# Package 'ClassifyR'

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Type Package

**Title** A framework for two-class classification problems, with applications to differential variability and differential distribution testing

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VignetteBuilder knitr

biocViews Classification, Survival

**Depends** R (>= 3.0.3), methods, Biobase, BiocParallel

Imports locfit, ROCR, grid

**Suggests** limma, edgeR, car, Rmixmod, ggplot2 (>= 2.0.0), gridExtra (>= 2.0.0), BiocStyle, pamr, sparsediscrim, PoiClaClu, curatedOvarianData, parathyroidSE, knitr, klaR, gtable, scales, e1071, rmarkdown, IRanges

Description The software formalises a framework for classification in R.

There are four stages; Data transformation, feature selection, classifier training, and prediction. The requirements of variable types and names are fixed, but specialised variables for functions can also be provided.

The classification framework is wrapped in a driver loop, that reproducibly carries out a number of cross-validation schemes.

Functions for differential expression, differential variability, and differential distribution are included. Additional functions may be developed by the user, by creating an interface to the framework.

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# License GPL-3

# ${\bf Needs Compilation} \ \ {\bf no}$

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# Description

Ranks features by largest Bartlett statistic and chooses the features which have best resubstitution performance.

# Usage

# **Arguments**

expression	Either a matrix or ExpressionSet containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	A vector of class labels.
	For the matrix method, variables passed to the ExpressionSet method.
datasetName	A name for the dataset used. Stored in the result.
trainParams	A container of class TrainParams describing the classifier to use for training.
predictParams	A container of class PredictParams describing how prediction is to be done.
resubstituteParams	
	An object of class ResubstituteParams describing the performance measure to consider and the numbers of top features to try for resubstitution classification.
selectionName	A name to identify this selection method by. Stored in the result.
verbose	A number between 0 and 3 for the amount of progress messages to give. This function only prints progress messages if the value is 3.

# **Details**

The calculation of the test statistic is performed by the bartlett.test function from the stats package.

# Value

An object of class SelectResult or a list of such objects, if the classifier which was used for determining resubstitution error rate made a number of prediction varieties.

# Author(s)

Dario Strbenac

4 calcPerformance

### **Examples**

calcPerformance

Add Performance Calculations to a ClassifyResult object

### **Description**

Annotates the results of calling runTests with different kinds of performance measures.

### Usage

```
## S4 method for signature 'ClassifyResult'
calcPerformance(result, performanceType, ...)
```

### **Arguments**

```
result An object of class ClassifyResult.

performanceType

Either "balanced" or one of the options provided by performance.

... Further arguments that may be used by performance.
```

### **Details**

If runTests was run in resampling mode, one performance measure is produced for every resampling. If the leave-out mode was used, then the predictions are concatenated, and one performance measure is calcuated for all predictions.

Because ROCR only provides calculations for two-class classification, this function is only suitable for two-class classification performance measures.

# Value

An updated ClassifyResult object, with new information in the performance slot.

### Author(s)

Dario Strbenac

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# **Examples**

classifyInterface

Interface for PoiClaClu Package's Classify Function

# **Description**

Passes along all parameters except verbose, from the framework to Classify.

# Usage

```
classifyInterface(..., verbose = 3)
```

# **Arguments**

... All parameters that Classify can accept and also verbose.

verbose A number between 0 and 3 for the amount of progress messages to give. This

function only prints a progress message if the value is 3.

# Value

A result list, the same as is returned by Classify.

# Author(s)

Dario Strbenac

```
if(require(PoiClaClu))
{
  readCounts <- CountDataSet(n = 100, p = 1000, 2, 5, 1)
  classifyInterface(readCounts[["x"]], readCounts[["y"]], readCounts[["xte"]], verbose = TRUE)
}</pre>
```

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ClassifyResult

Container for Storing Classification Results

### **Description**

Contains a table of actual sample classes and predicted classes, the indices of features selected for each fold of each bootstrap resampling or each hold-out classification, and error rates. This class is not intended to be created by the user, but could be used in another package. It is created by runTests.

### Constructor

ClassifyResult(datasetName, classificationName, originalNames, originalFeatures, rankedFeatures

datasetName A name associated with the dataset used.

classificationName A name associated with the classification.

originalNames Sample names.

originalFeatures Feature names.

rankedFeatures Indices or names of all features, from most to least important.

chosenFeatures Indices or names of features selected at each fold.

predictions A list of data. frame containing information about samples, their actual class and predicted class.

actualClasses Factor of class of each sample.

validation List with first elment being name of the validation scheme, and other elements providing details about scehme.

tune A description of the tuning parameters, and the value chosen of each parameter.

#### **Summary**

A method which summarises the results is available. result is a ClassifyResult object.

show(result)Prints a short summary of what result contains.

totalPredictions(ClassifyResult)Calculates the sum of the number of predictions.

#### Accessors

result is a ClassifyResult object.

predictions(result) Returns a list of data. frame. Each data.frame contains columns sample, predicted, and actual. For hold-out validation, only one data.frame is returned of all of the concatenated predictions.

actualClasses(result) Returns a factor class labels, one for each sample.

features(result) A list of the features selected for each training.

performance(result) Returns a list of performance measures. This is empty until calcPerformance has been used.

tunedParameters(result) Returns a list of tuned parameter values. If cross-validation is used, this list will be large, as it stores chosen values for every validation.

names(result) Returns a character vector of sample names.

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#### Author(s)

Dario Strbenac

# **Examples**

```
if(require(curatedOvarianData) && require(sparsediscrim))
{
    data(TCGA_eset)
    badOutcome <- which(pData(TCGA_eset)[, "vital_status"] == "deceased" & pData(TCGA_eset)[, "days_to_death"
    goodOutcome <- which(pData(TCGA_eset)[, "vital_status"] == "living" & pData(TCGA_eset)[, "days_to_death"]
    TCGA_eset <- TCGA_eset[, c(badOutcome, goodOutcome)]
    classes <- factor(rep(c("Poor", "Good"), c(length(badOutcome), length(goodOutcome))))
    pData(TCGA_eset)[, "class"] <- classes
    results <- runTests(TCGA_eset, "Ovarian Cancer", "Differential Expression", resamples = 2, folds = 2)
    show(results)
    predictions(results)
    actualClasses(results)
}</pre>
```

distribution

Get Frequencies of Feature Selection and Sample Errors

### **Description**

There are two modes. For aggregating feature selection results, the function counts the number of times each feature was selected in all cross-validations. For aggregating classification results, the error rate for each sample is calculated. This is useful in identifying outlier samples that are difficult to classify.

# Usage

## **Arguments**

result

plot

dataType Whether to calculate sample-wise error rate or the number of times a feature was selected.

plotType Whether to draw a probability density curve or a histogram.

summaryType Whether to summarise the feature selections as a percentage or count.

Whether to draw a plot of the frequency of selection or error rate.

An object of class ClassifyResult.

xMax Maximum data value to show in plot.
xLabel The label for the x-axis of the plot.
yLabel The label for the y-axis of the plot.

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title	An overall title for the plot.
fontSizes	A vector of length 3. The first number is the size of the title. The second number is the size of the axes titles. The third number is the size of the axes values.
	Further parameters, such as colour and fill, passed to geom_histogram or stat density, depending on the value of plotType.

### Value

If type is "features", a vector as long as the number of features that were chosen at least once containing the number of times the feature was chosen in cross validations or the percentage of times chosen. If type is "samples", a vector as long as the number of samples, containing the cross-validation error rate of the sample. If plot is TRUE, then a plot is also made on the current graphics device.

### Author(s)

Dario Strbenac

# **Examples**

DMDselection

Selection of Differential Distributions with Differences in Means or Medians and a Deviation Measure

# **Description**

Ranks features by largest Differences in Means/Medians and Deviations and chooses the features which have best resubstitution performance.

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#### **Usage**

# **Arguments**

expression Either a matrix or ExpressionSet containing the training data. For a matrix,

the rows are features, and the columns are samples.

classes A vector of class labels.

datasetName A name for the dataset used. Stored in the result.

trainParams A container of class TrainParams describing the classifier to use for training.

predictParams A container of class PredictParams describing how prediction is to be done.

resubstituteParams

An object of class ResubstituteParams describing the performance measure to consider and the numbers of top features to try for resubstitution classification.

... Either variables passed from the matrix method to the ExpressionSet method

or variables passed to  $\verb"getLocationsAndScales"$  from the  $\verb"ExpressionSet"$  method.

selectionName A name to identify this selection method by. Stored in the result.

verbose A number between 0 and 3 for the amount of progress messages to give. This

function only prints progress messages if the value is 3.

### **Details**

DMD is defined as  $|location_1 - location_2| + |scale_1 - scale_2|$ .

The subscripts denote the group which the parameter is calculated for.

# Value

An object of class SelectResult or a list of such objects, if the classifier which was used for determining resubstitution error rate made a number of prediction varieties.

# Author(s)

Dario Strbenac

# **Examples**

predictParams = PredictParams(function(){}, FALSE, getClasses = function(result) result),

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```
resubstituteParams = ResubstituteParams(nFeatures = seq(10, 100, 10), performanceType = "balance")
}
```

edgeRselection

Feature Selection Based on Differential Expression for RNA-seq

### **Description**

Performs a differential expression analysis between classes and chooses the features which have best resubstitution performance.

#### Usage

# **Arguments**

expression Either a matrix or ExpressionSet containing the expression values.

classes A vector of class labels.

.. Unused variables from the matrix method passed to the ExpressionSet method.

datasetName A name for the dataset used. Stored in the result.

 ${\tt normFactorsOptions}$ 

A named list of any options to be passed to calcNormFactors.

dispOptions A named list of any options to be passed to estimateDisp.

fitOptions A named list of any options to be passed to glmFit.

trainParams A container of class TrainParams describing the classifier to use for training.

predictParams A container of class PredictParams describing how prediction is to be done.

resubstituteParams

An object of class ResubstituteParams describing the performance measure to consider and the numbers of top features to try for resubstitution classification.

selectionName A name to identify this selection method by. Stored in the result.

verbose A number between 0 and 3 for the amount of progress messages to give. This

function only prints progress messages if the value is 3.

#### **Details**

The differential expression analysis follows the standard edgeR steps of estimating library size normalisation factors, calculating dispersion, in this case robustly, and then fitting a generalised linear model followed by a likelihood ratio test.

# Value

An object of class SelectResult or a list of such objects, if the classifier which was used for determining resubstitution error rate made a number of prediction varieties.

errorMap 11

#### Author(s)

Dario Strbenac

#### References

edgeR: a Bioconductor package for differential expression analysis of digital gene expression data, Mark D. Robinson, Davis McCarthy, and Gordon Smyth, 2010, Bioinformatics, Volume 26 Issue 1, bioinformatics.oxfordjournals.org/content/26/1/139.

#### **Examples**

errorMap

Plot a Grid of Sample Error Rates

### **Description**

A grid of coloured tiles is drawn. There is one column for each sample and one row for each classification result.

# Usage

# Arguments

```
results A list of ClassifyResult objects.

comparison The aspect of the experimental design to compare.

errorColours A vector of colours for error levels.
```

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classColours Either a vector of colours for class levels if both classes should have same colour,

or a list of length 2, with each component being a vector of the same length. The

vector has the colour gradient for each class.

fontSizes A vector of length 5. The first number is the size of the title. The second number

is the size of the axes titles. The third number is the size of the axes values. The fourth number is the size of the legends' titles. The fifth number is the font size

of the legend labels.

mapHeight Height of the map, relative to the height of the class colour bar.

title The title to place above the plot.

showLegends Logical. IF FALSE, the legend is not drawn.

xAxisLabel The name plotted for the x-axis. NULL suppresses label.

showXtickLabels

Logical. IF FALSE, the x-axis labels are hidden.

showYtickLabels

Logical. IF FALSE, the y-axis labels are hidden.

yAxisLabel The name plotted for the y-axis. NULL suppresses label.

legendSize The size of the boxes in the legends.

plot Logical. IF TRUE, a plot is produced on the current graphics device.

### **Details**

The names of results determine the row names that will be in the plot. The length of errorColours determines how many bins the error rates will be discretised to.

#### Value

A plot is produced and a grob is returned that can be saved to a graphics device.

### Author(s)

Dario Strbenac

fisherDiscriminant 13

fisherDiscriminant	Classification Using Fisher's LDA
ruiscriminant	Classification Using Fisher's LD.

# **Description**

Finds the decision boundary using the training set, and gives predictions for the test set.

# Usage

```
## S4 method for signature 'matrix'
fisherDiscriminant(expression, classes, ...)
   ## S4 method for signature 'ExpressionSet'
fisherDiscriminant(expression, test, returnType = c("label", "score", "both"), verbose = 3)
```

# **Arguments**

١	•	
	expression	Either a matrix or ExpressionSet containing the training data. For a matrix, the rows are features, and the columns are samples.
	classes	A vector of class labels.
		$Unused\ variables\ from\ the\ {\tt matrix}\ method\ passed\ to\ the\ {\tt ExpressionSet}\ method.$
	test	Either a matrix or ExpressionSet containing the test data.
	returnType	Either "label", "score", or "both". Sets the return value from the prediction to either a vector of class labels, score for a sample belonging to the second class, as determined by the factor levels, or both labels and scores in a data.frame.
	verbose	A number between 0 and 3 for the amount of progress messages to give. This function only prints progress messages if the value is 3.

### **Details**

Unlike ordinary LDA, Fisher's version does not have assumptions about the normality of the features.

# Value

A vector or data.frame of class prediction information, as long as the number of samples in the test data.

# Author(s)

Dario Strbenac

```
trainMatrix <- matrix(rnorm(1000, 8, 2), ncol = 10) trainMatrix[1:30, 1:5] <- trainMatrix[1:30, 1:5] + 5 # Make first 30 genes D.E. testMatrix <- matrix(rnorm(1000, 8, 2), ncol = 10) testMatrix[1:30, 6:10] <- testMatrix[1:30, 6:10] + 5 # Make first 30 genes D.E. classes <- factor(rep(c("Poor", "Good"), each = 5)) fisherDiscriminant(trainMatrix, classes, testMatrix)
```

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+111	ncti	$\cap$ n()i	rList

Union of Functions and List of Functions

### **Description**

Allows a slot to be either a function or a list of functions.

#### Author(s)

Dario Strbenac

# **Examples**

```
SelectParams(limmaSelection)
SelectParams(list(limmaSelection, leveneSelection), "Ensemble Selection")
```

getLocationsAndScales Calculate Location and Scale

# **Description**

Calculates the location and scale for each feature.

# Usage

# **Arguments**

expression Either a matrix or ExpressionSet containing data. For a matrix, the rows are features, and the columns are samples.

... Unused variables from the matrix method passed to the ExpressionSet method.

location The location to be calculated.

scale The scale to be calculated.

### **Details**

Location can be either "mean" or "median". Scale can be standard deviation, median absolute deviation, or  $Q_n$ .

# Value

A list of length 2. The first element contains the location for every feature. The second element contains the scale for every feature.

#### Author(s)

Dario Strbenac

#### References

```
Qn: http://www.tandfonline.com/doi/pdf/10.1080/01621459.1993.10476408
```

### **Examples**

```
genesMatrix <- matrix(rnorm(1000, 8, 4), ncol = 10)
getLocationsAndScales(genesMatrix, "median", "MAD")</pre>
```

KolmogorovSmirnovSelection

Selection of Differential Distributions with Kolmogorov-Smirnov Distance

# **Description**

Ranks features by largest Kolmogorov-Smirnov distance and chooses the features which have best resubstitution performance.

# Usage

### **Arguments**

expression Either a matrix or ExpressionSet containing the training data. For a matrix,

the rows are features, and the columns are samples.

classes A vector of class labels.

datasetName A name for the dataset used. Stored in the result.

trainParams A container of class TrainParams describing the classifier to use for training.

predictParams A container of class PredictParams describing how prediction is to be done.

resubstituteParams

An object of class ResubstituteParams describing the performance measure to consider and the numbers of top features to try for resubstitution classification.

... For the matrix method, variables passed to the ExpressionSet method. For

the ExpressionSet method, the options to be passed to function ks.test.

selectionName A name to identify this selection method by. Stored in the result.

verbose A number between 0 and 3 for the amount of progress messages to give. This

function only prints progress messages if the value is 3.

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#### **Details**

Features are sorted in order of biggest distance to smallest. The top number of features is used in a classifier, to determine which number of features has the best resubstitution performance.

#### Value

An object of class SelectResult or a list of such objects, if the classifier which was used for determining resubstitution error rate made a number of prediction varieties.

#### Author(s)

Dario Strbenac

# **Examples**

KullbackLeiblerSelection

Selection of Differential Distributions with Kullback Leibler Distance

# Description

Ranks features by largest Kullback-Leibler distance and chooses the features which have best resubstitution performance.

### Usage

#### **Arguments**

expression Either a matrix or ExpressionSet containing the training data. For a matrix,

the rows are features, and the columns are samples.

classes A vector of class labels.

datasetName A name for the dataset used. Stored in the result.

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trainParams A container of class TrainParams describing the classifier to use for training.

PredictParams A container of class PredictParams describing how prediction is to be done.

ResubstituteParams

An object of class ResubstituteParams describing the performance measure to consider and the numbers of top features to try for resubstitution classification.

Variables passed to getLocationsAndScales.

SelectionName A name to identify this selection method by. Stored in the result.

Verbose A number between 0 and 3 for the amount of progress messages to give. This

function only prints progress messages if the value is 3.

# **Details**

The distance is defined as  $1/2 * (location_1 - location_2)^2$ 

The subscripts denote the group which the parameter is calculated for.

#### Value

An object of class SelectResult or a list of such objects, if the classifier which was used for determining resubstitution error rate made a number of prediction varieties.

### Author(s)

Dario Strbenac

#### **Examples**

leveneSelection

Selection of Differential Variability with Levene Statistic

# **Description**

Ranks features by largest Levene statistic and chooses the features which have best resubstitution performance.

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#### **Usage**

# **Arguments**

expression Either a matrix or ExpressionSet containing the training data. For a matrix,

the rows are features, and the columns are samples.

classes A vector of class labels.

... For the matrix method, variables passed to the ExpressionSet method.

datasetName A name for the dataset used. Stored in the result.

trainParams A container of class TrainParams describing the classifier to use for training.

predictParams A container of class PredictParams describing how prediction is to be done.

resubstituteParams

An object of class ResubstituteParams describing the performance measure to consider and the numbers of top features to try for resubstitution classification.

selectionName A name to identify this selection method by. Stored in the result.

verbose A number between 0 and 3 for the amount of progress messages to give. This

function only prints progress messages if the value is 3.

# **Details**

Levene's statistic for unequal variance between groups is a robust version of Bartlett's statistic.

#### Value

An object of class SelectResult or a list of such objects, if the classifier which was used for determining resubstitution error rate made a number of prediction varieties.

# Author(s)

Dario Strbenac

likelihoodRatioSelection 19

```
performanceType = "balanced", better = "lower"))
}
```

likelihoodRatioSelection

Selection of Differential Distributions with Likelihood Ratio Statistic

### **Description**

Ranks features by largest ratio and chooses the features which have the best resubstitution performance.

### Usage

# **Arguments**

expression Either a matrix or ExpressionSet containing the training data. For a matrix, the rows are features, and the columns are samples. classes A vector of class labels. A name for the dataset used. Stored in the result. datasetName A container of class TrainParams describing the classifier to use for training. trainParams A container of class PredictParams describing how prediction is to be done. predictParams resubstituteParams An object of class ResubstituteParams describing the performance measure to consider and the numbers of top features to try for resubstitution classification. A vector of length 2. The first element specifies the location of the alternate alternative hypothesis. The second element specifies the scale of the alternate hypothesis. Acceptable values are "same" or "different". Either variables passed from the matrix method to the ExpressionSet method or variables passed to getLocationsAndScales from the ExpressionSet method. selectionName A name to identify this selection method by. Stored in the result. A number between 0 and 3 for the amount of progress messages to give. This verbose function only prints progress messages if the value is 3.

### **Details**

Likelihood ratio test of null hypothesis that the location and scale are the same for both groups, and an alternate hypothesis that is specified by parameters. The location and scale of features is calucated by getLocationsAndScales. The distribution fitted in the normal distribution.

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#### Value

A list of length 2. The first element has the features ranked from most important to least important. The second element has the features that were selected to be used for classification.

#### Author(s)

Dario Strbenac

# **Examples**

limmaSelection

Selection of Differentially Expressed Features

# **Description**

Uses a moderated t-test with empirical Bayes shrinkage to select differentially expressed features.

# Usage

# **Arguments**

expression Either a matrix or ExpressionSet containing the training data. For a matrix,

the rows are features, and the columns are samples.

classes A vector of class labels.

datasetName A name for the dataset used. Stored in the result.

trainParams A container of class TrainParams describing the classifier to use for training.

predictParams A container of class PredictParams describing how prediction is to be done.

resubstituteParams

An object of class ResubstituteParams describing the performance measure to consider and the numbers of top features to try for resubstitution classification.

For the matrix method, variables passed to the ExpressionSet method. For the ExpressionSet method, extra parameters that are passed to lmFit.

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selectionName A name to identify this selection method by. Stored in the result.

verbose A number between 0 and 3 for the amount of progress messages to give. This

function only prints progress messages if the value is 3.

### **Details**

This selection method looks for differential expression. It uses a moderated t-test.

#### Value

An object of class SelectResult or a list of such objects, if the classifier which was used for determining resubstitution error rate made a number of prediction varieties.

### Author(s)

Dario Strbenac

#### References

Limma: linear models for microarray data, Gordon Smyth, 2005, In: Bioinformatics and Computational Biology Solutions using R and Bioconductor, Springer, New York, pages 397-420.

# **Examples**

 ${\tt medianDifferenceSelection}$ 

Selection of Differential Expression by Comparing Differences in Medians of Groups

# Description

Ranks features by largest absolute difference of group medians and chooses the features which have best resubstitution performance.

#### **Usage**

### **Arguments**

expression Either a matrix or ExpressionSet containing the training data. For a matrix,

the rows are features, and the columns are samples.

classes A vector of class labels.

... For the matrix method, variables passed to the ExpressionSet method.

datasetName A name for the dataset used. Stored in the result.

trainParams A container of class TrainParams describing the classifier to use for training.

predictParams A container of class PredictParams describing how prediction is to be done.

resubstituteParams

An object of class ResubstituteParams describing the performance measure to consider and the numbers of top features to try for resubstitution classification.

selectionName A name to identify this selection method by. Stored in the result.

verbose A number between 0 and 3 for the amount of progress messages to give. This

function only prints progress messages if the value is 3.

### Value

An object of class SelectResult or a list of such objects, if the classifier which was used for determining resubstitution error rate made a number of prediction varieties.

# Author(s)

Dario Strbenac

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mixmodels

Selection of Differential Distributions with Mixtures of Normals

#### **Description**

Fits mixtures of normals for every gene, separately for each class.

# Usage

# **Arguments**

expression Either a matrix or ExpressionSet containing the training data. For a matrix,

the rows are features, and the columns are samples.

test Either a matrix or ExpressionSet containing the test data. For a matrix, the

rows are features, and the columns are samples.

classes A vector of class labels.

weighted In weighted mode, the difference in densities is summed over all features. If

unweighted mode, each features's vote is worth the same. To save computational

time, both can be calculated simultaneously.

weight The type of weight to calculate. For "height difference", the weight of

each prediction is equal to the sum of the verical distances for all of the mixture components within one class subtracted from the sum of the components of the other class, summed for each value of x. For "crossover distance", the x positions where two mixture densities cross is firstly calculated. The predicted class is the class with the highest mixture sum at the particular value of x and

the weight is the distance of x from the nearest density crossover point.

densityXvalues Only relevant when weight is "crossover distance". The number of equally-

spaced locations at which to calculate y values for each mixture density.

minDifference The minimum difference in sums of mixture densities within each class for a

feature to be allowed to vote. Can be a vector of cutoffs. If no features for a particular sample have a difference large enough, the class predicted is simply

the largest class.

For the training or testing function with matrix dispatch, arguments passed

to the function with ExpressionSet dispatch. For the training function with ExpressionSet dispatch, extra arguments passed to mixmodCluster. The ar-

gument nbCluster is mandatory.

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Malist of length 2 of models generated by the training function. The first element has mixture models the same length as the number of features in the expression data for one class. The second element has the same information for the other class.

returnType Either "label", "score", or "both". Sets the return value from the prediction

to either a vector of class labels, score for a sample belonging to the second class, as determined by the factor levels, or both labels and scores in a data. frame.

verbose A number between 0 and 3 for the amount of progress messages to give. A

higher number will produce more messages.

#### **Details**

If weighted is TRUE, then a sample's predicted class is the class with the largest sum of weights, scaled for the number of samples in the training data of each class. Otherwise, when weighted is FALSE, each feature has an equal vote, and votes for the class with the largest weight, scaled for class sizes in the training set.

If weight is "crossover distance", the crossover points are computed by considering the distance between y values of the two densities at every x value. x values for which the sign of the difference changes compared to the difference of the closest lower value of x are used as the crossover points. Setting weight to "sum differences" is intended to find a mix of features which are strongly differentially expressed and differentially variable.

#### Value

For mixModelsTrain, a list of trained models of class MixmodCluster. A vector or list of class prediction information, as long as the number of samples in the test data, or lists of such information, if both weighted and unweighted voting or a range of minDifference values was provided.

# Author(s)

Dario Strbenac

# **Examples**

```
# First 25 samples are mixtures of two normals. Last 25 samples are one normal.
genesMatrix <- sapply(1:25, function(geneColumn) c(rnorm(50, 5, 1), rnorm(50, 15, 1)))
genesMatrix <- cbind(genesMatrix, sapply(1:25, function(geneColumn) rnorm(100, 9, 3)))
classes <- factor(rep(c("Poor", "Good"), each = 25))
trained <- mixModelsTrain(genesMatrix, classes, nbCluster = 1:3)
mixModelsTest(trained, genesMatrix, minDifference = 1:3)</pre>
```

naiveBayesKernel

Classification Using A Bayes Classifier with Kernel Density Estimates

# **Description**

Kernel density estimates are fitted to the training data and a naive Bayes classifier is used to classify samples in the test data.

naiveBayesKernel 25

#### **Usage**

# **Arguments**

expression Either a matrix or ExpressionSet containing the training data. For a matrix,

the rows are features, and the columns are samples.

classes A vector of class labels.

.. Unused variables from the matrix method passed to the ExpressionSet method.

test Either a matrix or ExpressionSet containing the test data.

densityFunction

A function which will return a probability density, which is essentially a list with x and y coordinates.

densityParameters

A list of options for densityFunction.

weighted In weighted mode, the difference in densities is summed over all features. If

unweighted mode, each feature's vote is worth the same. To save computational

time, both can be calculated simultaneously.

weight The type of weight to calculate. For "height difference", the weight of each

prediction is equal to the verical distance between two densities, for a particular value of x. For "crossover distance", the x positions where two densities cross is firstly calculated. The predicted class is the class with the highest density at the particular value of x and the weight is the distance of x from the nearest density crossover point. For "sum differences", the weight is the sum of the

weights calculated by both types of distances.

minDifference The minimum difference in densities for a feature to be allowed to vote. Can be

a vector of cutoffs. If no features for a particular sample have a difference large

enough, the class predicted is simply the largest class.

returnType Either "label", "score", or "both". Sets the return value from the prediction

to either a vector of class labels, score for a sample belonging to the second class, as determined by the factor levels, or both labels and scores in a data.frame.

verbose A number between 0 and 3 for the amount of progress messages to give. This

function only prints progress messages if the value is 3.

# Details

If weighted is TRUE, then a sample's predicted class is the class with the largest sum of weights, scaled for the number of samples in the training data of each class. Otherwise, when weighted is FALSE, each feature has an equal vote, and votes for the class with the largest weight, scaled for class sizes in the training set.

The variable name of each feature's measurements in the iteration over all features is featureValues. This is important to know if each feature's measurements need to be referred to in the specification

of densityParameters, such as for specifying the range of x values of the density function to be computed.

If weight is "crossover distance", the crossover points are computed by considering the distance between y values of the two densities at every x value. x values for which the sign of the difference changes compared to the difference of the closest lower value of x are used as the crossover points.

Setting weight to "sum differences" is intended to find a mix of features which are strongly differentially expressed and differentially variable.

#### Value

A vector or list of class prediction information, as long as the number of samples in the test data, or lists of such information, if a variety of predictions is generated.

### Author(s)

Dario Strbenac, John Ormerod

# **Examples**

```
trainMatrix <- matrix(rnorm(1000, 8, 2), ncol = 10)
trainMatrix[1:30, 1:5] <- trainMatrix[1:30, 1:5] + 5 # Make first 30 genes D.E.
testMatrix <- matrix(rnorm(1000, 8, 2), ncol = 10)
testMatrix[1:30, 6:10] <- testMatrix[1:30, 6:10] + 5 # Make first 30 genes D.E.
classes <- factor(rep(c("Poor", "Good"), each = 5))
# Expected: Good Good Good Good Good Poor Poor Poor Poor
naiveBayesKernel(trainMatrix, classes, testMatrix)</pre>
```

nearestShrunkenCentroidPredictInterface

Interface for pamr.predict Function from pamr CRAN Package

# Description

Restructures variables from ClassifyR framework to be compatible with pamr.predict definition.

### Usage

```
## S4 method for signature 'pamrtrained,matrix'
nearestShrunkenCentroidPredictInterface(trained, test, ...)
## S4 method for signature 'pamrtrained,ExpressionSet'
nearestShrunkenCentroidPredictInterface(trained, test, ..., verbose = 3)
```

# Arguments

trained	An object of class pamrtrained.
test	Either a matrix or ExpressionSet containing the test data. For a matrix, the rows are features, and the columns are samples.
	For the function with matrix dispatch, arguments passed to the function with ExpressionSet dispatch. For the function with ExpressionSet dispatch, arguemnts passed to pamr.predict.
verbose	A number between 0 and 3 for the amount of progress messages to give. This function only prints progress messages if the value is 3.

#### **Details**

This function is an interface between the ClassifyR framework and pamr.predict.

### Value

A factor of predicted classes for the test data.

#### Author(s)

Dario Strbenac

### See Also

pamr.predict for the function that was interfaced to.

### **Examples**

nearestShrunkenCentroidSelectionInterface

Interface for pamr.listgenes Function from pamr CRAN Package

# **Description**

Restructures variables from ClassifyR framework to be compatible with pamr.listgenes definition.

# Usage

### **Arguments**

expression	Either a matrix or ExpressionSet containing the training data. For a matrix, the rows are features, and the columns are samples.
datasetName	A name for the dataset used. Stored in the result.
classes	A vector of class labels.
trained	The output of nearestShrunkenCentroidTrainInterface, which is identical to the output of pamr.listgenes.
•••	Extra arguments passed to pamr.listgenes or parameters not used by the matrix method that are passed to the ExpressionSet method.
selectionName	A name to identify this selection method by. Stored in the result.
verbose	A number between 0 and 3 for the amount of progress messages to give. This function only prints progress messages if the value is 3.

#### **Details**

This function is an interface between the ClassifyR framework and pamr.listgenes.

The set of features chosen is the obtained by considering the range of thresholds provided to nearestShrunkenCentroidTrainInterface and using the threshold that obtains the lowest cross-validation error rate on the training set.

### Value

An object of class SelectResult. The rankedFeatures slot will be empty.

# Author(s)

Dario Strbenac

# See Also

pamr.listgenes for the function that was interfaced to.

nearest Shrunken Centroid Train Interface

Interface for pamr.train Function from pamr CRAN Package

### **Description**

Restructures variables from ClassifyR framework to be compatible with pamr.train definition.

### Usage

```
## S4 method for signature 'matrix'
nearestShrunkenCentroidTrainInterface(expression, classes, ...)
## S4 method for signature 'ExpressionSet'
nearestShrunkenCentroidTrainInterface(expression, ..., verbose = 3)
```

### Arguments

expression	Either a matrix or ExpressionSet containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	A vector of class labels.
	Extra arguments passed to pamr. train.
verbose	A number between 0 and 3 for the amount of progress messages to give. This
	function only prints progress messages if the value is 3.

# **Details**

This function is an interface between the ClassifyR framework and pamr.train.

# Value

A list with elements as described in pamr. train.

#### Author(s)

Dario Strbenac

# See Also

pamr. train for the function that was interfaced to.

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pamrtrained

Trained pamr Object

#### **Description**

Enables dispatching on it.

#### **Summary**

A method which summarises the results is available. result is a ClassifyResult object.

show(result)Prints a short summary of what result contains.

#### Author(s)

Dario Strbenac

# **Examples**

performancePlot

Plot Performance Measures for Various Classifications

#### **Description**

Draws a graphical summary of a particular performance measure for a list of classifications

# Usage

margin = grid::unit(c(0, 0, 0, 0), "lines"), rotate90 = FALSE, showLegend = TRUE, p

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### **Arguments**

results A list of ClassifyResult objects.

aggregate A character vector of the levels of xVariable to aggregate to a single number

by taking the mean. This is partciularly meaningful when the cross-validation is

leave-k-out, when k is small.

xVariable The factor to make separate boxes for.

performanceName

The name of the performance measure to make comparisons of. This is one of the names printed in the Performance Measures field when a ClassifyResult

object is printed.

boxFillColouring

A factor to colour the boxes by.

boxFillColours A vector of colours, one for each level of boxFillColouring.

boxLineColouring

A factor to colour the box lines by.

boxLineColours A vector of colours, one for each level of boxLineColouring.

rowVariable The slot name that different levels of are plotted as separate rows of boxplots. columnVariable The slot name that different levels of are plotted as separate columns of boxplots.

yLimits The minimum and maximum value of the performance metric to plot.

fontSizes A vector of length 4. The first number is the size of the title. The second number

is the size of the axes titles. The third number is the size of the axes values. The fourth number is the font size of the titles of grouped plots, if any are produced.

In other words, when rowVariable or columnVariable are not NULL.

title An overall title for the plot.

xLabel Label to be used for the x-axis.

yLabel Label to be used for the y-axis of overlap percentages.

margin The margin to have around the plot.
rotate90 Logical. IF TRUE, the plot is horizontal.

showLegend If TRUE, a legend is plotted next to the plot. If FALSE, it is hidden.

plot Logical. IF TRUE, a plot is produced on the current graphics device.

### **Details**

Possible values for slot names are "datasetName", "classificationName", and "validation". If "None", then that graphic element is not used.

If there are multiple values for a performance measure in a single result object, it is plotted as a boxplot, unless aggregate is TRUE, in which case the all predictions in a single result object are considered simultaneously, so that only one performance number is calculated, and a barchart is plotted.

### Value

An object of class ggplot and a plot on the current graphics device, if plot is TRUE.

### Author(s)

Dario Strbenac

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#### **Examples**

```
predicted <- list(data.frame(sample = sample(10, 20, replace = TRUE),</pre>
                                                                               label = rep(c("Healthy", "Cancer"), each = 10)),
                                                    data.frame(sample = sample(10, 20, replace = TRUE),
                                                                                 label = rep(c("Healthy", "Cancer"), each = 10)),
                                                   data.frame(sample = sample(10, 20, replace = TRUE),
                                                                                  label = rep(c("Healthy", "Cancer"), each = 10)),
                                                    data.frame(sample = sample(10, 20, replace = TRUE),
                                                                                  label = rep(c("Healthy", "Cancer"), each = 10)))
actual <- factor(rep(c("Healthy", "Cancer"), each = 5))</pre>
result1 <- ClassifyResult("Example", "Differential Expression", "t-test", LETTERS[1:10], LETTERS[10:1], li
                                                                         predicted, actual, list("resampleFold", 2, 2))
result1 <- calcPerformance(result1, "f")</pre>
predicted <- data.frame(sample = sample(10, 100, replace = TRUE),</pre>
                                                                    label = rep(c("Healthy", "Cancer"), each = 50))
result2 <- ClassifyResult("Example", "Differential Variability", "F-test", LETTERS[1:10], LETTERS[10:1], l.
                                                                          list(predicted), actual, validation = list("leave", 1))
result2 <- calcPerformance(result2, "f")</pre>
performancePlot(list(result1, result2), performanceName = "Precision-Recall F measure", title = "Comparison of the comparison of the compa
```

plotFeatureClasses

Plot Density and Scatterplot for Genes By Class

### **Description**

Allows the visualisation of genes which were selected by a feature selection method.

# Usage

### **Arguments**

expression	Either a matrix or ExpressionSet containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	A vector of class labels.
	Unused variables from the matrix method passed to the ExpressionSet method.
rows	A vector specifying which rows of the matrix to plot.
whichPlots	Which plots to draw. Can draw either a density plot, stripchart, or both.
xAxisLabel	The axis label for the expression axis.
yAxisLabels	A character vector of length 2. The first value is the y-axis label for the density plot. The second value is the y-axis labels for the stripchart. Provide both labels, even if only plotting one kind of plot.

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expressionLimits

The minimum and maximum expression values to plot. Set to NULL to use range of data.

showXtickLabels

Logical. IF FALSE, the x-axis labels are hidden.

showYtickLabels

Logical. IF FALSE, the y-axis labels are hidden.

xLabelPositions

Either "auto" or a vector of values. The positions of labels on the x-axis. If "auto", the placement of labels is automatically calculated.

yLabelPositions

Either "auto" or a vector of values. The positions of labels on the y-axis. If "auto", the placement of labels is automatically calculated.

fontSizes

A vector of length 5. The first number is the size of the title. The second number is the size of the axes titles. The third number is the size of the axes values. The fourth number is the size of the legends' titles. The fifth number is the font size of the legend labels.

colours

The colours to plot data of each class in.

plot

Logical. If TRUE, a plot is produced on the current graphics device.

#### Value

Plots.

# Author(s)

Dario Strbenac

# **Examples**

```
# First 25 samples are mixtures of two normals. Last 25 samples are one normal. genesMatrix <- sapply(1:25, function(geneColumn) c(rnorm(50, 5, 1), rnorm(50, 15, 1))) genesMatrix <- cbind(genesMatrix, sapply(1:25, function(geneColumn) rnorm(100, 9, 3))) classes <- factor(rep(c("Poor", "Good"), each = 25), levels = c("Good", "Poor")) chosen <- 1:5 # First five genes in the data were chosen.
```

plotFeatureClasses(genesMatrix, classes, chosen, expressionLimits = NULL)

PredictParams

Parameters for Classifier Prediction

# Description

Collects the function to be used for making predictions and any associated parameters.

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#### Constructor

PredictParams() Creates a default PredictParams object. This assumes that the object returned by the classifier has a list element named "class".

PredictParams(predictor, transposeExpression, intermediate = character(0), getClasses, ...)

Creates a PredictParams object which stores the function which will do the class prediction and parameters that the function will use.

predictor A function to make predictions with. The first argument must accept the classifier made in the training step. The second argument must accept a matrix of new data.

transposeExpression Set to TRUE if classifier expects features as columns.

intermediate Character vector. Names of any variables created in prior stages by runTest that need to be passed to the prediction function.

getClasses A function to extract the vector of class predictions from the result object created by predictor.

... Other arguments that predictor may use.

### Author(s)

Dario Strbenac

### **Examples**

```
predictParams <- PredictParams(predictor = predict, TRUE, getClasses = function(result) result)
# For prediction by trained object created by dlda function.
PredictParams(predictor = function(){}, TRUE, getClasses = function(result) result)
# For when the training function also does prediction and directly returns vector of predictions.</pre>
```

previousSelection

Automated Selection of Previously Selected Features

# **Description**

Uses the feature selection of the same cross-validation iteration of a previous classification for the current classification task.

# Usage

# Arguments

expression Either a matrix or ExpressionSet containing the training data. For a matrix, the rows are features, and the columns are samples.

classes A vector of class labels.

For the matrix method, variables passed to the ExpressionSet method.

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datasetName A name for the dataset used. Stored in the result.

classifyResult An existing classification result from which to take the feature selections from. minimumOverlapPercent

If at least this many selected features can't be identified in the current dataset, then the selection stops with an error.

selectionName A name to identify this selection method by. Stored in the result.

.iteration Not to be set by the user.

verbose A number between 0 and 3 for the amount of progress messages to give. This

function only prints progress messages if the value is 3.

#### Value

An object of class SelectResult.

#### Author(s)

Dario Strbenac

```
if(require(sparsediscrim))
  # Genes 76 to 100 have differential expression.
 genesMatrix <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))</pre>
 genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample)</pre>
                                c(rnorm(75, 9, 2), rnorm(25, 14, 2))))
 rownames(genesMatrix) <- paste("Gene", 1:100)</pre>
 classes <- factor(rep(c("Poor", "Good"), each = 25))</pre>
 resubstitute <- ResubstituteParams(nFeatures = seq(10, 100, 10),
                                      performanceType = "err", better = "lower")
 result <- runTests(genesMatrix, classes, "Ovarian Cancer", "Differential Expression",
                     resamples = 2, fold = 2,
                 params = list(SelectParams(limmaSelection, resubstituteParams = resubstitute),
                     TrainParams(dlda, TRUE, FALSE),
                 PredictParams(predict, TRUE, getClasses = function(result) result[["class"]])))
 # Genes 74 to 98 have differential expression in new dataset.
 newDataset <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))</pre>
 newDataset <- cbind(newDataset, rbind(sapply(1:25, function(sample) rnorm(73, 9, 2)),</pre>
                                       sapply(1:25, function(sample) rnorm(25, 14, 2)),
                                       sapply(1:25, function(sample) rnorm(2, 14, 2))))
 newerResult <- runTests(newDataset, classes, "Ovarian Cancer Updated", "Differential Expression",</pre>
                     resamples = 2, fold = 2,
                 params = list(SelectParams(previousSelection, intermediate = ".iteration",
                                   classifyResult = result),
                     TrainParams(dlda, TRUE, FALSE),
                PredictParams(predict, TRUE, getClasses = function(result) result[["class"]])))
}
```

36 rankingPlot

rankingPlot

Plot Pair-wise Overlap of Ranked Features

#### **Description**

Pair-wise overlaps can be done for two types of analyses. Firstly, each cross-validation iteration can be considered within a single classification. This explores the feature ranking stability. Secondly, the overlap may be considered between different classification results. This approach compares the feature ranking commonality between different methods. Two types of commonality are possible to analyse. One summary is the average pair-wise overlap between a level of the comparison factor and the other summary is the pair-wise overlap of each level of the comparison factor that is not the reference level against the reference level. The overlaps are converted to percentages and plotted as lineplots.

### Usage

```
## S4 method for signature 'list'
rankingPlot(results, topRanked = seq(10, 100, 10),
                                                                      comparison = c("within", "classificationName", "validation", "datasetName"
                                                                                        referenceLevel = NULL,
                                                                      lineColourVariable = c("validation", "datasetName", "classificationName",
                                                                                                                                                                 "selectionName", "None"),
                                                                                        lineColours = NULL, lineWidth = 1,
                                                                      pointTypeVariable = c("datasetName", "classificationName", "validation",
                                                                                                                                                             "selectionName", "None"),
                                                                                        pointSize = 2, legendLinesPointsSize = 1,
                                                                       rowVariable = c("None", "datasetName", "classificationName", "validation",
                                                                       column Variable = c("classification Name", "dataset Name", "validation", "selection validation", "selection validation validation", "selection validation val
                                                                                        yMax = 100, fontSizes = c(24, 16, 12, 12, 16),
                                                                       title = if(comparison[1] == "within") "Feature Ranking Stability" else "Fea
                                                                                        xLabelPositions = seq(10, 100, 10),
                                                                      yLabel = if(is.null(referenceLevel)) "Average Common Features (%)" else pas
                                                                                        margin = grid::unit(c(0, 0, 0, 0), "lines"),
                                                                       showLegend = TRUE, plot = TRUE, parallelParams = bpparam())
```

### **Arguments**

results A list of ClassifyResult or SelectResult objects.

topRanked A sequence of thresholds of number of the best features to use for overlapping.

comparison The aspect of the experimental design to compare. See Details section for a

detailed description.

referenceLevel The level of the comparison factor to use as the reference to compare each non-

reference level to. If NULL, then each level has the average pairwise overlap

calculated to all other levels.

lineColourVariable

The slot name that different levels of are plotted as different line colours.

lineColours A vector of colours for different levels of the line colouring parameter. If NULL,

a default palette is used.

lineWidth A single number controlling the thickness of lines drawn.

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pointTypeVariable

The slot name that different levels of are plotted as different point shapes on the

lines.

pointSize A single number specifying the diameter of points drawn.

legendLinesPointsSize

A single number specifying the size of the lines and points in the legend, if a

legend is drawn.

rowVariable The slot name that different levels of are plotted as separate rows of lineplots. columnVariable The slot name that different levels of are plotted as separate columns of lineplots.

yMax The maximum value of the percentage to plot.

fontSizes A vector of length 6. The first number is the size of the title. The second

number is the size of the axes titles. The third number is the size of the axes values. The fourth number is the size of the legends' titles. The fifth number is the font size of the legend labels. The sixth number is the font size of the titles of grouped plots, if any are produced. In other words, when rowVariable or

columnVariable are not NULL.

title An overall title for the plot.

xLabelPositions

Locations where to put labels on the x-axis.

yLabel Label to be used for the y-axis of overlap percentages.

margin The margin to have around the plot.

showLegend If TRUE, a legend is plotted next to the plot. If FALSE, it is hidden. plot Logical. If TRUE, a plot is produced on the current graphics device.

parallelParams An object of class MulticoreParam or SnowParam.

## **Details**

Possible values for characteristics are "datasetName", "classificationName", "selectionName", and "validation". If "None", then that graphical element is not used.

If comparison is "within", then the feature rankings are compared within a particular analysis. The result will inform how stable the feature rankings are between different iterations of cross-validation for a particular analysis. If comparison is "classificationName", then the feature rankings are compared across different classification algorithm types, for each level of "datasetName", "selectionName" and "validation". The result will inform how stable the feature rankings are between different classification algorithms, for every cross-validation scheme, selction algorithm and dataset. If comparison is "selectionName", then the feature rankings are compared across different feature selection algorithms, for each level of "datasetName", "classificationName" and "validation". The result will inform how stable the feature rankings are between feature selection classification algorithms, for every dataset, classification algorithm, and cross-validation scheme. If comparison is "validation", then the feature rankings are compared across different cross-validation schemes, for each level of "classificationName", "selectionName" and "datasetName". The result will inform how stable the feature rankings are between different cross-validation schemes, for every selection algorithm, classification algorithm and every dataset. If comparison is "datasetName", then the feature rankings are compared across different datasets, for each level of "classificationName", "selectionName" and "validation". The result will inform how stable the feature rankings are between different datasets, for every classification algorithm and every dataset. This could be used to consider if different experimental studies have a highly overlapping feature ranking pattern.

Calculating all pair-wise set overlaps for a large cross-validation result can be time-consuming. This stage can be done on multiple CPUs by providing the relevant options to parallelParams.

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#### Value

An object of class ggplot and a plot on the current graphics device, if plot is TRUE.

## Author(s)

Dario Strbenac

# **Examples**

```
predicted <- data.frame(sample = sample(10, 100, replace = TRUE),</pre>
                         label = rep(c("Healthy", "Cancer"), each = 50))
actual <- factor(rep(c("Healthy", "Cancer"), each = 5))</pre>
rankList \leftarrow list(list(1:100, c(5:1, 6:100)), list(c(1:9, 11:101), c(1:50, 60:51, 61:100)))
result1 <- ClassifyResult("Example", "Differential Expression", "Example Selection", LETTERS[1:10], LETTERS
                           rankList,
                         list(list(rankList[[1]][[1]][1:15], rankList[[1]][[2]][1:15]),
                             list(rankList[[2]][[1]][1:10], rankList[[2]][[2]][1:10])),
                           list(predicted), actual, list("resampleFold", 2, 2))
predicted[, "label"] <- sample(predicted[, "label"])</pre>
rankList <- list(list(1:100, c(sample(20), 21:100)), list(c(1:9, 11:101), c(1:50, 60:51, 61:100)))
result2 <- ClassifyResult("Example", "Differential Variability", "Example Selection", LETTERS[1:10], LETTE
                           rankList,
                         list(list(rankList[[1]][[1]][1:15], rankList[[1]][[2]][1:15]),
                             list(rankList[[2]][[1]][1:10], rankList[[2]][[2]][1:10])),
                       list(predicted), actual, validation = list("resampleFold", 2, 2))
rankingPlot(list(result1, result2), pointTypeVariable = "classificationName")
oneRanking <- c(10, 8, 1, 2, 3, 4, 7, 9, 5, 6)
otherRanking \leftarrow c(8, 2, 3, 4, 1, 10, 6, 9, 7, 5)
oneResult <- SelectResult("Example", "One Method", list(oneRanking), list(oneRanking[1:5]))</pre>
otherResult <- SelectResult("Example", "Another Method", list(otherRanking), list(otherRanking[1:2]))
rankingPlot(list(oneResult, otherResult), comparison = "selectionName",
         referenceLevel = "One Method", topRanked = seq(2, 8, 2),
         lineColourVariable = "selectionName", columnVariable = "None",
         pointTypeVariable = "None", xLabelPositions = 1:10)
```

 ${\tt ResubstituteParams}$ 

Parameters for Resubstitution Error Calculation

# Description

Some feature selection functions provided in the framework use resubstitution error rate to choose the best number of features for classification. This class stores parameters related to that process

# Constructor

ResubstituteParams() Creates a default ResubstituteParams object. The number of features tried is 100, 200, 300, 400, 500. The performance measure used is the balanced error rate.

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ResubstituteParams(nFeatures, performanceType, better = c("lower", "higher"))
Creates a ResubstituteParams object, storing information about the number of top features to calculate the performance measure for, the performance measure to use, and if higher or lower values of the measure are better.

nFeatures A vector for the top number of features to test the resubstitution error for.

performanceType Either "balanced" or one of the options provided by performance.

better Either "lower" or "higher". Determines whether higher or lower values of the performance measure are desirable.

intermediate Character vector. Names of any variables created in prior stages by runTest that need to be passed to classifier.

... Other named parameters which will be used by the classifier.

# Author(s)

Dario Strbenac

# **Examples**

```
ResubstituteParams(nFeatures = seq(25, 1000, 25), performanceType = "err", better = "lower")
```

ROCplot

Plot Receiver Operating Curve Graphs for Classification Results

# Description

The average pair-wise overlap is computed for every pair of cross-validations. The overlap is converted to a percentage and plotted as lineplots.

# Usage

# Arguments

results A list of ClassifyResult objects.

nBins The number of intervals to group the samples' scores into. By default, there are

as many bins as there were predictions made, for each result object.

lineColourVariable

The slot name that different levels of are plotted as different line colours.

lineColours A vector of colours for different levels of the line colouring parameter. If NULL,

a default palette is used.

lineWidth A single number controlling the thickness of lines drawn.

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fontSizes A vector of length 5. The first number is the size of the title. The second number

is the size of the axes titles and AUC text, if it is not part of the legend. The third number is the size of the axes values. The fourth number is the size of the

legends' titles. The fifth number is the font size of the legend labels.

labelPositions Locations where to put labels on the x and y axes.

plotTitle An overall title for the plot.

legendTitle A default name is used if the value is NULL. Otherwise a character name can be

provided.

xLabel Label to be used for the x-axis of false positive rate.

yLabel Label to be used for the y-axis of true positive rate.

plot Logical. If TRUE, a plot is produced on the current graphics device.

showAUC Logical. If TRUE, the AUC value of each result is added to its legend text.

# **Details**

Possible values for slot names are "datasetName", "classificationName", and "validation". If "None", then any lines drawn will be black.

The scores stored in the results should be higher if the sample is more likely to be from the second class, based on the levels of the actual classes. The scores must be in a column named "score".

For cross-validated classification, all predictions from all iterations are considered simultaneously, to calculate one curve per classification.

The number of bins determines how many pairs of TPR and FPR points will be used to draw the plot. A higher number will result in a smoother ROC curve.

The AUC is calculated using the trapezoidal rule.

## Value

An object of class ggplot and a plot on the current graphics device, if plot is TRUE.

# Author(s)

Dario Strbenac

runTest 41

runTest	Perform a Single Classification	

# **Description**

For a dataset of features and samples, the classification process is run. It consists of data transformation, feature selection, training and testing.

# Usage

# Arguments

expression Either a matrix or ExpressionSet containing the training data. For a matrix,

the rows are features, and the columns are samples.

classes A vector of class labels.

datasetName A name associated with the dataset used.

classificationName

A name associated with the classification.

training A vector which specifies the training samples.
testing A vector which specifies the test samples.

params A list of objects of class of TransformParams, SelectParams, TrainParams,

or PredictParams. The order they are in the list determines the order in which

the stages of classification are done in.

... Unused variables from the matrix method passed to the ExpressionSet method.

verbose A number between 0 and 3 for the amount of progress messages to give. A

higher number will produce more messages.

.iteration Not to be set by a user. This value is used to keep track of the cross-validation

iteration, if called by runTests.

## **Details**

This function only performs one classification and prediction. See runTests for a driver function that does cross-validation and uses this function. datasetName and classificationName need to be provided.

## Value

A named list with five elements. The first element contains all of the features, ranked from most important to least important. The second element contains the indices of genes that were selected by the feature selection step. The third element contains the indices of the samples that were in the test set. The fourth element contains a vector of the classes predicted by the classifer. The fifth element contains the value of any tuning parameters tried and chosen.

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## Author(s)

Dario Strbenac

# **Examples**

runTests

Reproducibly Run Various Kinds of Cross-Validation

# **Description**

Enables doing classification schemes such as ordinary 10-fold, 100 resamples 5-fold, and leave one out cross-validaion. Processing in parallel is possible by leveraging the package BiocParallel.

# Usage

# **Arguments**

expression Either a matrix or ExpressionSet containing the training data. For a matrix,

the rows are features, and the columns are samples.

classes A vector the same length as the number of columns of expression data specifying

the class that the samples belong to.

datasetName A name associated with the dataset used.

classificationName

A name associated with the classification.

validation "bootstrap" for repeated resampling. "leaveOut" for leaving all combinations of

k samples as test samples. "fold" for folding of the dataset (no resampling).

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bootMode	Character. Either "fold" or "split". If "fold", then the samples are split into folds and in each iteration one is used as the test set. If "split", the samples are split into two groups, the sizes being based on the percent value. One group is used as the training set, the other is the test set. Has no effect if validation is not "bootstrap".
resamples	Relevant when repeated resampling is used. The number of times to do sampling with replacement.
percent	Used when bootstrap resampling with the split method is chosen. The percentage of samples to be in the test set.
folds	Relevant when repeated resampling is used with bootMode set to "fold" or when validation is set to "fold". The number of folds to break the dataset into. Each fold is used once as the test set.
leave	Relevant when leave k out validation is used. The number of samples to leave for testing.
seed	The random number generator used for repeated resampling will use this seed, if it is provided. Allows reproducibility of repeated usage on the same input data.
parallelParams	An object of class MulticoreParam or SnowParam.
params	A list of objects of class of TransformParams, SelectParams, TrainParams, or PredictParams. The order they are in the list determines the order in which the stages of classification are done in.
	$Unused\ variables\ from\ the\ {\tt matrix}\ method\ passed\ to\ the\ {\tt ExpressionSet}\ method.$
verbose	A number between 0 and 3 for the amount of progress messages to give. A higher number will produce more messages.

# Value

If the predictor function made a single prediction, then an object of class ClassifyResult. If the predictor function made a set of predictions, then a list of such objects.

## Author(s)

Dario Strbenac

```
if(require(curatedOvarianData) && require(sparsediscrim))
 data(TCGA_eset)
 badOutcome <- which(pData(TCGA_eset)[, "vital_status"] == "deceased" & pData(TCGA_eset)[, "days_to_death"</pre>
 goodOutcome <- which(pData(TCGA_eset)[, "vital_status"] == "living" & pData(TCGA_eset)[, "days_to_death"]</pre>
 TCGA_eset <- TCGA_eset[, c(badOutcome, goodOutcome)]</pre>
 {\tt classes} \gets {\tt factor(rep(c("Poor", "Good"), c(length(badOutcome), length(goodOutcome))))}
 pData(TCGA_eset)[, "class"] <- classes</pre>
 # Two datasets generated by resampling with replacement, each partitioned into two parts.
 runTests(TCGA_eset, "Ovarian Cancer", "Differential Expression", resamples = 2, fold = 2)
```

44 selectionPlot

selectionPlot	Plot Pair-wise Overlap or Selection Size Distribution of Selected Fea- tures
	tures

# **Description**

Pair-wise overlaps can be done for two types of analyses. Firstly, each cross-validation iteration can be considered within a single classification. This explores the feature selection stability. Secondly, the overlap may be considered between different classification results. This approach compares the feature selection commonality between different selection methods. Two types of commonality are possible to analyse. One summary is the average pair-wise overlap between a level of the comparison factor and the other summary is the pair-wise overlap of each level of the comparison factor that is not the reference level against the reference level. The overlaps are converted to percentages and plotted as lineplots.

Additionally, a heatmap of selection size frequencies can be made.

# Usage

```
## S4 method for signature 'list'
selectionPlot(results,
               comparison = c("within", "size", "classificationName", "validation", "datasetName"
                   referenceLevel = NULL,
               xVariable = c("classificationName", "datasetName", "validation", "selectionName")
               \verb|boxFillColouring| = \verb|c("classificationName", "size", "datasetName", "validation", \\
                                         "selectionName", "None"),
                   boxFillColours = NULL,
                   boxFillBinBoundaries = NULL, setSizeBinBoundaries = NULL,
               boxLineColouring = c("validation", "classificationName", "datasetName", "selection
                   boxLineColours = NULL,
               rowVariable = c("None", "validation", "datasetName", "classificationName", "select
               columnVariable = c("datasetName", "classificationName", "validation", "selectionName"
                   yMax = 100, fontSizes = c(24, 16, 12, 16),
                title = if(comparison[1] == "within") "Feature Selection Stability" else if(compar
                   xLabel = "Analysis",
               yLabel = if(is.null(referenceLevel) && comparison != "size") "Common Features (%)"
                  margin = grid::unit(c(0, 0, 0, 0), "lines"), rotate90 = FALSE,
                   showLegend = TRUE, plot = TRUE, parallelParams = bpparam())
```

# Arguments

results A list of ClassifyResult or SelectResult objects.

comparison The aspect of the experimental design to compare. See Details section for a

detailed description.

referenceLevel The level of the comparison factor to use as the reference to compare each non-

reference level to. If NULL, then each level has the average pairwise overlap

calculated to all other levels.

xVariable The factor to make separate boxes in the boxplot for.

boxFillColouring

A factor to colour the boxes by.

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boxFillColours A vector of colours, one for each level of boxFillColouring. If NULL, a default palette is used.

boxFillBinBoundaries

Used only if comparison is "size". A vector of integers, specifying the bin boundaries of percentages of size bins observed. e.g. 0, 10, 20, 30, 40, 50.

setSizeBinBoundaries

Used only if comparison is "size". A vector of integers, specifying the bin boundaries of set size bins. e.g. 50, 100, 150, 200, 250.

boxLineColouring

A factor to colour the box lines by.

boxLineColours A vector of colours, one for each level of boxLineColouring. If NULL, a default

palette is used.

rowVariable The slot name that different levels of are plotted as separate rows of boxplots. columnVariable The slot name that different levels of are plotted as separate columns of boxplots.

yMax The maximum value of the percentage to plot.

fontSizes A vector of length 4. The first number is the size of the title. The second number

is the size of the axes titles. The third number is the size of the axes values. The fourth number is the font size of the titles of grouped plots, if any are produced.

In other words, when rowVariable or columnVariable are not NULL.

title An overall title for the plot.

xLabel Label to be used for the x-axis.

yLabel Label to be used for the y-axis of overlap percentages.

margin The margin to have around the plot.

rotate90 Logical. If TRUE, the boxplot is horizontal.

showLegend If TRUE, a legend is plotted next to the plot. If FALSE, it is hidden.

plot Logical. If TRUE, a plot is produced on the current graphics device.

parallelParams An object of class MulticoreParam or SnowParam.

## Details

Possible values for characteristics are "datasetName", "classificationName", "size", "selectionName", and "validation". If "None", then that graphical element is not used.

If comparison is "within", then the feature selection overlaps are compared within a particular analysis. The result will inform how stable the selections are between different iterations of cross-validation for a particular analysis. If comparison is "classificationName", then the feature selections are compared across different classification algorithm types, for each level of "datasetName", "selectionName" and "validation". The result will inform how stable the feature selections are between different classification algorithms, for every cross-validation scheme, selction algorithm and dataset. If comparison is "selectionName", then the feature selections are compared across different feature selection algorithms, for each level of "datasetName", "classificationName" and "validation". The result will inform how stable the feature selections are between feature selection algorithms, for every dataset, classification algorithm, and cross-validation scheme. If comparison is "validation", then the feature selections are compared across different cross-validation schemes, for each level of "classificationName", "selectionName" and "datasetName". The result will inform how stable the feature selections are between different cross-validation schemes, for every selection algorithm, classification algorithm and every dataset. If comparison is "datasetName", then the feature selections are compared across different datasets, for each level of

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"classificationName", "selectionName", and "validation". The result will inform how stable the feature selections are between different datasets, for every classification algorithm and every dataset. This could be used to consider if different experimental studies have a highly overlapping feature selection pattern.

Calculating all pair-wise set overlaps can be time-consuming. This stage can be done on multiple CPUs by providing the relevant options to parallelParams. The percentage is calculated as the intersection of two sets of features divided by the union of the sets, multiplied by 100.

For the selection size mode, boxFillBins is used to create bins which include the lowest value for the first bin, and the highest value for the last bin using cut.

#### Value

An object of class ggplot and a plot on the current graphics device, if plot is TRUE.

## Author(s)

Dario Strbenac

```
predicted <- data.frame(sample = sample(10, 100, replace = TRUE),</pre>
                         label = rep(c("Healthy", "Cancer"), each = 50))
actual <- factor(rep(c("Healthy", "Cancer"), each = 5))</pre>
rankList <- list(list(1:100, c(5:1, 6:100)), list(c(1:9, 11:101), c(1:50, 60:51, 61:100)))
result1 <- ClassifyResult("Example", "Differential Expression", "Example Selection", LETTERS[1:10], LETTERS
                           rankList.
                         list(list(rankList[[1]][[1]][1:15], rankList[[1]][[2]][1:15]),
                             list(rankList[[2]][[1]][1:10], rankList[[2]][[2]][1:10])),
                           list(predicted), actual, list("resampleFold", 2, 2))
predicted[, "label"] <- sample(predicted[, "label"])</pre>
rankList <- list(list(1:100, c(sample(20), 21:100)), list(c(1:9, 11:101), c(1:50, 60:51, 61:100)))
result2 <- ClassifyResult("Example", "Differential Variability", "Example Selection", LETTERS[1:10], LETTE
                           rankList,
                         list(list(rankList[[1]][[1]][1:15], rankList[[1]][[2]][1:15]),
                             list(rankList[[2]][[1]][1:10], rankList[[2]][[2]][1:10])),
                      list(predicted), actual, validation = list("resampleFold", 2, 2))
selectionPlot(list(result1, result2), xVariable = "classificationName", xLabel = "Analysis", columnVariable
selectionPlot(list(result1, result2), comparison = "size", xVariable = "classificationName", xLabel = "Anal
setSizeBinBoundaries = seq(0, 25, 5), boxLineColouring = "None")
oneRanking \leftarrow c(10, 8, 1, 2, 3, 4, 7, 9, 5, 6)
otherRanking < c(8, 2, 3, 4, 1, 10, 6, 9, 7, 5)
oneResult <- SelectResult("Example", "One Method", list(oneRanking), list(oneRanking[1:5]))</pre>
otherResult <- SelectResult("Example", "Another Method", list(otherRanking), list(otherRanking[1:2]))
selectionPlot(list(oneResult, otherResult), comparison = "selectionName", xVariable = "selectionName", xLal
```

SelectParams 47

SelectParams

Parameters for Feature Selection

# **Description**

Collects and checks necessary parameters required for feature selection. The empty constructor is provided for convenience.

## Constructor

SelectParams() Creates a default SelectParams object. This uses a limma t-test and tries 100, 200, 300, 400, 500 features, and picks the number of features with the best resubstitution error rate. Users should create an appropriate SelectParams object for the characteristics of their data, once they are familiar with this software.

SelectParams(featureSelection, selectionName, minPresence = 1, intermediate = character(0), Creates a SelectParams object which stores the function which will do the selection and parameters that the function will use.

featureSelection Either a function which will do the selection or a list of such functions. For a particular function, the first argument must be an ExpressionSet object. The function's return value must be a SelectResult object.

selectionName A name to identify this selection method by.

minPresence If a list of functions was provided, how many of those must a feature have been selected by to be used in classification. 1 is equivalent to a set union and a number the same length as featureSelection is equivalent to set intersection.

intermediate Character vector. Names of any variables created in prior stages by runTest that need to be passed to a feature selection function.

subsetExpressionData Whether to subset the expression data, after selection has been done.

... Other named parameters which will be used by the selection function. If featureSelection was a list of functions, this must be a list of lists, as long as featureSelection.

## Author(s)

Dario Strbenac

48 subtractFromLocation

SelectResult

Container for Storing Feature Selection Results

# **Description**

Contains the ranked indices or names of features, from most discriminative to least discriminative and a list of indicies of feature selected for use in classification. This class is not intended to be created by the user, but could be used in another package.

## Constructor

```
SelectResult(datasetName, selectionName, rankedFeatures, chosenFeatures)
datasetName A name associated with the dataset used.
selectionName A name associated with the classification.
rankedFeatures Indices or names of all features, from most to least discriminative.
chosenFeatures Indices or names of features selected at each fold.
```

# **Summary**

A method which summarises the results is available. result is a SelectResult object.

show(result)Prints a short summary of what result contains.

# Author(s)

Dario Strbenac

# **Examples**

```
SelectResult("Melanoma", "Moderated t-test", list(1:50), list(1:10))
```

subtractFromLocation Subtract All Feature Measurements from Location

# Description

For each feature, calculates the location, and subtracts all measurements from that location.

# Usage

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## **Arguments**

expression	Either a matrix or ExpressionSet containing the data. For a matrix, the rows are features, and the columns are samples.
	Unused variables from the ${\tt matrix}$ method passed to the ${\tt ExpressionSet}$ method.
training	A vector specifying which samples are in the training set.
location	Character. Either "mean" or "median".
absolute	If TRUE, then absolute values of the differences are returned.
verbose	A number between 0 and 3 for the amount of progress messages to give. A higher number will produce more messages.

## **Details**

Only the samples specified by training are used in the calculation of the location. To use all samples for calculation of the location, simply provide indices of all the samples.

## Value

An ExpressionSet of the same dimension that was input, with values subtracted from the location specified.

# Author(s)

Dario Strbenac

# **Examples**

```
subtractFromLocation(matrix(1:100, ncol = 10), training = 1:5, "median")
```

TrainParams	Parameters for Classifier Training	

# Description

Collects and checks necessary parameters required for classifier training. The empty constructor is provided for convenience.

# Constructor

TrainParams() Creates a default TrainParams object. The classifier function is DLDA. Users should create an appropriate TrainParams object for the characteristics of their data, once they are familiar with this software.

TrainParams(classifier, transposeExpression, doesTests, ...) Creates a TrainParams object which stores the function which will do the classifier building and parameters that the function will use.

classifier A function which will construct a classifier, and also possibly make the predictions. The first argument must be a matrix object. The second argument must be a vector of classes. If doesTests is TRUE, the third argument must be a matrix of test data. The function must also accept a parameter named verbose The function's return value can be either a trained classifier when doesTests is FALSE or a vector of class predictions if doesTests is TRUE.

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transposeExpression Set to TRUE if classifier expects features as columns.

doesTests Set to TRUE if classifier also performs and returns predictions.

intermediate Character vector. Names of any variables created in prior stages by runTest that need to be passed to classifier.

... Other named parameters which will be used by the classifier.

## Author(s)

Dario Strbenac

if(require(sparsediscrim))

# **Examples**

```
trainParams <- TrainParams(dlda, transposeExpression = TRUE, doesTests = FALSE)
# sparsediscrim has a separate predict method for trained DLDA objects.
# dlda expects features in columns, and samples in rows.
# It doesn't formally have a verbose parameter, but it is effectively consumed by ... in its formal definition</pre>
```

TransformParams

Parameters for Data Transformation

# Description

Collects and checks necessary parameters required for transformation. The empty constructor is for when no data transformation is desired. One data transformation function is distributed. See subtractFromLocation.

## Constructor

TransformParams(transform, intermediate = character(0), ...) Creates a Transform-Params object which stores the function which will do the transformation and parameters that the function will use.

transform A function which will do the transformation. The first argument must be an ExpressionSet object.

intermediate Character vector. Names of any variables created in prior stages by runTest that need to be passed to a feature selection function.

... Other named parameters which will be used by the transformation function.

# Author(s)

Dario Strbenac

```
transforParams <- TransformParams(subtractFromLocation, location = "median")
# Subtract all values from training set median, to obtain absolute deviations.</pre>
```

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