# Package 'FRESA.CAD'

# November 27, 2018

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Author Jose Gerardo Tamez-Pena, Antonio Martinez-Torteya and Israel Alanis
Maintainer Jose Gerardo Tamez-Pena <jose.tamezpena@tec.mx></jose.tamezpena@tec.mx>
<b>Description</b> Contains a set of utilities for building and testing statistical models (linear, logistic,ordinal or COX) for Computer Aided Diagnosis/Prognosis applications. Utilities include data adjustment, univariate analysis, model building, model-validation, longitudinal analysis, reporting and visualization.
License LGPL (>= 2)
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# **Description**

Contains a set of utilities for building and testing formula-based models for Computer Aided Diagnosis/prognosis applications via feature selection. Bootstrapped Stage Wise Model Selection (B:SWiMS) controls the false selection (FS) for linear, logistic, or Cox proportional hazards regression models. Utilities include functions for: univariate/longitudinal analysis, data conditioning (i.e. covariate adjustment and normalization), model validation and visualization.

#### **Details**

Package: FRESA.CAD
Type: Package
Version: 3.1.0
Date: 2018-10-30
License: LGPL (>= 2)

Purpose: The design of diagnostic or prognostic multivariate models via the selection of significantly discriminant features. The models are selected via the bootstrapped step-wise selection of model features that offer a significant improvement in subject classification/error. The false selection control is achieved by train-test partitions, where train sets are used to select variables and test sets used to evaluate model performance. Variables that do not improve subject classification/error on the blind test are not included in the models. The main function of this package is the selection and cross-validation of diagnostic/prognostic linear, logistic, or Cox proportional hazards regression model constructed from a large set of candidate features. The variable selection may start by conditioning all variables via a covariate-adjustment and a z-inverse-rank-transformation. In order to integrate features with partial discriminant power, the package can be used to categorize the continuous variables and rank their discriminant power. Once ranked, each feature is bootstrap-tested in a multivariate model, and its blind performance is evaluated. Variables with a statistical significant improvement in classification/error are stored and finally inserted into the final model according to their relative store frequency. A cross-validation procedure may be used to diagnose the amount of model shrinkage produced by the selection scheme.

#### Author(s)

Jose Gerardo Tamez-Pena, Antonio Martinez-Torteya and Israel Alanis Maintainer: <jose.tamezpena@tec.mx>

#### References

Pencina, M. J., D'Agostino, R. B., & Vasan, R. S. (2008). Evaluating the added predictive ability of a new marker: from area under the ROC curve to reclassification and beyond. *Statistics in medicine* **27**(2), 157-172.

#### **Examples**

```
## Not run:
### Fresa Package Examples ####
library("epiR")
library("FRESA.CAD")
library(network)
library(GGally)
library("e1071")
# Start the graphics device driver to save all plots in a pdf format
pdf(file = "Fresa.Package.Example.pdf",width = 8, height = 6)
# Get the stage C prostate cancer data from the rpart package
data(stagec,package = "rpart")
options(na.action = 'na.pass')
dataCancer <- cbind(pgstat = stagec$pgstat,</pre>
                    pgtime = stagec$pgtime,
                    as.data.frame(model.matrix(Surv(pgtime,pgstat) ~ .,stagec))[-1])
#Impute missing values
dataCancerImputed <- nearestNeighborImpute(dataCancer)</pre>
# Remove the incomplete cases
dataCancer <- dataCancer[complete.cases(dataCancer),]</pre>
# Load a pre-stablished data frame with the names and descriptions of all variables
data(cancerVarNames)
# the Heat Map
hm <- heatMaps(cancerVarNames, varRank=NULL, Outcome="pgstat",</pre>
               data=dataCancer,title="Heat Map",hCluster=FALSE
               ,prediction=NULL,Scale=TRUE,
               theFiveColors=c("blue","cyan","black","yellow","red"),
               outcomeColors =
                 c("blue","lightgreen","yellow","orangered","red"),
               transpose=FALSE,cexRow=0.50,cexCol=0.80,srtCol=35)
# The univariate analysis
UniRankFeaturesRaw <- univariateRankVariables(variableList = cancerVarNames,</pre>
                                               formula = "pgstat ~ 1+pgtime",
                                               Outcome = "pgstat",
                                               data = dataCancer,
                                               categorizationType = "Raw",
```

```
rankingTest = "zIDI",
                                                description = "Description",
                                                uniType="Binary")
print(UniRankFeaturesRaw)
# A simple BSIWMS Model
BSWiMSModel <- BSWiMS.model(formula = Surv(pgtime, pgstat) ~ 1, dataCancerImputed)
# The Log-Rank Analysis using survdiff
lrsurvdiff <- survdiff(Surv(pgtime,pgstat)~</pre>
               BSWiMSModel$BSWiMS.model$back.model$linear.predictors > 0,
               data=dataCancerImputed)
# The Log-Rank Analysis EmpiricalSurvDiff and permutations of the null Chi distribution
lrp <- EmpiricalSurvDiff(dataCancerImputed$pgtime,dataCancerImputed$pgstat,</pre>
                          BSWiMSModel$BSWiMS.model$back.model$linear.predictors > 0,
                          type="Chi",plots=TRUE,samples=10000)
\hbox{\tt\# The Log-Rank Analysis Empirical Surv Diff and permutations of the null SLR distribution}\\
lrp <- EmpiricalSurvDiff(dataCancerImputed$pgtime,dataCancerImputed$pgstat,</pre>
                          BSWiMSModel$BSWiMS.model$back.model$linear.predictors > 0,
                          type="SLR",plots=TRUE,samples=10000)
# The Log-Rank Analysis EmpiricalSurvDiff and bootstrapping the SLR distribution
lrp <- EmpiricalSurvDiff(dataCancerImputed$pgtime,dataCancerImputed$pgstat,</pre>
                          BSWiMSModel$BSWiMS.model$back.model$linear.predictors > 0,
                          computeDist=TRUE,plots=TRUE)
#The performance of the final model using the summary function
sm <- summary(BSWiMSModel$BSWiMS.model$back.model)</pre>
print(sm$coefficients)
pv <- plot(sm$bootstrap)</pre>
# The equivalent model
eq <- reportEquivalentVariables(BSWiMSModel$BSWiMS.model$back.model,data=dataCancer,</pre>
                                  variableList=cancerVarNames,Outcome = "pgstat",
                                  timeOutcome="pgtime",
                                  type = "COX");
print(eq$equivalentMatrix)
#The list of all models of the bootstrap forward selection
print(BSWiMSModel$forward.selection.list)
#With FRESA.CAD we can do a leave-one-out using the list of models
pm <- ensemblePredict(BSWiMSModel$forward.selection.list,</pre>
                     dataCancer,predictType = "linear",type="LOGIT",Outcome="pgstat")
#Ploting the ROC with 95
```

type = "LOGIT",

```
pm <- plotModels.ROC(cbind(dataCancer$pgstat,</pre>
                     pm$ensemblePredict),main=("LOO Forward Selection Median Predict"))
#The plotModels.ROC provides the diagnosis confusion matrix.
summary(epi.tests(pm$predictionTable))
#FRESA.CAD can be used to create a bagged model using the forward selection formulas
bagging <- baggedModel(BSWiMSModel$forward.selection.list,dataCancer,useFreq=32)</pre>
pm <- predict(bagging$bagged.model)</pre>
pm <- plotModels.ROC(cbind(dataCancer$pgstat,pm),main=("Bagged"))</pre>
#Let's check the performance of the model
sm <- summary(bagging$bagged.model)</pre>
print(sm$coefficients)
#Using bootstrapping object I can check the Jaccard Index
print(bagging$Jaccard.SM)
#Ploting the evolution of the coefficient value
plot(bagging$coefEvolution$grade,main="Evolution of grade")
gplots::heatmap.2(bagging$formulaNetwork,trace="none",
                  mar=c(10,10),main="eB:SWIMS Formula Network")
barplot(bagging$frequencyTable,las = 2,cex.axis=1.0,
        cex.names=0.75,main="Feature Frequency")
n <- network::network(bagging$formulaNetwork, directed = FALSE,</pre>
                       ignore.eval = FALSE,names.eval = "weights")
ggnet2(n, label = TRUE, size = "degree", size.cut = 3, size.min = 1,
       mode = "circle",edge.label = "weights",edge.label.size=4)
# Get a Cox proportional hazards model using:
# - The default parameters
mdCOXs <- FRESA.Model(formula = Surv(pgtime, pgstat) ~ 1,data = dataCancer)</pre>
sm <- summary(mdCOXs$BSWiMS.model)</pre>
print(sm$coefficients)
# The model with singificant improvement in the residual error
mdCOXs <- FRESA.Model(formula = Surv(pgtime, pgstat) ~ 1,</pre>
                       data = dataCancer,OptType = "Residual" )
sm <- summary(mdCOXs$BSWiMS.model)</pre>
print(sm$coefficients)
# Get a Cox proportional hazards model using second order models:
mdCOX <- FRESA.Model(formula = Surv(pgtime, pgstat) ~ 1,</pre>
                      data = dataCancer,categorizationType="RawRaw")
sm <- summary(mdCOX$BSWiMS.model)</pre>
print(sm$coefficients)
```

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```

```
namesc <- names(mdCOX$BSWiMS.model$coefficients)[-1]</pre>
hm <- heatMaps(mdCOX$univariateAnalysis[namesc,],varRank=NULL,</pre>
                Outcome="pgstat",data=dataCancer,
                title="Heat Map", hCluster=FALSE, prediction=NULL, Scale=TRUE,
                theFiveColors=c("blue","cyan","black","yellow","red"),
                outcomeColors = c("blue", "lightgreen", "yellow", "orangered", "red"),
                transpose=FALSE,cexRow=0.50,cexCol=0.80,srtCol=35)
# The LOO estimation
pm <- ensemblePredict(mdCOX$BSWiMS.models$formula.list,dataCancer,</pre>
                        predictType = "linear",type="LOGIT",Outcome="pgstat")
pm <- plotModels.ROC(cbind(dataCancer$pgstat,pm$ensemblePredict),main=("LOO Median Predict"))</pre>
#Let us check the diagnosis performance
summary(epi.tests(pm$predictionTable))
# Get a Logistic model using FRESA.Model
# - The default parameters
dataCancer2 <-dataCancer</pre>
dataCancer2$pgtime <-NULL
mdLOGIT <- FRESA.Model(formula = pgstat ~ 1,data = dataCancer2)</pre>
if (!is.null(mdLOGIT$bootstrappedModel)) pv <- plot(mdLOGIT$bootstrappedModel)</pre>
sm <- summary(mdLOGIT$BSWiMS.model)</pre>
print(sm$coefficients)
## FRESA.Model with Cross Validation and Recursive Partitioning and Regression Trees
md <- FRESA.Model(formula = Surv(pgtime, pgstat) ~ 1,data = dataCancer,</pre>
                   CVfolds = 10,repeats = 5,equivalent = TRUE,usrFitFun=rpart::rpart)
colnames(md$cvObject$Models.testPrediction)
pm <- plotModels.ROC(md$cv0bject$LASSO.testPredictions,theCVfolds=10,main="CV LASSO",cex=0.90)
pm <- plotModels.ROC(md$cv0bject$KNN.testPrediction,theCVfolds=10,main="KNN",cex=0.90)</pre>
pm <- plotModels.ROC(md$cvObject$Models.testPrediction,theCVfolds=10,</pre>
                       predictor="Prediction", main="B:SWiMS Bagging", cex=0.90)
pm <- plotModels.ROC(md$cvObject$Models.testPrediction,theCVfolds=10,</pre>
                       predictor="Ensemble.B.SWiMS"
                       ,main="Forward Selection Median Ensemble",cex=0.90)
pm <- plotModels.ROC(md$cvObject$Models.testPrediction,theCVfolds=10,</pre>
                 predictor="Ensemble.Forward",main="Forward Selection Bagging",cex=0.90)
pm <- plotModels.ROC(md$cvObject$Models.testPrediction,theCVfolds=10,</pre>
                       predictor="eB.SWiMS",main="Equivalent Model",cex=0.90)
pm <- plotModels.ROC(md$cvObject$Models.testPrediction,theCVfolds=10,</pre>
                 predictor="Forward.Selection.Bagged",main="The Forward Bagging",cex=0.90)
pm <- plotModels.ROC(md$cvObject$Models.testPrediction,theCVfolds=20,</pre>
                      predictor="usrFitFunction",
                      main="Recursive Partitioning and Regression Trees",cex=0.90)
pm <- plotModels.ROC(md$cvObject$Models.testPrediction,theCVfolds=20,</pre>
                       predictor="usrFitFunction_Sel",
                  main="Recursive Partitioning and Regression Trees with FS",cex=0.90)
```

```
## FRESA.Model with Cross Validation, LOGISTIC and Support Vector Machine
   md <- FRESA.Model(formula = pgstat ~ 1,data = dataCancer2,</pre>
                      CVfolds = 10,repeats = 5,equivalent = TRUE,usrFitFun=svm)
   pm <- plotModels.ROC(md$cv0bject$LASSO.testPredictions,theCVfolds=10,main="CV LASSO",cex=0.90)
   pm <- plotModels.ROC(md$cvObject$KNN.testPrediction,theCVfolds=10,main="KNN",cex=0.90)
   pm <- plotModels.ROC(md$cvObject$Models.testPrediction,theCVfolds=10,</pre>
                         predictor="Prediction", main="B:SWiMS Bagging", cex=0.90)
   md$cvObject$Models.testPrediction[,"usrFitFunction"] <-</pre>
                      md$cvObject$Models.testPrediction[,"usrFitFunction"] - 0.5
   md$cvObject$Models.testPrediction[,"usrFitFunction_Sel"] <-</pre>
                      md$cvObject$Models.testPrediction[,"usrFitFunction_Sel"] - 0.5
   pm <- plotModels.ROC(md$cvObject$Models.testPrediction,theCVfolds=10,</pre>
                         predictor="usrFitFunction",
                         main="SVM", cex = 0.90)
   pm <- plotModels.ROC(md$cvObject$Models.testPrediction,theCVfolds=10,</pre>
                         predictor="usrFitFunction_Sel",
                         main="SVM with FS", cex = 0.90)
    # Shut down the graphics device driver
   dev.off()
## End(Not run)
```

backVarElimination\_Bin

IDI/NRI-based backwards variable elimination

# **Description**

This function removes model terms that do not significantly affect the integrated discrimination improvement (IDI) or the net reclassification improvement (NRI) of the model.

## Usage

#### **Arguments**

object An object of class 1m, g1m, or coxph containing the model to be analyzed The maximum p-value, associated to either IDI or NRI, allowed for a term in pvalue

the model

Outcome The name of the column in data that stores the variable to be predicted by the

model

data A data frame where all variables are stored in different columns

startOffset Only terms whose position in the model is larger than the startOffset are

candidates to be removed

Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX") type selectionType

The type of index to be evaluated by the improveProb function (Hmisc pack-

age): z-score of IDI or of NRI

#### **Details**

For each model term  $x_i$ , the IDI or NRI is computed for the Full model and the reduced model( where the term  $x_i$  removed). The term whose removal results in the smallest drop in improvement is selected. The hypothesis: the term adds classification improvement is tested by checking the pvalue of improvement. If p(IDIorNRI) > pvalue, then the term is removed. In other words, only model terms that significantly aid in subject classification are kept. The procedure is repeated until no term fulfils the removal criterion.

## Value

back.model An object of the same class as object containing the reduced model

loops The number of loops it took for the model to stabilize

reclas.info A list with the NRI and IDI statistics of the reduced model, as given by the

getVar.Bin function

An object of class formula with the formula used to fit the reduced model back.formula The name of the last term that was removed (-1 if all terms were removed) lastRemoved

at.opt.model the model before the BH procedure

beforeFSC.formula

the string formula of the model before the BH procedure

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

#### References

Pencina, M. J., D'Agostino, R. B., & Vasan, R. S. (2008). Evaluating the added predictive ability of a new marker: from area under the ROC curve to reclassification and beyond. Statistics in medicine **27**(2), 157-172.

#### See Also

backVarElimination\_Res, bootstrapVarElimination\_Bin, bootstrapVarElimination\_Res

backVarElimination\_Res

NeRI-based backwards variable elimination

# **Description**

This function removes model terms that do not significantly improve the "net residual" (NeRI)

#### **Usage**

## **Arguments**

object	An object of class 1m, g1m, or coxph containing the model to be analyzed
pvalue	The maximum p-value, associated to the NeRI, allowed for a term in the model
Outcome	The name of the column in data that stores the variable to be predicted by the model
data	A data frame where all variables are stored in different columns
startOffset	Only terms whose position in the model is larger than the startOffset are candidates to be removed
type	Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")
testType	Type of non-parametric test to be evaluated by the improvedResiduals function: Binomial test ("Binomial"), Wilcoxon rank-sum test ("Wilcox"), Student's <i>t</i> -test ("tStudent"), or <i>F</i> -test ("Ftest")
setIntersect	The intersect of the model (To force a zero intersect, set this value to 0)

## **Details**

For each model term  $x_i$ , the residuals are computed for the Full model and the reduced model (where the term  $x_i$  removed). The term whose removal results in the smallest drop in residuals improvement is selected. The hypothesis: the term improves residuals is tested by checking the pvalue of improvement. If p(residualsbetterthanreducedresiduals) > pvalue, then the term is removed. In other words, only model terms that significantly aid in improving residuals are kept. The procedure is repeated until no term fulfils the removal criterion. The p-values of improvement can be computed via a sign-test (Binomial) a paired Wilcoxon test, paired t-test or f-test. The first three tests compare the absolute values of the residuals, while the f-test test if the variance of the residuals is improved significantly.

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# Value

back.model	An object of the same class as object containing the reduced model
loops	The number of loops it took for the model to stabilize
reclas.info	A list with the NeRI statistics of the reduced model, as given by the ${\tt getVar}$ . Res function
back.formula	An object of class formula with the formula used to fit the reduced model
lastRemoved	The name of the last term that was removed (-1 if all terms were removed)
at.opt.model	the model with before the FSR procedure.
beforeFSC.formu	ula
	the string formula of the the FSR procedure

# Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

## See Also

backVarElimination\_Bin, bootstrapVarElimination\_Bin bootstrapVarElimination\_Res

baggedModel	Get the bagged model from a list of models	
-------------	--	--

# Description

This function will take the frequency-ranked of variables and the list of models to create a single bagged model

# Usage

12 baggedModel

# **Arguments**

modelFormulas The name of the column in data that stores the variable to be predicted by the

model

data A data frame with two columns. The first one must have the names of the can-

didate variables and the other one the description of such variables

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")

Outcome The name of the column in data that stores the time to outcome

timeOutcome The name of the column in data that stores the time to event (needed only for a

Cox proportional hazards regression model fitting)

frequencyThreshold

set the frequency the threshold of the frequency of features to be included in the

model)

univariate The FFRESA.CAD univariate analysis matrix

useFreq Use the feature frequency to order the formula terms. If set to a positive value is

the number of estimation loops

n\_bootstrap if greater than 1, defines the number of bootstraps samples to be used

#### Value

bagged.model the bagged model

formula the formula of the model

frequencyTable the table of variables ranked by their model frequency

faverageSize the average size of the models

formulaNetwork The matrix of interaction between formulas

Jaccard Stability Measure of the formulas

coefEvolution The evolution of the coefficients

avgZvalues The average Z value of each coefficient

featureLocation

The average location of the feature in the formulas

# Author(s)

Jose G. Tamez-Pena

#### See Also

ensemblePredict

barPlotCiError 13

## **Description**

Ranked Plot a set of measurements with error bars or confidence intervals (CI)

# Usage

# **Arguments**

ciTable A matrix with three columns: the value, the low CI value and the high CI value

metricname The name of the plotted values

thesets A character vector with the names of the sets
themethod A character vector with the names of the methods

main The plot title

angle The angle of the x labels offsets The offset of the x-labels

scoreDirection Indicates how to aggregate the supMethod score and the ingMethod score.

ho the null hypothesis

... Extra parametrs pased to the barplot function

## Value

barplot the x-location of the bars

ciTable the ordered matrix with the 95 CI

barMatrix the mean values of the bars

supMethod A superiority score equal to the numbers of methods that were inferior infMethod A inferiority score equal to the number of methods that were superior

interMethodScore

the sum of supMethod and infMethod defined by the score direction.

# Author(s)

Jose G. Tamez-Pena

benchmarking

Compare performance of different model fitting/filtering algorithms

## **Description**

Evaluates a data set with a set of fitting/filtering methods and returns the observed cross-validation performance

# Usage

# **Arguments**

theData The data frame
theOutcome The outcome feature

reps The number of times that the random cross-validation will be performed

trainFraction The fraction of the data used for training.

referenceCV A user supplied random cross-validation object to be benchmarked referenceName The name of the reference classifier to be used in the reporting tables referenceFilterName

The name of the reference filter to be used in the reporting tables

#### **Details**

The benchmark functions provide the performance of different classification algorithms (Binary-Benchmark), registration algorithms (RegresionBenchmark) or ordinal regression algorithms (OrdinalBenchmark) The evaluation method is based on applying the random cross-validation method (randomCV) that randomly splits the data into train and test sets. The user can provide a Cross validated object that will define the train-test partitions.

The BinaryBenchmark compares: BSWiMS,Random Forest ,RPART,LASSO,SVM/mRMR,KNN and the ensemble of them in their ability to correctly classify the test data. Furthermore, it evaluates the ability of the following feature selection algorithms: BSWiMS or ReferenceCV, LASSO, RPART, RF/BSWiMS, IDI, NRI, t-test, Wilcoxon, Kendall, and mRMR in their ability to select the best set of features for the following classification methods: SVM, KNN, Naive Bayes, Random Forest Nearest Centroid (NC) with root sum square (RSS), and NC with Spearman correlation

The RegresionBenchmark compares: BSWiMS,Random Forest ,RPART,LASSO,SVM/mRMR and the ensemble of them in their ability to correctly predict the test data. Furthermore, it evaluates the ability of the following feature selection algorithms: BSWiMS or referenceCV, LASSO, RPART, RF/BSWiMS, F-Test, W-Test, Pearson Kendall, and mRMR in their ability to select the best set of features for the following regression methods: Linear Regression, Robust Regression, Ridge Regression, LASSO, SVM, and Random Forest.

The OrdinalBenchmark compares: BSWiMS,Random Forest ,RPART,LASSO,KNN ,SVM and the ensemble of them in their ability to correctly predict the test data. Furthermore, it evaluates the ability of the following feature selection algorithms: BSWiMS or referenceCV, LASSO, RPART, RF/BSWiMS, F-Test, Kendall, and mRMR in their ability to select the best set of features for the following regression methods: Ordinal, KNN, SVM, Random Forest, and Naive Bayes.

#### Value

errorciTable the matrix of the balanced error with the 95 CI

accciTable the matrix of the classification accuracy with the 95 CI

aucTable the matrix of the ROC AUC with the 95 CI senTable the matrix of the sensitivity with the 95 CI speTable the matrix of the specificity with the 95 CI

errorciTable\_filter

the matrix of the balanced error with the 95 CI for filter methods

accciTable\_filter

the matrix of the classification accuracy with the 95 CI for filter methods

senciTable\_filter

the matrix of the classification sensitivity with the 95 CI for filter methods

speciTable\_filter

the matrix of the classification specificity with the 95 CI for filter methods

aucTable\_filter

the matrix of the ROC AUC with the 95 CI for filter methods

CorTable the matrix of the Pearson correlation with the 95 CI

RMSETable the matrix of the root mean square error (RMSE) with the 95 CI

BiasTable the matrix of the prediction bias with the 95 CI

CorTable\_filter

the matrix of the Pearson correlation with the 95 CI for filter methods

RMSETable\_filter

the matrix of the root mean square error (RMSE) with the 95 CI for filter meth-

ods

BiasTable\_filter

the matrix of the prediction bias with the 95 CI for filter methods

BMAETable the matrix of the balanced mean absolute error (MEA) with the 95 CI for filter

methods

KappaTable the matrix of the Kappa value with the 95 CI

BiasTable the matrix of the prediction Bias with the 95 CI

KendallTable the matrix of the Kendall correlation with the 95 CI

MAETable\_filter

the matrix of the mean absolute error (MEA) with the 95 CI for filter methods

KappaTable\_filter

the matrix of the Kappa value with the 95 CI for filter methods

BiasTable\_filter

the matrix of the prediction Bias with the 95 CI for filter methods

KendallTable\_filter

the matrix of the Kendall correlation with the 95 CI for filter methods

times The average CPU time used by the method

jaccard\_filter The average Jaccard Index of the feature selection methods

TheCVEvaluations

The output of the randomCV (randomCV) evaluations of the different methods

testPredictions

A matrix with all the test predictions

featureSelectionFrequency

The frequency of feature selection

cpuElapsedTimes

The mean elapsed times

cpuElapsedTimes

#### Author(s)

Jose G. Tamez-Pena

## See Also

randomCV

## **Examples**

```
### Not run:
### Binary Classification Example ####
# Start the graphics device driver to save all plots in a pdf format
pdf(file = "BinaryClassificationExample.pdf",width = 8, height = 6)
# Get the stage C prostate cancer data from the rpart package

data(stagec,package = "rpart")

# Prepare the data. Create a model matrix without the event time
stagec$pgtime <- NULL
stagec$eet <- as.factor(stagec$eet)</pre>
```

```
options(na.action = 'na.pass')
stagec_mat <- cbind(pgstat = stagec$pgstat,</pre>
as.data.frame(model.matrix(pgstat ~ .,stagec))[-1])
# Impute the missing data
        dataCancerImputed <- nearestNeighborImpute(stagec_mat)</pre>
      dataCancerImputed[,1:ncol(dataCancerImputed)] <- sapply(dataCancerImputed,as.numeric)</pre>
# Cross validating a LDA classifier.
# 80
cv <- randomCV(dataCancerImputed, "pgstat", MASS::lda, trainFraction = 0.8,</pre>
repetitions = 10,featureSelectionFunction = univariate_tstudent,
featureSelection.control = list(limit = 0.5,thr = 0.975));
# Compare the LDA classifier with other methods
cp <- BinaryBenchmark(referenceCV = cv,referenceName = "LDA",</pre>
                      referenceFilterName="t.Student")
pl <- plot(cp,prefix = "StageC: ")</pre>
# Default Benchmark classifiers method (BSWiMS) and filter methods.
cp <- BinaryBenchmark(theData = dataCancerImputed,</pre>
theOutcome = "pgstat", reps = 10, fraction = 0.8)
# plot the Cross Validation Metrics
pl <- plot(cp,prefix = "Stagec:");</pre>
# Shut down the graphics device driver
dev.off()
#### Regression Example #####
# Start the graphics device driver to save all plots in a pdf format
pdf(file = "RegressionExample.pdf", width=8, height=6)
# Get the body fat data from the TH package
data("bodyfat", package = "TH.data")
# Benchmark regression methods and filter methods.
cp <- RegresionBenchmark(theData = bodyfat,</pre>
theOutcome = "DEXfat", reps = 10, fraction = 0.8)
# plot the Cross Validation Metrics
pl <- plot(cp,prefix = "Body Fat:");</pre>
# Shut down the graphics device driver
dev.off()
#### Ordinal Regression Example #####
# Start the graphics device driver to save all plots in a pdf format
pdf(file = "OrdinalRegressionExample.pdf", width=8, height=6)
```

```
# Get the GBSG2 data
data("GBSG2", package = "TH.data")

# Prepare the model frame for benchmarking
GBSG2$time <- NULL;
GBSG2$cens <- NULL;
GBSG2_mat <- cbind(tgrade = as.numeric(GBSG2$tgrade),
as.data.frame(model.matrix(tgrade~.,GBSG2))[-1])

# Benchmark regression methods and filter methods.
#30
cp <- OrdinalBenchmark(theData = GBSG2_mat,
theOutcome = "tgrade", reps = 10, fraction = 0.3)

# plot the Cross Validation Metrics
pl <- plot(cp,prefix = "GBSG:");
# Shut down the graphics device driver
dev.off()

## End(Not run)</pre>
```

bootstrapValidation\_Bin

Bootstrap validation of binary classification models

# Description

This function bootstraps the model n times to estimate for each variable the empirical distribution of model coefficients, area under ROC curve (AUC), integrated discrimination improvement (IDI) and net reclassification improvement (NRI). At each bootstrap the non-observed data is predicted by the trained model, and statistics of the test prediction are stored and reported. The method keeps track of predictions and plots the bootstrap-validated ROC. It may plots the blind test accuracy, sensitivity, and specificity, contrasted with the bootstrapped trained distributions.

# Usage

#### **Arguments**

fraction The fraction of data (sampled with replacement) to be used as train

loops The number of bootstrap loops

model.formula An object of class formula with the formula to be used

Outcome The name of the column in data that stores the variable to be predicted by the

model

data A data frame where all variables are stored in different columns

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")

plots Logical. If TRUE, density distribution plots are displayed

best.model.formula

An object of class formula with the formula to be used for the best model

## **Details**

The bootstrap validation will estimate the confidence interval of the model coefficients and the NRI and IDI. The non-sampled values will be used to estimate the blind accuracy, sensitivity, and specificity. A plot to monitor the evolution of the bootstrap procedure will be displayed if plots is set to TRUE. The plot shows the train and blind test ROC. The density distribution of the train accuracy, sensitivity, and specificity are also shown, with the blind test results drawn along the y-axis.

#### Value

data The data frame used to bootstrap and validate the model

outcome A vector with the predictions made by the model blind.accuracy The accuracy of the model in the blind test set

blind.sensitivity

The sensitivity of the model in the blind test set

blind.specificity

The specificity of the model in the blind test set

train.ROCAUC A vector with the AUC in the bootstrap train sets

blind.ROCAUC An object of class roc containing the AUC in the bootstrap blind test set

boot.ROCAUC An object of class roc containing the AUC using the mean of the bootstrapped

coefficients

fraction The fraction of data that was sampled with replacement loops

The number of loops it took for the model to stabilize

base. Accuracy The accuracy of the original model

base.sensitivity

The sensitivity of the original model

base.specificity

The specificity of the original model

accuracy A vector with the accuracies in the bootstrap test sets

sensitivities	A vector with the sensitivities in the bootstrap test sets
specificities	A vector with the specificities in the bootstrap test sets
train.accuracy	A vector with the accuracies in the bootstrap train sets
train.sensitivi	ity
	A vector with the sensitivities in the bootstrap train sets
train.specifici	ity
	A vector with the specificities in the bootstrap train sets
s.coef	A matrix with the coefficients in the bootstrap train sets
boot.model	An object of class 1m, g1m, or coxph containing a model whose coefficients are the median of the coefficients of the bootstrapped models
boot.accuracy	The accuracy of the mboot.model model
boot.sensitivit	ty
	The sensitivity of the mboot.model model
boot.specificit	ty
	The specificity of the mboot.model model
z.NRIs	A matrix with the <i>z</i> -score of the NRI for each model term, estimated using the bootstrap train sets
z.IDIs	A matrix with the <i>z</i> -score of the IDI for each model term, estimated using the bootstrap train sets
test.z.NRIs	A matrix with the <i>z</i> -score of the NRI for each model term, estimated using the bootstrap test sets
test.z.IDIs	A matrix with the <i>z</i> -score of the IDI for each model term, estimated using the bootstrap test sets
NRIs	A matrix with the NRI for each model term, estimated using the bootstrap test sets
IDIs	A matrix with the IDI for each model term, estimated using the bootstrap test sets
testOutcome	A vector that contains all the individual outcomes used to validate the model in the bootstrap test sets
testPrediction	A vector that contains all the individual predictions used to validate the model

# Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

in the bootstrap test sets

# See Also

 $bootstrap Validation\_Res, plot.bootstrap Validation\_Bin, summary.bootstrap Validation\_Bin$ 

```
bootstrapValidation_Res
```

Bootstrap validation of regression models

# **Description**

This function bootstraps the model *n* times to estimate for each variable the empirical bootstrapped distribution of model coefficients, and net residual improvement (NeRI). At each bootstrap the non-observed data is predicted by the trained model, and statistics of the test prediction are stores and reported.

## **Usage**

# **Arguments**

fraction The fraction of data (sampled with replacement) to be used as train

loops The number of bootstrap loops

model.formula An object of class formula with the formula to be used

Outcome The name of the column in data that stores the variable to be predicted by the

model

data A data frame where all variables are stored in different columns

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")

plots Logical. If TRUE, density distribution plots are displayed

bestmodel.formula

An object of class formula with the best formula to be compared

## **Details**

The bootstrap validation will estimate the confidence interval of the model coefficients and the NeRI. It will also compute the train and blind test root-mean-square error (RMSE), as well as the distribution of the NeRI *p*-values.

#### Value

data The data frame used to bootstrap and validate the model

outcome A vector with the predictions made by the model

boot.model An object of class 1m, g1m, or coxph containing a model whose coefficients are

the median of the coefficients of the bootstrapped models

NeRIs A matrix with the NeRI for each model term, estimated using the bootstrap test

sets

tStudent.pvalues

A matrix with the t-test p-value of the NeRI for each model term, estimated

using the bootstrap train sets

wilcox.pvalues A matrix with the Wilcoxon rank-sum test p-value of the NeRI for each model

term, estimated using the bootstrap train sets

bin.pvalues A matrix with the binomial test p-value of the NeRI for each model term, esti-

mated using the bootstrap train sets

F. pvalues A matrix with the F-test p-value of the NeRI for each model term, estimated

using the bootstrap train sets

test.tStudent.pvalues

A matrix with the t-test p-value of the NeRI for each model term, estimated

using the bootstrap test sets

test.wilcox.pvalues

A matrix with the Wilcoxon rank-sum test p-value of the NeRI for each model

term, estimated using the bootstrap test sets

test.bin.pvalues

A matrix with the binomial test p-value of the NeRI for each model term, esti-

mated using the bootstrap test sets

test.F.pvalues A matrix with the F-test p-value of the NeRI for each model term, estimated

using the bootstrap test sets

testPrediction A vector that contains all the individual predictions used to validate the model

in the bootstrap test sets

testOutcome A vector that contains all the individual outcomes used to validate the model in

the bootstrap test sets

testResiduals A vector that contains all the residuals used to validate the model in the bootstrap

test sets

trainPrediction

A vector that contains all the individual predictions used to validate the model

in the bootstrap train sets

trainOutcome A vector that contains all the individual outcomes used to validate the model in

the bootstrap train sets

trainResiduals A vector that contains all the residuals used to validate the model in the bootstrap

train sets

testRMSE The global RMSE, estimated using the bootstrap test sets

trainRMSE The global RMSE, estimated using the bootstrap train sets

```
trainSampleRMSE
```

A vector with the RMSEs in the bootstrap train sets

testSampledRMSE

A vector with the RMSEs in the bootstrap test sets

#### Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

#### See Also

bootstrapValidation\_Bin, plot.bootstrapValidation\_Res

```
bootstrapVarElimination_Bin
```

IDI/NRI-based backwards variable elimination with bootstrapping

# **Description**

This function removes model terms that do not improve the bootstrapped integrated discrimination improvement (IDI) or net reclassification improvement (NRI) significantly.

#### Usage

## **Arguments**

object	An object of class 1m, g1m, or coxph containing the model to be analyzed
pvalue	The maximum $p$ -value, associated to either IDI or NRI, allowed for a term in the model

Outcome The name of the column in data that stores the variable to be predicted by the

model

data A data frame where all variables are stored in different columns

startOffset Only terms whose position in the model is larger than the startOffset are

candidates to be removed

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX") selectionType The type of index to be evaluated by the improveProb function (Hmisc pack-

age): z-score of IDI or of NRI

loops The number of bootstrap loops

print Logical. If TRUE, information will be displayed

plots Logical. If TRUE, plots are displayed

#### **Details**

For each model term  $x_i$ , the IDI or NRI is computed for the Full model and the reduced model (where the term  $x_i$  removed). The term whose removal results in the smallest drop in bootstrapped improvement is selected. The hypothesis: the term adds classification improvement is tested by checking the p value of average improvement. If p(IDIorNRI) > pvalue, then the term is removed. In other words, only model terms that significantly aid in subject classification are kept. The procedure is repeated until no term fulfils the removal criterion.

#### Value

back.model An object of the same class as object containing the reduced model

loops The number of loops it took for the model to stabilize

reclas.info A list with the NRI and IDI statistics of the reduced model, as given by the

getVar.Bin function

bootCV An object of class bootstrapValidation\_Bin containing the results of the

bootstrap validation in the reduced model

back.formula An object of class formula with the formula used to fit the reduced model lastRemoved The name of the last term that was removed (-1 if all terms were removed)

at.opt.model The model will have the fitted model that had close to maximum bootstrapped

test accuracy

beforeFSC.formula

The formula of the model before False Selection Correction

at.Accuracy.formula

the string formula of the model that had the best or close to the best test accuracy

# Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

#### References

Pencina, M. J., D'Agostino, R. B., & Vasan, R. S. (2008). Evaluating the added predictive ability of a new marker: from area under the ROC curve to reclassification and beyond. *Statistics in medicine* **27**(2), 157-172.

### See Also

 $bootstrap Var Elimination\_Res,\ back Var Elimination\_Bin,\ back Var Elimination\_Res$ 

 $bootstrap Var Elimination\_Res$ 

NeRI-based backwards variable elimination with bootstrapping

# Description

This function removes model terms that do not improve the bootstrapped net residual improvement (NeRI) significantly.

# Usage

## **Arguments**

plots

object	An object of class 1m, g1m, or coxph containing the model to be analysed
pvalue	The maximum p-value, associated to the NeRI, allowed for a term in the model
Outcome	The name of the column in data that stores the variable to be predicted by the model
data	A data frame where all variables are stored in different columns
startOffset	Only terms whose position in the model is larger than the startOffset are candidates to be removed
type	Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")
testType	Type of non-parametric test to be evaluated by the improvedResiduals function: Binomial test ("Binomial"), Wilcoxon rank-sum test ("Wilcox"), Student's <i>t</i> -test ("tStudent"), or <i>F</i> -test ("Ftest")
loops	The number of bootstrap loops
setIntersect	The intersect of the model (To force a zero intersect, set this value to 0)
print	Logical. If TRUE, information will be displayed

Logical. If TRUE, plots are displayed

#### **Details**

For each model term  $x_i$ , the residuals are computed for the Full model and the reduced model (where the term  $x_i$  removed). The term whose removal results in the smallest drop in bootstrapped test residuals improvement is selected. The hypothesis: the term improves residuals is tested by checking the p-value of average improvement. If p(residualsbetterthanreducedresiduals) > pvalue, then the term is removed. In other words, only model terms that significantly aid in improving residuals are kept. The procedure is repeated until no term fulfils the removal criterion. The p-values of improvement can be computed via a sign-test (Binomial) a paired Wilcoxon test, paired t-test or f-test. The first three tests compare the absolute values of the residuals, while the f-test test if the variance of the residuals is improved significantly.

#### Value

back.model An object of the same class as object containing the reduced model

loops The number of loops it took for the model to stabilize

reclas.info A list with the NeRI statistics of the reduced model, as given by the getVar.Res

function

bootCV An object of class bootstrapValidation\_Res containing the results of the

bootstrap validation in the reduced model

hack.formula An object of class formula with the formula used to fit the reduced model lastRemoved

The name of the last term that was removed (-1 if all terms were removed)

at.opt.model The model with close to minimum bootstrapped RMSE

beforeFSC.formula

The formula of the model before the FSC stage

 $\verb"at.RMSE.formula"\\$ 

the string formula of the model that had the minimum or close to minimum RMSE

# Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

#### See Also

bootstrapVarElimination\_Bin, backVarElimination\_Res, bootstrapValidation\_Res

BSWiMS.model	BSWiMS model selection

## **Description**

This function returns a set of models that best predict the outcome. Based on a Bootstrap Stage Wise Model Selection algorithm.

# Usage

```
BSWiMS.model(formula,
            data,
            type = c("Auto","LM","LOGIT","COX"),
            testType = c("Auto","zIDI",
                          "zNRI",
                          "Binomial",
                          "Wilcox",
                          "tStudent",
                          "Ftest"),
            pvalue=0.05,
            variableList=NULL,
            size=0,
            loops=32,
            elimination.bootstrap.steps = 100,
            fraction=1.0,
            maxTrainModelSize=20,
            maxCycles=20,
            print=FALSE,
            plots=FALSE,
            featureSize=0,
NumberofRepeats=1
            )
```

# Arguments

formula	An object of class formula with the formula to be fitted				
data	A data frame where all variables are stored in different columns				
type	The fit type. Auto will determine the fitting based on the formula				
testType	For an Binary-based optimization, the type of index to be evaluated by the improveProb function (Hmisc package): <i>z</i> -value of Binary or of NRI. For a NeRI-based optimization, the type of non-parametric test to be evaluated by the improvedResiduals function: Binomial test ("Binomial"), Wilcoxon rank-sum test ("Wilcox"), Student's <i>t</i> -test ("tStudent"), or <i>F</i> -test ("Ftest")				
pvalue	The maximum $p$ -value, associated to the testType, allowed for a term in the model (it will control the false selection rate)				
variableList	A data frame with two columns. The first one must have the names of the candidate variables and the other one the description of such variables				
size	The number of candidate variables to be tested (the first size variables from variableList)				
loops	The number of bootstrap loops for the forward selection procedure				
elimination.bootstrap.steps					
	The number of bootstrap loops for the backwards elimination procedure				
fraction	The fraction of data (sampled with replacement) to be used as train				

maxTrainModelSize

Maximum number of terms that can be included in the each forward selection

model

maxCycles The maximum number of model generation cycles

print Logical. If TRUE, information will be displayed

plots Logical. If TRUE, plots are displayed

featureSize The original number of features to be explored in the data frame.

NumberofRepeats

How many times the BSWiMS search will be repeated

#### **Details**

This is a core function of FRESA.CAD. The function will generate a set of B:SWiMS models from the data based on the provided baseline formula. The function will loop extracting a models whose all terms are statistical significant. After each loop it will remove the significant terms, and it will repeat the model generation until no mode significant models are found or the maximum number of cycles is reached.

#### Value

BSWiMS.model the output of the bootstrap backwards elimination step

forward.model The output of the forward selection step update.model The output of the forward selection step

univariate The univariate ranking of variables if no list of features was provided

bagging The model after bagging the set of models

formula.list The formulas extracted at each cycle

forward.selection.list

All formulas generated by the forward selection procedure

oridinal Models A list of scores, the data and a formulas vector required for ordinal scores pre-

dictions

## Author(s)

Jose G. Tamez-Pena

## References

Pencina, M. J., D'Agostino, R. B., & Vasan, R. S. (2008). Evaluating the added predictive ability of a new marker: from area under the ROC curve to reclassification and beyond. *Statistics in medicine* **27**(2), 157-172.

## **Examples**

```
## Not run:
# Start the graphics device driver to save all plots in a pdf format
pdf(file = "BSWiMS.model.Example.pdf",width = 8, height = 6)
# Get the stage C prostate cancer data from the rpart package
data(stagec,package = "rpart")
options(na.action = 'na.pass')
stagec_mat <- cbind(pgstat = stagec$pgstat,</pre>
             pgtime = stagec$pgtime,
             as.data.frame(model.matrix(Surv(pgtime,pgstat) ~ .*.,stagec))[-1])
fnames <- colnames(stagec_mat)</pre>
fnames <- str_replace_all(fnames,":","__")</pre>
colnames(stagec_mat) <- fnames</pre>
dataCancerImputed <- nearestNeighborImpute(stagec_mat)</pre>
# Get a Cox proportional hazards model using:
# - The default parameters
md <- BSWiMS.model(formula = Surv(pgtime, pgstat) ~ 1,</pre>
  data = dataCancerImputed)
#Plot the bootstrap validation
pt <- plot(md$BSWiMS.model$bootCV)</pre>
#Get the coefficients summary
sm <- summary(md)</pre>
print(sm$coefficients)
#Plot the bagged model
pl <- plotModels.ROC(cbind(dataCancerImputed$pgstat,</pre>
  predict(md, dataCancerImputed)),
 main = "Bagging Predictions")
# Get a Cox proportional hazards model using:
# - The default parameters but repeated 10 times
md <- BSWiMS.model(formula = Surv(pgtime, pgstat) ~ 1,</pre>
   data = dataCancerImputed,
   NumberofRepeats = 10)
#Get the coefficients summary
sm <- summary(md)</pre>
print(sm$coefficients)
#Check all the formulas
print(md$formula.list)
#Plot the bagged model
pl <- plotModels.ROC(cbind(dataCancerImputed$pgstat,</pre>
   predict(md,dataCancerImputed)),
```

```
main = "Bagging Predictions")
# Get a regression of the survival time
timeSubjects <- dataCancerImputed</pre>
timeSubjects$pgtime <- log(timeSubjects$pgtime)</pre>
md <- BSWiMS.model(formula = pgtime ~ 1,</pre>
  data = timeSubjects,
  )
pt <- plot(md$BSWiMS.model$bootCV)</pre>
sm <- summary(md)</pre>
print(sm$coefficients)
# Get a logistic regression model using
# - The default parameters and removing time as possible predictor
data(stagec,package = "rpart")
stagec$pgtime <- NULL</pre>
stagec_mat <- cbind(pgstat = stagec$pgstat,</pre>
                       as.data.frame(model.matrix(pgstat ~ .*.,stagec))[-1])
fnames <- colnames(stagec_mat)</pre>
fnames <- str_replace_all(fnames,":","__")</pre>
colnames(stagec_mat) <- fnames</pre>
dataCancerImputed <- nearestNeighborImpute(stagec_mat)</pre>
md <- BSWiMS.model(formula = pgstat ~ 1,</pre>
  data = dataCancerImputed)
pt <- plot(md$BSWiMS.model$bootCV)</pre>
sm <- summary(md)</pre>
print(sm$coefficients)
# Get a ordinal regression of grade model using GBSG2 data
# - The default parameters and removing the
# time and status as possible predictor
data("GBSG2", package = "TH.data")
# Prepare the model frame for prediction
GBSG2$time <- NULL;</pre>
GBSG2$cens <- NULL;</pre>
GBSG2_mat <- cbind(tgrade = as.numeric(GBSG2$tgrade),</pre>
                         as.data.frame(model.matrix(tgrade~.*.,GBSG2))[-1])
fnames <- colnames(GBSG2_mat)</pre>
fnames <- str_replace_all(fnames,":","__")</pre>
colnames(GBSG2_mat) <- fnames</pre>
md <- BSWiMS.model(formula = tgrade ~ 1,</pre>
   data = GBSG2_mat)
```

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```
sm <- summary(md$oridinalModels$theBaggedModels[[1]]$bagged.model)
print(sm$coefficients)
sm <- summary(md$oridinalModels$theBaggedModels[[2]]$bagged.model)
print(sm$coefficients)

print(table(GBSG2_mat$tgrade,predict(md,GBSG2_mat)))

# Shut down the graphics device driver
dev.off()

## End(Not run)</pre>
```

cancerVarNames

Data frame used in several examples of this package

# **Description**

This data frame contains two columns, one with names of variables, and the other with descriptions of such variables. It is used in several examples of this package. Specifically, it is used in examples working with the stage C prostate cancer data from the rpart package

# Usage

```
data(cancerVarNames)
```

## **Format**

A data frame with names and descriptions of the variables used in several examples

Var A column with the names of the variables

Description A column with a short description of the variables

# **Examples**

```
data(cancerVarNames)
```

crossValidationFeatureSelection\_Bin

IDI/NRI-based selection of a linear, logistic, or Cox proportional hazards regression model from a set of candidate variables

## **Description**

This function performs a cross-validation analysis of a feature selection algorithm based on the integrated discrimination improvement (IDI) or the net reclassification improvement (NRI) to return a predictive model. It is composed of an IDI/NRI-based feature selection followed by an update procedure, ending with a bootstrapping backwards feature elimination. The user can control how many train and blind test sets will be evaluated.

### Usage

```
crossValidationFeatureSelection_Bin(size = 10,
                                 fraction = 1.0,
                                 pvalue = 0.05,
                                 loops = 100,
                                 covariates = "1",
                                 Outcome,
                                 timeOutcome = "Time",
                                 variableList,
                                 data,
                                 maxTrainModelSize = 20,
                                 type = c("LM", "LOGIT", "COX"),
                                 selectionType = c("zIDI", "zNRI"),
                                 startOffset = 0,
                                 elimination.bootstrap.steps = 100,
                                 trainFraction = 0.67,
                                 trainRepetition = 9,
                                 bootstrap.steps = 100,
                                 nk = 0,
                                 unirank = NULL,
                                 print=TRUE,
                                 plots=TRUE,
                                 lambda="lambda.1se",
                                 equivalent=FALSE,
                                 bswimsCycles=10,
                                 usrFitFun=NULL,
                                 featureSize=0)
```

#### **Arguments**

size The number of candidate variables to be tested (the first size variables from

variableList)

fraction The fraction of data (sampled with replacement) to be used as train

pvalue The maximum p-value, associated to either IDI or NRI, allowed for a term in

the model

loops The number of bootstrap loops

covariates A string of the type "1 + var1 + var2" that defines which variables will always

be included in the models (as covariates)

Outcome The name of the column in data that stores the variable to be predicted by the

model

timeOutcome The name of the column in data that stores the time to event (needed only for a

Cox proportional hazards regression model fitting)

variableList A data frame with two columns. The first one must have the names of the can-

didate variables and the other one the description of such variables

data A data frame where all variables are stored in different columns

maxTrainModelSize

Maximum number of terms that can be included in the model

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")

selectionType The type of index to be evaluated by the improveProb function (Hmisc pack-

age): z-score of IDI or of NRI

startOffset Only terms whose position in the model is larger than the startOffset are

candidates to be removed

elimination.bootstrap.steps

The number of bootstrap loops for the backwards elimination procedure

trainFraction The fraction of data (sampled with replacement) to be used as train for the cross-

validation procedure

trainRepetition

The number of cross-validation folds (it should be at least equal to 1/trainFraction

for a complete cross-validation)

bootstrap.steps

The number of bootstrap loops for the confidence intervals estimation

nk The number of neighbours used to generate a k-nearest neighbours (KNN) clas-

sification. If zero, k is set to the square root of the number of cases. If less than

zero, it will not perform the KNN classification

unirank A list with the results yielded by the uniRankVar function, required only if the

rank needs to be updated during the cross-validation procedure

print Logical. If TRUE, information will be displayed

plots Logical. If TRUE, plots are displayed

lambda The passed value to the s parameter of the glmnet cross validation coefficient

equivalent Is set to TRUE CV will compute the equivalent model

bswimsCycles The maximum number of models to be returned by BSWiMS.model

usrFitFun A user fitting function to be evaluated by the cross validation procedure

featureSize The original number of features to be explored in the data frame.

#### **Details**

This function produces a set of data and plots that can be used to inspect the degree of over-fitting or shrinkage of a model. It uses bootstrapped data, cross-validation data, and, if possible, retrain data. During each cycle, a train and a test ROC will be generated using bootstrapped data. At the end of the cross-validation feature selection procedure, a set of three plots may be produced depending on the specifications of the analysis. The first plot shows the ROC for each cross-validation blind test. The second plot, if enough samples are given, shows the ROC of each model trained and tested in the blind test partition. The final plot shows ROC curves generated with the train, the bootstrapped blind test, and the cross-validation test data. Additionally, this plot will also contain the ROC of the cross-validation mean test data, and of the cross-validation coherence. These set of plots may be used to get an overall perspective of the expected model shrinkage. Along with the plots, the function provides the overall performance of the system (accuracy, sensitivity, and specificity). The function also produces a report of the expected performance of a KNN algorithm trained with the selected features of the model, and an elastic net algorithm. The test predictions obtained with these algorithms can then be compared to the predictions generated by the logistic, linear, or Cox proportional hazards regression model.

#### Value

formula.list A list containing objects of class formula with the formulas used to fit the models found at each cycle

Models.testPrediction

A data frame with the blind test set predictions (Full B:SWiMS,Median,Bagged,Forward,Backwards Eliminations) made at each fold of the cross validation, where the models used to generate such predictions (formula.list) were generated via a feature selection process which included only the train set. It also includes a column with the Outcome of each prediction, and a column with the number of the fold at which the prediction was made.

FullBSWiMS.testPrediction

A data frame similar to Models.testPrediction, but where the model used to generate the predictions was the Full model, generated via a feature selection process which included all data.

TestRetrained.blindPredictions

A data frame similar to Models.testPrediction, but where the models were retrained on an independent set of data (only if enough samples are given at each fold)

 ${\tt LastTrainBSWiMS.bootstrapped}$ 

An object of class bootstrapValidation\_Bin containing the results of the bootstrap validation in the last trained model

Test.accuracy The global blind test accuracy of the cross-validation procedure

Test.sensitivity

The global blind test sensitivity of the cross-validation procedure

Test.specificity

The global blind test specificity of the cross-validation procedure

Train.correlationsToFull

The Spearman  $\rho$  rank correlation coefficient between the predictions made with each model from formula.list and the Full model in the train set

Blind.correlationsToFull

The Spearman  $\rho$  rank correlation coefficient between the predictions made with each model from formula.1ist and the Full model in the test set

FullModelAtFoldAccuracies

The blind test accuracy for the Full model at each cross-validation fold

FullModelAtFoldSpecificties

The blind test specificity for the Full model at each cross-validation fold

FullModelAtFoldSensitivities

The blind test sensitivity for the Full model at each cross-validation fold FullModelAtFoldAUC

The blind test ROC AUC for the Full model at each cross-validation fold AtCVFoldModelBlindAccuracies

The blind test accuracy for the Full model at each final cross-validation fold

 ${\tt AtCVFoldModelBlindSpecificities}$ 

The blind test specificity for the Full model at each final cross-validation fold

AtCVFoldModelBlindSensitivities

The blind test sensitivity for the Full model at each final cross-validation fold

CVTrain.Accuracies

The train accuracies at each fold

CVTrain.Sensitivity

The train sensitivity at each fold

CVTrain.Specificity

The train specificity at each fold

CVTrain. AUCs The train ROC AUC for each fold

forwardSelection

A list containing the values returned by ForwardSelection.Model.Bin using all data

updateforwardSelection

A list containing the values returned by updateModel.Bin using all data and the model from forwardSelection

BSWiMS A list containing the values returned by bootstrapVarElimination\_Bin using all data and the model from updateforwardSelection

FullBSWiMS.bootstrapped

An object of class bootstrapValidation\_Bin containing the results of the bootstrap validation in the Full model

Models.testSensitivities

A matrix with the mean ROC sensitivities at certain specificities for each train and all test cross-validation folds using the cross-validation models (i.e. 0.95, 0.90, 0.80, 0.70, 0.60, 0.50, 0.40, 0.30, 0.20, 0.10, and 0.05)

FullKNN.testPrediction

A data frame similar to Models.testPrediction, but where a KNN classifier with the same features as the Full model was used to generate the predictions

KNN.testPrediction

A data frame similar to Models.testPrediction, but where KNN classifiers with the same features as the cross-validation models were used to generate the predictions at each cross-validation fold

Fullenet An object of class cv.glmnet containing the results of an elastic net cross-validation fit

LASSO.testPredictions

A data frame similar to Models.testPrediction, but where the predictions were made by the elastic net model

LASSOVariables A list with the elastic net Full model and the models found at each cross-validation fold

uniTrain.Accuracies

The list of accuracies of an univariate analysis on each one of the model variables in the train sets

uniTest.Accuracies

The list of accuracies of an univariate analysis on each one of the model variables in the test sets

uniTest.TopCoherence

The accuracy coherence of the top ranked variable on the test set

uniTrain.TopCoherence

The accuracy coherence of the top ranked variable on the train set

Models.trainPrediction

A data frame with the outcome and the train prediction of every model

FullBSWiMS.trainPrediction

A data frame with the outcome and the train prediction at each CV fold for the main model

LASSO.trainPredictions

A data frame with the outcome and the prediction of each enet lasso model

BSWiMS.ensemble.prediction

The ensemble prediction by all models on the test data

AtOptFormulas.list

The list of formulas with "optimal" performance

ForwardFormulas.list

The list of formulas produced by the forward procedure

baggFormulas.list

The list of the bagged models

LassoFilterVarList

The list of variables used by LASSO fitting

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

## References

Pencina, M. J., D'Agostino, R. B., & Vasan, R. S. (2008). Evaluating the added predictive ability of a new marker: from area under the ROC curve to reclassification and beyond. *Statistics in medicine* **27**(2), 157-172.

## See Also

crossValidationFeatureSelection\_Res, ForwardSelection.Model.Bin, ForwardSelection.Model.Res

crossValidationFeatureSelection\_Res

NeRI-based selection of a linear, logistic, or Cox proportional hazards regression model from a set of candidate variables

## **Description**

This function performs a cross-validation analysis of a feature selection algorithm based on net residual improvement (NeRI) to return a predictive model. It is composed of a NeRI-based feature selection followed by an update procedure, ending with a bootstrapping backwards feature elimination. The user can control how many train and blind test sets will be evaluated.

### Usage

```
crossValidationFeatureSelection_Res(size = 10,
                                     fraction = 1.0,
                                     pvalue = 0.05,
                                     loops = 100,
                                     covariates = "1",
                                     Outcome,
                                     timeOutcome = "Time",
                                     variableList,
                                     maxTrainModelSize = 20,
                                     type = c("LM", "LOGIT", "COX"),
                                     testType = c("Binomial",
                                                   "Wilcox",
                                                   "tStudent",
                                                   "Ftest"),
                                     startOffset = 0,
                                     elimination.bootstrap.steps = 100,
                                     trainFraction = 0.67,
                                     trainRepetition = 9,
                                     setIntersect = 1,
                                     unirank = NULL,
                                     print=TRUE,
                                     plots=TRUE,
                                     lambda="lambda.1se",
                                     equivalent=FALSE,
                                     bswimsCycles=10,
                                     usrFitFun=NULL,
                                     featureSize=0)
```

#### **Arguments**

size

The number of candidate variables to be tested (the first size variables from variableList)

fraction The fraction of data (sampled with replacement) to be used as train

pvalue The maximum p-value, associated to the NeRI, allowed for a term in the model

loops The number of bootstrap loops

covariates A string of the type "1 + var1 + var2" that defines which variables will always

be included in the models (as covariates)

Outcome The name of the column in data that stores the variable to be predicted by the

model

timeOutcome The name of the column in data that stores the time to event (needed only for a

Cox proportional hazards regression model fitting)

variableList A data frame with two columns. The first one must have the names of the can-

didate variables and the other one the description of such variables

data A data frame where all variables are stored in different columns

maxTrainModelSize

Maximum number of terms that can be included in the model

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")

testType Type of non-parametric test to be evaluated by the improvedResiduals func-

tion: Binomial test ("Binomial"), Wilcoxon rank-sum test ("Wilcox"), Student's

t-test ("tStudent"), or F-test ("Ftest")

startOffset Only terms whose position in the model is larger than the startOffset are

candidates to be removed

elimination.bootstrap.steps

The number of bootstrap loops for the backwards elimination procedure

trainFraction The fraction of data (sampled with replacement) to be used as train for the cross-

validation procedure

setIntersect The intersect of the model (To force a zero intersect, set this value to 0)

trainRepetition

The number of cross-validation folds (it should be at least equal to 1/trainFraction

for a complete cross-validation)

unirank A list with the results yielded by the uniRankVar function, required only if the

rank needs to be updated during the cross-validation procedure

print Logical. If TRUE, information will be displayed

plots Logical. If TRUE, plots are displayed

lambda The passed value to the s parameter of the glmnet cross validation coefficient

equivalent Is set to TRUE CV will compute the equivalent model

bswimsCycles The maximum number of models to be returned by BSWiMS.model

usrFitFun A user fitting function to be evaluated by the cross validation procedure

featureSize The original number of features to be explored in the data frame.

### **Details**

This function produces a set of data and plots that can be used to inspect the degree of over-fitting or shrinkage of a model. It uses bootstrapped data, cross-validation data, and, if possible, retrain data.

#### Value

formula.list A list containing objects of class formula with the formulas used to fit the models found at each cycle

Models.testPrediction

A data frame with the blind test set predictions made at each fold of the cross validation (Full B:SWiMS,Median,Bagged,Forward,Backward Elimination), where the models used to generate such predictions (formula.list) were generated via a feature selection process which included only the train set. It also includes a column with the Outcome of each prediction, and a column with the number of the fold at which the prediction was made.

FullBSWiMS.testPrediction

A data frame similar to Models.testPrediction, but where the model used to generate the predictions was the Full model, generated via a feature selection process which included all data.

BSWiMS A list containing the values returned by bootstrapVarElimination\_Res using all data and the model from updatedforwardModel

forwardSelection

A list containing the values returned by ForwardSelection.Model.Res using all data

updatedforwardModel

A list containing the values returned by updateModel.Res using all data and the model from forwardSelection

testRMSE The global blind test root-mean-square error (RMSE) of the cross-validation

procedure

testPearson The global blind test Pearson r product-moment correlation coefficient of the

cross-validation procedure

testSpearman The global blind test Spearman  $\rho$  rank correlation coefficient of the cross-validation

procedure

FulltestRMSE The global blind test RMSE of the Full model

FullTestPearson

The global blind test Pearson r product-moment correlation coefficient of the Full model

FullTestSpearman

The global blind test Spearman  $\rho$  rank correlation coefficient of the Full model

train RMSE at each fold of the cross-validation procedure

trainPearson The train Pearson r product-moment correlation coefficient at each fold of the

cross-validation procedure

trainSpearman The train Spearman  $\rho$  rank correlation coefficient at each fold of the cross-

validation procedure

FullTrainRMSE The train RMSE of the Full model at each fold of the cross-validation procedure

FullTrainPearson

The train Pearson r product-moment correlation coefficient of the Full model at each fold of the cross-validation procedure

FullTrainSpearman

The train Spearman  $\rho$  rank correlation coefficient of the Full model at each fold of the cross-validation procedure

 ${\tt testRMSEAtFold} \quad The \ blind \ test \ RMSE \ at \ each \ fold \ of \ the \ cross-validation \ procedure \\ {\tt FullTestRMSEAtFold}$ 

The blind test RMSE of the Full model at each fold of the cross-validation procedure

Fullenet An object of class cv.glmnet containing the results of an elastic net cross-validation fit

LASSO.testPredictions

A data frame similar to Models.testPrediction, but where the predictions were made by the elastic net model

LASSOVariables A list with the elastic net Full model and the models found at each cross-validation fold

byFoldTestMS A vector with the Mean Square error for each blind fold byFoldTestSpearman

A vector with the Spearman correlation between prediction and outcome for each blind fold

byFoldTestPearson

A vector with the Pearson correlation between prediction and outcome for each blind fold

byFoldCstat A vector with the C-index (Somers' Dxy rank correlation:rcorr.cens) between prediction and outcome for each blind fold

CVBlindPearson A vector with the Pearson correlation between the outcome and prediction for each repeated experiment

CVBlindSpearman

A vector with the Spearm correlation between the outcome and prediction for each repeated experiment

CVBlindRMS A vector with the RMS between the outcome and prediction for each repeated experiment

Models.trainPrediction

A data frame with the outcome and the train prediction of every model

FullBSWiMS.trainPrediction

A data frame with the outcome and the train prediction at each CV fold for the main model

LASSO.trainPredictions

A data frame with the outcome and the prediction of each enet lasso model

uniTrainMSS A data frame with mean square of the train residuals from the univariate models of the model terms

uniTestMSS A data frame with mean square of the test residuals of the univariate models of the model terms

BSWiMS.ensemble.prediction

The ensemble prediction by all models on the test data

AtOptFormulas.list

The list of formulas with "optimal" performance

CVsignature 41

ForwardFormulas.list

The list of formulas produced by the forward procedure

baggFormulas.list

The list of the bagged models

LassoFilterVarList

The list of variables used by LASSO fitting

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

### See Also

crossValidationFeatureSelection\_Bin, improvedResiduals, bootstrapVarElimination\_Res

CVsignature

Cross-validated Signature

## **Description**

A formula based wrapper of the getSignature function

## Usage

```
CVsignature(formula = formula,data=NULL,...)
```

## **Arguments**

formula The base formula

data The data to be used for training the signature method

... Parameters for the getSignature function

### Value

fit A getSignature object.
method The distance method

variable.importance

The named vector of relevant features

### Author(s)

Jose G. Tamez-Pena

# See Also

getSignature,signatureDistance

42 EmpiricalSurvDiff

EmpiricalSurvDiff Estimate the LR value and its associated p-values

### **Description**

Permutations or Bootstrapping computation of the standardized log-rank (SLR) or the Chi=SLR^2 p-values for differences in survival times

### Usage

### **Arguments**

times A numeric vector with he observed times to event
status A numeric vector indicating if the time to event is censored

groups A numeric vector indicating the label of the two survival groups

samples The number of bootstrap samples

type The type of log-rank statistics. SLR or Chi

plots If TRUE, the Kaplan-Meier plot will be plotted

minAproxSamples

The number of tail samples used for the normal-distribution approximation

computeDist If TRUE, it will compute the bootstrapped distribution of the SLR

... Additional parameters for the plot

#### **Details**

It will compute the null distribution of the SRL or the square SLR (Chi) via permutations, and it will return the p-value of differences between survival times between two groups. It may also be used to compute the empirical distribution of the difference in SLR using bootstrapping. (computeDist=TRUE) The p-values will be estimated based on the sampled distribution, or normal-approximated along the tails.

EmpiricalSurvDiff 43

## Value

pvalue	the minimum one-tailed p-value : $\min[p(SRL < 0), p(SRL > 0)]$ for type="SLR" or the two tailed p-value: 1-p( SRL  > 0) for type="Chi"
LR	A list of LR statistics: LR=Expected, VR=Variance, SLR=Standardized LR.
p.equal	The two tailed p-value: $1-p( SRL  > 0)$
p.sup	The one tailed p-value: p(SRL < 0), return NA for type="Chi"
p.inf	The one tailed p-value: $p(SRL > 0)$ , return NA for type="Chi"
nullDist	permutation derived probability density function of the null distribution
LRDist	bootstrapped derived probability density function of the SLR (computeDist=TRUE)

### Author(s)

Jose G. Tamez-Pena

# Examples

```
## Not run:
     library(rpart)
      data(stagec)
     # The Log-Rank Analysis using survdiff
     lrsurvdiff <- survdiff(Surv(pgtime,pgstat)~grade>2,data=stagec)
     print(lrsurvdiff)
      # The Log-Rank Analysis: permutations of the null Chi distribution
     lrp <- EmpiricalSurvDiff(stagec$pgtime,stagec$pgstat,stagec$grade>2,
                         type="Chi",plots=TRUE,samples=10000,
                         main="Chi Null Distribution")
     print(list(unlist(c(lrp$LR,lrp$pvalue))))
      # The Log-Rank Analysis: permutations of the null SLR distribution
     lrp <- EmpiricalSurvDiff(stagec$pgtime, stagec$pgstat, stagec$grade>2,
                         type="SLR",plots=TRUE,samples=10000,
                         main="SLR Null Distribution")
     print(list(unlist(c(lrp$LR,lrp$pvalue))))
      # The Log-Rank Analysis: Bootstraping the SLR distribution
     lrp <- EmpiricalSurvDiff(stagec$pgtime,stagec$pgstat,stagec$grade>2,
                         computeDist=TRUE,plots=TRUE,samples=100000,
                         main="SLR Null and SLR bootrapped")
     print(list(unlist(c(lrp$LR,lrp$pvalue))))
## End(Not run)
```

44 ensemblePredict

ensemblePredict T

The median prediction from a list of models

#### **Description**

Given a list of model formulas, this function will train such models and return the a single(ensemble) prediction from the list of formulas on a test data set. It may also provides a *k*-nearest neighbors (KNN) prediction using the features listed in such models.

## Usage

### **Arguments**

formulaList A list made of objects of class formula, each representing a model formula to

be fitted and predicted with

trainData A data frame with the data to train the model, where all variables are stored in

different columns

testData A data frame similar to trainData, but with the data set to be predicted. If

NULL, trainData will be used

predictType Prediction type: Probability ("prob") or linear predictor ("linear")

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")

Outcome The name of the column in data that stores the variable to be predicted by the

model

nk The number of neighbors used to generate the KNN classification. If zero, k is

set to the square root of the number of cases. If less than zero, it will not perform

the KNN classification

## Value

ensemblePredict

A vector with the median prediction for the testData data set, using the models

from formulaList

medianKNNPredict

A vector with the median prediction for the testData data set, using the KNN

models

predictions A matrix, where each column represents the predictions made with each model

from formulaList

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KNNpredictions A matrix, where each column represents the predictions made with a different

KNN model

wPredict A vector with the weighted mean ensemble

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

featureAdjustment Adjust each listed variable to the provided set of covariates

## **Description**

This function fits the candidate variables to the provided model, for each strata, on a control population. If the variance of the residual (the fitted observation minus the real observation) is reduced significantly, then, such residual is used in the resulting data frame. Otherwise, the control mean is subtracted to the observation.

## Usage

## **Arguments**

variableList A data frame with two columns. The first one must have the names of the can-

didate variables and the other one the description of such variables

baseModel A string of the type "1 + var1 + var2" that defines the model to which variables

will be fitted

strata The name of the column in data that stores the variable that will be used to

stratify the model

data A data frame where all variables are stored in different columns referenceframe A data frame similar to data, but with only the control population

type Fit type: linear fitting ("LM"), or generalized least squares fitting ("GLS")

pvalue The maximum p-value, associated to the F-test, for the model to be allowed to

reduce variability

correlationGroup

The name of the column in data that stores the variable to be used to group the

data (only needed if type defined as "GLS")

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#### Value

A data frame, where each input observation has been adjusted from data at each strata

#### Note

This function prints the residuals and the F-statistic for all candidate variables

#### Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

FilterUnivariate	Univariate Filters
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## Description

Returns the top set of features that are statistically associated with the outcome.

## Usage

# **Arguments**

limit

The data frame
The outcome feature
The threshold pvalue used after the p.adjust method
The method used by the p.adjust method
The unitTest to be performed by the linear fitting model
The type of linear model: LM or LOGIT
The correlation method: pearson, spearman or kendall.

The samples-wise fraction of features to return.

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fnames	The list of features to test inside the correlated_Remove function
thr	The maximum correlation to allow between features
	Parameters to be passed to the correlated Remove function

#### Value

Named vector with the adjusted p-values or the list of no-correlated features for the correlated\_Remove

### Author(s)

Jose G. Tamez-Pena

# Examples

```
## Not run:
    library("FRESA.CAD")
    ### Univariate Filter Examples ####
    # Get the stage C prostate cancer data from the rpart package
    data(stagec,package = "rpart")
   # Prepare the data. Create a model matrix without the event time and interactions
    stagec$pgtime <- NULL</pre>
    stagec$eet <- as.factor(stagec$eet)</pre>
    options(na.action = 'na.pass')
    stagec_mat <- cbind(pgstat = stagec$pgstat,</pre>
                         as.data.frame(model.matrix(pgstat ~ .*.,stagec))[-1])
    fnames <- colnames(stagec_mat)</pre>
    fnames <- str_replace_all(fnames,":","__")</pre>
    colnames(stagec_mat) <- fnames</pre>
    # Impute the missing data
    dataCancerImputed <- nearestNeighborImpute(stagec_mat)</pre>
  dataCancerImputed[,1:ncol(dataCancerImputed)] <- sapply(dataCancerImputed,as.numeric)</pre>
    # Get the top Features associated to pgstat
    q_values <- univariate_Logit(data=dataCancerImputed,</pre>
                                  Outcome="pgstat",
                                  pvalue = 0.05)
    qValueMatrix <- q_values
    idiqValueMatrix <- q_values</pre>
    barplot(-log(q_values),las=2,cex.names=0.4,ylab="-log(Q)",
    main="Association with PGStat: IDI Test")
    q_values <- univariate_Logit(data=dataCancerImputed,</pre>
                                 Outcome="pgstat",
                                  uniTest="zNRI",pvalue = 0.05)
    qValueMatrix <- cbind(idiqValueMatrix,q_values[names(idiqValueMatrix)])</pre>
```

```
q_values <- univariate_residual(data=dataCancerImputed,</pre>
                                      Outcome="pgstat",
                                      pvalue = 0.05,type="LOGIT")
        qValueMatrix <- cbind(qValueMatrix,q_values[names(idiqValueMatrix)])</pre>
        q_values <- univariate_tstudent(data=dataCancerImputed,</pre>
                                         Outcome="pgstat",
                                         pvalue = 0.05)
        qValueMatrix <- cbind(qValueMatrix,q_values[names(idiqValueMatrix)])</pre>
        q_values <- univariate_Wilcoxon(data=dataCancerImputed,</pre>
                                         Outcome="pgstat",
                                         pvalue = 0.05)
        qValueMatrix <- cbind(qValueMatrix,q_values[names(idiqValueMatrix)])</pre>
        q_values <- univariate_correlation(data=dataCancerImputed,</pre>
                                         Outcome="pgstat",
                                         pvalue = 0.05)
        qValueMatrix <- cbind(qValueMatrix,q_values[names(idiqValueMatrix)])</pre>
        q_values <- univariate_correlation(data=dataCancerImputed,</pre>
                                            Outcome="pgstat",
                                             pvalue = 0.05,
                                             method = "pearson")
        #The qValueMatrix has the qValues of all filter methods.
        qValueMatrix <- cbind(qValueMatrix,q_values[names(idiqValueMatrix)])</pre>
        colnames(qValueMatrix) <- c("IDI","NRI","F","t","W","K","P")</pre>
        #Do the log transform to display the heatmap
        qValueMatrix <- -log10(qValueMatrix)</pre>
        #the Heatmap of the q-values
        gplots::heatmap.2(qValueMatrix,Rowv = FALSE,dendrogram = "col",
        main = "Method q.values",cexRow = 0.4)
## End(Not run)
```

ForwardSelection.Model.Bin

IDI/NRI-based feature selection procedure for linear, logistic, and Cox proportional hazards regression models

## Description

This function performs a bootstrap sampling to rank the variables that statistically improve prediction. After the frequency rank, the function uses a forward selection procedure to create a final model, whose terms all have a significant contribution to the integrated discrimination improvement (IDI) or the net reclassification improvement (NRI). For each bootstrap, the IDI/NRI is computed and the variable with the largest statically significant IDI/NRI is added to the model. The procedure

is repeated at each bootstrap until no more variables can be inserted. The variables that enter the model are then counted, and the same procedure is repeated for the rest of the bootstrap loops. The frequency of variable-inclusion in the model is returned as well as a model that uses the frequency of inclusion.

#### Usage

#### **Arguments**

size	The number of candidate variables to be tested (the first size variables from
	. 13 1 . ()

variableList)

fraction The fraction of data (sampled with replacement) to be used as train

pvalue The maximum p-value, associated to either IDI or NRI, allowed for a term in

the model

loops The number of bootstrap loops

covariates A string of the type "1 + var1 + var2" that defines which variables will always

be included in the models (as covariates)

Outcome The name of the column in data that stores the variable to be predicted by the

model

variableList A data frame with two columns. The first one must have the names of the can-

didate variables and the other one the description of such variables

data A data frame where all variables are stored in different columns

maxTrainModelSize

Maximum number of terms that can be included in the model

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")

timeOutcome The name of the column in data that stores the time to event (needed only for a

Cox proportional hazards regression model fitting)

selectionType The type of index to be evaluated by the improveProb function (Hmisc pack-

age): z-score of IDI or of NRI

cores Cores to be used for parallel processing

randsize	the model size of a random outcome. If randsize is less than zero. It will estimate

the size

featureSize The original number of features to be explored in the data frame.

### Value

final.model	An object of class 1m, g1m, or coxph containing the final model
var.names	A vector with the names of the features that were included in the final model
formula	An object of class formula with the formula used to fit the final model
ranked.var	An array with the ranked frequencies of the features
z.selection	A vector in which each term represents the $z$ -score of the index defined in selectionType obtained with the Full model and the model without one term
formula.list	A list containing objects of class formula with the formulas used to fit the models found at each cycle
variableList	A list of variables used in the forward selection

### Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

#### References

Pencina, M. J., D'Agostino, R. B., & Vasan, R. S. (2008). Evaluating the added predictive ability of a new marker: from area under the ROC curve to reclassification and beyond. *Statistics in medicine* **27**(2), 157-172.

### See Also

ForwardSelection.Model.Res

ForwardSelection.Model.Res

NeRI-based feature selection procedure for linear, logistic, or Cox proportional hazards regression models

# Description

This function performs a bootstrap sampling to rank the most frequent variables that statistically aid the models by minimizing the residuals. After the frequency rank, the function uses a forward selection procedure to create a final model, whose terms all have a significant contribution to the net residual improvement (NeRI).

### **Usage**

## Arguments

size	The number of	candidate	variables to	he	tested (	(the	first	Si76	variables from	m
3120	THE HUILIDEL OF	candidate	variables u	, 00	icsicu (	(uic	mst	3120	variables iioi	.11

variableList)

fraction The fraction of data (sampled with replacement) to be used as train

pvalue The maximum p-value, associated to the NeRI, allowed for a term in the model

(controls the false selection rate)

loops The number of bootstrap loops

covariates A string of the type "1 + var1 + var2" that defines which variables will always

be included in the models (as covariates)

Outcome The name of the column in data that stores the variable to be predicted by the

model

variableList A data frame with two columns. The first one must have the names of the can-

didate variables and the other one the description of such variables

data A data frame where all variables are stored in different columns

 ${\tt maxTrainModelSize}$ 

Maximum number of terms that can be included in the model

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")

testType Type of non-parametric test to be evaluated by the improvedResiduals func-

tion: Binomial test ("Binomial"), Wilcoxon rank-sum test ("Wilcox"), Student's

t-test ("tStudent"), or F-test ("Ftest")

timeOutcome The name of the column in data that stores the time to event (needed only for a

Cox proportional hazards regression model fitting)

cores Cores to be used for parallel processing

randsize the model size of a random outcome. If randsize is less than zero. It will estimate

the size

featureSize The original number of features to be explored in the data frame.

### Value

final.model	An object of class 1m, g1m, or coxph containing the final model
var.names	A vector with the names of the features that were included in the final model
formula	An object of class formula with the formula used to fit the final model
ranked.var	An array with the ranked frequencies of the features
formula.list	A list containing objects of class formula with the formulas used to fit the models found at each cycle
variableList	A list of variables used in the forward selection

### Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

#### See Also

ForwardSelection.Model.Bin

FRESA.Model

Automated model selection

## **Description**

This function uses a wrapper procedure to select the best features of a non-penalized linear model that best predict the outcome, given the formula of an initial model template (linear, logistic, or Cox proportional hazards), an optimization procedure, and a data frame. A filter scheme may be enabled to reduce the search space of the wrapper procedure. The false selection rate may be empirically controlled by enabling bootstrapping, and model shrinkage can be evaluated by cross-validation.

## Usage

```
"Categorical",
                        "ZCategorical",
                        "RawZCategorical",
                        "RawTail",
                        "RawZTail",
                        "Tail",
                        "RawRaw"),
cateGroups = c(0.1, 0.9),
raw.dataFrame = NULL.
var.description = NULL,
testType = c("zIDI",
              "zNRI"
              "Binomial",
              "Wilcox",
             "tStudent"
             "Ftest"),
lambda="lambda.1se",
equivalent=FALSE,
bswimsCycles=20,
usrFitFun=NULL
)
```

### **Arguments**

formula An object of class formula with the formula to be fitted

data A data frame where all variables are stored in different columns

OptType Optimization type: Based on the integrated discrimination improvement (Bi-

nary) index for binary classification ("Binary"), or based on the net residual

improvement (NeRI) index for linear regression ("Residual")

pvalue The maximum p-value, associated to the testType, allowed for a term in the

model (it will control the false selection rate)

filter.p.value The maximum p-value, for a variable to be included to the feature selection

procedure

loops The number of bootstrap loops for the forward selection procedure

 ${\tt maxTrainModelSize}$ 

Maximum number of terms that can be included in the model

elimination.bootstrap.steps

The number of bootstrap loops for the backwards elimination procedure

bootstrap.steps

The number of bootstrap loops for the bootstrap validation procedure

print Logical. If TRUE, information will be displayed

plots Logical. If TRUE, plots are displayed

CVfolds The number of folds for the final cross-validation

repeats The number of times that the cross-validation procedure will be repeated

nk The number of neighbors used to generate a k-nearest neighbors (KNN) classi-

fication. If zero, k is set to the square root of the number of cases. If less than

zero, it will not perform the KNN classification

categorizationType

How variables will be analyzed: As given in data ("Raw"); broken into the *p*-value categories given by cateGroups ("Categorical"); broken into the *p*-value categories given by cateGroups, and weighted by the *z*-score ("ZCategorical"); broken into the *p*-value categories given by cateGroups, weighted by the *z*-score, plus the raw values ("RawZCategorical"); raw values, plus the tails ("RawTail"); or raw values, weighted by the *z*-score, plus the tails ("RawZTail")

cateGroups A vector of percentiles to be used for the categorization procedure

raw.dataFrame A data frame similar to data, but with unadjusted data, used to get the means

and variances of the unadjusted data

var.description

A vector of the same length as the number of columns of data, containing a

description of the variables

testType For an Binary-based optimization, the type of index to be evaluated by the

improveProb function (Hmisc package): z-value of Binary or of NRI. For a NeRI-based optimization, the type of non-parametric test to be evaluated by the improvedResiduals function: Binomial test ("Binomial"), Wilcoxon rank-sum

test ("Wilcox"), Student's t-test ("tStudent"), or F-test ("Ftest")

lambda The passed value to the s parameter of the glmnet cross validation coefficient

equivalent Is set to TRUE CV will compute the equivalent model

bswimsCycles The maximum number of models to be returned by BSWiMS.model

usrFitFun An optional user provided fitting function to be evaluated by the cross validation

procedure: fitting: usrFitFun(formula,data), with a predict function

#### **Details**

This important function of FRESA.CAD will model or cross validate the models. Given an outcome formula, and a data.frame this function will do an univariate analysis of the data (univariateRankVariables), then it will select the top ranked variables; after that it will select the model that best describes the outcome. At output it will return the bootstrapped performance of the model (bootstrapValidation\_Bin or bootstrapValidation\_Res). It can be set to report the cross-validation performance of the selection process which will return either a crossValidationFeatureSelection\_Bin or a crossValidationFeatureSelect object.

#### Value

BSWiMS.model An object of class lm, glm, or coxph containing the final model reducedModel The resulting object of the backward elimination procedure univariateAnalysis

A data frame with the results from the univariate analysis

forwardModel The resulting object of the feature selection function.

updatedforwardModel

The resulting object of the the update procedure

#### bootstrappedModel

The resulting object of the bootstrap procedure on final.model

cvObject The resulting object of the cross-validation procedure used.variables The number of terms that passed the filter procedure

call the function call

#### Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

#### References

Pencina, M. J., D'Agostino, R. B., & Vasan, R. S. (2008). Evaluating the added predictive ability of a new marker: from area under the ROC curve to reclassification and beyond. *Statistics in medicine* **27**(2), 157-172.

### **Examples**

```
## Not run:
# Start the graphics device driver to save all plots in a pdf format
pdf(file = "FRESA.Model.Example.pdf", width = 8, height = 6)
# Get the stage C prostate cancer data from the rpart package
data(stagec,package = "rpart")
options(na.action = 'na.pass')
stagec_mat <- cbind(pgstat = stagec$pgstat,</pre>
    pgtime = stagec$pgtime,
    as.data.frame(model.matrix(Surv(pgtime,pgstat) ~ .,stagec))[-1])
data(cancerVarNames)
dataCancerImputed <- nearestNeighborImpute(stagec_mat)</pre>
# Get a Cox proportional hazards model using:
# - The default parameters
md <- FRESA.Model(formula = Surv(pgtime, pgstat) ~ 1,</pre>
  data = dataCancerImputed,
  var.description = cancerVarNames[,2])
pt <- plot(md$bootstrappedModel)</pre>
sm <- summary(md$BSWiMS.model)</pre>
print(sm$coefficients)
# Get a 10 fold CV Cox proportional hazards model using:
# - Repeat 10 times de CV
md <- FRESA.Model(formula = Surv(pgtime, pgstat) ~ 1,</pre>
  data = dataCancerImputed, CVfolds = 10,
  repeats = 10,
  var.description = cancerVarNames[,2])
pt <- plotModels.ROC(md$cvObject$Models.testPrediction,theCVfolds = 10)</pre>
print(pt$predictionTable)
```

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```
pt <- plotModels.ROC(md$cvObject$LASSO.testPredictions,theCVfolds = 10)</pre>
pt <- plotModels.ROC(md$cvObject$KNN.testPrediction,theCVfolds = 10)</pre>
# Get a regression of the survival time
timeSubjects <- dataCancerImputed</pre>
timeSubjects$pgtime <- log(timeSubjects$pgtime)</pre>
md <- FRESA.Model(formula = pgtime ~ 1,</pre>
  data = timeSubjects,
  var.description = cancerVarNames[,2])
pt <- plot(md$bootstrappedModel)</pre>
sm <- summary(md$BSWiMS.model)</pre>
print(sm$coefficients)
# Get a logistic regression model using
# - The default parameters and removing time as possible predictor
dataCancerImputed$pgtime <- NULL
md <- FRESA.Model(formula = pgstat ~ 1,</pre>
  data = dataCancerImputed,
  var.description = cancerVarNames[,2])
pt <- plot(md$bootstrappedModel)</pre>
sm <- summary(md$BSWiMS.model)</pre>
print(sm$coefficients)
# Get a logistic regression model using:
# - residual-based optimization
md \leftarrow FRESA.Model(formula = pgstat \sim 1,
  data = dataCancerImputed,
  OptType = "Residual",
  var.description = cancerVarNames[,2])
pt <- plot(md$bootstrappedModel)</pre>
sm <- summary(md$BSWiMS.model)</pre>
print(sm$coefficients)
# Shut down the graphics device driver
dev.off()
## End(Not run)
```

FRESAScale

Data frame normalization

## **Description**

All features from the data will be normalized based on the distribution of the reference data-frame

### Usage

```
FRESAScale(data,refFrame=NULL,method=c("Norm","Order","RankInv"),
    refMean=NULL,refDisp=NULL)
```

#### **Arguments**

data The dataframe to be normalized

refFrame The reference frame that will be used to extract the feature distribution

method The normalization method. Norm: Mean and Std, Order: Median and IQR,

RankInv: rankInverseNormalDataFrame

refMean The mean vector of the reference frame

refDisp the data dispersion method of the reference frame

#### **Details**

The data-frame will be normalized according to the distribution of the reference frame or the mean vector(refMean) scaled by the reference dispersion vector(refDisp).

## Value

scaledData The scaled data set

refMean The mean or median vector of the reference frame refDisp The data dispersion (standard deviation or IQR)

## Author(s)

Jose G. Tamez-Pena

### See Also

rankInverseNormalDataFrame

getKNNpredictionFromFormula

Predict classification using KNN

# Description

This function will return the classification of the samples of a test set using a k-nearest neighbors (KNN) algorithm with euclidean distances, given a formula and a train set.

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### Usage

### **Arguments**

model.formula An object of class formula with the formula to be used

trainData A data frame with the data to train the model, where all variables are stored in

different columns

testData A data frame similar to trainData, but with the data set to be predicted

Outcome The name of the column in trainData that stores the variable to be predicted

by the model

nk The number of neighbors used to generate the KNN classification

#### Value

prediction A vector with the predicted outcome for the testData data set

The proportion of k neighbors that predicted the class to be the one being re-

ported in prediction

binProb The proportion of k neighbors that predicted the class of the outcome to be equal

to 1

featureList A vector with the names of the features used by the KNN procedure

### Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

#### See Also

```
predict.fitFRESA, knn
```

etSignature Returns a CV signature template
---

## Description

This function returns the matrix template [mean,sd,IQR] that maximizes the ROC AUC between cases of controls.

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### Usage

## Arguments

data A data frame whose rows contains the sampled "subject" data, and each column

is a feature.

varlist The varlist is a character vector that list all the features to be searched by the

Backward elimination forward selection procedure.

Outcome The name of the column that has the binary outcome. 1 for cases, 0 for controls

target The target template that will be used to maximize the AUC.

CVFolds The number of folds to be used

repeats how many times the CV procedure will be repeated

distanceFunction

The function to be used to compute the distance between the template and each

sample

... the parameters to be passed to the distance function

## Details

The function repeats full cycles of a Cross Validation (RCV) procedure. At each CV cycle the algorithm estimate the mean template and the distance between the template and the test samples. The ROC AUC is computed after the RCV is completed. A forward selection scheme. The set of features that maximize the AUC during the Forward loop is returned.

#### Value

 ${\tt controlTemplate}$ 

the control matrix with quantile probs[0.025, 0.25, 0.5, 0.75, 0.975] that maximized

the AUC (template of controls subjects)

caseTamplate the case matrix with quantile probs[0.025,0.25,0.5,0.75,0.975] that maximized

the AUC (template of case subjects)

AUCevolution The AUC value at each cycle

featureSizeEvolution

The number of features at each cycle

featureList The final list of features

getVar.Bin

CVOutput A data frame with four columns: ID, Outcome, Case Distances, Control Dis-

tances. Each row contains the CV test results

MaxAUC The maximum ROC AUC

### Author(s)

Jose G. Tamez-Pena

getVar.Bin	Analysis of the effect of each term of a binary classification model by
	analysing its reclassification performance

# Description

This function provides an analysis of the effect of each model term by comparing the binary classification performance between the Full model and the model without each term. The model is fitted using the train data set, but probabilities are predicted for the train and test data sets. Reclassification improvement is evaluated using the improveProb function (Hmisc package). Additionally, the integrated discrimination improvement (IDI) and the net reclassification improvement (NRI) of each model term are reported.

### Usage

## **Arguments**

object	An object of class 1m, g1m, or coxph containing the model to be analysed
data	A data frame where all variables are stored in different columns
Outcome	The name of the column in data that stores the variable to be predicted by the model
type	$Fit \ type: \ Logistic \ ("LOGIT"), \ linear \ ("LM"), \ or \ Cox \ proportional \ hazards \ ("COX")$
testData	A data frame similar to data, but with a data set to be independently tested. If NULL, data will be used.
callCpp	is set to true it will use the c++ implementation of improvement.

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## Value

z.IDIs	A vector in which each term represents the <i>z</i> -score of the IDI obtained with the Full model and the model without one term	
z.NRIs	A vector in which each term represents the <i>z</i> -score of the NRI obtained with the Full model and the model without one term	
IDIs	A vector in which each term represents the IDI obtained with the Full model and the model without one term	
NRIs	A vector in which each term represents the NRI obtained with the Full model and the model without one term	
testData.z.IDIs		
	A vector similar to z.IDIs, where values were estimated in testdata	
testData.z.NRIs		
	A vector similar to z.NRIs, where values were estimated in testdata	
testData.IDIs	A vector similar to IDIs, where values were estimated in testdata	
testData.NRIs uniTrainAccura	A vector similar to NRIs, where values were estimated in testdata cy	
	A vector with the univariate train accuracy of each model variable	
uniTestAccuracy		
	A vector with the univariate test accuracy of each model variable	

#### Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

## References

Pencina, M. J., D'Agostino, R. B., & Vasan, R. S. (2008). Evaluating the added predictive ability of a new marker: from area under the ROC curve to reclassification and beyond. Statistics in medicine **27**(2), 157-172.

## See Also

getVar.Res

getVar.Res	Analysis of the effect of each term of a linear regression model by analysing its residuals

## **Description**

This function provides an analysis of the effect of each model term by comparing the residuals of the Full model and the model without each term. The model is fitted using the train data set, but analysis of residual improvement is done on the train and test data sets. Residuals are compared by a paired t-test, a paired Wilcoxon rank-sum test, a binomial sign test and the F-test on residual variance. Additionally, the net residual improvement (NeRI) of each model term is reported.

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#### Usage

#### Arguments

object An object of class 1m, g1m, or coxph containing the model to be analyzed

data A data frame where all variables are stored in different columns

Outcome The name of the column in data that stores the variable to be predicted by the

model

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")

testData A data frame similar to data, but with a data set to be independently tested. If

NULL, data will be used.

callCpp is set to true it will use the c++ implementation of residual improvement.

#### Value

tP. value A vector in which each element represents the single sided p-value of the paired

t-test comparing the absolute values of the residuals obtained with the Full

model and the model without one term

BinP. value A vector in which each element represents the p-value associated with a signifi-

cant improvement in residuals according to the binomial sign test

WilcoxP. value A vector in which each element represents the single sided p-value of the Wilcoxon

rank-sum test comparing the absolute values of the residuals obtained with the

Full model and the model without one term

FP. value A vector in which each element represents the single sided p-value of the F-test

comparing the residual variances of the residuals obtained with the Full model

and the model without one term

NeRIs A vector in which each element represents the net residual improvement be-

tween the Full model and the model without one term

testData.tP.value

A vector similar to tP. value, where values were estimated in testdata

testData.BinP.value

A vector similar to BinP. value, where values were estimated in testdata

testData.WilcoxP.value

A vector similar to WilcoxP. value, where values were estimated in testdata

testData.FP.value

A vector similar to FP. value, where values were estimated in testdata

testData.NeRIs A vector similar to NeRIs, where values were estimated in testdata

unitestMSE A vector with the univariate residual mean sum of squares of each model vari-

able on the test data

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unitrainMSE A vector with the univariate residual mean sum of squares of each model vari-

able on the train data

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

#### See Also

```
getVar.Bin
```

heatMaps

Plot a heat map of selected variables

## Description

This function creates a heat map for a data set based on a univariate or frequency ranking

## Usage

## **Arguments**

variableList A data frame with two columns. The first	rst one must have the names of the can-
---	---

didate variables and the other one the description of such variables

varRank A data frame with the name of the variables in variableList, ranked according

to a certain metric

Outcome The name of the column in data that stores the variable to be predicted by the

model

data A data frame where all variables are stored in different columns

title The title of the plot

hCluster Logical. If TRUE, variables will be clustered

prediction A vector with a prediction for each subject, which will be used to rank the heat

map

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Scale An optional value to force the data normalization outcome

theFiveColors the colors of the heatmap
outcomeColors the colors of the outcome bar

transpose the heatmap

. . . additional parameters for the heatmap.2 function

#### Value

dataMatrix A matrix with all the terms in data described by variableList

orderMatrix A matrix similar to dataMatrix, where rows are ordered according to the outcome

heatMap A list with the values returned by the heatmap. 2 function (gplots package)

#### Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

## **Examples**

```
## Not run:
library(rpart)
data(stagec)
# Set the options to keep the na
options(na.action='na.pass')
# create a model matrix with all the NA values imputed
stagecImputed \leftarrow as.data.frame(nearestNeighborImpute(model.matrix(~.,stagec)[,-1]))
# the simple heat map
hm <- heatMaps(Outcome="pgstat",data=stagecImputed,title="Heat Map",Scale=TRUE)</pre>
# transposing the heat-map with clustered colums
hm <- heatMaps(Outcome="pgstat",data=stagecImputed,title="Heat Map",Scale=TRUE,</pre>
   transpose= TRUE,hCluster = TRUE,
   cexRow=0.80,cexCol=0.50,srtCol=35)
# transposing the heat-map with reds and time to event as outcome
hm <- heatMaps(Outcome="pgtime",data=stagecImputed,title="Heat Map",Scale=TRUE,
   theFiveColors=c("black","red","orange","yellow","white"),
  cexRow=0.50,cexCol=0.80,srtCol=35)
## End(Not run)
```

improvedResiduals 65

improvedResiduals	Estimate the significance of the reduction of predicted residuals

## **Description**

This function will test the hypothesis that, given a set of two residuals (new vs. old), the new ones are better than the old ones as measured with non-parametric tests. Four p-values are provided: one for the binomial sign test, one for the paired Wilcoxon rank-sum test, one for the paired t-test, and one for the F-test. The proportion of subjects that improved their residuals, the proportion that worsen their residuals, and the net residual improvement (NeRI) will be returned.

### Usage

#### Arguments

oldResiduals	A vector with the residuals of the original model
newResiduals	A vector with the residuals of the new model
testType	Type of non-parametric test to be evaluated: Binomial test ("Binomial"), Wilcoxon

rank-sum test ("Wilcox"), Student's *t*-test ("tStudent"), or *F*-test ("Ftest")

#### Details

This function will test the hypothesis that the new residuals are "better" than the old residuals. To test this hypothesis, four types of tests are performed:

- 1. The paired *t*-test, which compares the absolute value of the residuals
- 2. The paired Wilcoxon rank-sum test, which compares the absolute value of residuals
- 3. The binomial sign test, which evaluates whether the number of subjects with improved residuals is greater than the number of subjects with worsened residuals
- 4. The *F*-test, which is the standard test for evaluating whether the residual variance is "better" in the new residuals.

The proportions of subjects that improved and worsen their residuals are returned, and so is the NeRI.

## Value

p1	Proportion of subjects that improved their residuals to the total number of subjects
p2	Proportion of subjects that worsen their residuals to the total number of subjects
NeRI	The net residual improvement (p1-p2)
p.value	The one tail p-value of the test specified in testType

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BinP. value The *p*-value associated with a significant improvement in residuals

WilcoxP. value The single sided *p*-value of the Wilcoxon rank-sum test comparing the absolute

values of the new and old residuals

tP. value The single sided p-value of the paired t-test comparing the absolute values of

the new and old residuals

FP. value The single sided p-value of the F-test comparing the residual variances of the

new and old residuals

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

KNN\_method KNN Setup for KNN prediction

## **Description**

Prepares the KNN function to be used to predict the class of a new set

### Usage

```
KNN_method(formula = formula,data=NULL,...)
```

### **Arguments**

formula the base formula to extract the outcome

data the data to be used for training the KNN method

... parameters for the KNN function and the data scaling method

### Value

trainData The data frame to be used to train the KNN prediction

scaledData The scaled training set

classData A vector with the outcome to be used by the KNN function

outcome The name of the outcome

usedFeatures The list of features to be used by the KNN method mean\_col A vector with the mean of each training feature disp\_col A vector with the dispesion of each training feature

kn The number of neigbors to be used by the predict function scaleMethod The scaling method to be used by FRESAScale() function

## Author(s)

Jose G. Tamez-Pena

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### See Also

```
class::knn,FRESAScale
```

LASS0

CV LASSO fit with s="lambda.min" or s="lambda.1se"

# Description

Fits a glmnet::cv.glmnet object to the data, and sets the prediction to use the features that created the minimum CV error or one SE.

## Usage

```
LASSO_MIN(formula = formula,data=NULL,...)
LASSO_1SE(formula = formula,data=NULL,...)
```

# Arguments

formula The base formula to extract the outcome
data The data to be used for training the KNN method
... Parameters to be passed to the cv.glmnet function

### Value

fit The glmnet::cv.glmnet fitted object

s The s. Set to "lambda.min" or "lambda.1se" for prediction

formula The formula

outcome The name of the outcome

usedFeatures The list of features to be used

# Author(s)

```
Jose G. Tamez-Pena
```

#### See Also

```
glmnet::cv.glmnet
```

listTopCorrelatedVariables

List the variables that are highly correlated with each other

## **Description**

This function computes the Pearson, Spearman, or Kendall correlation for each specified variable in the data set and returns a list of the variables that are correlated to them. It also provides a short variable list without the highly correlated variables.

# Usage

### **Arguments**

variableList A data frame with two columns. The first one must have the names of the candidate variables and the other one the description of such variables

data A data frame where all variables are stored in different columns

pvalue The maximum p-value, associated to method, allowed for a pair of variables to

be defined as significantly correlated

corthreshold The minimum correlation score, associated to method, allowed for a pair of

variables to be defined as significantly correlated

method Correlation method: Pearson product-moment ("pearson"), Spearman's rank

("spearman"), or Kendall rank ("kendall")

#### Value

correlated.variables

A data frame with two columns:

1. cor.var.names: The variables that are correlated

2. cor.var.value: The correlation value

short.list A vector with a list of variables that are not correlated to each other. For every

correlated pair, only the variable that first entered the correlation analysis was

kept

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

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### **Examples**

```
## Not run:
# Start the graphics device driver to save all plots in a pdf format
pdf(file = "Example.pdf")
# Get the stage C prostate cancer data from the rpart package
library(rpart)
data(stagec)
# Split the stages into several columns
dataCancer <- cbind(stagec[,c(1:3,5:6)],</pre>
                    gleason4 = 1*(stagec[,7] == 4),
                    gleason5 = 1*(stagec[,7] == 5),
                    gleason6 = 1*(stagec[,7] == 6),
                    gleason7 = 1*(stagec[,7] == 7),
                    gleason8 = 1*(stagec[,7] == 8),
                    gleason910 = 1*(stagec[,7] >= 9),
                    eet = 1*(stagec[,4] == 2),
                    diploid = 1*(stagec[,8] == "diploid"),
                    tetraploid = 1*(stagec[,8] == "tetraploid"),
                    notAneuploid = 1-1*(stagec[,8] == "aneuploid"))
# Remove the incomplete cases
dataCancer <- dataCancer[complete.cases(dataCancer),]</pre>
# Load a pre-stablished data frame with the names and descriptions of all variables
data(cancerVarNames)
# Get the variables that have a correlation coefficient larger
# than 0.65 at a p-value of 0.05
cor <- listTopCorrelatedVariables(variableList = cancerVarNames,</pre>
                                   data = dataCancer,
                                   pvalue = 0.05,
                                   corthreshold = 0.65,
                                   method = "pearson")
# Shut down the graphics device driver
dev.off()
## End(Not run)
```

LM\_RIDGE\_MIN

Ridge Linear Models

## **Description**

FRESA wrapper to fit MASS::lm.ridge object to the data and returning the coef with minimum GCV

# Usage

```
LM_RIDGE_MIN(formula = formula,data=NULL,...)
```

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## Arguments

formula The base formula to extract the outcome data The data to be used for training the method

. . . Parameters to be passed to the MASS::lm.ridge function

### Value

fit The MASS::lm.ridge fitted object

## Author(s)

Jose G. Tamez-Pena

#### See Also

MASS::lm.ridge

modelFitting

Fit a model to the data

## **Description**

This function fits a linear, logistic, or Cox proportional hazards regression model to given data

## Usage

# Arguments

model.formula An object of class formula with the formula to be used data A data frame where all variables are stored in different columns

A data frame where all variables are stored in different columns

type Fit type: Logistic ("LOGIT"), linear ("LM"), Cox proportional hazards ("COX")

or "SVM"

fitFRESA if true it will perform use the FRESA cpp code for fitting . . . Additional parameters for fitting a default glm object

# Value

A fitted model of the type defined in type

#### Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

mRMR.classic\_FRESA

FRESA.CAD wrapper of mRMRe::mRMR.classic

## **Description**

Returns the positive MI-scored set of maximum relevance minimum redundancy (mRMR) features returned by the mMRM.classic function

### Usage

```
mRMR.classic_FRESA(data=NULL, Outcome=NULL, feature_count=0,...)
```

# Arguments

data The data frame

Outcome The outcome feature

Extra parameters to be passed to the mRMRe::mMRM.classic function

## Value

Named vector with the MI-score of the selected features

## Author(s)

Jose G. Tamez-Pena

## See Also

mRMRe::mRMR.classic

NAIVE\_BAYES

Naive Bayes Modeling

## **Description**

FRESA wrapper to fit naivebayes::naive\_bayes object to the data

### Usage

```
NAIVE_BAYES(formula = formula,data=NULL,...)
```

### **Arguments**

formula The base formula to extract the outcome data The data to be used for training the method

. . . Parameters to be passed to the naivebayes::naive\_bayes function

#### Value

fit The naivebayes::naive\_bayes fitted object

## Author(s)

Jose G. Tamez-Pena

### See Also

naivebayes::naive\_bayes

nearestNeighborImpute nearest neighbor NA imputation

### **Description**

The function will replace any NA present in the data-frame with the median values of the nearest neighbours.

# Usage

# Arguments

tobeimputed a data frame with missing values (NA values)

referenceSet An optional data frame with a set of complete observations. This data frame will

be added to the search set

distol The tolerance used to define if a particular set of row observations is similar to

the minimum distance

#### Details

This function will find any NA present in the data set and it will search for the row set of complete observations that have the closest IQR normalized Manhattan distance to the row with missing values. If a set of rows have similar minimum distances (toldis\*(minimum distance) > row set distance) the median value will be used.

## Value

A data frame, where each NA has been replaced with the value of the nearest neighbors

## Author(s)

```
Jose G. Tamez-Pena
```

## **Examples**

```
## Not run:
# Get the stage C prostate cancer data from the rpart package
library(rpart)
data(stagec)
# Set the options to keep the na
options(na.action='na.pass')
# create a model matrix with all the NA values imputed
stagecImputed <- nearestNeighborImpute(model.matrix(~.,stagec)[,-1])
## End(Not run)</pre>
```

```
plot.bootstrapValidation_Bin
```

Plot ROC curves of bootstrap results

# **Description**

This function plots ROC curves and a Kaplan-Meier curve (when fitting a Cox proportional hazards regression model) of a bootstrapped model.

## Usage

## **Arguments**

X	A bootstrapValidation_Bin object
xlab	The label of the <i>x</i> -axis
ylab	The label of the <i>y</i> -axis
strata.levels	stratification level for the Kaplan-Meier plots
main	Main Plot title

cex The text cex

... Additional parameters for the generic plot function

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

## See Also

```
plot.bootstrapValidation_Res
```

```
plot.bootstrapValidation_Res
```

Plot ROC curves of bootstrap results

# Description

This function plots ROC curves and a Kaplan-Meier curve (when fitting a Cox proportional hazards regression model) of a bootstrapped model.

## Usage

## **Arguments**

```
    x A bootstrapValidation_Res object
    xlab The label of the x-axis
    ylab The label of the y-axis
    ... Additional parameters for the plot
```

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

## See Also

```
plot.bootstrapValidation_Bin
```

## **Description**

The different output metrics of the benchmark (BinaryBenchmark,RegresionBenchmark or OrdinalBenchmark) are plotted. It returns data matrices that describe the different plots.

## Usage

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

## **Arguments**

x A FRESA\_benchmark object

... Additional parameters for the generic plot function

#### Value

metrics The model test performance based on the predictionStats\_binary, predictionStats\_regression

or predictionStats\_ordinal functions.

barPlotsCI The barPlotCiError outputs for each metric.

metrics\_filter The model test performance for each filter method based on the predictionStats\_binary

function.

barPlotsCI\_filter

The barPlotCiError outputs for each metric on the filter methods

minMaxMetrics Reports the min and maximum value for each reported metric.

# Author(s)

```
Jose G. Tamez-Pena
```

#### See Also

BinaryBenchmark, predictionStats\_binary

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plotModels.ROC

Plot test ROC curves of each cross-validation model

## **Description**

This function plots test ROC curves of each model found in the cross validation process. It will also aggregate the models into a single prediction performance, plotting the resulting ROC curve (models coherence). Furthermore, it will plot the mean sensitivity for a given set of specificities.

#### Usage

```
plotModels.ROC(modelPredictions,
    number.of.models=0,
    specificities=c(0.975,0.95,0.90,0.80,0.70,0.60,0.50,0.40,0.30,0.20,0.10,0.05),
    theCVfolds=1,
    predictor="Prediction",
cex=1.0,
    ...)
```

## **Arguments**

modelPredictions

A data frame returned by the crossValidationFeatureSelection\_Bin function, either the Models.testPrediction, the FullBSWiMS.testPrediction, the Models.CVtestPredictions, the TestRetrained.blindPredictions, the KNN.testPrediction, or the LASSO.testPredictions value

number.of.models

The maximum number of models to plot

specificities Vector containing the specificities at which the ROC sensitivities will be calcu-

lated

the CV folds The number of folds performed in a Cross-validation experiment

predictor The name of the column to be plotted

cex Controlling the font size of the text inside the plots

... Additional parameters for the roc function (pROC package)

#### Value

ROC. AUCS A vector with the AUC of each ROC

mean.sensitivities

A vector with the mean sensitivity at the specificities given by specificities model.sensitivities

A matrix where each row represents the sensitivity at the specificity given by specificities for a different ROC

specificities The specificities used to calculate the sensitivities

senAUC The AUC of the ROC curve that resulted from using mean.sensitivities

predict.fitFRESA 77

```
predictionTable
```

 $\label{thm:confusion} The \ confusion \ matrix \ between \ the \ outcome \ and \ the \ ensemble \ prediction$   $\ ensemble \ Prediction$ 

The ensemble (median prediction) of the repeated predictions

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

predict.fitFRESA

Linear or probabilistic prediction

# **Description**

This function returns the predicted outcome of a specific model. The model is used to generate linear predictions. The probabilistic values are generated using the logistic transformation on the linear predictors.

# Usage

# Arguments

object An object of class fitFRESA containing the model to be analyzed

A list with: testdata=testdata;predictType=c("linear","prob") and impute=FALSE.

If impute is set to TRUE it will use the object model to impute missing data

#### Value

A vector with the predicted values

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

#### See Also

```
nearestNeighborImpute
```

# Description

This function predicts the outcome from a FRESAKNN model

## Usage

```
## S3 method for class 'FRESAKNN'
predict(object,...)
```

## **Arguments**

object An object of class FRESAKNN containing the KNN train set

... A list with: testdata=testdata

#### Value

A vector of the predicted values

## Author(s)

```
Jose G. Tamez-Pena
```

# See Also

```
KNN_method, class::knn
```

```
predict.FRESAsignature
```

Predicts CV signature models

# **Description**

This function predicts the outcome from a FRESAsignature model

#### **Usage**

```
## S3 method for class 'FRESAsignature'
predict(object,...)
```

# Arguments

object An object of class FRESAsignature
... A list with: testdata=testdata

## Value

A vector of the predicted values

# Author(s)

Jose G. Tamez-Pena

## See Also

CVsignature,getSignature,signatureDistance

predict.FRESA\_LASSO

Predicts LASSO fitted objects

# Description

This function predicts the outcome from a FRESA\_LASSO fitted object

## Usage

```
## S3 method for class 'FRESA_LASSO'
predict(object,...)
```

# Arguments

object An object of class FRESA\_LASSO containing the model to be analyzed

... A list with: testdata=testdata

## Value

A vector of the predicted values

## Author(s)

Jose G. Tamez-Pena

# See Also

LASS0

```
predict.FRESA_NAIVEBAYES
```

Predicts NAIVE\_BAYES models

## **Description**

This function predicts the outcome from a FRESA\_NAIVEBAYES model

## Usage

```
## S3 method for class 'FRESA_NAIVEBAYES'
predict(object,...)
```

# **Arguments**

object An object of class FRESA\_NAIVEBAYES

. . . A list with: testdata=testdata

## Value

A vector of the predicted values

## Author(s)

Jose G. Tamez-Pena

# See Also

NAIVE\_BAYES

# **Description**

This function predicts the outcome from a LM\_RIDGE\_MIN model

#### Usage

```
## S3 method for class 'FRESA_RIDGE'
predict(object,...)
```

# Arguments

object An object of class FRESA\_RIDGE
... A list with: testdata=testdata

predictionStats 81

## Value

A vector of the predicted values

## Author(s)

Jose G. Tamez-Pena

## See Also

LM\_RIDGE\_MIN

predictionStats

Prediction Evaluation

## **Description**

This function returns the statistical metrics describing the association between model predictions and the ground truth outcome

#### Usage

```
predictionStats_binary(predictions, plotname="", center=FALSE,...)
predictionStats_regression(predictions, plotname="",...)
predictionStats_ordinal(predictions, plotname="",...)
```

# Arguments

predictions A matrix whose first column is the ground truth, and the second is the model prediction

The main title to be used by the plot function. If empty, no plot will be provided center

For binary predictions indicates if the prediction is around zero

... Extra parameters to be passed to the plot function.

#### **Details**

These functions will analyze the prediction outputs and will compare to the ground truth. The output will depend on the prediction task: Binary classification, Linear Regression or Ordinal regression.

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#### Value

accc The classification accuracy with its95% confidence intervals (95/

berror The balanced error rate with its 95%CI

aucs The ROC area under the curve (ROC AUC) of the binary classifier with its

95%CI

specificity The specificity with its 95%CI sensitivity The sensitivity with its 95%CI ROC.analysis The output of the ROC function

CM. analysis The output of the epiR::epi.tests function

corci the Pearson correlation with its 95%CI

biasci the regression bias and its 95%CI

RMSEci the root mean square error (RMSE) and its 95%CI

spearmanci the Spearman correlation and its 95%CI

MAEci the mean absolute difference(MAE) and its 95%CI

pearson the output of the cor.test function

Kendall the Kendall correlation and its 95%CI

Bias the ordinal regression bias and its 95%CI

BMAE the balanced mean absolute difference for ordinal regression

class95ci the output of the bootstrapped estimation of accuracy, sensitivity, and ROC AUC

KendallTauB the output of the DescTools::KendallTauB function

Kappa.analysis the output of the irr::kappa2 function

## Author(s)

Jose G. Tamez-Pena

#### See Also

randomCV

randomCV Cross Validation of Prediction Models

## **Description**

The data set will be divided into a random train set and a test sets. The train set will be modeled by the user provided fitting method. Each fitting method must have a prediction function that will be used to predict the outcome of the test set.

randomCV 83

## Usage

#### **Arguments**

theData The data-frame for cross-validation

theOutcome The name of the outcome

fittingFunction

The fitting function used to model the data

trainFraction The percentage of the data to be used for training

repetitions The number of times that the CV process will be repeated

trainSampleSets

A set of train samples

featureSelectionFunction

The feature selection function to be used to filter out irrelevant features

featureSelection.control

The parameters to control the feature selection function

asFactor Set theOutcome as factor addNoise if TRUE will add 0.1

. . . Parameters to be passed to the fitting function

#### Value

testPredictions

All the predicted outcomes. Is a data matrix with three columns c("Outcome", "Model", "Prediction").

Each row has a prediction for a given test subject

trainPredictions

All the predicted outcomes in the train data set. Is a data matrix with three columns c("Outcome", "Model", "Prediction"). Each row has a prediction for a

given test subject

medianTest The median of the test prediction for each subject medianTrain The median of the prediction for each train subject

boxstaTest The statistics of the boxplot for test data boxstaTrain The statistics of the boxplot for train data

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trainSamplesSets

The id of the subjects used for training

selectedFeaturesSet

A list with all the features used at each training cycle

featureFrequency

A order table object that describes how many times a feature was selected.

jaccard The jaccard index of the features as well as the average number of features used

for prediction

theTimes The CPU time analysis

## Author(s)

Jose G. Tamez-Pena

# Examples

```
## Not run:
        ### Cross Validation Example ####
        # Start the graphics device driver to save all plots in a pdf format
        pdf(file = "CrossValidationExample.pdf", width = 8, height = 6)
        # Get the stage C prostate cancer data from the rpart package
        data(stagec,package = "rpart")
        # Prepare the data. Create a model matrix with interactions but no event time
        stagec$pgtime <- NULL</pre>
        stagec$eet <- as.factor(stagec$eet)</pre>
        options(na.action = 'na.pass')
        stagec_mat <- cbind(pgstat = stagec$pgstat,</pre>
                          as.data.frame(model.matrix(pgstat ~ .*.,stagec))[-1])
        fnames <- colnames(stagec_mat)</pre>
        fnames <- str_replace_all(fnames,":","__")</pre>
        colnames(stagec_mat) <- fnames</pre>
        # Impute the missing data
        dataCancerImputed <- nearestNeighborImpute(stagec_mat)</pre>
      dataCancerImputed[,1:ncol(dataCancerImputed)] <- sapply(dataCancerImputed,as.numeric)</pre>
        # Cross validating a Random Forest classifier
        cvRF <- randomCV(dataCancerImputed, "pgstat",</pre>
                          randomForest::randomForest,
                          trainFraction = 0.8,
                          repetitions = 10,
                          asFactor = TRUE);
        # Evaluate the prediction performance of the Random Forest classifier
        RFStats <- predictionStats_binary(cvRF$medianTest,</pre>
        plotname = "Random Forest",cex = 0.9);
        # Cross validating a BSWiMS with the same train/test set
```

```
cvBSWiMS <- randomCV(fittingFunction = BSWiMS.model,</pre>
         trainSampleSets = cvRF$trainSamplesSets);
        # Evaluate the prediction performance of the BSWiMS classifier
        BSWiMSStats <- predictionStats_binary(cvBSWiMS$medianTest,</pre>
        plotname = "BSWiMS",cex = 0.9);
        # Cross validating a LDA classifier with a t-student filter
        cvLDA <- randomCV(dataCancerImputed, "pgstat", MASS::lda,</pre>
                          trainSampleSets = cvRF$trainSamplesSets,
                           featureSelectionFunction = univariate_tstudent,
                          featureSelection.control = list(limit = 0.5,thr = 0.975));
        # Evaluate the prediction performance of the LDA classifier
        LDAStats <- predictionStats_binary(cvLDA$medianTest,plotname = "LDA",cex = 0.9);
      # Cross validating a QDA classifier with LDA t-student features and RF train/test set
        cvQDA <- randomCV(fittingFunction = MASS::qda,</pre>
                          trainSampleSets = cvRF$trainSamplesSets,
                           featureSelectionFunction = cvLDA$selectedFeaturesSet);
        # Evaluate the prediction performance of the QDA classifier
        QDAStats <- predictionStats_binary(cvQDA$medianTest,plotname = "QDA",cex = 0.9);
        #Create a barplot with 95
        errorciTable <- rbind(RFStats$berror,</pre>
        BSWiMSStats$berror,
        LDAStats$berror,
         QDAStats$berror)
        bpCI <- barPlotCiError(as.matrix(errorciTable), metricname = "Balanced Error",</pre>
                             thesets = c("Classifier Method"),
                             themethod = c("RF", "BSWiMS", "LDA", "QDA"),
                             main = "Balanced Error",
                             offsets = c(0.5, 0.15),
                             scoreDirection = "<",</pre>
                             ho = 0.5,
                             args.legend = list(bg = "white",x = "topright"),
                             col = terrain.colors(4));
        dev.off()
## End(Not run)
```

 ${\tt rankInverseNormalDataFrame}$ 

rank-based inverse normal transformation of the data

## **Description**

This function takes a data frame and a reference control population to return a *z*-transformed data set conditioned to the reference population. Each sample data for each feature column in the data frame is conditionally *z*-transformed using a rank-based inverse normal transformation, based on the rank of the sample in the reference frame.

# Usage

## **Arguments**

variableList A data frame with two columns. The first one must have the names of the can-

didate variables and the other one the description of such variables

data A data frame where all variables are stored in different columns referenceframe A data frame similar to data, but with only the control population

strata The name of the column in data that stores the variable that will be used to

stratify the model

#### Value

A data frame where each observation has been conditionally z-transformed, given control data

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

## **Examples**

```
## Not run:
# Start the graphics device driver to save all plots in a pdf format
pdf(file = "Example.pdf")
# Get the stage C prostate cancer data from the rpart package
library(rpart)
data(stagec)
# Split the stages into several columns
dataCancer <- cbind(stagec[,c(1:3,5:6)],</pre>
                    gleason4 = 1*(stagec[,7] == 4),
                    gleason5 = 1*(stagec[,7] == 5),
                    gleason6 = 1*(stagec[,7] == 6),
                    gleason7 = 1*(stagec[,7] == 7),
                    gleason8 = 1*(stagec[,7] == 8),
                    gleason910 = 1*(stagec[,7] >= 9),
                    eet = 1*(stagec[,4] == 2),
                    diploid = 1*(stagec[,8] == "diploid"),
                    tetraploid = 1*(stagec[,8] == "tetraploid"),
                    notAneuploid = 1-1*(stagec[,8] == "aneuploid"))
```

reportEquivalentVariables

Report the set of variables that will perform an equivalent IDI discriminant function

## **Description**

Given a model, this function will report a data frame with all the variables that may be interchanged in the model without affecting its classification performance. For each variable in the model, this function will loop all candidate variables and report all of which result in an equivalent or better zIDI than the original model.

## Usage

# Arguments

object	An object of class 1m, g1m, or coxph containing the model to be analyzed
pvalue	The maximum $p$ -value, associated to the IDI , allowed for a pair of variables to be considered equivalent
data	A data frame where all variables are stored in different columns
variableList	A data frame with two columns. The first one must have the names of the candidate variables and the other one the description of such variables

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Outcome The name of the column in data that stores the variable to be predicted by the

model

timeOutcome The name of the column in data that stores the time to event

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")

description The name of the column in variableList that stores the variable description

method The method used by the p-value adjustment algorithm osize The number of features used for p-value adjustment fitFRESA if TRUE it will use the cpp based fitting method

#### Value

pvalueList A list with all the unadjusted p-values of the equivalent features per model vari-

able

equivalentMatrix

A data frame with three columns. The first column is the original variable of the model. The second column lists all variables that, if interchanged, will not statistically affect the performance of the model. The third column lists the

corresponding z-scores of the IDI for each equivalent variable.

formulaList a character vector with all the equivalent formulas

equivalentModel

a bagged model that used all the equivalent formulas. The model size is limited

by the number of observations

## Author(s)

Jose G. Tamez-Pena

residualForFRESA Return residuals from prediction

## **Description**

Given a model and a new data set, this function will return the residuals of the predicted values. When dealing with a Cox proportional hazards regression model, the function will return the Martingale residuals.

# Usage

signatureDistance 89

## **Arguments**

object An object of class 1m, g1m, or coxph containing the model to be analyzed

testData A data frame where all variables are stored in different columns, with the data

set to be predicted

Outcome The name of the column in data that stores the variable to be predicted by the

model

eta The weight of the contribution of the Martingale residuals, or 1 - the weight of

the contribution of the classification residuals (only needed if object is of class

coxph)

#### Value

A vector with the residuals (i.e. the differences between the predicted and the real outcome)

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

signatureDistance Distance to the signature template

## **Description**

This function returns a normalized distance to the signature template

#### Usage

#### **Arguments**

template A list with a template matrix of the signature described with quantiles = [0.025, 0.25, 0.5, 0.75, 0.975]

data A data frame that will be used to compute the distance

method The distance method.

# **Details**

The distance to the template: "pearson", "spearman" and "kendall" distances are computed using the correlation function i.e. 1-r. "RSS" distance is the root sum square distance "MAN" Manhattan. The standardized L^1 distance

#### Value

result the distance to the template

#### Author(s)

Jose G. Tamez-Pena

summary.bootstrapValidation\_Bin

Generate a report of the results obtained using the bootstrapValidation\_Bin function

## **Description**

This function prints two tables describing the results of the bootstrap-based validation of binary classification models. The first table reports the accuracy, sensitivity, specificity and area under the ROC curve (AUC) of the train and test data set, along with their confidence intervals. The second table reports the model coefficients and their corresponding integrated discrimination improvement (IDI) and net reclassification improvement (NRI) values.

## Usage

## **Arguments**

object An object of class bootstrapValidation\_Bin

... Additional parameters for the generic summary function

#### Value

performance A vector describing the results of the bootstrapping procedure

summary An object of class summary.lm, summary.glm, or summary.coxph containing a

summary of the analyzed model

coef A matrix with the coefficients, IDI, NRI, and the 95% confidence intervals ob-

tained via bootstrapping

performance.table

A matrix with the tabulated results of the blind test accuracy, sensitivity, speci-

ficities, and area under the ROC curve

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

summary.fitFRESA 91

## See Also

summaryReport

summary.fitFRESA

Returns the summary of the fit

## **Description**

Returns a summary of fitted model created by the modelFitting function with the fitFRESA parameter set to TRUE

# Usage

```
## $3 method for class 'fitFRESA'
summary(object,
type=c("Improvement","Residual"),
ci=c(0.025,0.975),
data=NULL,
...)
```

# **Arguments**

 ${\tt object} \qquad \qquad {\tt fitted} \ {\tt model} \ {\tt with} \ {\tt the} \ {\tt modelFitting} \ {\tt function}$ 

type the type of coefficient estimation

ci lower and upper limit of the ci estimation

data the data to be used for 95

... parameters of the boostrap method

## Value

a list with the analysis results.

## Author(s)

Jose G. Tamez-Pena

# See Also

modelFitting,bootstrapValidation\_Bin,bootstrapValidation\_Res

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correlation analysis	summaryReport	Report the univariate analysis, the cross-validation analysis and the correlation analysis
----------------------	---------------	--

## **Description**

This function takes the variables of the cross-validation analysis and extracts the results from the univariate and correlation analyses. Then, it prints the cross-validation results, the univariate analysis results, and the correlated variables. As output, it returns a list of each one of these results.

## Usage

#### **Arguments**

univariateObject

A data frame that contains the results of the univariateRankVariables function

summaryBootstrap

A list that contains the results of the  $summary.bootstrapValidation\_Bin function$ 

listOfCorrelatedVariables

A matrix that contains the correlated.variables value from the results obtained with the listTopCorrelatedVariables function

digits The number of significant digits to be used in the print function

## Value

performance.table

A matrix with the tabulated results of the blind test accuracy, sensitivity, specificities, and area under the ROC curve

coefStats A data frame that lists all the model features along with its univariate statistics

and bootstrapped coefficients

cor.varibles A matrix that lists all the features that are correlated to the model variables

# Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

# See Also

```
summary.bootstrap Validation\_Bin
```

timeSerieAnalysis 93

timeSerieAnalysis

Fit the listed time series variables to a given model

## **Description**

This function plots the time evolution and does a longitudinal analysis of time dependent features. Features listed are fitted to the provided time model (mixed effect model) with a generalized least squares (GLS) procedure. As output, it returns the coefficients, standard errors, *t*-values, and corresponding *p*-values.

# Usage

## **Arguments**

catgo.names

variableList	A data frame with two columns. The first one must have the names of the candidate variables and the other one the description of such variables
baseModel	A string of the type $"1 + var1 + var2"$ that defines the model to which variables will be fitted
data	A data frame where all variables are stored in different columns
timevar	The name of the column in data that stores the visit ID
contime	The name of the column in data that stores the continuous time (e.g. days or months) that has elapsed since the baseline visit
Outcome	The name of the column in data that stores an optional binary outcome that may be used to show the stratified analysis
description	The name of the column in variableList that stores the variable description
Ptoshow	Index of the <i>p</i> -values to be shown in the plot
plegend	Legend of the <i>p</i> -values to be shown in the plot
timesign	The direction of the arrow of time

Additional parameters to be passed to the gls function

The legends of the binary categories

94 uniRankVar

#### **Details**

This function will plot the evolution of the mean value of the listed variables with its corresponding error bars. Then, it will fit the data to the provided time model with a GLS procedure and it will plot the fitted values. If a binary variable was provided, the plots will contain the case and control data. As output, the function will return the model coefficients and their corresponding *t*-values, and the standard errors and their associated *p*-values.

#### Value

coef A matrix with the coefficients of the GLS fitting

std. Errors A matrix with the standardized error of each coefficient

t.values A matrix with the *t*-value of each coefficient p.values A matrix with the *p*-value of each coefficient sigmas The root-mean-square error of the fitting

#### Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

uniRankVar Univariate analysis of features (additional values returned)

## Description

This function reports the mean and standard deviation for each feature in a model, and ranks them according to a user-specified score. Additionally, it does a Kolmogorov-Smirnov (KS) test on the raw and *z*-standardized data. It also reports the raw and *z*-standardized *t*-test score, the *p*-value of the Wilcoxon rank-sum test, the integrated discrimination improvement (IDI), the net reclassification improvement (NRI), the net residual improvement (NeRI), and the area under the ROC curve (AUC). Furthermore, it reports the *z*-value of the variable significance on the fitted model. Besides reporting an ordered data frame, this function returns all arguments as values, so that the results can be updates with the update.uniRankVar if needed.

## Usage

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```
"RawRaw"),
type = c("LOGIT", "LM",
                         "COX"),
rankingTest = c("zIDI",
                 "zNRI".
                "IDI",
                "NRI",
                "NeRI",
                "Ztest"
                "AUC",
                "CStat"
                "Kendall"),
cateGroups = c(0.1, 0.9),
raw.dataFrame = NULL,
description = ".",
uniType = c("Binary", "Regression"),
FullAnalysis=TRUE,
acovariates = NULL,
timeOutcome = NULL)
```

#### **Arguments**

variableList A data frame with two columns. The first one must have the names of the can-

didate variables and the other one the description of such variables

formula An object of class formula with the formula to be fitted

Outcome The name of the column in data that stores an optional binary outcome that may

be used to show the stratified analysis

data A data frame where all variables are stored in different columns

 ${\tt categorizationType}$ 

How variables will be analyzed: As given in data ("Raw"); broken into the *p*-value categories given by cateGroups ("Categorical"); broken into the *p*-value categories given by cateGroups, and weighted by the *z*-score ("ZCategorical"); broken into the *p*-value categories given by cateGroups, weighted by the *z*-score, plus the raw values ("RawZCategorical"); raw values, plus the tails ("RawTail"); or raw values, weighted by the *z*-score, plus the tails ("RawZTail")

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")

rankingTest Variables will be ranked based on: The z-score of the IDI ("zIDI"), the z-score of

the NRI ("zNRI"), the IDI ("IDI"), the NRI ("NRI"), the NeRI ("NeRI"), the z-score of the model fit ("Ztest"), the AUC ("AUC"), the Somers' rank correlation

("Cstat"), or the Kendall rank correlation ("Kendall")

cateGroups A vector of percentiles to be used for the categorization procedure

raw.dataFrame A data frame similar to data, but with unadjusted data, used to get the means

and variances of the unadjusted data

description The name of the column in variableList that stores the variable description

uniType Type of univariate analysis: Binary classification ("Binary") or regression ("Re-

gression")

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FullAnalysis If FALSE it will only order the features according to its z-statistics of the linear

model

acovariates the list of covariates

timeOutcome the name of the Time to event feature

#### **Details**

This function will create valid dummy categorical variables if, and only if, data has been *z*-standardized. The *p*-values provided in cateGroups will be converted to its corresponding *z*-score, which will then be used to create the categories. If non *z*-standardized data were to be used, the categorization analysis would return wrong results.

## Value

orderframe A sorted list of model variables stored in a data frame

formula The argument formula
Outcome The argument Outcome
data The argument data

categorizationType

The  $argument\ categorizationType$ 

type The argument type

rankingTest The argument rankingTest
cateGroups The argument cateGroups
raw.dataFrame The argument raw.dataFrame

description The argument description

uniType The argument uniType

# Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

## References

Pencina, M. J., D'Agostino, R. B., & Vasan, R. S. (2008). Evaluating the added predictive ability of a new marker: from area under the ROC curve to reclassification and beyond. *Statistics in medicine* **27**(2), 157-172.

## See Also

update.uniRankVar, univariateRankVariables

univariateRankVariables

Univariate analysis of features

## **Description**

This function reports the mean and standard deviation for each feature in a model, and ranks them according to a user-specified score. Additionally, it does a Kolmogorov-Smirnov (KS) test on the raw and z-standardized data. It also reports the raw and z-standardized t-test score, the p-value of the Wilcoxon rank-sum test, the integrated discrimination improvement (IDI), the net reclassification improvement (NRI), the net residual improvement (NeRI), and the area under the ROC curve (AUC). Furthermore, it reports the z-value of the variable significance on the fitted model.

## Usage

```
univariateRankVariables(variableList,
                         formula,
                         Outcome,
                         data,
                         categorizationType = c("Raw",
                                                  "Categorical",
                                                  "ZCategorical",
                                                  "RawZCategorical",
                                                 "RawTail",
                                                  "RawZTail",
                                                  "Tail",
                                                  "RawRaw"),
                         type = c("LOGIT", "LM", "COX"),
                         rankingTest = c("zIDI",
                                          "zNRI",
                                          "IDI",
                                          "NRI",
                                          "NeRI"
                                          "Ztest"
                                          "AUC",
                                          "CStat",
                                          "Kendall"),
                         cateGroups = c(0.1, 0.9),
                         raw.dataFrame = NULL,
                         description = ".",
                         uniType = c("Binary", "Regression"),
                         FullAnalysis=TRUE,
                         acovariates = NULL,
                         timeOutcome = NULL
```

)

#### **Arguments**

variableList A data frame with the candidate variables to be ranked formula

An object of class formula with the formula to be fitted

Outcome The name of the column in data that stores the variable to be predicted by the

model

data A data frame where all variables are stored in different columns

categorizationType

How variables will be analyzed: As given in data ("Raw"); broken into the *p*-value categories given by cateGroups ("Categorical"); broken into the *p*-value categories given by cateGroups, and weighted by the *z*-score ("ZCategorical"); broken into the *p*-value categories given by cateGroups, weighted by the *z*-score, plus the raw values ("RawZCategorical"); raw values, plus the tails ("RawTail"); or raw values, weighted by the *z*-score, plus the tails ("RawZTail")

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")

rankingTest Variables will be ranked based on: The z-score of the IDI ("zIDI"), the z-score of

the NRI ("zNRI"), the IDI ("IDI"), the NRI ("NRI"), the NeRI ("NeRI"), the z-score of the model fit ("Ztest"), the AUC ("AUC"), the Somers' rank correlation

("Cstat"), or the Kendall rank correlation ("Kendall")

cateGroups A vector of percentiles to be used for the categorization procedure

raw.dataFrame A data frame similar to data, but with unadjusted data, used to get the means

and variances of the unadjusted data

description The name of the column in variableList that stores the variable description

uniType Type of univariate analysis: Binary classification ("Binary") or regression ("Re-

gression")

FullAnalysis If FALSE it will only order the features according to its z-statistics of the linear

model

acovariates the list of covariates

timeOutcome the name of the Time to event feature

#### **Details**

This function will create valid dummy categorical variables if, and only if, data has been *z*-standardized. The *p*-values provided in cateGroups will be converted to its corresponding *z*-score, which will then be used to create the categories. If non *z*-standardized data were to be used, the categorization analysis would return wrong results.

#### Value

A sorted data frame. In the case of a binary classification analysis, the data frame will have the following columns:

Name Name of the raw variable or of the dummy variable if the data has been catego-

rized

parent Name of the raw variable from which the dummy variable was created

descrip	Description of the parent variable, as defined in description
cohortMean	Mean value of the variable
cohortStd	Standard deviation of the variable
cohortKSD	D statistic of the KS test when comparing a normal distribution and the distribution of the variable
cohortKSP	Associated <i>p</i> -value to the cohortKSD
caseMean	Mean value of cases (subjects with Outcome equal to 1)
caseStd	Standard deviation of cases
caseKSD	D statistic of the KS test when comparing a normal distribution and the distribution of the variable only for cases
caseKSP	Associated <i>p</i> -value to the caseKSD
caseZKSD	D statistic of the KS test when comparing a normal distribution and the distribution of the <i>z</i> -standardized variable only for cases
caseZKSP	Associated <i>p</i> -value to the caseZKSD
controlMean	Mean value of controls (subjects with Outcome equal to 0)
controlStd	Standard deviation of controls
controlKSD	D statistic of the KS test when comparing a normal distribution and the distribution of the variable only for controls
controlKSP	Associated $p$ -value to the controlsKSD
controlZKSD	D statistic of the KS test when comparing a normal distribution and the distribution of the <i>z</i> -standardized variable only for controls
controlZKSP	Associated $p$ -value to the controlsZKSD
t.Rawvalue	Normal inverse $p$ -value ( $z$ -value) of the $t$ -test performed on raw.dataFrame
t.Zvalue	z-value of the <i>t</i> -test performed on data
wilcox.Zvalue	z-value of the Wilcoxon rank-sum test performed on data
ZGLM	z-value returned by the 1m, g1m, or coxph functions for the z-standardized variable
zNRI	$z\mbox{-}{\mbox{value}}$ returned by the improve Prob function (Hmisc package) when evaluating the NRI
zIDI	z-value returned by the improveProb function (Hmisc package) when evaluating the IDI
zNeRI	z-value returned by the improvedResiduals function when evaluating the NeRI
ROCAUC	Area under the ROC curve returned by the roc function (pROC package)
cStatCorr	c index of Somers' rank correlation returned by the <code>rcorr.cens</code> function (Hmisc package) $$
NRI	NRI returned by the improveProb function (Hmisc package)
IDI	IDI returned by the improveProb function (Hmisc package)
NeRI	NeRI returned by the improvedResiduals function
kendall.r	Kendall $\boldsymbol{\tau}$ rank correlation coefficient between the variable and the binary out-

come

kendall.p Associated *p*-value to the kendall.r

TstudentRes.p p-value of the improvement in residuals, as evaluated by the paired t-test

WilcoxRes.p p-value of the improvement in residuals, as evaluated by the paired Wilcoxon

rank-sum test

FRes.p p-value of the improvement in residual variance, as evaluated by the F-test

caseN\_Z\_Low\_Tail

Number of cases in the low tail

caseN\_Z\_Hi\_Tail

Number of cases in the top tail

controlN\_Z\_Low\_Tail

Number of controls in the low tail

controlN\_Z\_Hi\_Tail

Number of controls in the top tail

In the case of regression analysis, the data frame will have the following columns:

Name of the raw variable or of the dummy variable if the data has been catego-

rized

parent Name of the raw variable from which the dummy variable was created

descrip Description of the parent variable, as defined in description

cohortMean Mean value of the variable

cohortStd Standard deviation of the variable

cohortKSD D statistic of the KS test when comparing a normal distribution and the distri-

bution of the variable

cohortKSP Associated *p*-value to the cohortKSP

cohortZKSD D statistic of the KS test when comparing a normal distribution and the distri-

bution of the z-standardized variable

cohortZKSP Associated *p*-value to the cohortZKSD

ZGLM z-value returned by the glm or Cox procedure for the z-standardized variable

zNRI z-value returned by the improveProb function (Hmisc package) when evaluating

the NRI

NeRI NeRI returned by the improvedResiduals function

cStatCorr c index of Somers' rank correlation returned by the rcorr.cens function (Hmisc

package)

spearman.r Spearman  $\rho$  rank correlation coefficient between the variable and the outcome

pearson.r Pearson r product-moment correlation coefficient between the variable and the

outcome

kendall.r Kendall au rank correlation coefficient between the variable and the outcome

kendall.p Associated p-value to the kendall.r

TstudentRes.p p-value of the improvement in residuals, as evaluated by the paired t-test

WilcoxRes.p p-value of the improvement in residuals, as evaluated by the paired Wilcoxon

rank-sum test

FRes.p p-value of the improvement in residual variance, as evaluated by the F-test

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## Author(s)

Jose G. Tamez-Pena

## References

Pencina, M. J., D'Agostino, R. B., & Vasan, R. S. (2008). Evaluating the added predictive ability of a new marker: from area under the ROC curve to reclassification and beyond. *Statistics in medicine* **27**(2), 157-172.

update.uniRankVar

Update the univariate analysis using new data

# **Description**

This function updates the results from an univariate analysis using a new data set

## Usage

## **Arguments**

object A list with the results from the uniRankVar function

... Additional parameters to be passed to the uniRankVar function, used to update

the univariate analysis

## Value

A list with the same format as the one yielded by the uniRankVar function

## Author(s)

Jose G. Tamez-Pena

## See Also

uniRankVar

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values	updateModel.Bin	Update the IDI/NRI-based model using new data or new threshold values
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## **Description**

This function will take the frequency-ranked set of variables and will generate a new model with terms that meet either the integrated discrimination improvement (IDI), or the net reclassification improvement (NRI), threshold criteria.

# Usage

```
updateModel.Bin(Outcome,
            covariates = "1",
            pvalue = c(0.025, 0.05),
            VarFrequencyTable,
            variableList,
            data,
            type = c("LM", "LOGIT", "COX"),
            lastTopVariable = 0,
            timeOutcome = "Time",
            selectionType = c("zIDI","zNRI"),
            maxTrainModelSize = 0,
            zthrs = NULL
            )
```

## Arguments

Outcome	The name of the column in data that stores the variable to be predicted by the model	
covariates	A string of the type $"1 + var1 + var2"$ that defines which variables will always be included in the models (as covariates)	
pvalue	The maximum $p$ -value, associated to either IDI or NRI, allowed for a term in the model	
VarFrequencyTable		
	An array with the ranked frequencies of the features, (e.g. the ranked.var value returned by the ForwardSelection.Model.Bin function)	

A data frame with two columns. The first one must have the names of the can-

variableList didate variables and the other one the description of such variables

A data frame where all variables are stored in different columns

Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX") type

lastTopVariable

data

The maximum number of variables to be tested

The name of the column in data that stores the time to event (needed only for a timeOutcome

Cox proportional hazards regression model fitting)

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 ${\tt selectionType} \quad \text{The type of index to be evaluated by the improveProb function (Hmisc pack-}$ 

age): z-score of IDI or of NRI

maxTrainModelSize

Maximum number of terms that can be included in the model

zthrs The z-thresholds estimated in forward selection

#### Value

final.model An object of class lm, glm, or coxph containing the final model

var.names A vector with the names of the features that were included in the final model

formula An object of class formula with the formula used to fit the final model

z.selectionType

A vector in which each term represents the *z*-score of the index defined in selectionType obtained with the Full model and the model without one term

## Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

#### See Also

updateModel.Res

updateModel.Res

Update the NeRI-based model using new data or new threshold values

## **Description**

This function will take the frequency-ranked set of variables and will generate a new model with terms that meet the net residual improvement (NeRI) threshold criteria.

## Usage

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#### **Arguments**

Outcome The name of the column in data that stores the variable to be predicted by the

model

covariates A string of the type "1 + var1 + var2" that defines which variables will always

be included in the models (as covariates)

pvalue The maximum p-value, associated to the NeRI, allowed for a term in the model

VarFrequencyTable

An array with the ranked frequencies of the features, (e.g. the ranked.var value

returned by the ForwardSelection. Model. Res function)

variableList A data frame with two columns. The first one must have the names of the can-

didate variables and the other one the description of such variables

data A data frame where all variables are stored in different columns

type Fit type: Logistic ("LOGIT"), linear ("LM"), or Cox proportional hazards ("COX")

testType Type of non-parametric test to be evaluated by the improvedResiduals func-

tion: Binomial test ("Binomial"), Wilcoxon rank-sum test ("Wilcox"), Student's

*t*-test ("tStudent"), or *F*-test ("Ftest")

lastTopVariable

The maximum number of variables to be tested

timeOutcome The name of the column in data that stores the time to event (needed only for a

Cox proportional hazards regression model fitting)

maxTrainModelSize

Maximum number of terms that can be included in the model

p. thresholds The p.value thresholds estimated in forward selection

#### Value

final.model An object of class lm, glm, or coxph containing the final model

var.names A vector with the names of the features that were included in the final model

formula An object of class formula with the formula used to fit the final model

z.NeRI A vector in which each element represents the z-score of the NeRI, associated

to the testType, for each feature found in the final model

#### Author(s)

Jose G. Tamez-Pena and Antonio Martinez-Torteya

#### See Also

updateModel.Bin

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