## Package ‘MCRestimate’

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**Title**  Misclassification error estimation with cross-validation  
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**Author**  Marc Johannes, Markus Ruschhaupt, Holger Froehlich, Ulrich Mansmann, Andreas Buness, Patrick Warnat, Wolfgang Huber, Axel Benner, Tim Beissbarth  
**Description**  This package includes a function for combining preprocessing and classification methods to calculate misclassification errors  
**Maintainer**  Marc Johannes <m.johannes@dkfz.de>  
**License**  GPL (>= 2)  
**Depends**  R (>= 2.7.2), golubEsets (>= 1.4.6)  
**Imports**  e1071 (>= 1.5-12), pamr (>= 1.22), randomForest (>= 3.9-6), RColorBrewer (>= 0.1-3), Biobase (>= 2.5.5), graphics, grDevices, stats, utils  
**Suggests**  xtable (>= 1.2-1), ROC (>= 1.8.0), genefilter (>= 1.12.0), gpls (>= 1.6.0)  
**LazyLoad**  yes  
**biocViews**  Classification  
**NeedsCompilation**  no

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class.factor.format

A function for creating a factor from the phenoData slot of an exprSet

Description

This function creates a factor whose levels represent the different classes for a classification problem. It is derived from the column specified in the argument class.column. If the factor has more than two levels, the argument reference.class can be used to transform this into a two-class problem: reference class versus the rest.

Usage

class.factor.format(x, class.column, reference.class=NULL)

Arguments

x an exprSet
class.column either a number or a character string specifying the relevant column of the phenoData slot in x
reference.class character vector. If specified the result will be a factor with only 2 levels: the reference class(es) versus all other

Value

A factor of length nrow(pData(x))

Author(s)

Markus Ruschhaupt mailto:m.ruschhaupt@dkfz.de

Examples

library(golubEsets)
data(Golub_Train)
class.factor.format(Golub_Train[,28:35], "FAB", reference="M1")
ClassifierBuild

Building a classifier as a combination of preprocessing and classification method

Description

builds a classifier as a combination of preprocessing and classification methods

Usage

ClassifierBuild(eset,
    class.column,
    reference.class=NULL,
    classification.fun,
    variableSel.fun = "identity",
    cluster.fun = "identity",
    poss.parameters=list(),
    cross.inner=10,
    rand=123,
    information=TRUE,
    thePreprocessingMethods=c(variableSel.fun,cluster.fun))

Arguments

eset an object of class exprSet or exprSetRG
class.column a number or a character string which indicated the column of the expression set’s phenodata containing the class label
reference.class a character string with the name of one class - if specified the class will form the first class and all the other classes will form the second class
classification.fun a character string which names the function that should be used for the classification
variableSel.fun character string which names the function that should be used for variable selection
cluster.fun character string which names the function that should be used for clustering the variables
thePreprocessingMethods vector of character with the names of all preprocessing functions- can be used instead of ‘variableSel.fun’ and ‘cluster.fun’ - see details
poss.parameters a list of possible values for the parameter of the classification method
cross.inner integer - the number of nearly equal sized parts the train set should be divided into
rand integer - the random number generator will be put in a reproducible state
information information - should classifier specific data be given (depends on the wrapper for the classification method)
**important.variable.names**

**Value**

a list with the following arguments:

- **classifier.for.matrix**
- **classifier.for.exprSet**

**parameter** a list consisting of the estimated 'best' parameter for each cross-validation part

**class.method** string which names the function used for the classification

**thePreprocessingMethods** character string - name of the preprocessing functions that have been used

**cross.inner** number of blocks for a the inner cross-validation

**information** classifier specific data

**Author(s)**

Markus Ruschhaupt  
mailto:m.ruschhaupt@dkfz.de

**Examples**

```r
library(golubEsets)
data(Golub_Train)

class.column <- "ALL.AML"
Preprocessingfunctions <- c("varSel.highest.var")
list.of.poss.parameter <- list(var.numbers = c(250,1000))
classification.funct <- "RF.wrap"
cross.inner <- 5

RF.classifier <- ClassifierBuild(Golub_Train,  
class.column,  
classification.fun = classification.funct,  
thePreprocessingMethods = Preprocessingfunctions,  
poss.parameters = list.of.poss.parameter,  
cross.inner = cross.inner)
```

---

**important.variable.names**

*Writing tables with variable information*

**Description**

The information slot of a MCRestimate object may contain lists of variable names that are important for each classification. This function produces summary tables of these variables. It is assumed that the first column of each information list contains the variable names if not otherwise specified with the argument listName. This is important if someone wants to write a new wrapper for a classification method.
**Usage**

```r
important.variable.names(mcr, file="important_variables", listName=NULL, writeFile=TRUE,...)
```

**Arguments**

- `mcr`: an object of class `MCRestimate`
- `file`: a character string specifying the name of the output files
- `listName`: a character string specifying the variable names vector in the information list
- `writeFile`: Should the files be written?
- `...`: Further arguments that are passed on to `plot.default`

**Value**

The function is called for its side effect, writing two tables with variable information.

**Author(s)**

Markus Ruschhaupt [mailto:m.ruschhaupt@dkfz.de](mailto:m.ruschhaupt@dkfz.de)

**Examples**

```r
library(golubEsets)
data(Golub_Train)

class.column <- "ALL.AML"
list.of.poss.parameter <- list(var.numbers = c(250,1000))
Preprocessingfunctions <- c("identity")
list.of.poss.parameter <- list(threshold = 6)
class.function <- "PAM.wrap"
plot.label <- "Samples"

cross.outer <- 10
cross.repeat <- 7
cross.inner <- 5

PAM.estimate <- MCRestimate(Golub_Train, 
class.column, 
classification.fun = class.function, 
thePreprocessingMethods = Preprocessingfunctions, 
poss.parameters = list.of.poss.parameter, 
cross.outer = cross.outer, 
cross.inner = cross.inner, 
cross.repeat = cross.repeat, 
plot.label = plot.label)

important.variable.names(PAM.estimate)
```
intersectList

A function for creating all possible intersects for a list of sets.

Description
The list contains several sets. The function calculates all possible intersections.

Usage
intersectList(x)

Arguments
x a list

Value
A list containing all possible intersections.

Author(s)
Markus Ruschhauptmailto:m.ruschhaupt@dkfz.de

Examples
a <- list(x=1:5,y=3:4,z=c(1,3,3))
intersectList(a)

MCRconfusion

Summary tables for MCRestimate objects

Description
MCRwrongsamples returns a matrix with all the samples that have a higher frequency of being predicted as a member of a wrong class than of the correct class for at least one classification method. MCRconfusion summarizes the result of the vote matrices

Usage
MCRwrongsamples(x,  
col.names=names(x),  
rownames.from.object=TRUE,  
subgroup=NULL,  
freq=FALSE)

MCRconfusion(x,  
col.names=names(x),  
row.names=NULL)
**MCRestimate**

**Arguments**

- **x**: List of objects of S3 class `MCRestimate`
- **col.names**: Vector of strings used for column names. The length must match the number of objects in `x`
- **rownames.from.object**: Logical. If TRUE then the sample names of the `MCRestimate` object in `x` are used as row names
- **subgroup**: Logical. If TRUE then only the samples which belongs to the specified group are listed in the table
- **freq**: Logical. If TRUE then the frequency with which each sample in the table has been misclassified will be printed.
- **row.names**: Vector of strings used for row names. If not specified the names of the groups are used

**Value**

`MCRwrongsamples` returns a matrix and `MCRconfusion` returns a confusion matrix.

**Author(s)**

Markus Ruschhaupt [mailto:m.ruschhaupt@dkfz.de](mailto:m.ruschhaupt@dkfz.de)

**See Also**

`MCRestimate`

**Examples**

```r
library(golubEsets)
data(Golub_Train)
exSet <- Golub_Train[1:500,]
result1 <- MCRestimate(exSet,"ALL.AML",classification.fun="RF.wrap",cross.outer=3,cross.repeat=2)
result2 <- MCRestimate(exSet,"ALL.AML",classification.fun="PAM.wrap",poss.parameters=list(threshold=c(0.5,1)),cross.inner=3,cross.outer=3,cross.repeat=2)
MCRwrongsamples(list(result1,result2),subgroup="AML",col.names=c("Random Forest","PAM"))
MCRconfusion(list(result1,result2),col.names=c("Random Forest","PAM"))
```

**Description**

Several repetitions of a cross-validation are performed to get 'votes' how stable a method is against different partitions into training and test set
Usage

MCRestimate(eset,
class.column,
reference.class=NULL,
classification.fun,
variableSel.fun="identity",
cluster.fun="identity",
poss.parameters=list(),
cross.outer=10,
cross.repeat=3,
cross.inner=cross.outer,
plot.label=NULL,
rand=123,
stratify=FALSE,
information=TRUE,
block.column=NULL,
thePreprocessingMethods=c(variableSel.fun,cluster.fun))

Arguments

eset	an object of class ExpressionSet
class.column	a number or a character string which indicates the column of the expression set’s phenodata containing the class label
reference.class	a character string - the name of one class - if specified, the class will form the first class and all the other classes will form the second class
classification.fun	character string which names the function that should be used for the classification
variableSel.fun	character string which names the function that should be used for the variable selection
cluster.fun	character string which names the function that should be used for the clustering of variables
thePreprocessingMethods	vector of character with the names of all preprocessing functions - can be used instead of ‘variableSel.fun’ and ‘cluster.fun’ - see details
poss.parameters	a list of possible values for the parameter of the classification, variable selection, and cluster methods
cross.outer	integer - the number of nearly equal sized parts the sample set should be divided into (outer cross-validation)
cross.repeat	integer - the number of repetitions of the cross-validation procedure
cross.inner	integer - the number of nearly equal sized parts the train set should be divided into (inner cross-validation)
plot.label	name of one column of the phenodata- if specified, the content of this column will form the labels of the x-axis if the ‘votematrix’ will be plotted with plot.MCRestimate
rand	integer - the random number generator will be put in a reproducible state
stratify	should a stratified version be used for the cross validation?
block.column a character string which indicates the column of the expression set’s phenodata containing the blocking covariate, which sets a constrain on the cross-validation splits: each block is either completely assigned to the test or to the training set

information information - should classifier specific data be given (depends on the wrapper for the classification method)

Details

The argument ‘thePreprocessingMethods’ can be used instead of ’variableSel.fun’ and ’cluster.fun’. In the first versions of MCRestimate it was only possible to have one variable selection and one cluster functions. Now it is possible to have more than two functions and the ordering is arbitrary, e.g. you can have a variable selection function, then a cluster function and then a second variable selection function.

If MCRestimate is used with an object of class exprSetRG-class, the preprocessing steps can use the green and the red channel separately but the classification methods works with green channel - red channel.

Note: ‘correct prediction’ means that a sample was predicted to be a member of the correct class at least as often as it was predicted to be a member of each other class. So in the two class problem a sample is also ‘correct’ if it has been predicted correctly half of the time.

Value

an object of class MCRestimate which is a list with fourteen arguments:

votes a matrix consisting of the different votes for each sample

classes the class of each sample

table a ‘confusion’ table, shows the number of ‘correct prediction’ for each class

correct.prediction a logical vector - indicates if a sample was predicted to be a member of the correct class at least as often as it was predicted to be a member of each other class.

correct.class.vote vector that contains for every sample the vote for it’s correct class

parameter a list consisting of the estimated ‘best’ parameter for each cross-validation part

class.method string which names the function used for the classification

thePreprocessingMethods character string - name of the preprocessing functions that have been used

cross.outer number of blocks for a the outer cross-validation

cross.repeat number of outer cross-validation repetitions

cross.inner number of blocks for a the inner cross-validation

sample.names names of the sample

information classifier specific data (if information is TRUE)

Author(s)

Markus Ruschhaupt mailto:m.ruschhaupt@dkfz.de, contributions from Andreas Buness and Patrick Warnat
Examples

```r
library(golubEsets)
data(Golub_Test)
G2 <- Golub_Test[1:500,]
result <- MCRestimate(G2, "ALL.AML", classification.fun="RF.wrap",
                      cross.outer=4, cross.repeat=3)
result
if (interactive()) {
  x11(width=9, height=4)}
plot(result)
```

MCRestimateMerge  Merging objects of class MCRestimate

Description

MCRestimateMerge merges objects of S3 class MCRestimate. See vignette MCRestimateBlueprint.Rnw for details.

Usage

```r
MCRestimateMerge(MCRestimateList)
```

Arguments

- **MCRestimateList**
  - list of objects of S3 class MCRestimate

Value

- An objects of S3 class MCRestimate

Author(s)

- Markus Ruschhaupt <mailto:m.ruschhaupt@dkfz.de>

See Also

- MCRestimate
**MCRindError**

*Individual Error of the outer cross-validations*

**Description**

MCRindError returns a vector with the individual number of incorrect classified samples for each cross-validation. plotIndGroupVotes plots the individual group votes.

**Usage**

```r
MCRindError(MCRe, perGroup=FALSE)

plotIndGroupVotes(MCRest, PvD= 0.5, dotCol="red", errCol="black", xlab="", ylab="# misclassified samples (mean + SD)", ...)
```

**Arguments**

- `MCRe`: Object of S3 class MCRestimate
- `perGroup`: returns a vector with the individual number of incorrect classified samples for each group
- `MCRest`: Object of S3 class MCRestimate
- `PvD`: Offset of the text that belongs to a specific point in the plot
- `dotCol`: Color of the dots
- `errCol`: Line color between points
- `xlab`: Label of X-Axis
- `ylab`: Label of Y-Axis
- `...`: Advanced options to the plot command

**Value**

MCRindError returns a vector of individual errors.

**Author(s)**

Markus Ruschhaupt [mailto:m.ruschhaupt@dkfz.de](mailto:m.ruschhaupt@dkfz.de)

**See Also**

MCRestimate
Examples

```r
library(golubEsets)
data(Golub_Train)
exSet <- Golub_Train[1:500]  
result1 <- MCRestimate(exSet,"ALL.AML",classification.fun="RF.wrap",cross.outer=3,cross.repeat=3)
MCRindError(result1)
```

Description

plot.MCRestimate visualizes a 'vote matrix'. A 'vote matrix' is the result of a classification procedure. For every sample (=row) i and every class (=column) j the matrix element [i,j] is the probability or frequency the classification method predicts sample i as a member of class j.

Usage

```r
## S3 method for class 'MCRestimate'
plot(x,  
class.factor=NULL,  
rownames.from.object=FALSE,  
sample.order=TRUE,  
legend=FALSE,  
mypalette=NULL,  
shading=NULL,  
xlab="Sample ID",  
ylab="Frequency of correct classification",  
cex.axis=1,...)
```

Arguments

- `x` Object of S3 class MCRestimate or a matrix
- `class.factor` Factor. Its length must match the number of rows in x and the levels must be the same as the colnames in x. If x is of class MCRestimate this argument will be ignored.
- `rownames.from.object` Logical. If TRUE then the rownames of the matrix or the sample names of MCRestimate in x are used as labels for the x-axis
- `sample.order` Logical. If TRUE then the samples are ordered by class membership
- `legend` Logical. If TRUE then there will be a small legend in the output
- `mypalette` vector with length equal to the number of classes. The vector specifies the color for the bar representing the classes. If 'NULL' colors chosen by the author are used.
- `shading` the density of shading lines for the rectangles that indicate the groups, in lines per inch. The default value of 'NULL' means that no shading lines are drawn.
- `xlab` Character
- `ylab` Character
- `cex.axis` numeric
- `...` Further arguments that are passed on to plot.default
PLR

A function which performs penalised logistic regression classification for two groups

Description

A function which performs penalised logistic regression.

Usage

PLR(trainmatrix, resultvector, kappa=0, eps=1e-4)

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

Arguments

resultvector a vector which contains the labeling of the samples
trainmatrix a matrix which includes the data. The rows corresponds to the observations and the columns to the variables.
kappa value range for penalty parameter. If more that one parameter is specified the one with the lowest AIC will be used.
eps precision of convergence
object a fitted PLR model
... here a data matrix from samples that should be predicted
Value

a list with three arguments

a
Intercept estimate of the linear predictor

b
vector of estimated regression coefficients

factorlevel
levels of grouping variable

aics
vector of AIC values with respect to penalty parameter kappa

trs
vector of effective degrees of freedom with respect to penalty parameter kappa

Author(s)

Axel Benner, Ulrich Mansmann, based on MathLab code by Paul Eilers

Examples

library(golubEsets)
data(Golub_Merge)
eSet<-Golub_Merge
X0 <- t(exprs(eSet))
m <- nrow(X0); n <- ncol(X0)
y <- pData(eSet)$ALL.AML
f <- PLR(X0, y,kappa=10^seq(0, 7, 0.5))
if (interactive()) {
x11(width=9, height=4)
par(mfrow=c(1,2))
plot(log10(f$kappas), f$aics, type="l",main="Akaike’s Information Criterion", xlab="log kappa", ylab="AIC")
plot(log10(f$kappas), f$trs, type="l",xlab="log kappa", ylab="Dim",main="Effective dimension")
}

replace.NA(x, replacement, byRow = TRUE)

Argument

x numeric input matrix
replacement numeric vector containing the values which are used for NA replacement. If byRow = TRUE, this vector must contain as many values as matrix X has rows. Else, this vector must contain as many elements as matrix X has columns.
byRow logical. If TRUE, then NA values in row n are replaced by the value at position n in the vector ‘replacement’. Else, NA values are replaced according to their column position.
RF.wrap

Value

The numeric input matrix with replaced NA values.

Author(s)

Patrick Warnat mailto:p.warnat@dkfz-heidelberg.de

Description

Wrapper function for different classification methods used by MCRestimator. These functions are mainly used within the function MCRestimate

Usage

RF.wrap(x,y,...)
PAM.wrap(x,y,threshold,...)
PLR.wrap(x,y,kappa=0,eps=1e-4,...)
SVM.wrap(x,y,gamma = NULL, kernel = "radial", ...)
GPLS.wrap(x,y,...)

Arguments

x, y x is a matrix where each row refers to a sample a each column refers to a gene; y is a factor which includes the class for each sample

threshold the threshold for PAM

kappa the penalty parameter for the penalised logistic regression

eps precision of convergence

gamma parameter for support vector machines

kernel parameter for support vector machines

... Further parameters

Value

Every function return a predict function which can be used to predict the classes for a new data set.

Author(s)

Markus Ruschhaupt mailto:m.ruschhaupt@dkfz.de

See Also

MCRestimate
select.NA.elements

Selects NA values of a given numeric matrix

Description

Selects of a given numeric matrix rows or columns containing more NA values than defined by a
given threshold.

Usage

select.NA.elements(x, NAthreshold, byRow = TRUE)

Arguments

x numeric input matrix

NAthreshold numeric value between 0 and 1, determining the allowed percentage of NA val-
ues per row or column. Rows or columns containing more NA values are se-
lected.

byRow logical. If TRUE, then rows with more NA values than determined by the argu-
ment threshold are selected, else columns.

Value

logical vector containing the row or column selection. If argument byRow = TRUE, then value
contains as many values as the input matrix contains rows, else it contains as many values as the
input matrix contains columns.

Examples

library(golubEsets)
data(Golub_Train)

class.column <- "ALL.AML"
Preprocessingfunctions <- c("varSel.highest.var")
list.of.poss.parameter <- list(threshold = 6)

Preprocessingfunctions <- c("identity")
class.function <- "PAM.wrap"
plot.label <- "Samples"

cross.outer <- 10
cross.repeat <- 7
cross.inner <- 5

PAM.estimate <- MCRestimate(Golub_Train,
class.column,
classification.fun = class.function,
thePreprocessingMethods = Preprocessingfunctions,
poss.parameters = list.of.poss.parameter,
cross.outer = cross.outer, cross.inner = cross.inner,
cross.repeat = cross.repeat, plot.label = plot.label)
**Author(s)**

Patrick Warnat mailto:p.warnat@dkfz-heidelberg.de

---

**SVM.OVA.wrap**  
*SVM with 'One-Versus-All' multiclass approach*

---

**Description**

Multiclass approach where k binary SVM classifiers are constructed for a classification problem with k classes: Every classifier is trained to distinguish samples of one class from samples of all other classes. For prediction of the class of a new sample, the sample is classified by all k classifiers, and the class corresponding to the classifier with the maximum decision value is chosen.

**Usage**

SVM.OVA.wrap(x, y, gamma = NULL, kernel = "radial", ...)

**Arguments**

- **x**, **y**  
  x is a matrix where each row refers to a sample and each column refers to a gene; y is a factor which includes the class for each sample

- **gamma**  
  parameter for support vector machines

- **kernel**  
  parameter for support vector machines

- **...**  
  Further parameters

**Value**

A predict function which can be used to predict the classes for a new data set.

**Author(s)**

Patrick Warnat mailto:p.warnat@dkfz-heidelberg.de

**See Also**

MCRestimate

**Examples**

```r
## Not run:
library(golubEsets)
data(Golub_Train)

class.column <- "ALL.AML"
Preprocessingfunctions <- c("varSel.highest.var")
list.of.poss.parameter <- list(var.numbers = c(250, 1000))

Preprocessingfunctions <- c("identity")
class.function <- "SVM.OVA.wrap"
list.of.poss.parameter <- list(gamma = 6)
plot.label <- "Samples"
```
cross.outer <- 10
cross.repeat <- 20
cross.inner <- 5
SVM.estimate <- MCRestimate(Golub_Train,
class.column,
classification.fun = class.function,
thePreprocessingMethods = Preprocessingfunctions,
poss.parameters = list.of.poss.parameter,
cross.outer = cross.outer, cross.inner = cross.inner,
cross.repeat = cross.repeat, plot.label = plot.label)
## End(Not run)

varSel.highest.var Variable selection and cluster functions

Description
Different functions for a variable selection and clustering methods. These functions are mainly used for the function MCRestimate

Usage
identity(sample.gene.matrix, classfactor,...)
varSel.highest.t.stat(sample.gene.matrix, classfactor, theParameter=NULL, var.numbers=500,...)
varSel.highest.var(sample.gene.matrix, classfactor, theParameter=NULL, var.numbers=2000,...)
varSel.AUC(sample.gene.matrix, classfactor, theParameter=NULL, var.numbers=200,...)
cluster.kmeans.mean(sample.gene.matrix, classfactor, theParameter=NULL, number.clusters=500,...)
varSel.removeManyNA(sample.gene.matrix, classfactor, theParameter=NULL, NAthreshold=0.25,...)
varSel.impute.NA(sample.gene.matrix, classfactor, theParameter=NULL,...)

Arguments
sample.gene.matrix
a matrix in which the rows corresponds to genes and the columns corresponds to samples
classfactor
a factor containing the values that should be predicted
theParameter
Parameter that depends on the function. For 'cluster.kmeans.mean' either NULL or an output of the function kmeans. If it is NULL then kmeans will be used to form clusters of the genes. Otherwise the already existing clusters will be used. In both ways there will be a calculation of the metagene intensities afterwards. For the other functions either NULL or a logical vector which indicates for every gene if it should be left out from further analysis or not
number.clusters
parameter which specifies the number of clusters
var.numbers
some methods needs an argument which specifies how many variables should be taken
**Details**

`metagene.kmeans.mean` performs a kmeans clustering with a number of clusters specified by `number clusters` and takes the mean of each cluster. `varSel.highest.var` selects a number (specified by `var.numbers`) of variables with the highest variance. `varSel.AUC` chooses the most discriminating variables due to the AUC criterium (the library ROC is required).

**Value**

Every function returns a list consisting of two arguments:

- **matrix**: the result matrix of the variable reduction or the clustering
- **parameter**: The parameter which are used to reproduce the algorithm, i.e. a vector which indicates for every gene if it will be left out from further analysis or not if a gene reduction is performed or the output of the function kmeans for the clustering algorithm.

**Author(s)**

Markus Ruschhaupt [mailto:m.ruschhaupt@dkfz.de](mailto:m.ruschhaupt@dkfz.de)

**See Also**

`MCRestimate`

**Examples**

```r
m <- matrix(c(rnorm(10,2,0.5),rnorm(10,4,0.5),rnorm(10,7,0.5),rnorm(10,2,0.5),rnorm(10,4,0.5),rnorm(10,2,0.5),
  rnorm(10,4,0.5),rnorm(10,4,0.5),rnorm(10,2,0.5)),ncol=2)
cluster.kmeans.mean(m ,number.clusters=3)
```
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