# Package 'CrossValidate'

July 6, 2017

Version 2.2.2
<b>Date</b> 2016-05-09
Title Classes and Methods for Cross Validation of ``Class Prediction" with Microarrays or Proteomics
Author Kevin R. Coombes
Maintainer Kevin R. Coombes <a href="https://krc@silicovore.com">krc@silicovore.com</a>
<b>Depends</b> R (>= 3.0), Modeler
Imports methods, oompaBase (>= 3.0.1)
Suggests Biobase
<b>Description</b> Defines classes and methods to cross validate methods for ``class prediction".
<b>License</b> Apache License (== 2.0)
LazyLoad yes
biocViews Microarray, Clustering
URL
NeedsCompilation no
R topics documented:
CrossValidate-package2balancedSplit3CrossValidate4CrossValidate-class6CrossValSummary-class7
Index 8

CrossValidate-package Cross validation of high-throughput prediction algorithms

#### **Description**

The CrossValidate package provides generic tools for performing cross-validation on classification methods in the context of high-throughput data sets such as those produced by gene expression microarrays. In order to use a classifier with this implementation of cross-validation, you must first prepare a pair of functions (one for learning models from training data, and one for making predictions on test data). These functions, along with any required meta-parameters, are used to create an object of the Modeler-class. That object is then passed to the CrossValidate function along with the full training data set. The full data set is then repeatedly split into its own training and test sets; you can specify the fraction to be used for training and the number of iterations. The result is a detailed look at the accuracy, sensitivity, specificity, and positive and negative predictive value of the model, as estimated by cross-validation.

#### **Details**

Package: CrossValidate
Type: Package
Version: 1.0.1
Date: 2012-05-04
License: Artistic-2.0
LazyLoad: yes

## Author(s)

Kevin R. Coombes < krc@silicovore.com>

#### References

Braga-Neto U, Dougherty ER.

Is cross-validation valid for small-sample microarray classification?

Bioinformatics, 2004; 20:374-380.

Jiang W, Varma S, Simon R.

Calculating confidence intervals for prediction error in microarray classification using resampling. Stat Appl Genet Mol Biol. 2008; 7:Article8.

Fu LM, Youn ES.

Improving reliability of gene selection from microarray functional genomics data.

IEEE Trans Inf Technol Biomed. 2003; 7:191-6.

Man MZ, Dyson G, Johnson K, Liao B.

Evaluating methods for classifying expression data.

J Biopharm Stat. 2004; 14:1065-84.

Fu WJ, Carroll RJ, Wang S.

Estimating misclassification error with small samples via bootstrap cross-validation.

Bioinformatics, 2005; 21:1979-86.

balancedSplit 3

Ancona N, Maglietta R, Piepoli A, D'Addabbo A, Cotugno R, Savino M, Liuni S, Carella M, Pesole G, Perri F.

On the statistical assessment of classifiers using DNA microarray data.

BMC Bioinformatics, 2006; 7:387.

Lecocke M, Hess K.

An empirical study of univariate and genetic algorithm-based feature selection in binary classification with microarray data.

Cancer Inform, 2007; 2:313-27.

Lee S.

Mistakes in validating the accuracy of a prediction classifier in high-dimensional but small-sample microarray data.

Stat Methods Med Res, 2008; 17:635-42.

#### See Also

The following classification methods have been adapted to work within the general cross-validation framework: K nearest neighbors (learnKNN), recursive partitioning and regression trees (learnRPART),

balancedSplit

Split a dataset into training and testing sets, balancing a factor

#### **Description**

When performing cross-validation on a dataset, it often becomes necessary to split the data into training and test sets that are balanced for a certain binary outcome. This function implements such a balanced split.

## Usage

balancedSplit(fac, size)

## **Arguments**

fac A factor that should be balnced between the two subsets.

size A number between 0 and 1 indicating the fraction of the dataset to be used for

training.

#### **Details**

Stuff should go here

## Value

Returns a logical vector with length equal to the length of fac. TRUE values designate samples selected for the training set.

#### Author(s)

Kevin R. Coombes <a href="mailto:krc@silicovore.com">krc@silicovore.com</a>

4 Cross Validate

#### See Also

CrossValidate, CrossValidate-class, CrossValidate-package.

#### **Examples**

```
nFeatures <- 40
nSamples <- 2*10
dataset <- matrix(rnorm(nSamples*nFeatures), ncol=nSamples)
groups <- factor(rep(c("A", "B"), each=10))
balancedSplit(dataset, groups)</pre>
```

CrossValidate

Creating CrossValidate objects

#### **Description**

Given a model classifier and a data set, this function performs cross-valiadtion by repeatedly splitting the data into training and testing subsets in order to estimate the performance of this kind of classifier on new data.

#### Usage

```
CrossValidate(model, data, status, frac, nLoop, verbose=TRUE)
```

## Arguments

model
data
status
frac
nLoop
verbose

#### **Details**

The CrossValidate package provides generic tools for performing cross-validation on classification methods in the context of high-throughput data sets such as those produced by gene expression microarrays. In order to use a classifier with this implementation of cross-validation, you must first prepare a pair of functions (one for learning models from training data, and one for making predictions on test data). These functions, along with any required meta-parameters, are used to create an object of the Modeler-class. That object is then passed to the CrossValidate function along with the full training data set. The full data set is then repeatedly split into its own training and test sets; you can specify the fraction to be used for training and the number of iterations. The result is a detailed look at the accuracy, sensitivity, specificity, and positive and negative predictive value of the model, as estimated by cross-validation.

#### Value

An object of the CrossValidate-class.

Cross Validate 5

#### Author(s)

Kevin R. Coombes <a href="mailto:krcoombes@mdanderson.org">krcoombes@mdanderson.org</a>

#### References

See the manual page for the CrossValidate-package for a list of related references.

#### See Also

See the manual page for the CrossValidate-package for a list of classifiers that have been adapted to work with this cross-validation mechanism.

See CrossValidate-class for a description of the slots in the object created by this function.

#### **Examples**

```
##---- Should be DIRECTLY executable !! ----
##-- ==> Define data, use random,
##--or do help(data=index) for the standard data sets.
## The function is currently defined as
function(model, data, status, frac, nLoop, verbose=TRUE) {
  if (length(status) != ncol(data)) {
    stop("The length of the status vector must match the size of the data set.")
  temp <- balancedSplit(status, frac) # just to compute sizes</pre>
  nTrain <- sum(temp)
  nTest <- sum(!temp)</pre>
  # allocate space to hold the results
  trainOutcome <- data.frame(matrix(NA, ncol=nLoop, nrow=nTrain))</pre>
  validOutcome <- data.frame(matrix(NA, ncol=nLoop, nrow=nTest))</pre>
  trainPredict <- data.frame(matrix(NA, ncol=nLoop, nrow=nTrain))</pre>
  validPredict <- data.frame(matrix(NA, ncol=nLoop, nrow=nTest))</pre>
  extras <- list()
  for (i in 1:nLoop) {
    # show that we are still alive
    if(verbose) print(i)
    # split into training and test
    tr <- balancedSplit(status, frac)</pre>
    # record the true status for each split so we can get
    # statistics on the performance later
    trainOutcome[,i] <- status[tr]</pre>
    validOutcome[,i] <- status[!tr]</pre>
    # train the model
    thisModel <- learn(model, data[,tr], status[tr])</pre>
    # record anything interesting about the model
    extras[[i]] <- thisModel@extras</pre>
    # save the predictions on the training set
    trainPredict[,i] <- predict(thisModel)</pre>
    # now make the predictions using the logistic model
    validPredict[,i] <- predict(thisModel, newdata=data[, !tr])</pre>
  new("CrossValidate",
      nIterations=nLoop,
```

6 Cross Validate-class

```
trainPercent=frac,
  outcome=status,
  trainOutcome=trainOutcome,
  validOutcome=validOutcome,
  trainPredict=trainPredict,
  validPredict=validPredict,
  extras=extras)
}
```

CrossValidate-class

Class "CrossValidate"

## **Description**

```
~~ A concise (1-5 lines) description of what the class is. ~~
```

## **Objects from the Class**

Objects can be created by calls to the constructor function, CrossValidate.

#### **Slots**

```
nIterations: Object of class "numeric" ~~
trainPercent: Object of class "numeric" ~~
outcome: Object of class "factor" ~~
trainOutcome: Object of class "data.frame" ~~
trainPredict: Object of class "data.frame" ~~
validOutcome: Object of class "data.frame" ~~
validPredict: Object of class "data.frame" ~~
extras: Object of class "list" ~~
```

## Methods

```
summary signature(object = "CrossValidate"): ...
```

## Author(s)

Kevin R. Coombes <a href="mailto:kreoombes@mdanderson.org">kreoombes@mdanderson.org</a>

## References

See the manual page for the CrossValidate-package for a list of related references.

## See Also

See CrossValidate-package for an overview, and see CrossValidate for the constructor function.

#### **Examples**

```
showClass("CrossValidate")
```

CrossValSummary" Class "CrossValSummary"

## **Description**

```
~~ A concise (1-5 lines) description of what the class is. ~~
```

## **Objects from the Class**

Objects are almost always created automatically by applying the summary method to an object oif the CrossValidate-class.

#### **Slots**

```
call: Object of class "call" ~~
parent: Object of class "character" ~~
trainAcc: Object of class "list" ~~
validAcc: Object of class "list" ~~
```

#### Methods

```
show signature(object = "CrossValSummary"): ...
```

## Author(s)

Kevin R. Coombes <a href="mailto:kreoombes@mdanderson.org">kreoombes@mdanderson.org</a>

## See Also

```
CrossValidate-class
```

## **Examples**

```
showClass("CrossValSummary")
```

## **Index**

```
*Topic \textasciitildekwd1
    CrossValidate, 4
*Topic \textasciitildekwd2
    CrossValidate, 4
*Topic classes
    CrossValidate-class, 6
    CrossValSummary-class, 7
*Topic classif
    balancedSplit, 3
    CrossValidate-package, 2
*Topic multivariate
    CrossValidate-package, 2
*Topic package
    CrossValidate-package, 2
balancedSplit, 3
CrossValidate, 2, 4, 4, 6
CrossValidate-class, 6
CrossValidate-package, 2
CrossValSummary-class, 7
learnKNN, 3
learnRPART, 3
show,CrossValSummary-method
        (CrossValSummary-class), 7
summary,CrossValidate-method
        (CrossValidate-class), 6
```