drop=FALSE]

mypriors <- priors.ras[goi, goi, drop=FALSE]

mydemo <- demo.ras

mypert <- pert[, goi, drop=FALSE]
```

netinf.predict

Function to make prediction of a node values given its parents using an inferred network

Description

This function predict the value of a node given its parents using an inferred network

Usage

netinf.predict(net, data, categories, perturbations, subset, predn, method=c("linear", "linear.penalized", "cpt"))

Arguments

net
a network object with local regression models.
data
matrix of continuous or categorical values (gene expressions for example); observations in rows, features in columns.
categories
if this parameter missing, 'data' should be already discretize; otherwise either a single integer or a vector of integers specifying the number of categories used to discretize each variable (data are then discretized using equal-frequency bins) or a list of cutoffs to use to discretize each of the variables in 'data' matrix. If method='bayesnet', this parameter should be specified by the user.
perturbations
matrix of 0, 1 specifying whether a gene has been perturbed (e.g., knockdown, overexpression) in some experiments. Dimensions should be the same than data.
subset
vector of indices to select only subset of the observations.
netinf2gml

Function to create an igraph object and export a network to a GML readable by Cytoscape

Description
This function creates, from a network inferred from netinf or netinf.cv, an igraph object and export this network to a GML readable by Cytoscape.

Usage
netinf2gml(object, edge.info, node.info, file = "predictionet")
Arguments

object          object returns by netinf or netinf.cv
edge.info      matrix of values representing the statistics for each edge; parents in rows, children in columns. A list of matrices could be provided, names of the list will then be used to describe the statistics in Cytoscape
node.info      vector of values representing the statistics for each node; parents in rows, children in columns. A list of vectors could be provided, names of the list will then be used to describe the statistics in Cytoscape
file            name of the GML file to be saved.

Details

The GML file created by this function has been tested on Cytoscape 2.8.1; a Vizmap property file of the same name is also created and could be imported into Cytoscape ("preditionet_vizmap2") so the information for each node and edge are displayed correctly.

Value

an igraph object

Author(s)

Benjamin Haibe-Kains

See Also

\code{RCytoscape}

Examples

```r
## load gene expression data for colon cancer data, list of genes related to RAS signaling pathway and the corresponding priors
data(expO.colon.ras)
## number of genes to select for the analysis
genen <- 10
## select only the top genes
goi <- dimnames(annot.ras)[[1]][order(abs(log2(annot.ras[, "fold.change"])), decreasing=TRUE)[1:genen]]
mydata <- data.ras[, goi, drop=FALSE]
myannot <- annot.ras[goi, , drop=FALSE]
mypriors <- priors.ras[goi, goi, drop=FALSE]
mydemo <- demo.ras
## infer global network from data and priors
mynet <- netinf.cv(data=mydata, categories=3, priors=mypriors, priors.count=TRUE, priors.weight=0.5, maxparents=3, method="regrnet", nfold=3, seed=54321)
## create an igraph object and export it into a GML file
### Not run: netinf2gml(object=mynet, file = "predictionet")
```
pred.score  

Function computing performance of prediction; methods include r2, nrmse and mcc

Description

This function computes prediction performance; methods include r2, nrmse and mcc.

Usage

```r
pred.score(data, pred, categories, method = c("r2", "nrmse", "mcc"))
```

Arguments

data  

pred

categories  

if this parameter missing, 'data' should be already discretize; otherwise either a single integer or a vector of integers specifying the number of categories used to discretize each variable (data are then discretized using equal-frequency bins) or a list of cutoffs to use to discretize each of the variables in 'data' matrix. If method='bayesnet', this parameter should be specified by the user.

method

Value

A vector of performance scores, one for each node

Author(s)

Benjamin Haibe-Kains, Catharina Olsen

See Also

netinf.predict

Examples

```r
set.seed(54321)
xx <- runif(100)
## R2
pred.score(data=xx, pred=xx+rnorm(100)/10, method="r2")
## NRMSE
pred.score(data=xx, pred=xx+rnorm(100)/10, method="nrmse")
## MCC
pred.score(data=xx, pred=xx+rnorm(100)/10, categories=3, method="mcc")
```
predictionet.press.statistic

Function computing the press statistic for all target variables in topology

Description

The function `predictionet.press.statistic` computes the press statistic for all target variables in the provided topology.

Usage

`predictionet.press.statistic(topo, data, ensemble=FALSE, perturbations=NULL)`

Arguments

topo  
adjacency matrix of 0,1 indicating whether two variables are connected

data  
matrix of continuous or categorical values (gene expressions for example); observations in rows, features in columns.

perturbations  
matrix of 0, 1 specifying whether a gene has been perturbed (e.g., knockdown, overexpression) in some experiments. Dimensions should be the same than data.

ensemble  
TRUE if the ensemble approach should be used, FALSE otherwise.

Value

A vector of press statistics, one for every target variable.

Author(s)

Benjamin Haibe-Kains, Catharina Olsen

Examples

```r
## load gene expression data for colon cancer data, list of genes related to RAS signaling pathway and the corresponding priors
data(expO.colon.ras)
## create matrix of perturbations (no perturbations in this dataset)
pert <- matrix(0, nrow=nrow(data.ras), ncol=ncol(data.ras), dimnames=dimnames(data.ras))

# number of genes to select for the analysis
gen = 10
# select only the top genes
goi <- dimnames(annot.ras)[[1]][order(abs(log2(annot.ras[,"fold.change"])), decreasing=TRUE)[1:gen]]
mydata <- data.ras[, goi, drop=FALSE]
myannot <- annot.ras[goi, , drop=FALSE]
mypriors <- priors.ras[goi, goi, drop=FALSE]
mydemo <- demo.ras
mypert <- pert[, goi, drop=FALSE]

# regression-based network inference
```

predictionet.stability.cv

Function inferring networks in cross-validation

Description

The function predictionet.stability.cv infers networks in cross-validation (compared to netinf.cv no regression is carried out, thus less computational cost but no prediction scores)

Usage

predictionet.stability.cv(data, categories, perturbations, priors, predn, priors.count = TRUE, priors.weight = 0.5, ... = FALSE, ensemble.maxnsol = 3, nfold = 10, causal = TRUE, seed, bayesnet.maxcomplexity = 0, bayesnet.maxiter = 100)

Arguments

data: matrix of continuous or categorical values (gene expressions for example); observations in rows, features in columns.
categories: if this parameter missing, 'data' should be already discretized; otherwise either a single integer or a vector of integers specifying the number of categories used to discretize each variable (data are then discretized using equal-frequency bins) or a list of cutoffs to use to discretize each of the variables in 'data' matrix. If method='bayesnet', this parameter should be specified by the user.
perturbations: matrix of 0, 1 specifying whether a gene has been perturbed (e.g., knockdown, overexpression) in some experiments. Dimensions should be the same than data.
priors: matrix of prior information available for gene-gene interaction (parents in rows, children in columns). Values may be probabilities or any other weights (citations count for instance). If priors counts are used the parameter priors.count should be TRUE so the priors are scaled accordingly.
predictionet.stability.cv

predn  indices or names of variables to fit during network inference. If missing, all the variables will be used for network inference.

priors.count  TRUE if priors specified by the user are number of citations (count) for each interaction, FALSE if probabilities or any other weight in [0,1] are reported instead.

priors.weight  real value in [0,1] specifying the weight to put on the priors (0=only the data are used, 1=only the priors are used to infer the topology of the network).

maxparents  maximum number of parents allowed for each gene.

subset  vector of indices to select only subset of the observations.

method  regrnet for regression-based network inference, bayesnet for bayesian network inference with the catnet package.

ensemble  TRUE if the ensemble approach should be used, FALSE otherwise.

ensemble.maxnsol  Number of equivalent solutions chosen at each step.

nfold  number of folds for the cross-validation.

causal  'TRUE' if the causality should be inferred from the data, 'FALSE' otherwise

seed  set the seed to make the cross-validation and network inference deterministic.

bayesnet.maxcomplexity  maximum complexity for bayesian network inference, see Details.

bayesnet.maxiter  maximum number of iterations for bayesian network inference, see Details.

Value

method name of the method used for network inference.

topology topology of the model inferred using the entire dataset.

topology.cv topology of the networks inferred at each fold of the cross-validation.

edge.stability stability of the edges inferred during cross-validation; only the stability of the edges present in the network inferred using the entire dataset is reported.

edge.stability.cv stability of the edges inferred during cross-validation.

Author(s)

Benjamin Haibe-Kains, Catharina Olsen

Examples

## load gene expression data for colon cancer data, list of genes related to RAS signaling pathway and the corresponding priors
data(expO.colon.ras)

## create matrix of perturbations (no perturbations in this dataset)
pert <- matrix(0, nrow=nrow(data.ras), ncol=ncol(data.ras), dimnames=dimnames(data.ras))

## number of genes to select for the analysis
genen <- 10

## select only the top genes
goi <- dimnames(annot.ras[[1]])[order(abs(log2(annot.ras[,"fold.change"])), decreasing=TRUE)[1:genen]]

mydata <- data.ras[, goi, drop=FALSE]

myannot <- annot.ras[goi, , drop=FALSE]

mypriors <- priors.ras[goi, goi, drop=FALSE]
mydemo <- demo.ras
mypert <- pert[ , goi, drop=FALSE]

##################################
## regression-based network inference
##################################
## number of fold for cross-validation
res <- netinf.cv(data=mydata, categories=3, perturbations=mypert, priors=mypriors, priors.weight=0.5, method="regrnet", nfold=3, seed=54321)

## MCC for predictions in cross-validation
print(res$prediction.score.cv)

## export network as a 'gml' file that you can import into Cytoscape
## Not run: rr <- netinf2gml(object=res, file="predictionet_regrnet")

##################################
## bayesian network inference
##################################
## infer a bayesian network network from data and priors
## number of fold for cross-validation
## Not run: res <- netinf.cv(data=mydata, categories=3, perturbations=mypert, priors=mypriors, priors.count=TRUE, priors.weight=0.5, method="bayesnet", nfold=3, seed=54321)

## MCC for predictions in cross-validation
## Not run: print(res$prediction.score.cv)

## export network as a 'gml' file that you can import into Cytoscape
## Not run: rr <- netinf2gml(object=res, file="predictionet_bayesnet")
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