

Package ‘GroupBN’

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Title Inferring Group Bayesian Networks using Hierarchical Feature Clustering

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Description Group Bayesian Networks: This package implements the inference of group Bayesian networks based on hierarchical feature clustering, and the adaptive refinement of the grouping regarding an outcome of interest, as described in Becker et. al (2021) <[doi:10.1371/journal.pcbi.1008735](https://doi.org/10.1371/journal.pcbi.1008735)>.

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cross.en	<i>cross.en</i>
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Description

Calculates the weighted cross entropy / log-loss for a vector of observations and predicted probabilities (weighted by class proportions)

Usage

```
cross.en(pred, obs, sdpred=NULL, weighted=T)
```

Arguments

pred	a numeric vector, the predicted probabilities of the reference class
obs	the vector of observations, a categorical variable with 2-4 levels
sdpred	either NULL or a vector containing the standard deviations of every estimate
weighted	a boolean, if FALSE, the unweighted logloss is calculated. By default, the weighted cross entropy is calculated.

Details

if sdpred contains the standard deviations for each estimated probability, then a lower bound of the log loss is returned.

Value

a numeric value: cross entropy / log loss for comparison of classifiers. The smaller, the better.

Author(s)

Ann-Kristin Becker

Examples

```

#observations
obs<-as.factor(c("A","A","B"))
#correct prediction
pred1<-c(1,1,0)
#wrong prediction
pred2<-c(0,0,1)

cross.en(pred=pred1, obs=obs) #small
cross.en(pred=pred2, obs=obs) #large

#prediction of only majority class
pred3<-c(1,1,1)
#prediction of only minority class
pred4<-c(0,0,0)

cross.en(pred=pred3, obs=obs, weighted=TRUE)
cross.en(pred=pred4, obs=obs, weighted=TRUE)
#both equal (as weighted)

cross.en(pred=pred3, obs=obs, weighted=FALSE)
cross.en(pred=pred4, obs=obs, weighted=FALSE)
#unweighted, majority class is favored

```

discretize.dens

discretize.dens

Description

density approximative discretization. Significant peaks in the density are determined and used as starting points for k-means based discretization. If only one peak is present, distribution quartiles are used for binning.

Usage

```

discretize.dens(data, graph=F, title="Density-approxmative Discretization",
  rename.level=F, return.all=T, cluster=F, seed=NULL)

```

Arguments

data	a vector containing the data that may be discretized
graph	a boolean value, if TRUE, the density and the determined binning are plotted
title	a title for the plot
rename.level	a boolean value, if TRUE, factor levels are replaced by integers 1:n
return.all	a boolean value, if FALSE, only the discretized data are returned.
cluster	a boolean value, if data is a cluster variable and may already be discrete or not
seed	a random seed number

Value

discretized	the discretized data
levels	the factor levels
optima	the x and y coordinates of the determined peaks

Author(s)

Ann-Kristin Becker

Examples

```
testdata = c(rnorm(100,-3,1), rnorm(100,3,1))
d<-discretize.dens(testdata, graph=TRUE)
summary(d$discretized)
```

groupbn

groupbn

Description

creates groupbn object (determines an initial clustering based on a hierarchy with target variable and 'separated' variables separated, learns a Bayesian network from grouped data and saves discretization and pca parameters)

Usage

```
groupbn(hierarchy, k, target, separate=NULL, separate.as.roots=FALSE,
X.quantitative=NULL, X.qualitative=NULL, struct.alg="hc", boot=TRUE,
discretize=TRUE, arc.thresh=NULL,
debug=FALSE, R=100, seed=NULL)
```

Arguments

hierarchy	a cluster object from ClustOfVar.
k	a positive integer number, the number of initial clusters.
target	a string, the name of the target variable.
separate	a vector of strings, names of variables that should be separated from the groups, such as age, sex,...
separate.as.roots	a boolean; if TRUE separated variables are used as roots in the network. Can be ignored if separate is empty.
X.quantitative	a numeric matrix of data, or an object that can be coerced to such a matrix (such as a numeric vector or a data frame with all numeric columns).
X.qualitative	a categorical matrix of data, or an object that can be coerced to such a matrix (such as a character vector, a factor or a data frame with all factor columns).

struct.alg	structure learning algorithm according to bnlearn
arc.thresh	threshold for bootstrap arcs
discretize	a boolean, if a network variables should be discretized before network learning
boot	boolean, if TRUE, a bootstrap based network averaging approach is used
debug	a boolean, if TRUE, debugging messages are printed
R	number of bootstrap replicates for model averaging, default is 100
seed	a random seed number

Value

an object of class groupbn

bn	a Bayesian Network structure of bn class from bnlearn.
fit	a Bayesian Network with fitted parameters of bn.fit class from bnlearn.
X.quant i	a data.frame containing only the quantitative variables.
X.qual i	a data.frame containing only the qualitative variables.
grouping	a vector of positive integers, giving the cluster assignment.
k	the number of clusters.
group.data	a data.frame containing the cluster representants.
target	a string, the name of the target variable.
separate	a vector of strings, names of variables that should be separated from the groups.
pca.param	the PCAmix used to determine the cluster representants.
disc.param	the cutpoints used to discretize the cluster representants.
score	Different prediction scores for the target variable using the fitted network.

Author(s)

Ann-Kristin Becker

References

Becker A-K, Dörr M, Felix SB, Frost F, Grabe HJ, Lerch MM, et al. (2021) From heterogeneous healthcare data to disease-specific biomarker networks: A hierarchical Bayesian network approach. PLoS Comput Biol 17(2): e1008735. <https://doi.org/10.1371/journal.pcbi.1008735>

See Also

[groupbn_refinement](#)

Examples

```
#load example data
data(wine)
wine.test<-wine[wine$Soil%in%c("Reference", "Env1"),1:29]
wine.test$Soil<-factor(wine.test$Soil)
levels(wine.test$Soil)<-c("0", "1")

#cluster data
hierarchy<-hclustvar(X.quanti=wine.test[,3:29], X.quali=wine.test[,1:2])

#Learn group network among 5 clusters with "Soil" as target variable
wine.groupbn<-groupbn(hierarchy, k=5, target="Soil", separate=NULL,
X.quanti=wine.test[,3:29], X.quali=wine.test[,1:2], seed=321)

#Plot network
plot(wine.groupbn)
```

groupbn.output.table *groupbn.output.table*

Description

Create an output table with clusters and included variables with similarity scores

Usage

```
groupbn.output.table(res, with.scores=TRUE)
```

Arguments

res	gn object
with.scores	if TRUE, similarity scores of every cluster member to the cluster center are added to the table

Value

a table with one column per group, similarity scores to cluster centers are calculated for each variable

Author(s)

Ann-Kristin Becker

See Also

[groupbn](#) [groupbn_refinement](#)

Examples

```
data("wine.groupbn.refined")
df<-groupbn.output.table(wine.groupbn.refined)
```

`groupbn.vis.html.plot` *groupbn.vis.html.plot*

Description

Create an interactive html network object with visNet (displaying similarity scores and number of variables in a score)

Usage

```
groupbn.vis.html.plot(res, df=NULL, save.file=TRUE, save.name=NULL,
  hierarchical=FALSE, nodecolor.all="#E0F3F8",
  nodecolor.special="cornflowerblue", main=NULL)
```

Arguments

<code>res</code>	a groupbn object
<code>df</code>	output from output.table if already calculated, otherwise the same table is calculated internally
<code>save.file</code>	boolean; if TRUE a html file is produced
<code>save.name</code>	name for saving html object, date is additionally used
<code>hierarchical</code>	boolean; if TRUE the network is plotted with a hierarchical layout
<code>nodecolor.all</code>	a color for "normal" nodes
<code>nodecolor.special</code>	a color for the target variable and all separated nodes, if any.
<code>main</code>	optionally a title for the plot

Details

Plots an interactive network plot using visNetwork package

Value

an html widget of class visNetwork

Author(s)

Ann-Kristin Becker

See Also

[groupbn.refinement](#)

Examples

```
data("wine.groupbn.refined")
groupbn.vis.html.plot(wine.groupbn.refined, hierarchical=TRUE, save.file=FALSE)
```

groupbn_refinement *groupbn_refinement*

Description

Adaptive Refinement of a group Bayesian Network using hierarchical Clustering

Usage

```
groupbn_refinement(res, hierarchy, refinement.part="mb", restart=0, perturb=1,
max.step=10, max.min=Inf, R=100,
return.all=FALSE, arc.thresh=NULL, debug=FALSE, seed=NULL)
```

Arguments

res	an object of class groupbn
hierarchy	a cluster object from ClustOfVar
refinement.part	"mb", "mb2", "arc.confid" or "all", selects if the refinement steps should be done only within the markov blanket of the target variable (mb), within the second-order markov blanket (mb2), in all clusters with an arcconfidence to target >0 (arc.confid) or within all clusters (all). Default: "mb"
restart	a positive integer number, the number of restarts
perturb	a positive integer number, the number of perturbations (splits) in each restart
max.step	a positive integer number, the maximal number of refinement steps, default is 10
max.min	a positive integer number, the maximal run time in minutes, default is unlimited
R	number of bootstrap replicates for model averaging, default is 100
return.all	a boolean, if TRUE, the output is a whole list of group models, if FALSE, the output is only the best-scoring model.
arc.thresh	threshold for bootstrap arcs
debug	a boolean, if TRUE, debugging messages are printed
seed	a random seed number

Details

Based on a variable grouping, data are aggregated and a Bayesian network is learned. The target variable is kept separated during this procedure, so that the resulting network model can be used for risk prediction and classification. Starting from a coarse group network, groups are iteratively refined to smaller groups. The heuristic refinement happens downwards along the dendrogram, and stops, if it no longer improves the predictive performance of the model. The refinement part is implemented using a hill-climbing procedure.

Value

returns an object of class groupbn

Author(s)

Ann-Kristin Becker

References

Becker A-K, Dörr M, Felix SB, Frost F, Grabe HJ, Lerch MM, et al. (2021) From heterogeneous healthcare data to disease-specific biomarker networks: A hierarchical Bayesian network approach. PLoS Comput Biol 17(2): e1008735. <https://doi.org/10.1371/journal.pcbi.1008735>

See Also

[groupbn](#) [groupbn.output.table](#)

Examples

```
#load example data
data(wine)
wine.test<-wine[wine$Soil%in%c("Reference", "Env1"),1:29]
wine.test$Soil<-factor(wine.test$Soil)
levels(wine.test$Soil)<-c("0", "1")

#cluster data
hierarchy<-hclustvar(X.quanti=wine.test[,3:29], X.quali=wine.test[,1:2])

#Learn group network among 5 clusters with "Soil" as target variable
wine.groupbn<-groupbn(hierarchy, k=5, target="Soil", separate=NULL,
X.quanti=wine.test[,3:29], X.quali=wine.test[,1:2], seed=321)

#Do one refinement step
#Set max.step higher to optimize completely
wine.groupbn.refined<-groupbn_refinement(wine.groupbn, hierarchy,
refinement.part="mb", max.step = 1, seed=321)

#Plot refined network
plot(wine.groupbn.refined)
```

groupbn_refine_manually

groupbn_refine_manually

Description

Based on a GroupBN, a cluster can be selected manually, that is split and the refined model is learned.

Usage

```
groupbn_refine_manually(res, hierarchy, refine, arc.thresh=NULL,  
R=100, debug=FALSE, seed=NULL)
```

Arguments

res	an object of class groupbn
hierarchy	a cluster object from ClustOfVar
refine	name of group to be refined
arc.thresh	threshold for bootstrap arcs
R	number of bootstrap replicates for model averaging, default is 100
debug	a boolean, if TRUE, debugging messages are printed
seed	a random seed number

Value

returns an object of class groupbn

Author(s)

Ann-Kristin Becker

Examples

```
#load example data  
data(wine)  
wine.test<-wine[wine$Soil%in%c("Reference", "Env1"),1:29]  
wine.test$Soil<-factor(wine.test$Soil)  
levels(wine.test$Soil)<-c("0", "1")  
  
#cluster data  
hierarchy<-hclustvar(X.quanti=wine.test[,3:29], X.quali=wine.test[,1:2])  
  
#Learn group network among 5 clusters with "Soil" as target variable  
wine.groupbn<-groupbn(hierarchy, k=5, target="Soil", separate=NULL,  
X.quanti=wine.test[,3:29], X.quali=wine.test[,1:2], seed=321)  
  
#Refine cluster 2  
wine.groupbn.refined<-groupbn_refine_manually(wine.groupbn, hierarchy,  
refine = "cl2", seed=321)  
  
#Plot refined network  
plot(wine.groupbn.refined)
```

is.groupbn *is.groupbn*

Description

Generic function for groupbn objects

Usage

`is.groupbn(x)`

Arguments

`x` an object of class groupbn

Value

A boolean; TRUE if `x` is of class groupbn, FALSE otherwise.

Author(s)

Ann-Kristin Becker

See Also

[groupbn](#)

Examples

```
data("wine.groupbn.refined")
is.groupbn(wine.groupbn.refined)
```

plot.groupbn *plot.groupbn*

Description

generic plot function for class groupbn

Usage

```
## S3 method for class 'groupbn'
plot(x, ...)
```


<code>new.fit</code>	a boolean; if TRUE, the parameters are newly fit using the test data.
<code>debug</code>	a boolean, if TRUE, debugging messages are printed
<code>...</code>	further arguments

Value

Returns a dataframe with a column of predictions and a column of the target data. If the target is discrete, class probabilities are returned. Otherwise continuous scores are returned. If `return.data` is TRUE, additionally the transformed group data are returned.

Author(s)

Ann-Kristin Becker

Examples

```
#load example data
data(wine)
wine.test<-wine[wine$Soil%in%c("Reference", "Env1"),1:29]
wine.test$Soil<-factor(wine.test$Soil)
levels(wine.test$Soil)<-c("0", "1")

data(wine.groupbn.refined)
predict(wine.groupbn.refined, X.quanti=wine.test[,3:29], X.quali=wine.test[,1:2])
```

<code>print.groupbn</code>	<i>print.groupbn</i>
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Description

This is a method for the function `print` for objects of the class `groupbn`.

Usage

```
## S3 method for class 'groupbn'
print(x, ...)
```

Arguments

<code>x</code>	An object of class <code>groupbn</code> generated by the functions <code>groupbn</code> or <code>groupbn_refinement</code>
<code>...</code>	further arguments

Value

No return value, prints a description of the object

Author(s)

Ann-Kristin Becker

See Also[groupbn](#)**Examples**

```
data("wine.groupbn.refined")
print(wine.groupbn.refined)
```

```
wine.groupbn.refined  wine.groupbn.refined
```

Description

A refined group Bayesian network with 8 groups learned from dataset 'wine'.

Usage

```
data("wine.groupbn.refined")
```

Format

```
group Bayesian network (class 'groupbn')
```

name of target variable: Soil number of groups: 8 achieved scoring: F1: 0.92 ; Precision: 1 ; Recall: 0.86 ; AUC-PR: 1 ; AUC-ROC: 1 ; cross-entr.: 1.43; BIC (netw.): -77.21

name description "\$bn" "Bayesian network structure" "\$fit" "fitted Bayesian network (multinomial)" "\$arc.confid" "arc confidence" "\$X.quali" "qualitative variables in a data.frame" "\$X.quant" "quantitative variables in a data.frame" "\$grouping" "group memberships" "\$k" "number of groups of initial grouping" "\$group.data" "group representatives used for network inference" "\$target" "name of target variable" "\$separate" "name of any other separated variables" "\$pca.param" "pca parameters of each group" "\$disc.param" "discretization intervals of each group" "\$score" "cross entropy and additional scoring information"

Examples

```
data(wine.groupbn.refined)
```

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