Package 'ClassifyR'

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Type Package

Title A framework for cross-validated classification problems, with
applications to differential variability and differential
distribution testing

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Author Dario Strbenac, John Ormerod, Graham Mann, Jean Yang

Maintainer Dario Strbenac <dario.strbenac@sydney.edu.au>

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Imports locfit, grid, utils, plyr

Suggests limma, genefilter, edgeR, car, Rmixmod, ggplot2 (>= 3.0.0),
gridExtra (>= 2.0.0), cowplot, BiocStyle, pamr, PoiClaClu,
parathyroidSE, knitr, htmltools, gtable, scales, e1071,
rmarkdown, IRanges, randomForest, robustbase, glmnet, class

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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R **topics documented:**

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asthma   *Asthma RNA Abundance and Patient Classes*

Description

Data set consists of a matrix of abundances of 2000 most variable gene expression measurements for 190 samples and a factor vector of classes for those samples.

Usage

```
data(asthma)
```

Format

measurements has a row for each gene and a column for each sample. classes is a factor vector.

Source

A Nasal Brush-based Classifier of Asthma Identified by Machine Learning Analysis of Nasal RNA Sequence Data, *Scientific Reports*, 2018. Webpage: http://www.nature.com/articles/s41598-018-27189-4

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bartlettSelection   *Selection of Differential Variability with Bartlett Statistic*

Description

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

Usage

```
   ## S4 method for signature 'matrix'
bartlettSelection(measurements, classes, ...)
   ## S4 method for signature 'DataFrame'
bartlettSelection(measurements, classes, datasetName,
                  trainParams, predictParams, resubstituteParams,
                  selectionName = "Bartlett Test", verbose = 3)
   ## S4 method for signature 'MultiAssayExperiment'
bartlettSelection(measurements, targets, ...)
```

Arguments

measurements	Either a [matrix](#), [DataFrame](#) or [MultiAssayExperiment](#) containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	Either a vector of class labels of class [factor](#) of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
targets	If measurements is a MultiAssayExperiment, the names of the data tables to be used. "clinical" is also a valid value and specifies that numeric variables from the clinical data table will be used.
...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method.
datasetName	A name for the data set 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	Default: 3. 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.

Data tables which consist entirely of non-numeric data cannot be analysed. If measurements is an object of class MultiAssayExperiment, the factor of sample classes must be stored in the DataFrame accessible by the colData function with column name "class".

Value

An object of class [SelectResult](#) or a list of such objects, if the classifier which was used for determining the specified performance metric made a number of prediction varieties.

Author(s)

Dario Strbenac

Examples

```
# Samples in one class with differential variability to other class.
# First 20 genes are DV.
genesRNAmatrix <- sapply(1:25, function(sample) c(rnorm(100, 9, 1)))
moreVariable <- sapply(1:25, function(sample) rnorm(20, 9, 5))
genesRNAmatrix <- cbind(genesRNAmatrix, rbind(moreVariable,
```

```
                              sapply(1:25, function(sample) rnorm(80, 9, 1))))
    colnames(genesRNAmatrix) <- paste("Sample", 1:50)
    rownames(genesRNAmatrix) <- paste("Gene", 1:100)
    genesSNPmatrix <- matrix(sample(c("None", "Missense"), 250, replace = TRUE),
                             ncol = 50)
    colnames(genesSNPmatrix) <- paste("Sample", 1:50)
    rownames(genesSNPmatrix) <- paste("Gene", 1:5)
    classes <- factor(rep(c("Poor", "Good"), each = 25))
    names(classes) <- paste("Sample", 1:50)
    genesDataset <- MultiAssayExperiment(list(RNA = genesRNAmatrix, SNP = genesSNPmatrix),
                                         colData = DataFrame(class = classes))
    # Wait for update to MultiAssayExperiment wideFormat function.
    trainIDs <- paste("Sample", c(1:20, 26:45))
    genesDataset <- subtractFromLocation(genesDataset, training = trainIDs,
                                         targets = "RNA") # Exclude SNP data.

    resubstituteParams <- ResubstituteParams(nFeatures = seq(10, 100, 10),
                                             performanceType = "balanced error",
                                             better = "lower")
    bartlettSelection(genesDataset, datasetName = "Example", targets = "RNA",
                      trainParams = TrainParams(fisherDiscriminant),
                      predictParams = PredictParams(NULL),
                      resubstituteParams = resubstituteParams)
```

---

calcPerformance   *Add Performance Calculations to a ClassifyResult Object or Calculate*
                                for a Pair of Factor Vectors

Description

If calcExternalPerformance is used, such as when having a vector of known classes and a vector
of predicted classes determined outside of the ClassifyR package, a single metric value is calculated.
If calcCVperformance is used, annotates the results of calling runTests with one of the user-
specified performance measures.

Usage

```
    ## S4 method for signature 'factor,factor'
calcExternalPerformance(actualClasses, predictedClasses,
                        performanceType = c("error", "accuracy", "balanced error", "balanced accuracy",
                                            "micro precision", "micro recall",
                                            "micro F1", "macro precision",
                                            "macro recall", "macro F1", "matthews"))
    ## S4 method for signature 'ClassifyResult'
calcCVperformance(result, performanceType = c("error", "accuracy", "balanced error", "balanced accurac
                                              "sample error", "sample accuracy",
                                              "micro precision", "micro recall",
                                              "micro F1", "macro precision",
                                              "macro recall", "macro F1", "matthews"))
```

Arguments

result   An object of class [`ClassifyResult`](#).

performanceType

A character vector of length 1. Default: `"balanced error"`.
Must be one of the following options:

- `"error"`: Ordinary error rate.
- `"accuracy"`: Ordinary accuracy.
- `"balanced error"`: Balanced error rate.
- `"balanced accuracy"`: Balanced accuracy.
- `"sample error"`: Error rate for each sample in the data set.
- `"sample accuracy"`: Accuracy for each sample in the data set.
- `"micro precision"`: Sum of the number of correct predictions in each class, divided by the sum of number of samples in each class.
- `"micro recall"`: Sum of the number of correct predictions in each class, divided by the sum of number of samples predicted as belonging to each class.
- `"micro F1"`: F1 score obtained by calculating the harmonic mean of micro precision and micro recall.
- `"macro precision"`: Sum of the ratios of the number of correct predictions in each class to the number of samples in each class, divided by the number of classes.
- `"macro recall"`: Sum of the ratios of the number of correct predictions in each class to the number of samples predicted to be in each class, divided by the number of classes.
- `"macro F1"`: F1 score obtained by calculating the harmonic mean of macro precision and macro recall.
- `"matthews"`: Matthews Correlation Coefficient (MCC). A score between -1 and 1 indicating how concordant the predicted classes are to the actual classes. Only defined if there are two classes.

actualClasses   A factor vector specifying each sample's correct class.

predictedClasses

A factor vector of the same length as `actualClasses` specifying each sample's predicted class.

Details

All metrics except Matthews Correlation Coefficient are suitable for evaluating classification scenarios with more than two classes and are reimplementations of those available from Intel DAAL.

If [`runTests`](#) was run in resampling mode, one performance measure is produced for every resampling. If the leave-k-out mode was used, then the predictions are concatenated, and one performance measure is calculated for all classifications.

`"balanced error"` calculates the balanced error rate and is better suited to class-imbalanced data sets than the ordinary error rate specified by `"error"`. `"sample error"` calculates the error rate of each sample individually. This may help to identify which samples are contributing the most to the

overall error rate and check them for confounding factors. Precision, recall and F1 score have micro and macro summary versions. The macro versions are preferable because the metric will not have a good score if there is substantial class imbalance and the classifier predicts all samples as belonging to the majority class.

Value

If calcCVperformance was run, an updated [ClassifyResult](#) object, with new metric values in the performance slot. If calcExternalPerformance was run, the performance metric value itself.

Author(s)

Dario Strbenac

Examples

```
predictTable <- data.frame(sample = paste("A", 1:10, sep = ''),
                           class = factor(sample(LETTERS[1:2], 50, replace = TRUE)))
actual <- factor(sample(LETTERS[1:2], 10, replace = TRUE))
result <- ClassifyResult("Example", "Differential Expression", "A Selection",
                         paste("A", 1:10, sep = ''), paste("Gene", 1:50, sep = ''),
                       50, list(1:50, 1:50), list(1:5, 6:15), list(function(oracle){}),
                         list(predictTable), actual, list("leave", 2))
result <- calcCVperformance(result, "balanced error")
performance(result)
```

---

characterOrDataFrame   *Union of a Character and a DataFrame*

Description

Allows a slot to be either a character or a DataFrame.

Author(s)

Dario Strbenac

Examples

```
setClass("Selections", representation(features = "characterOrDataFrame"))
selections <- new("Selections", features = c("BRAF", "NRAS"))
featuresTable <- DataFrame(assay = c("RNA-seq", "Mass spectrometry"),
                           feature = c("PD-1", "MITF"))
omicsSelections <- new("Selections", features = featuresTable)
```

---

classifyInterface   *An Interface for PoiClaClu Package's Classify Function*

Description

More details of Poisson LDA are available in the documentation of [`Classify`](#).

Usage

```
   ## S4 method for signature 'matrix'
classifyInterface(measurements, classes, test, ...)
   ## S4 method for signature 'DataFrame'
classifyInterface(measurements, classes, test, ..., returnType = c("class", "score", "both"), verbose =
   ## S4 method for signature 'MultiAssayExperiment'
classifyInterface(measurements, test, targets = names(measurements), ...)
```

Arguments

measurements	Either a [`matrix`](#), [`DataFrame`](#) or [`MultiAssayExperiment`](#) containing the training data. For a `matrix`, the rows are features, and the columns are samples. If of type [`DataFrame`](#), the data set is subset to only those features of type `integer`.
classes	Either a vector of class labels of class [`factor`](#) of the same length as the number of samples in `measurements` or if the measurements are of class DataFrame a character vector of length 1 containing the column name in `measurement` is also permitted. Not used if `measurements` is a MultiAssayExperiment object.
test	An object of the same class as `measurements` with no samples in common with `measurements` and the same number of features as it.
targets	If measurements is a MultiAssayExperiment, the names of the data tables to be used. `"clinical"` is also a valid value and specifies that integer variables from the clinical data table will be used.
...	Variables not used by the `matrix` nor the `MultiAssayExperiment` method which are passed into and used by the DataFrame method or parameters that [`Classify`](#) can accept.
returnType	Default: `"class"`. Either `"class"`, `"score"` or `"both"`. Sets the return value from the prediction to either a vector of class labels, matrix of scores for each class, or both labels and scores in a `data.frame`.
verbose	Default: 3. 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

Data tables which consist entirely of non-integer data cannot be analysed. If `measurements` is an object of class `MultiAssayExperiment`, the factor of sample classes must be stored in the DataFrame accessible by the `colData` function with column name `"class"`.

Value

Either a factor vector of predicted classes, a matrix of scores for each class, or a table of both the class labels and class scores, depending on the setting of returnType.

Author(s)

Dario Strbenac

Examples

```
if(require(PoiClaClu))
{
  readCounts <- CountDataSet(n = 100, p = 1000, 2, 5, 0.1)
  # Rows are for features, columns are for samples.
  trainData <- t(readCounts[['x']])
  classes <- factor(paste("Class", readCounts[['y']]))
  testData <- t(readCounts[['xte']])
  storage.mode(trainData) <- storage.mode(testData) <- "integer"
  classified <- classifyInterface(trainData, classes, testData)

 setNames(table(paste("Class", readCounts[["yte"]]) == classified), c("Incorrect", "Correct"))
}
```

ClassifyResult   *Container for Storing Classification Results*

Description

Contains a table of actual sample classes and predicted classes, the identifiers of features selected for each fold of each permutation 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, selectionName, originalNames, originalFeatures,
            rankedFeatures, chosenFeatures, predictions, actualClasses, models,
                validation, tune = list(NULL))
```

datasetName A name associated with the dataset used.

classificationName A name associated with the classification.

seletionName A name associated with the feature selection.

originalNames All sample names.

originalFeatures All feature names. Character vector or DataFrame with one row for each feature if the data set is a MultiAssayExperiment.

rankedFeatures All features, from most to least important. Character vector or DataFrame if data set is a MultiAssayExperiment.

chosenFeatures Features selected at each fold. Character vector or DataFrame if data set is a MultiAssayExperiment.

predictions A [list](#) of [data.frame](#) containing information about samples, their actual class and predicted class.

actualClasses Factor of class of each sample.

models All of the models fitted to the training data.

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

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.

sampleNames(result) Returns a vector of sample names present in the data set.

featureNames(result) Returns a vector of features present in the data set.

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.

models(result) A list of the models fitted for each training.

performance(result) Returns a list of performance measures. This is empty until calcCVperformance 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 iteration.

sampleNames(result) Returns a [character](#) vector of sample names.

Author(s)

Dario Strbenac

Examples

```
#if(require(sparsediscrim))
#{
  data(asthma)

  resubstituteParams <- ResubstituteParams(nFeatures = seq(5, 25, 5),
                                      performanceType = ”balanced error”,
                                      better = ”lower”)
  classified <-
  runTests(measurements, classes, datasetName = ”Asthma”,
          classificationName = ”Different Means”, validation = ”leaveOut”, leave = 1,
          params = list(SelectParams(limmaSelection, ”Moderated t Statistic”,
                                  resubstituteParams = resubstituteParams),
                      TrainParams(DLDAtrainInterface),
                      PredictParams(DLDApredictInterface)))
  class(classified)
#}
```

---

differentMeansSelection

Selection of Differentially Abundant Features

Description

Uses an ordinary t-test if the data set has two classes or one-way ANOVA if the data set has three or more classes to select differentially expressed features.

Usage

```
  ## S4 method for signature 'matrix'
differentMeansSelection(measurements, classes, ...)
  ## S4 method for signature 'DataFrame'
differentMeansSelection(measurements, classes, datasetName,
                trainParams, predictParams, resubstituteParams,
                selectionName = ”Difference in Means”, verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
differentMeansSelection(measurements, targets = NULL, ...)
```

Arguments

measurements	Either a [matrix](#), [DataFrame](#) or [MultiAssayExperiment](#) containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	A vector of class labels of class [factor](#) of the same length as the number of samples in measurements. Not used if measurements is a MultiAssayExperiment object.
targets	Names of data tables to be combined into a single table and used in the analysis.

...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method.
datasetName	A name for the data set 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	Default: 3. 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 changes in means and uses rowttests to rank the features if there are two classes or rowFtests if there are three or more classes. The choice of features is based on the best resubstitution performance.

Value

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

Author(s)

Dario Strbenac

Examples

```
#if(require(sparsediscrim))
#{
  # Genes 76 to 100 have differential expression.
  genesMatrix <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))
  genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample)
                                    c(rnorm(75, 9, 2), rnorm(25, 14, 2))))
  classes <- factor(rep(c("Poor", "Good"), each = 25))
  colnames(genesMatrix) <- paste("Sample", 1:ncol(genesMatrix))
  rownames(genesMatrix) <- paste("Gene", 1:nrow(genesMatrix))

  resubstituteParams <- ResubstituteParams(nFeatures = seq(10, 100, 10),
                          performanceType = "balanced error", better = "lower")
  selected <- differentMeansSelection(genesMatrix, classes, "Example",
                        trainParams = TrainParams(), predictParams = PredictParams(),
                            resubstituteParams = resubstituteParams)

  selected@chosenFeatures
#}
```

---

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

```
   ## S4 method for signature 'ClassifyResult'
distribution(result, dataType = c("features", "samples"),
           plotType = c("density", "histogram"), summaryType = c("percentage", "count"),
            plot = TRUE, xMax = NULL, xLabel = "Percentage of Cross-validations",
               yLabel = "Density", title = "Distribution of Feature Selections",
              fontSizes = c(24, 16, 12), ...)
```

Arguments

result	An object of class [ClassifyResult]().
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.
plot	Whether to draw a plot of the frequency of selection or error rate.
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.
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

```
#if(require(sparsediscrim))
#{
  data(asthma)
  resubstituteParams <- ResubstituteParams(nFeatures = seq(5, 25, 5),
                                    performanceType = "balanced error",
                                    better = "lower")

  result <- runTests(measurements, classes, datasetName = "Asthma",
                     classificationName = "Different Means",
                     permutations = 5,
               params = list(SelectParams(limmaSelection, "Moderated t Statistic",
                                      resubstituteParams = resubstituteParams),
                             TrainParams(DLDAtrainInterface),
                             PredictParams(DLDApredictInterface)
                             )
                    )
  featureDistribution <- distribution(result, "features", summaryType = "count",
                                    plotType = "histogram",
                             xLabel = "Number of Cross-validations", yLabel = "Count",
                                    binwidth = 1)
  print(head(featureDistribution))
#}
```

---

dlda   *Trained dlda Object*

Description

Enables S4 method dispatching on it.

Author(s)

Dario Strbenac

DLDAinterface   *An Interface for sparsediscrim Package's dlda Function*

Description

`DLDAtrainInterface` generates a trained diagonal LDA classifier and `DLDApredictInterface` uses it to make predictions on a test data set.

Usage

```
  ## S4 method for signature 'matrix'
DLDAtrainInterface(measurements, classes, ...)
  ## S4 method for signature 'DataFrame'
DLDAtrainInterface(measurements, classes, verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
DLDAtrainInterface(measurements, targets = names(measurements), ...)
  ## S4 method for signature 'dlda,matrix'
DLDApredictInterface(model, test, ...)
  ## S4 method for signature 'dlda,DataFrame'
DLDApredictInterface(model, test, returnType = c("class", "score", "both"),
                                  verbose = 3)
  ## S4 method for signature 'dlda,MultiAssayExperiment'
DLDApredictInterface(model, test, targets = names(test), ...)
```

Arguments

measurements	Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training data. For a matrix, the rows are features, and the columns are samples. If of type [DataFrame](), the data set is subset to only those features of type integer.
classes	Either a vector of class labels of class [factor]() of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
model	A fitted model as returned by DLDAtrainInterface.
test	An object of the same class as measurements with no samples in common with measurements and the same number of features as it. Also, if a DataFrame, the class column must be absent.
targets	If measurements is a MultiAssayExperiment, the names of the data tables to be used. "clinical" is also a valid value and specifies that integer variables from the clinical data table will be used.
...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method (e.g. verbose).
returnType	Default: "class". Either "class", "score" or "both". Sets the return value from the prediction to either a vector of class labels, matrix of scores for each class, or both labels and scores in a data.frame.
verbose	Default: 3. 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 measurements is an object of class MultiAssayExperiment, the factor of sample classes must be stored in the DataFrame accessible by the colData function with column name "class".

Value

For `DLDAtrainInterface`, a trained DLDA classifier. For `DLDApredictInterface`, either a factor vector of predicted classes, a matrix of scores for each class, or a table of both the class labels and class scores, depending on the setting of `returnType`.

Author(s)

Dario Strbenac

Examples

```
# if(require(sparsediscrim)) Package currently removed from CRAN.
#{
  # Genes 76 to 100 have differential expression.
  genesMatrix <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))
  genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample)
                                    c(rnorm(75, 9, 2), rnorm(25, 14, 2))))
  classes <- factor(rep(c("Poor", "Good"), each = 25))
  colnames(genesMatrix) <- paste("Sample", 1:ncol(genesMatrix))
  rownames(genesMatrix) <- paste("Gene", 1:nrow(genesMatrix))
  selected <- rownames(genesMatrix)[91:100]
  trainingSamples <- c(1:20, 26:45)
  testingSamples <- c(21:25, 46:50)

  classifier <- DLDAtrainInterface(genesMatrix[selected, trainingSamples],
                                   classes[trainingSamples])
  DLDApredictInterface(classifier, genesMatrix[selected, testingSamples])
#}
```

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.

Usage

```
   ## S4 method for signature 'matrix'
DMDselection(measurements, classes, ...)
   ## S4 method for signature 'DataFrame'
DMDselection(measurements, classes, datasetName, differences = c("both", "location", "scale"),
             trainParams, predictParams, resubstituteParams, ...,
             selectionName = "Differences of Medians and Deviations",
             verbose = 3)
   ## S4 method for signature 'MultiAssayExperiment'
DMDselection(measurements, targets = names(measurements), ...)
```

Arguments

measurements	Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	A vector of class labels.
targets	If measurements is a MultiAssayExperiment, the names of the data tables to be used. "clinical" is also a valid value and specifies that numeric variables from the clinical data table will be used.
...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method or parameters for [getLocationsAndScales](), such as location, scale.
datasetName	Default: "Differences of Medians and Deviations". A name for the data set used. Stored in the result.
differences	Default: "both". Either "both", "location", or "scale". The type of differences to consider. If both are considered then the absolute difference in location and the absolute difference in scale are summed.
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	Default: 3. 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 $\sum_{i=1}\sum_{j=i+1}|location_i - location_j| + |scale_i - scale_j|$. The subscripts denote the class for which the parameter is calculated for.

Data tables which consist entirely of non-numeric data cannot be analysed. If measurements is an object of class MultiAssayExperiment, the factor of sample classes must be stored in the DataFrame accessible by the colData function with column name "class".

Value

An object of class [SelectResult]() or a list of such objects, if the classifier which was used for determining the specified performance metric made a number of prediction varieties.

Author(s)

Dario Strbenac

Examples

```
# First 20 features have bimodal distribution for Poor class.
# Other 80 features have normal distribution for both classes.
genesMatrix <- sapply(1:25, function(sample)
                              {
                                randomMeans <- sample(c(8, 12), 20, replace = TRUE)
                                c(rnorm(20, randomMeans, 1), rnorm(80, 10, 1))
                              }
                      )
genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample) rnorm(100, 10, 1)))
classes <- factor(rep(c("Poor", "Good"), each = 25))

resubstituteParams <- ResubstituteParams(nFeatures = seq(10, 100, 10),
                                         performanceType = "balanced error",
                                         better = "lower")
DMDselection(genesMatrix, classes, datasetName = "Example",
             trainParams = TrainParams(naiveBayesKernel),
             predictParams = PredictParams(NULL),
             resubstituteParams = resubstituteParams)
```

EasyHardClassifier   *Container for a Pair of Trained Classifiers*

Description

Stores two classifiers and the ID of the data set each one of them was trained on. Not intended for end-user.

Constructor

EasyHardClassifier(easyClassifier, hardClassifier, datasetIDs)

Creates a EasyHardClassifier object which stores the details of the two underlying classification models.

easyClassifier A classifier trained on the easy-to-collect data set by easyHardClassifier-Train. Represented as a list of rules, each of which is also a list.

hardClassifier A list of two with names "selected" and "model". The "selected" element should contain the chosen features and the "model" element is for the trained model on the hard-to-collect data set or simply a character vector of length 1 containing a class name, if the prediction of the samples left over from the easy classifier all or all except one belonged to a particular class.

datasetIDs A vector of length 2 with names "easy" and "hard" containing the data set IDs from the original MultiAssayExperiment input data object for the easy data set and the hard data set.

Author(s)

Dario Strbenac

Examples

```
    predictiveRules <- list(list(feature = "age", relation = "<", value = 18, predict = "Risk"))
     hardClassifier <- DLDAtrainInterface(matrix(rnorm(400), ncol = 20),
                            classes = factor(sample(c("Safe", "Risk"), 20, replace = TRUE)))
    EasyHardClassifier(predictiveRules, list(selected = LETTERS[1:5], model = hardClassifier),
                       setNames(c("clinical", "RNA-seq"), c("easy", "hard")))
```

---

easyHardClassifier	*Two-stage Classification Using Easy-to-collect Data Set and Hard-to-collect data set.*

Description

An alternative implementation to the previously published easy-hard classifier that doesn't do nested cross-validation for speed. In the first stage, each numeric variable is split on all possible midpoints between consecutive ordered values and the samples below the split and above the split are checked to see if they mostly belong to one class. Categorical varaibles are tabulated on factor levels and the count of samples in each class is determined. If any partitions of samples are pure for a class, based on a purity threshold, prediction rules are created. The samples not classified by any rule or classified to two or more classes the same number of times are left to be trained by the hard classifier.

Usage

```
   ## S4 method for signature 'MultiAssayExperiment'
easyHardClassifierTrain(measurements, easyDatasetID = "clinical", hardDatasetID = names(measurements)
         featureSets = NULL, metaFeatures = NULL, minimumOverlapPercent = 80,
         datasetName = NULL, classificationName = "Easy-Hard Classifier",
         easyClassifierParams = list(minCardinality = 10, minPurity = 0.9),
      hardClassifierParams = list(SelectParams(), TrainParams(), PredictParams()),
         verbose = 3)
   ## S4 method for signature 'EasyHardClassifier,MultiAssayExperiment'
easyHardClassifierPredict(model, test, predictParams, verbose = 3)
```

Arguments

measurements	A [MultiAssayExperiment](#) object containing the data set The sample classes must be in a column of the DataFrame accessed by colData named "class".
easyDatasetID	The name of a data set in measurements or "clinical" to indicate the patient information in the column data be used.
hardDatasetID	The name of a data set in measurements different to the value of easyDatasetID to be used for classifying the samples not classified by the easy classifier.
featureSets	An object of type [FeatureSetCollection](#) which defines sets of features or sets of edges.
metaFeatures	Either NULL or a DataFrame which has meta-features of the numeric data of interest.

minimumOverlapPercent

> If `featureSets` stores sets of features, the minimum overlap of feature IDs with `measurements` for a feature set to be retained in the analysis. If `featureSets` stores sets of network edges, the minimum percentage of edges with both vertex IDs found in `measurements` that a set has to have to be retained in the analysis.

datasetName   A name associated with the data set used.

classificationName

> A name associated with the classification.

easyClassifierParams

> A list of length 2 with names "minCardinality" and "minPurity". The first parameter specifies what the minimum number of samples after a split has to be and the second specifies the minimum proportion of samples in a partition belonging to a particular class.

hardClassifierParams

> A list of objects defining the classification to do on the samples which were not predicted by the easy classifier Objects must of of class `TransformParams`, `SelectParams`, `TrainParams` or `PredictParams`.

model   A trained `EasyHardClassifier` object.

test   A `MultiAssayExperiment` object containing the test data.

predictParams An object of class `PredictParams`. It specifies the classifier used to make the hard predictions.

verbose   Default: 3. 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 easy classifier may be `NULL` if there are no rules that predicted the sample well using the easy data set. The hard classifier may be `NULL` if all of the samples could be predicted with rules generated using the easy data set or it will simply be a character if all or almost all of the remaining samples belong to one class.

Value

For `EasyHardClassifierTrain`, the trained two-stage classifier. For `EasyHardClassifierPredict`, a factor vector of predicted classes.

Author(s)

Dario Strbenac

References

Inspired by: Stepwise Classification of Cancer Samples Using Clinical and Molecular Data, Askar Obulkasim, Gerrit Meijer and Mark van de Wiel 2011, *BMC Bioinformatics*, Volume 12 article 422, https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-12-422.

Examples

```
genesMatrix <- matrix(c(rnorm(90, 9, 1),
                        9.5, 9.4, 5.2, 5.3, 5.4, 9.4, 9.6, 9.9, 9.1, 9.8),
        ncol = 10, byrow = TRUE)
colnames(genesMatrix) <- paste("Sample", 1:10)
rownames(genesMatrix) <- paste("Gene", 1:10)
genders <- factor(c("Male", "Male", "Female", "Female", "Female",
                    "Female", "Female", "Female", "Female", "Female"))

# Scenario: Male gender can predict the hard-to-classify Sample 1 and Sample 2.
clinical <- DataFrame(age = c(31, 34, 32, 39, 33, 38, 34, 37, 35, 36),
                      gender = genders,
                      class = factor(rep(c("Poor", "Good"), each = 5)),
        row.names = colnames(genesMatrix))
dataset <- MultiAssayExperiment(ExperimentList(RNA = genesMatrix), clinical)
selParams <- SelectParams(featureSelection = differentMeansSelection, selectionName = "Difference in Means",
                resubstituteParams = ResubstituteParams(1:10, "balanced error", "lower"))
trained <- easyHardClassifierTrain(dataset, easyClassifierParams = list(minCardinality = 2, minPurity = 0.9),
                        hardClassifierParams = list(selParams, TrainParams(), PredictParams()))

predictions <- easyHardClassifierPredict(trained, dataset, PredictParams())
```

---

easyHardFeatures   *Extract Chosen Features from an EasyHardClassifier Object*

Description

The features are described by a data frame. One column is named "dataset" and the other is named "feature". This provides identifiability in case when multiple types of data have features with the same name.

Usage

```
   ## S4 method for signature 'EasyHardClassifier'
easyHardFeatures(easyHardClassifier)
```

Arguments

easyHardClassifier

               An [EasyHardClassifier](#) object.

Details

If any of the features are from the colun data of the input [MultiAssayExperiment](#), the dataset value will be "clinical".

Value

To be consistent with other functions for extracting features from a trained model, a list of length two. The first element is for feature rankings, which is not meaningful for an easy-hard classifier, so it is NULL. The second element is the selected features.

Author(s)

Dario Strbenac

Examples

```
genesMatrix <- matrix(c(rnorm(90, 9, 1),
                         9.5, 9.4, 5.2, 5.3, 5.4, 9.4, 9.6, 9.9, 9.1, 9.8),
       ncol = 10, byrow = TRUE)
colnames(genesMatrix) <- paste("Sample", 1:10)
rownames(genesMatrix) <- paste("Gene", 1:10)
genders <- factor(c("Male", "Male", "Female", "Female", "Female",
                    "Female", "Female", "Female", "Female", "Female"))

# Scenario: Male gender can predict the hard-to-classify Sample 1.
clinical <- DataFrame(age = c(31, 34, 32, 39, 33, 38, 34, 37, 35, 36),
                      gender = genders,
                      class = factor(rep(c("Poor", "Good"), each = 5)),
       row.names = colnames(genesMatrix))
dataset <- MultiAssayExperiment(ExperimentList(RNA = genesMatrix), clinical)
trained <- easyHardClassifierTrain(dataset, easyClassifierParams = list(minCardinality = 2, minPurity = 0.9),
                     hardClassifierParams = list(SelectParams(featureSelection = differentMeansSelection,
                                                 selectionName = "Difference in Means",
                                       resubstituteParams = ResubstituteParams(1:10, "balanced error", "lowe

easyHardFeatures(trained)
```

---

edgeRselection   *Feature Selection Based on Differential Expression for Count Data*

Description

Performs a differential expression analysis between classes and chooses the features which have best resubstitution performance. The data may have overdispersion and this is modelled.

Usage

```
  ## S4 method for signature 'matrix'
edgeRselection(counts, classes, ...)
  ## S4 method for signature 'DataFrame'
edgeRselection(counts, classes, datasetName,
               normFactorsOptions = NULL, dispOptions = NULL, fitOptions = NULL,
               trainParams, predictParams, resubstituteParams,
```

```
                    selectionName = "edgeR LRT", verbose = 3)
   ## S4 method for signature 'MultiAssayExperiment'
edgeRselection(counts, targets = NULL, ...)
```

Arguments

counts	Either a [matrix](#) or [MultiAssayExperiment](#) containing the unnormalised counts.
classes	A vector of class labels of class [factor](#) of the same length as the number of samples in measurements. Not used if measurements is a MultiAssayExperiment object.
targets	If measurements is a MultiAssayExperiment, the names of the data tables of counts to be used.
...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method.
datasetName	A name for the data set used. Stored in the result.
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	Default: 3. 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.

Data tables which consist entirely of non-numeric data cannot be analysed. If measurements is an object of class MultiAssayExperiment, the factor of sample classes must be stored in the DataFrame accessible by the colData function with column name "class".

Value

An object of class [SelectResult](#) or a list of such objects, if the classifier which was used for determining the specified performance metric made a number of prediction varieties.

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, <https://academic.oup.com/bioinformatics/article/26/1/139/182458>.

Examples

```
if(require(parathyroidSE) && require(PoiClaClu))
{
  data(parathyroidGenesSE)
  expression <- assays(parathyroidGenesSE)[[1]]
  sampleNames <- paste("Sample", 1:ncol(parathyroidGenesSE))
  colnames(expression) <- sampleNames
  DPN <- which(colData(parathyroidGenesSE)[, "treatment"] == "DPN")
  control <- which(colData(parathyroidGenesSE)[, "treatment"] == "Control")
  expression <- expression[, c(control, DPN)]
  classes <- factor(rep(c("Contol", "DPN"), c(length(control), length(DPN))))
  expression <- expression[rowSums(expression > 1000) > 8, ] # Make small data set.

  selected <- edgeRselection(expression, classes, "DPN Treatment",
                 trainParams = TrainParams(classifyInterface),
                 predictParams = PredictParams(NULL),
                 resubstituteParams = ResubstituteParams(nFeatures = seq(10, 100, 10),
                                  performanceType = "balanced error", better = "lower"))

  head(selected@rankedFeatures[[1]])
  plotFeatureClasses(expression, classes, "ENSG00000044574",
                     dotBinWidth = 500, xAxisLabel = "Unnormalised Counts")
}
```

---

edgesToHubNetworks	*Convert a Two-column Matrix or Data Frame into a Hub Node List*

Description

Interactions between pairs of features (typically a protein-protein interaction, commonly abbreviated as PPI, database) are restructured into a named list. The name of the each element of the list is a feature and the element contains all features which have an interaction with it.

Usage

```
edgesToHubNetworks(edges, minCardinality = 5)
```

Arguments

edges   A two-column `matrix` or `data.frame` for which each row specifies a known interaction betwen two interactors. If feature X appears in the first column and feature Y appears in the second, there is no need for feature Y to appear in the first column and feature X in the second.

minCardinality   An integer specifying the minimum number of features to be associated with a
                  hub feature for it to be present in the result.

Value

An object of type [FeatureSetCollection](#).

Author(s)

Dario Strbenac

References

VAN: an R package for identifying biologically perturbed networks via differential variability analysis, Vivek Jayaswal, Sarah-Jane Schramm, Graham J Mann, Marc R Wilkins and Yee Hwa Yang, 2010, *BMC Research Notes*, Volume 6 Article 430, https://bmcresnotes.biomedcentral.com/articles/10.1186/1756-0500-6-430.

Examples

```
interactor <- c("MITF", "MITF", "MITF", "MITF", "MITF", "MITF",
                "KRAS", "KRAS", "KRAS", "KRAS", "KRAS", "KRAS",
                "PD-1")
otherInteractor <- c("HINT1", "LEF1", "PSMD14", "PIAS3", "UBE2I", "PATZ1",
                     "ARAF", "CALM1", "CALM2", "CALM3", "RAF1", "HNRNPC",
                     "PD-L1")
edges <- data.frame(interactor, otherInteractor, stringsAsFactors = FALSE)

edgesToHubNetworks(edges, minCardinality = 4)
```

---

elasticNetFeatures   *Extract Vectors of Ranked and Selected Features From an Elastic Net*
                            GLM Object

Description

Provides a ranking of features based on the magnitude of fitted GLM coefficients. Also provides the selected features which are those with a non-zero coefficient.

Usage

```
   ## S4 method for signature 'multnet'
elasticNetFeatures(model)
```

Arguments

model   A fitted multinomial GLM which was created by [glmnet](#).

Value

An `list` object. The first element is a vector or data frame of ranked features, the second is a vector or data frame of selected features.

Author(s)

Dario Strbenac

Examples

```
if(require(glmnet))
{
  # Genes 76 to 100 have differential expression.
  genesMatrix <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))
  genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample)
                                    c(rnorm(75, 9, 2), rnorm(25, 14, 2))))
  classes <- factor(rep(c("Poor", "Good"), each = 25))
  colnames(genesMatrix) <- paste("Sample", 1:ncol(genesMatrix))
  rownames(genesMatrix) <- paste("Gene", 1:nrow(genesMatrix))

  resubstituteParams <- ResubstituteParams(nFeatures = seq(10, 100, 10),
                                            performanceType = "balanced error",
                                            better = "lower")

  # alpha is a user-specified tuning parameter.
  # lambda is automatically tuned, based on glmnet defaults, if not user-specified.
  trainParams <- TrainParams(elasticNetGLMtrainInterface, nlambda = 500)
  predictParams <- PredictParams(elasticNetGLMpredictInterface)
  classified <- runTests(genesMatrix, classes, datasetName = "Example",
                         classificationName = "Differential Expression",
                         validation = "fold",
                         params = list(trainParams, predictParams))

  elasticNetFeatures(models(classified)[[1]])
}
```

---

elasticNetGLMinterface

An Interface for glmnet Package's glmnet Function

Description

An elastic net GLM classifier uses a penalty which is a combination of a lasso penalty and a ridge penalty, scaled by a lambda value, to fit a sparse linear model to the data.

Usage

```
  ## S4 method for signature 'matrix'
elasticNetGLMtrainInterface(measurements, classes, ...)
  ## S4 method for signature 'DataFrame'
elasticNetGLMtrainInterface(measurements, classes, lambda = NULL,
                           ..., verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
elasticNetGLMtrainInterface(measurements, targets = names(measurements), ...)
  ## S4 method for signature 'multnet,matrix'
elasticNetGLMpredictInterface(model, test, ...)
  ## S4 method for signature 'multnet,DataFrame'
elasticNetGLMpredictInterface(model, test, classes = NULL, lambda, ..., returnType = c("class", "score"
  ## S4 method for signature 'multnet,MultiAssayExperiment'
elasticNetGLMpredictInterface(model, test, targets = names(test), ...)
```

Arguments

measurements	Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training data. For a `matrix`, the rows are features, and the columns are samples. If of type [DataFrame](), the data set is subset to only those features of type `integer`.
classes	Either a vector of class labels of class [factor]() of the same length as the number of samples in `measurements` or if the measurements are of class `DataFrame` a character vector of length 1 containing the column name in `measurement` is also permitted. Not used if `measurements` is a `MultiAssayExperiment` object.
lambda	The lambda value passed directly to [glmnet]() if the training function is used or passed as s to [predict.glmnet]() if the prediction function is used.
test	An object of the same class as `measurements` with no samples in common with `measurements` and the same number of features as it.
targets	If `measurements` is a `MultiAssayExperiment`, the names of the data tables to be used. `"clinical"` is also a valid value and specifies that integer variables from the clinical data table will be used.
...	Variables not used by the `matrix` nor the `MultiAssayExperiment` method which are passed into and used by the `DataFrame` method (e.g. `verbose`) or, for the training function, options that are used by the `glmnet` function. For the testing function, this variable simply contains any parameters passed from the classification framework to it which aren't used by glmnet's `predict` fuction.
model	A trained elastic net GLM, as created by the `glmnet` function.
returnType	Default: `"class"`. Either `"class"`, `"score"` or `"both"`. Sets the return value from the prediction to either a vector of class labels, matrix of scores for each class, or both labels and scores in a `data.frame`.
verbose	Default: 3. 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 `measurements` is an object of class `MultiAssayExperiment`, the factor of sample classes must be stored in the DataFrame accessible by the `colData` function with column name `"class"`.

The value of the `family` parameter is fixed to "multinomial" so that classification with more than 2 classes is possible and `type.multinomial` is fixed to "grouped" so that a grouped lasso penalty is used. During classifier training, if more than one lambda value is considered by specifying a vector of them as input or leaving the default value of NULL, then the chosen value is determined based on classifier resubstitution error rate.

Value

For `elasticNetGLMtrainInterface`, an object of type `glmnet`. For `elasticNetGLMpredictInterface`, either a factor vector of predicted classes, a matrix of scores for each class, or a table of both the class labels and class scores, depending on the setting of `returnType`.

Author(s)

Dario Strbenac

Examples

```
if(require(glmnet))
{
  # Genes 76 to 100 have differential expression.
  genesMatrix <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))
  genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample)
                                    c(rnorm(75, 9, 2), rnorm(25, 14, 2))))
  classes <- factor(rep(c("Poor", "Good"), each = 25))
  colnames(genesMatrix) <- paste("Sample", 1:ncol(genesMatrix))
  rownames(genesMatrix) <- paste("Gene", 1:nrow(genesMatrix))

  resubstituteParams <- ResubstituteParams(nFeatures = seq(10, 100, 10),
                                           performanceType = "balanced error",
                                           better = "lower")

  # lambda is automatically tuned, based on glmnet defaults, if not user-specified.
  trainParams <- TrainParams(elasticNetGLMtrainInterface, nlambda = 500,
                             getFeatures = elasticNetFeatures)
  predictParams <- PredictParams(elasticNetGLMpredictInterface)
  classified <- runTests(genesMatrix, classes, datasetName = "Example",
                         classificationName = "Differential Expression",
                         validation = "fold",
                         params = list(trainParams, predictParams))

  classified <- calcCVperformance(classified, "balanced error")
  head(tunedParameters(classified))
  performance(classified)
}
```

FeatureSetCollection   *Container for Storing A Collection of Sets*

Description

This container is the required storage format for a collection of sets. Typically, the elements of a set will either be a set of proteins (i.e. character vector) which perform a particular biological process or a set of binary interactions (i.e. Two-column matrix of feature identifiers).

Constructor

`FeatureSetCollection(sets)`

`sets` A named list. The names of the list describe the sets and the elements of the list specify the features which comprise the sets.

Summary

A method which summarises the results is available. `featureSets` is a `FeatureSetCollection` object.

`show(featureSets)`Prints a short summary of what `featureSets` contains.

Subsetting

The FeatureSetCollection may be subsetted or a single set may be extracted as a vector. `featureSets` is a `FeatureSetCollection` object.

`featureSets[i:j]`: Reduces the object to a subset of the feature sets between elements `i` and `j` of the collection.

`featureSets[[i]]`: Extract the feature set identified by `i`. `i` may be a numeric index or the character name of a feature set.

Author(s)

Dario Strbenac

Examples

```
ontology <- list(c("SESN1", "PRDX1", "PRDX2", "PRDX3", "PRDX4", "PRDX5", "PRDX6",
                   "LRRK2", "PARK7"),
                 c("ATP7A", "CCS", "NQO1", "PARK7", "SOD1", "SOD2", "SOD3",
                   "SZT2", "TNF"),
                 c("AARS", "AIMP2", "CARS", "GARS", "KARS", "NARS", "NARS2",
                   "LARS2", "NARS", "NARS2", "RGN", "UBA7"),
                 c("CRY1", "CRY2", "ONP1SW", "OPN4", "RGR"),
                 c("ESRRG", "RARA", "RARB", "RARG", "RXRA", "RXRB", "RXRG"),
                 c("CD36", "CD47", "F2", "SDC4"),
                 c("BUD31", "PARK7", "RWDD1", "TAF1")
```

```
                              )
          names(ontology) <- c("Peroxiredoxin Activity", "Superoxide Dismutase Activity",
                               "Ligase Activity", "Photoreceptor Activity",
                               "Retinoic Acid Receptor Activity",
                               "Thrombospondin Receptor Activity",
                               "Regulation of Androgen Receptor Activity")

          featureSets <- FeatureSetCollection(ontology)
          featureSets
          featureSets[3:5]
          featureSets[["Photoreceptor Activity"]]

          subNetworks <- list(MAPK = matrix(c("NRAS", "NRAS", "NRAS", "BRAF", "MEK",
                                              "ARAF", "BRAF", "CRAF", "MEK", "ERK"), ncol = 2),
                              P53 = matrix(c("ATM", "ATR", "ATR", "P53",
                                             "CHK2", "CHK1", "P53", "MDM2"), ncol = 2)
                             )
          networkSets <- FeatureSetCollection(subNetworks)
          networkSets
```

FeatureSetCollectionOrNULL

Union of a FeatureSetCollection and NULL

Description

Allows a slot to be either a FeatureSetCollectionOrNULL object or empty.

Author(s)

Dario Strbenac

Examples

```
    TrainParams(DLDAtrainInterface, transform = NULL) # Use the input data as-is.
```

---

featureSetSummary   *Transform a Table of Feature Abundances into a Table of Feature Set*
                           Abundances.

Description

Represents a feature set by the mean or median feature measurement of a feature set for all features belonging to a feature set.

Usage

```
   ## S4 method for signature 'matrix'
featureSetSummary(measurements, location = c("median", "mean"),
                    featureSets, minimumOverlapPercent = 80, verbose = 3)
   ## S4 method for signature 'DataFrame'
featureSetSummary(measurements, location = c("median", "mean"),
                           featureSets, minimumOverlapPercent = 80, verbose = 3)
   ## S4 method for signature 'MultiAssayExperiment'
featureSetSummary(measurements, target = NULL, location = c("median", "mean"),
                    featureSets, minimumOverlapPercent = 80, verbose = 3)
```

Arguments

measurements   Either a [matrix](#) or [DataFrame](#) containing the training data. For a matrix, the
                 rows are features, and the columns are samples.

target   If the input is a [MultiAssayExperiment](#), this specifies which data set will be
                 transformed. Can either be an integer or a character string specifying the name
                 of the table. Must have length 1.

location   Default: The median. The type of location to summarise a set of features be-
                 longing to a feature set by.

featureSets   An object of type [FeatureSetCollection](#) which defines the feature sets.

minimumOverlapPercent
                 The minimum percentage of overlapping features between the data set and a
                 feature set defined in featureSets for that feature set to not be discarded from
                 the anaylsis.

verbose   Default: 3. 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 feature transformation method is unusual because the mean or median feature of a feature
set for one sample may be different to another sample, whereas most other feature transformation
methods do not result in different features being compared between samples during classification.

Value

The same class of variable as the input variable measurements is, with the individual features
summarised to feature sets. The number of samples remains unchanged, so only one dimension of
measurements is altered.

Author(s)

Dario Strbenac

References

Network-based biomarkers enhance classical approaches to prognostic gene expression signatures, Rebecca L Barter, Sarah-Jane Schramm, Graham J Mann and Yee Hwa Yang, 2014, *BMC Systems Biology*, Volume 8 Supplement 4 Article S5, `https://bmcsystbiol.biomedcentral.com/articles/10.1186/1752-0509-8-S4-S5`.

Examples

```
sets <- list(Adhesion = c("Gene 1", "Gene 2", "Gene 3"),
             `Cell Cycle` = c("Gene 8", "Gene 9", "Gene 10"))
featureSets <- FeatureSetCollection(sets)

# Adhesion genes have a median gene difference between classes.
genesMatrix <- matrix(c(rnorm(5, 9, 0.3), rnorm(5, 7, 0.3), rnorm(5, 8, 0.3),
                        rnorm(5, 6, 0.3), rnorm(10, 7, 0.3), rnorm(70, 5, 0.1)),
                        ncol = 10, byrow = TRUE)
rownames(genesMatrix) <- paste("Gene", 1:10)
colnames(genesMatrix) <- paste("Patient", 1:10)
classes <- factor(rep(c("Poor", "Good"), each = 5)) # But not used for transformation.

featureSetSummary(genesMatrix, featureSets = featureSets)
```

---

fisherDiscriminant *Classification Using Fisher's LDA*

Description

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

Usage

```
  ## S4 method for signature 'matrix'
fisherDiscriminant(measurements, classes, test, ...)
  ## S4 method for signature 'DataFrame'
fisherDiscriminant(measurements, classes, test, returnType = c("class", "score", "both"),
                   verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
fisherDiscriminant(measurements, test, targets = names(measurements), ...)
```

Arguments

measurements Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training data. For a `matrix`, the rows are features, and the columns are samples.

classes Either a vector of class labels of class [factor]() of the same length as the number of samples in `measurements` or if the measurements are of class `DataFrame` a character vector of length 1 containing the column name in `measurement` is also permitted. Not used if `measurements` is a `MultiAssayExperiment` object.

test	An object of the same class as `measurements` with no samples in common with `measurements` and the same number of features as it.
targets	If measurements is a `MultiAssayExperiment`, the names of the data tables to be used. `"clinical"` is also a valid value and specifies that integer variables from the clinical data table will be used.
...	Variables not used by the `matrix` nor the `MultiAssayExperiment` method which are passed into and used by the `DataFrame` method.
returnType	Default: `"class"`. Either `"class"`, `"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	Default: 3. 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.

Data tables which consist entirely of non-numeric data cannot be analysed. If `measurements` is an object of class `MultiAssayExperiment`, the factor of sample classes must be stored in the DataFrame accessible by the `colData` function with column name `"class"`.

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

Examples

```
trainMatrix <- matrix(rnorm(1000, 8, 2), ncol = 10)
classes <- factor(rep(c("Poor", "Good"), each = 5))

# Make first 30 genes increased in value for poor samples.
trainMatrix[1:30, 1:5] <- trainMatrix[1:30, 1:5] + 5

testMatrix <- matrix(rnorm(1000, 8, 2), ncol = 10)

# Make first 30 genes increased in value for sixth to tenth samples.
testMatrix[1:30, 6:10] <- testMatrix[1:30, 6:10] + 5

fisherDiscriminant(trainMatrix, classes, testMatrix)
```

---

forestFeatures	*Extract Vectors of Ranked and Selected Features From a Random Forest Object*

Description

Provides a ranking of features based on the total decrease in node impurities from splitting on the variable, averaged over all trees. Also provides the selected features which are those that were used in at least one tree of the forest.

Usage

```
   ## S4 method for signature 'randomForest'
forestFeatures(forest)
```

Arguments

forest   A trained random forest which was created by randomForest.

Value

An list object. The first element is a vector or data frame of features, ranked from best to worst using the Gini index. The second element is a vector or data frame of features used in at least one tree.

Author(s)

Dario Strbenac

Examples

```
    if(require(randomForest))
    {
      genesMatrix <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))
      genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample)
                                       c(rnorm(75, 9, 2), rnorm(25, 14, 2))))
      classes <- factor(rep(c("Poor", "Good"), each = 25))
      colnames(genesMatrix) <- paste("Sample", 1:ncol(genesMatrix))
      rownames(genesMatrix) <- paste("Gene", 1:nrow(genesMatrix))
      trainingSamples <- c(1:20, 26:45)
      testingSamples <- c(21:25, 46:50)

      trained <- randomForestTrainInterface(genesMatrix[, trainingSamples],
                                           classes[trainingSamples], ntree = 10)

      forestFeatures(trained)
    }
```

---

functionOrList *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")
```

---

functionOrNULL *Union of A Function and NULL*

Description

Allows a slot to be either a function or empty.

Author(s)

Dario Strbenac

Examples

```
PredictParams(NULL)
PredictParams(predict)
```

---

getLocationsAndScales *Calculate Location and Scale*

Description

Calculates the location and scale for each feature.

Usage

```
    ## S4 method for signature 'matrix'
getLocationsAndScales(measurements, ...)
    ## S4 method for signature 'DataFrame'
getLocationsAndScales(measurements, location = c("mean", "median"),
                        scale = c("SD", "MAD", "Qn"))
    ## S4 method for signature 'MultiAssayExperiment'
getLocationsAndScales(measurements, targets = names(measurements), ...)
```

Arguments

measurements	Either a matrix, DataFrame or MultiAssayExperiment containing the data. For a `matrix`, the rows are features, and the columns are samples.
targets	If measurements is a `MultiAssayExperiment`, the names of the data tables to be used. `"clinical"` is also a valid value and specifies that numeric variables from the clinical data table will be used.
...	Variables not used by the `matrix` nor the `MultiAssayExperiment` method which are passed into and used by the `DataFrame` method.
location	The type of location to be calculated.
scale	The type of scale to be calculated.

Details

`"SD"` is used to represent standard deviation and `"MAD"` is used to represent median absolute deviation.

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)
    distributionInfo <- getLocationsAndScales(genesMatrix, "median", "MAD")

    mean(distributionInfo[["median"]]) # Typical median.
    mean(distributionInfo[["MAD"]]) # Typical MAD.
```

---

integerOrNumeric   *Union of a Integer and a Numeric*

Description

Allows the same S4 subsetting function to be specified for `object[i]` and `object[i:j]`, where `i` and `j` are integers.

Author(s)

Dario Strbenac

Examples

```
setClass("Container", representation(scores = "numeric"))
setMethod("[", c("Container", "integerOrNumeric", "missing", "ANY"),
          function(x, i, j, ..., drop = TRUE)
          {
            new("Container", scores = x@scores[i])
          })

dataset <- new("Container", scores = 1:10)
dataset[1] # 1 is numeric.
dataset[4:6] # 4:6 is a sequence of integers.
```

---

interactorDifferences   *Convert Individual Features into Differences Between Binary Interactors Based on Known Sub-networks*

Description

This conversion is useful for creating a meta-feature table for classifier training and prediction based on sub-networks that were selected based on their differential correlation between classes.

Usage

```
  ## S4 method for signature 'matrix'
interactorDifferences(measurements, ...)
  ## S4 method for signature 'DataFrame'
interactorDifferences(measurements, networkSets = NULL, absolute = FALSE, verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
interactorDifferences(measurements, target = NULL, ...)
```

Arguments

measurements	Either a `matrix`, `DataFrame` or `MultiAssayExperiment` containing the training data. For a `matrix`, the rows are features, and the columns are samples.
networkSets	A object of type `FeatureSetCollection`. The `sets` slot must contain a list of two-column matrices with each row corresponding to a binary interaction. Such sub-networks may be determined by a community detection algorithm.
absolute	If TRUE, then the absolute values of the differences are returned.
target	If `measurements` is a `MultiAssayExperiment`, the name of the data table to be used.
...	Variables not used by the `matrix` nor the `MultiAssayExperiment` method which are passed into and used by the `DataFrame` method.
verbose	Default: 3. 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 pairs of features known to interact with each other are specified by `networkSets`.

Value

An object of class `DataFrame` with one column for each interactor pair difference and one row for each sample. Additionally, mcols(resultTable) prodvides a `DataFrame` with a column named "original" containing the name of the sub-network each meta-feature belongs to.

Author(s)

Dario Strbenac

References

Dynamic modularity in protein interaction networks predicts breast cancer outcome, Ian W Taylor, Rune Linding, David Warde-Farley, Yongmei Liu, Catia Pesquita, Daniel Faria, Shelley Bull, Tony Pawson, Quaid Morris and Jeffrey L Wrana, 2009, *Nature Biotechnology*, Volume 27 Issue 2, https://www.nature.com/articles/nbt.1522.

Examples

```
networksList <- list(`A Hub` = matrix(c('A', 'A', 'A', 'B', 'C', 'D'), ncol = 2),
                     `G Hub` = matrix(c('G', 'G', 'G', 'H', 'I', 'J'), ncol = 2))
netSets <- FeatureSetCollection(networksList)

# Differential correlation for sub-network with hub A.
measurements <- matrix(c(5.7, 10.1, 6.9, 7.7, 8.8, 9.1, 11.2, 6.4, 7.0, 5.5,
                         5.6, 9.6, 7.0, 8.4, 10.8, 12.2, 8.1, 5.7, 5.4, 12.1,
                         4.5, 9.0, 6.9, 7.0, 7.3, 6.9, 7.8, 7.9, 5.7, 8.7,
                         8.1, 10.6, 7.4, 7.15, 10.4, 6.1, 7.3, 2.7, 11.0, 9.1,
                         round(rnorm(60, 8, 1), 1)), ncol = 10, byrow = TRUE)
```

```
rownames(measurements) <- LETTERS[1:10]
colnames(measurements) <- paste("Patient", 1:10)

interactorDifferences(measurements, netSets)
```

---

kNNinterface   *An Interface for class Package's knn Function*

Description

More details of k Nearest Neighbours are available in the documentation of [knn](#).

Usage

```
  ## S4 method for signature 'matrix'
kNNinterface(measurements, classes, test, ...)
  ## S4 method for signature 'DataFrame'
kNNinterface(measurements, classes, test, ..., verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
kNNinterface(measurements, test, targets = names(measurements), ...)
```

Arguments

measurements	Either a [matrix](#), [DataFrame](#) or [MultiAssayExperiment](#) containing the training data. For a matrix, the rows are features, and the columns are samples. If of type [DataFrame](#), the data set is subset to only those features of type integer.
classes	Either a vector of class labels of class [factor](#) of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
test	An object of the same class as measurements with no samples in common with measurements and the same number of features as it.
targets	If measurements is a MultiAssayExperiment, the names of the data tables to be used. "clinical" is also a valid value and specifies that integer variables from the clinical data table will be used.
...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method or parameters that [knn](#) can accept.
verbose	Default: 3. 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

Data tables which consist entirely of non-numeric data cannot be analysed. If measurements is an object of class MultiAssayExperiment, the factor of sample classes must be stored in the DataFrame accessible by the colData function with column name "class".

Value

A factor vector, the same as is returned by [knn](knn).

Author(s)

Dario Strbenac

Examples

```
if(require(class))
{
  classes <- factor(rep(c("Healthy", "Disease"), each = 5),
                    levels = c("Healthy", "Disease"))
  measurements <- matrix(c(rnorm(50, 10), rnorm(50, 5)), ncol = 10)
  colnames(measurements) <- paste("Sample", 1:10)
  rownames(measurements) <- paste("mRNA", 1:10)
}

kNNinterface(measurements[, 1:9], classes[1:9], measurements[, 10, drop = FALSE])
```

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

```
  ## S4 method for signature 'matrix'
KolmogorovSmirnovSelection(measurements, classes, ...)
  ## S4 method for signature 'DataFrame'
KolmogorovSmirnovSelection(measurements, classes, datasetName,
                             trainParams, predictParams, resubstituteParams, ...,
                           selectionName = "Kolmogorov-Smirnov Test", verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
KolmogorovSmirnovSelection(measurements, targets = names(measurements), ...)
```

Arguments

measurements	Either a matrix, DataFrame or MultiAssayExperiment containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	Either a vector of class labels of class factor of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.

targets   If measurements is a MultiAssayExperiment, the names of the data tables to
                 be used. "clinical" is also a valid value and specifies that numeric variables
                 from the clinical data table will be used.

...   Variables not used by the matrix nor the MultiAssayExperiment method which
                 are passed into and used by the DataFrame method or options which are ac-
                 cepted by the function ks.test.

datasetName   A name for the data set 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   Default: 3. 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

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.

Data tables which consist entirely of non-numeric data cannot be analysed. If measurements is
an object of class MultiAssayExperiment, the factor of sample classes must be stored in the
DataFrame accessible by the colData function with column name "class".

Value

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

Author(s)

Dario Strbenac

Examples

```
# First 20 features have bimodal distribution for Poor class.
# Other 80 features have normal distribution for both classes.
set.seed(1984)
genesMatrix <- sapply(1:25, function(sample)
                              {
                                randomMeans <- sample(c(8, 12), 20, replace = TRUE)
                                c(rnorm(20, randomMeans, 1), rnorm(80, 10, 1))
                              }
                      )
genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample) rnorm(100, 10, 1)))
rownames(genesMatrix) <- paste("Gene", 1:nrow(genesMatrix))
classes <- factor(rep(c("Poor", "Good"), each = 25))
```

```
resubstituteParams <- ResubstituteParams(nFeatures = seq(5, 25, 5),
                                          performanceType = "balanced error",
                                          better = "lower")
selected <- KolmogorovSmirnovSelection(genesMatrix, classes, "Example",
                          trainParams = TrainParams(naiveBayesKernel),
                          predictParams = PredictParams(NULL),
                          resubstituteParams = resubstituteParams)

head(selected@chosenFeatures)
plotFeatureClasses(genesMatrix, classes, "Gene 13", dotBinWidth = 0.25,
                   xAxisLabel = bquote(log[2]*'(expression)'))
```

---

kTSPclassifier   *Classification Using k Pairs of Features With Relative Differences Be-*
                      tween Classes

Description

Each pair of features votes for a class based on whether the value of one feature is less than the
other feature.

Usage

```
  ## S4 method for signature 'matrix'
kTSPclassifier(measurements, classes, test, featurePairs = NULL, ...)
  ## S4 method for signature 'DataFrame'
kTSPclassifier(measurements, classes, test, featurePairs = NULL,
                  weighted = c("unweighted", "weighted", "both"),
            minDifference = 0, returnType = c("class", "score", "both"), verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
kTSPclassifier(measurements, test, target = names(measurements)[1],
                  featurePairs = NULL, ...)
```

Arguments

measurements	Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	Either a vector of class labels of class [factor]() of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
test	An object of the same class as measurements with no samples in common with measurements and the same number of features as it.
featurePairs	An object of class as [Pairs]() containing the pairs of features to determine whether the inequality of the first feature being less than the second feature holds, indiciating evidence for the second level of the classes factor.

target   If measurements is a MultiAssayExperiment, the name of the data table to be
                     used. "clinical" is also a valid value and specifies that integer variables from
                     the clinical data table will be used.

...   Unused variables by the methods for a matrix or a MultiAssayExperiment
                     passed to the DataFrame method which does the classification.

weighted   Default: "both". Either "both", "unweighted" or "weighted". In weighted
                     mode, the difference in densities is summed over all features. If unweighted
                     mode, each feature's vote is worth the same. Both can be calculated simultane-
                     ously.

minDifference   Default: 0. 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   Default: "class". Either "class", "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   Default: 3. 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 based on the sum of differences of measure-
ments for each feature pair. Otherwise, when weighted is FALSE, each pair of features has an equal
vote, the predicted class is the one with the most votes. If the voting is tied, the the class with the
most samples in the training set is voted for.

Because this method compares different features, they need to have comparable measurements.
For example, RNA-seq counts would be unsuitable since these depend on the length of a feature,
whereas F.P.K.M. values would be suitable.

The featurePairs to use is recommended to be determined in conjunction with pairsDifferencesSelection.

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

See Also

[pairsDifferencesSelection](#) for a function which could be used to do feature selection before
the k-TSP classifier is run.

Examples

```
    # Difference in differences for features A and C between classes.
    measurements <- matrix(c(9.9, 10.5, 10.1, 10.9, 11.0, 6.6, 7.7, 7.0, 8.1, 6.5,
                             8.5, 10.5, 12.5, 10.5, 9.5, 8.5, 10.5, 12.5, 10.5, 9.5,
                             6.6, 7.7, 7.0, 8.1, 6.5, 11.2, 11.0, 11.1, 11.4, 12.0,
                             8.1, 10.6, 7.4, 7.1, 10.4, 6.1, 7.3, 2.7, 11.0, 9.1,
                             round(rnorm(60, 8, 1), 1)), ncol = 10, byrow = TRUE)
    classes <- factor(rep(c("Good", "Poor"), each = 5))

    rownames(measurements) <- LETTERS[1:10]
    colnames(measurements) <- names(classes) <- paste("Patient", 1:10)

    trainIndex <- c(1:4, 6:9)
    trainMatrix <- measurements[, trainIndex]
    testMatrix <- measurements[, c(5, 10)]

   featurePairs <- Pairs('A', 'C') # Could be selected by pairsDifferencesSelection function.
   kTSPclassifier(trainMatrix, classes[trainIndex], testMatrix, featurePairs)
```

KullbackLeiblerSelection

Selection of Differential Distributions with Kullback-Leibler Distance

---

Description

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

Usage

```
   ## S4 method for signature 'matrix'
KullbackLeiblerSelection(measurements, classes, ...)
   ## S4 method for signature 'DataFrame'
KullbackLeiblerSelection(measurements, classes, datasetName,
                          trainParams, predictParams, resubstituteParams, ...,
                      selectionName = "Kullback-Leibler Divergence", verbose = 3)
   ## S4 method for signature 'MultiAssayExperiment'
KullbackLeiblerSelection(measurements, targets = names(measurements), ...)
```

Arguments

measurements	Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	Either a vector of class labels of class [factor]() of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.

targets   If measurements is a MultiAssayExperiment, the names of the data tables to be used. "clinical" is also a valid value and specifies that numeric variables from the clinical data table will be used.

...   Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method or options which are accepted by the function getLocationsAndScales.

datasetName   A name for the data set 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   Default: 3. 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 $\frac{1}{2} \times \left(\frac{(location_1 - location_2)^2}{scale_1^2} + \frac{(location_1 - location_2)^2}{scale_2^2} + \frac{scale_2^2}{scale_1^2} + \frac{scale_1^2}{scale_2^2} \right)$

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

Data tables which consist entirely of non-numeric data cannot be analysed. If measurements is an object of class MultiAssayExperiment, the factor of sample classes must be stored in the DataFrame accessible by the colData function with column name "class".

Value

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

Author(s)

Dario Strbenac

Examples

```
# First 20 features have bimodal distribution for Poor class.
# Other 80 features have normal distribution for both classes.
genesMatrix <- sapply(1:25, function(sample)
                            {
                              randomMeans <- sample(c(8, 12), 20, replace = TRUE)
                              c(rnorm(20, randomMeans, 1), rnorm(80, 10, 1))
                            }
                      )
genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample) rnorm(100, 10, 1)))
classes <- factor(rep(c("Poor", "Good"), each = 25))

resubstituteParams <- ResubstituteParams(nFeatures = seq(5, 25, 5),
                                          performanceType = "balanced error",
```

```
                                        better = "lower")
  KullbackLeiblerSelection(genesMatrix, classes, "Example",
                           trainParams = TrainParams(naiveBayesKernel),
                           predictParams = PredictParams(NULL),
                           resubstituteParams = resubstituteParams
                          )
```

---

leveneSelection   *Selection of Differential Variability with Levene Statistic*

Description

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

Usage

```
  ## S4 method for signature 'matrix'
leveneSelection(measurements, classes, ...)
  ## S4 method for signature 'DataFrame'
leveneSelection(measurements, classes, datasetName,
                trainParams, predictParams, resubstituteParams,
                selectionName = "Levene Test", verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
leveneSelection(measurements, targets = names(measurements), ...)
```

Arguments

measurements	Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	Either a vector of class labels of class [factor]() of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
targets	If measurements is a MultiAssayExperiment, the names of the data tables to be used. "clinical" is also a valid value and specifies that numeric variables from the clinical data table will be used.
...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method.
datasetName	A name for the data set 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   Default: 3. 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.

Data tables which consist entirely of non-numeric data cannot be analysed. If `measurements` is
an object of class MultiAssayExperiment, the factor of sample classes must be stored in the
DataFrame accessible by the `colData` function with column name `"class"`.

Value

An object of class [SelectResult](#) or a list of such objects, if the classifier which was used for
determining the specified performance metric made a number of prediction varieties.

Author(s)

Dario Strbenac

Examples

```
# First 20 features have bimodal distribution for Poor class.
# Other 80 features have normal distribution for both classes.
set.seed(1984)
genesMatrix <- sapply(1:25, function(sample)
                            {
                              randomMeans <- sample(c(8, 12), 20, replace = TRUE)
                              c(rnorm(20, randomMeans, 1), rnorm(80, 10, 1))
                            }
                      )
genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample) rnorm(100, 10, 1)))
rownames(genesMatrix) <- paste("Gene", 1:nrow(genesMatrix))
classes <- factor(rep(c("Poor", "Good"), each = 25))
genesMatrix <- subtractFromLocation(genesMatrix, 1:ncol(genesMatrix))

resubstituteParams <- ResubstituteParams(nFeatures = seq(10, 100, 10),
                                          performanceType = "balanced error",
                                          better = "lower")
selected <- leveneSelection(genesMatrix, classes, "Example",
                            trainParams = TrainParams(fisherDiscriminant),
                            predictParams = PredictParams(NULL),
                            resubstituteParams = resubstituteParams)
selected@chosenFeatures
```

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

```
  ## S4 method for signature 'matrix'
likelihoodRatioSelection(measurements, classes, ...)
  ## S4 method for signature 'DataFrame'
likelihoodRatioSelection(measurements, classes, datasetName,
                        trainParams, predictParams, resubstituteParams,
                     alternative = c(location = "different", scale = "different"),
                       ..., selectionName = "Likelihood Ratio Test (Normal)", verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
likelihoodRatioSelection(measurements, targets = names(measurements), ...)
```

Arguments

measurements	Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	Either a vector of class labels of class [factor]() of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
targets	If measurements is a MultiAssayExperiment, the names of the data tables to be used. "clinical" is also a valid value and specifies that numeric variables from the clinical data table will be used.
...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method or options which are accepted by the function [getLocationsAndScales]().
datasetName	A name for the data set 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.
alternative	Default: c("different","different"). A vector of length 2. The first element specifies the location of the alternate hypothesis. The second element specifies the scale of the alternate hypothesis. Valid values in each element are "same" or "different".

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

verbose   Default: 3. 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

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 calcu-
lated by getLocationsAndScales. The distribution fitted to the data is the normal distribution.

Data tables which consist entirely of non-numeric data cannot be analysed. If measurements is
an object of class MultiAssayExperiment, the factor of sample classes must be stored in the
DataFrame accessible by the colData function with column name "class".

Value

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

Author(s)

Dario Strbenac

Examples

```
# First 20 features have bimodal distribution for Poor class.
# Other 80 features have normal distribution for both classes.
set.seed(1984)
genesMatrix <- sapply(1:25, function(sample)
                             {
                               randomMeans <- sample(c(8, 12), 20, replace = TRUE)
                               c(rnorm(20, randomMeans, 1), rnorm(80, 10, 1))
                             }
                       )
genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample) rnorm(100, 10, 1)))
rownames(genesMatrix) <- paste("Gene", 1:nrow(genesMatrix))
classes <- factor(rep(c("Poor", "Good"), each = 25))

resubstituteParams <- ResubstituteParams(nFeatures = seq(10, 100, 10),
                                         performanceType = "balanced error",
                                         better = "lower")
selected <- likelihoodRatioSelection(genesMatrix, classes, "Example",
                                     trainParams = TrainParams(naiveBayesKernel),
                          predictParams = PredictParams(NULL),
                          resubstituteParams = resubstituteParams)

head(selected@chosenFeatures[[1]])
```

limmaSelection   *Selection of Differentially Abundant Features*

Description

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

Usage

```
  ## S4 method for signature 'matrix'
limmaSelection(measurements, classes, ...)
  ## S4 method for signature 'DataFrame'
limmaSelection(measurements, classes, datasetName,
               trainParams, predictParams, resubstituteParams, ...,
               selectionName = "Moderated t-test", verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
limmaSelection(measurements, targets = NULL, ...)
```

Arguments

measurements	Either a `matrix`, `DataFrame` or `MultiAssayExperiment` containing the training data. For a `matrix`, the rows are features, and the columns are samples.
classes	A vector of class labels of class `factor` of the same length as the number of samples in `measurements`. Not used if `measurements` is a `MultiAssayExperiment` object.
targets	Names of data tables to be combined into a single table and used in the analysis.
...	Variables not used by the `matrix` nor the `MultiAssayExperiment` method which are passed into and used by the `DataFrame` method or optional settings that are passed to `lmFit`.
datasetName	A name for the data set 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	Default: 3. 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 changes in means and 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 the specified performance metric 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

```
#if(require(sparsediscrim))
#{
  # Genes 76 to 100 have differential expression.
  genesMatrix <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))
  genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample)
                                c(rnorm(75, 9, 2), rnorm(25, 14, 2))))
  classes <- factor(rep(c("Poor", "Good"), each = 25))
  colnames(genesMatrix) <- paste("Sample", 1:ncol(genesMatrix))
  rownames(genesMatrix) <- paste("Gene", 1:nrow(genesMatrix))

  resubstituteParams <- ResubstituteParams(nFeatures = seq(10, 100, 10),
                          performanceType = "balanced error", better = "lower")
  selected <- limmaSelection(genesMatrix, classes, "Example",
                        trainParams = TrainParams(), predictParams = PredictParams(),
                            resubstituteParams = resubstituteParams)

  selected@chosenFeatures
#}
```

---

listOrCharacterOrNULL   *Union of a List and a Character Vector and NULL*

Description

Allows a slot to be either a list, character or a NULL.

Author(s)

Dario Strbenac

Examples

```
setClass("HardClassifier", representation(model = "listOrCharacterOrNULL"))
classifier <- new("HardClassifier", model = "Good") # Optimistic classifier.
```

---

listOrNULL   *Union of a List and NULL*

Description

Allows a slot to be either a list or a NULL.

Author(s)

Dario Strbenac

Examples

```
setClass("EasyClassifier", representation(model = "listOrNULL"))
classifier <- new("EasyClassifier", model = NULL) # Optimistic classifier.
```

---

mixmodels   *Classification based on Differential Distribution utilising Mixtures of Normals*

Description

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

Usage

```
   ## S4 method for signature 'matrix'
mixModelsTrain(measurements, ...)
   ## S4 method for signature 'DataFrame'
mixModelsTrain(measurements, classes, ..., verbose = 3)
   ## S4 method for signature 'MultiAssayExperiment'
mixModelsTrain(measurements, targets = names(measurements), ...)
   ## S4 method for signature 'MixModelsListsSet,matrix'
mixModelsPredict(models, test, ...)
   ## S4 method for signature 'MixModelsListsSet,DataFrame'
mixModelsPredict(models, test, weighted = c("unweighted", "weighted", "both"),
                 weight = c("height difference", "crossover distance", "both"),
             densityXvalues = 1024, minDifference = 0,
             returnType = c("class", "score", "both"), verbose = 3)
   ## S4 method for signature 'MixModelsListsSet,MultiAssayExperiment'
mixModelsPredict(models, test, targets = names(test), ...)
```

Arguments

measurements	Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	Either a vector of class labels of class [factor]() of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
test	An object of the same class as measurements with no samples in common with measurements and the same number of features as it. Also, if a DataFrame, the class column must be absent.
targets	If measurements is a MultiAssayExperiment, the names of the data tables to be used. "clinical" is also a valid value and specifies that numeric variables from the clinical data table will be used.
...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method or extra arguments for training passed to [mixmodCluster](). The argument nbCluster is mandatory.
models	A [MixModelsListsSet]() of models generated by the training function and training class information. There is one element for each class. Another element at the end of the list has the class sizes of the classes in the training data.
weighted	Default: "unweighted". Either "unweighted", "weighted" or "both". In weighted mode, the difference in densities is summed over all features. If unweighted mode, each feature's vote is worth the same. Both can be calculated simultaneously.
weight	Default: "both". Either "both", "height difference", or "crossover distance". The type of weight to calculate. For "height difference", the weight of each prediction is equal to the sum of the vertical 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 the mixture density of the class being considered crosses another class' density 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	Default: 1024. Only relevant when weight is "crossover distance". The number of equally-spaced locations at which to calculate y values for each mixture density.
minDifference	Default: 0. The minimum difference in sums of mixture densities between the class with the highest sum and the class with the second highest sum 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	Default: "class". Either "class", "score" or "both". Sets the return value from the prediction to either a vector of predicted classes, a matrix of scores with columns corresponding to classes, as determined by the factor levels of classes, or both a column of predicted classes and columns of class scores in a data.frame.

verbose	Default: 3. 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, each 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.

Value

For `mixModelsTrain`, a list of trained models of class `MixmodCluster`. For `mixModelsPredict`, a vector or list of class prediction information (i.e. classes and/or scores), as long as the number of samples in the test data, or lists of such information, if both weighted and unweighted voting was used or a range of `minDifference` values was provided.

Author(s)

Dario Strbenac

Examples

```
# First 25 samples and first 5 genes are mixtures of two normals. Last 25 samples are
# one normal.

genesMatrix <- sapply(1:25, function(geneColumn) c(rnorm(5, sample(c(5, 15), replace = TRUE, 5))))
genesMatrix <- cbind(genesMatrix, sapply(1:25, function(geneColumn) c(rnorm(5, 9, 1))))
genesMatrix <- rbind(genesMatrix, sapply(1:50, function(geneColumn) rnorm(5, 9, 1)))
rownames(genesMatrix) <- paste("Gene", 1:10)
colnames(genesMatrix) <- paste("Sample", 1:50)
classes <- factor(rep(c("Poor", "Good"), each = 25), levels = c("Good", "Poor"))

trainSamples <- c(1:15, 26:40)
testSamples <- c(16:25, 41:50)
selected <- 1:5

trained <- mixModelsTrain(genesMatrix[selected, trainSamples], classes[trainSamples],
                          nbCluster = 1:3)
mixModelsPredict(trained, genesMatrix[selected, testSamples], minDifference = 0:3)
```

MixModelsListsSet   *Container for a List of Lists Containing Mixture Models*

Description

Stores a list of lists of trained mixture models, to prevent them being unintentionally being unlisted during cross-validation. Not intended for end-user.

Constructor

```
MixModelsListsSet(set)
```

Creates a MixModelsListsSet object which stores the mixture models.

set A list as long as the number of classes in the data set. Each element is a list, which each element of is a mixture model trained on one feature.

Author(s)

Dario Strbenac

Examples

```
if(require(Rmixmod))
{
  mixModels <- list(Good = list(mixmodCluster(rnorm(20), nbCluster = 1:2)),
                    Poor = list(mixmodCluster(rnorm(20), nbCluster = 1:2)))
  MixModelsListsSet(mixModels)
}
```

---

multnet   *Trained multnet Object*

Description

Enables S4 method dispatching on it.

Author(s)

Dario Strbenac

---

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.

Usage

```
  ## S4 method for signature 'matrix'
naiveBayesKernel(measurements, classes, test, ...)
  ## S4 method for signature 'DataFrame'
naiveBayesKernel(measurements, classes, test,
                 densityFunction = density,
                 densityParameters = list(bw = "nrd0", n = 1024,
                                          from = expression(min(featureValues)),
                                          to = expression(max(featureValues))),
                 weighted = c("unweighted", "weighted", "both"),
                 weight = c("height difference", "crossover distance", "both"),
             minDifference = 0, returnType = c("class", "score", "both"), verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
naiveBayesKernel(measurements, test, targets = names(measurements), ...)
```

Arguments

measurements	Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	Either a vector of class labels of class [factor]() of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
test	An object of the same class as measurements with no samples in common with measurements and the same number of features as it.
targets	If measurements is a MultiAssayExperiment, the names of the data tables to be used. "clinical" is also a valid value and specifies that integer variables from the clinical data table will be used.
...	Unused variables by the three top-level methods passed to the internal method which does the classification.
densityFunction	
	Default: [density](). 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. Default: list(bw = "nrd0", n = 1024, from = expression(min(featureValues)), to = expression(max(featureValues)).

weighted   Default: ″unweighted″. Either ″unweighted″, ″weighted″ or ″both″. In
                weighted mode, the difference in densities is summed over all features. If un-
                weighted mode, each feature's vote is worth the same. Both can be calculated
                simultaneously.

weight   Default: ″both″. Either ″both″, ″height difference″, or ″crossover distance″.
                The type of weight to calculate. For ″height difference″, the weight of each
                prediction is equal to the vertical distance between the highest density and the
                second-highest, 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.

minDifference   Default: 0. The minimum difference in density height between the highest den-
                sity and second-highest 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   Default: ″class″. Either ″class″, ″score″ or ″both″. Sets the return value
                from the prediction to either a vector of predicted classes, a matrix of scores
                with columns corresponding to classes, as determined by the factor levels of
                classes, or both a column of predicted classes and columns of class scores in a
                data.frame.

verbose   Default: 3. 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,
each 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. For example, see the default value of densityParameters above.

If weight is ″crossover distance″, the crossover points are computed by considering the distance
between y values of all of the densities at every x value. x values for which a class density crosses
any other class' density are used as the crossover points for that class.

Value

A vector or list of class prediction information (i.e. classes and/or scores), as long as the number of
samples in the test data, or lists of such information, if both weighted and unweighted voting was
used or a range of minDifference values was provided.

Author(s)

Dario Strbenac, John Ormerod

Examples

```
    trainMatrix <- matrix(rnorm(1000, 8, 2), ncol = 10)
    classes <- factor(rep(c("Poor", "Good"), each = 5))

    # Make first 30 genes increased in value for poor samples.
    trainMatrix[1:30, 1:5] <- trainMatrix[1:30, 1:5] + 5

    testMatrix <- matrix(rnorm(1000, 8, 2), ncol = 10)

    # Make first 30 genes increased in value for sixth to tenth samples.
    testMatrix[1:30, 6:10] <- testMatrix[1:30, 6:10] + 5

    naiveBayesKernel(trainMatrix, classes, testMatrix)
```

---

networkCorrelationsSelection

Selection of Differentially Correlated Hub Sub-networks

Description

Ranks sub-networks by largest within-class to between-class correlation variability and chooses the sub-networks which have the best resubstitution performance.

Usage

```
    ## S4 method for signature 'matrix'
networkCorrelationsSelection(measurements, classes, metaFeatures = NULL, ...)
    ## S4 method for signature 'DataFrame'
networkCorrelationsSelection(measurements, classes, metaFeatures = NULL,
              featureSets, datasetName, trainParams, predictParams, resubstituteParams,
              selectionName = "Differential Correlation of Sub-networks", verbose = 3)
    ## S4 method for signature 'MultiAssayExperiment'
networkCorrelationsSelection(measurements, target = NULL, metaFeatures = NULL, ...)
```

Arguments

measurements	Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	Either a vector of class labels of class [factor]() of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
metaFeatures	A DataFrame with the same number of samples as the numeric table of interest. The number of derived features in this table will be different to the original input data table. The command mcols(metaFeatureMeasurements) must return a DataFrame which has an "original" column with as many rows as there are meta-features and specifies the feature which the meta-feature is originally derived from (e.g. network name).

featureSets   A object of type [FeatureSetCollection](). The sets slot must contain a list of
                     two-column matrices with each row corresponding to a binary interaction. Such
                     sub-networks may be determined by a community detection algorithm. This
                     will be used to determine which features belong to which sub-networks before
                     calculating a statistic for each sub-network.

target   If measurements is a MultiAssayExperiment, the name of the data table to be
                     used.

...   Variables not used by the matrix nor the MultiAssayExperiment method which
                     are passed into and used by the DataFrame method.

datasetName   A name for the data set 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   Default: 3. 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 selection of sub-networks is based on the average difference in correlations between each pair
of interactors, considering the samples within each class separately. Such differences of correlations
within each of the two classes are scaled by the average difference of correlations within each class.

More formally, let $C_{i,j}$ be the correlation of the jth edge using all samples belonging to to class i.
Then, let $\overline{C}_{i\bullet}$ be defined as $\frac{C_{i,1}+C_{i,2}+...+C_{i,e}}{n}$ where e is the number of edges in the sub-network
being considered. Also, let $\overline{C}_{\bullet\bullet}$, the average overall correlation, be $\frac{C_{1\bullet}+C_{2\bullet}}{2}$. Then, the between-
class sum-of-squares (BSS) is $\sum_{i=1}^{2} e(\overline{C}_{i\bullet} - \overline{C}_{\bullet\bullet})^2$. Also the within-class sum-of-squares (WSS)
is $\sum_{i=1}^{2} \sum_{j=1}^{e} (C_{i,j} - \overline{C}_{i\bullet})^2$. The sub-networks are ranked in decreasing order of $\frac{BSS}{WSS}$.

The classifier specified by trainParams and predictParams is used to calculate resubtitution error
rates using the transformation of the data set provided by metaFeatures. The set of top-ranked sub-
networks which give the lowest resubstitution error rate are finally selected.

Data tables which consist entirely of non-numeric data cannot be analysed. If measurements is
an object of class MultiAssayExperiment, the factor of sample classes must be stored in the
DataFrame accessible by the colData function with column name "class".

Value

An object of class [SelectResult]() or a list of such objects, if the classifier which was used for
determining the specified performance metric made a number of prediction varieties.

Author(s)

Dario Strbenac

References

Network-based biomarkers enhance classical approaches to prognostic gene expression signatures, Rebecca L Barter, Sarah-Jane Schramm, Graham J Mann and Yee Hwa Yang, 2014, *BMC Systems Biology*, Volume 8 Supplement 4 Article S5, https://bmcsystbiol.biomedcentral.com/articles/10.1186/1752-0509-8-S4-S5.

See Also

interactorDifferences for an example of a function which can turn the measurements into meta-features for classification.

Examples

```
networksList <- list(`A Hub` = matrix(c('A', 'A', 'A', 'B', 'C', 'D'), ncol = 2),
                     `G Hub` = matrix(c('G', 'G', 'G', 'H', 'I', 'J'), ncol = 2))
netSets <- FeatureSetCollection(networksList)

# Differential correlation for sub-network with hub A.
measurements <- matrix(c(5.7, 10.1, 6.9, 7.7, 8.8, 9.1, 11.2, 6.4, 7.0, 5.5,
                         5.6, 9.6, 7.0, 8.4, 10.8, 12.2, 8.1, 5.7, 5.4, 12.1,
                         4.5, 9.0, 6.9, 7.0, 7.3, 6.9, 7.8, 7.9, 5.7, 8.7,
                         8.1, 10.6, 7.4, 7.1, 10.4, 6.1, 7.3, 2.7, 11.0, 9.1,
                         round(rnorm(60, 8, 1), 1)), ncol = 10, byrow = TRUE)
classes <- factor(rep(c("Good", "Poor"), each = 5))

rownames(measurements) <- LETTERS[1:10]
colnames(measurements) <- names(classes) <- paste("Patient", 1:10)

Idifferences <- interactorDifferences(measurements, netSets)

# The features are sub-networks and there are only two in this example.
resubstituteParams <- ResubstituteParams(nFeatures = 1:2,
                               performanceType = "balanced error", better = "lower")

predictParams <- PredictParams(NULL)
networkCorrelationsSelection(measurements, classes, metaFeatures = Idifferences,
                             featureSets = netSets, datasetName = "Example",
                             trainParams = TrainParams(naiveBayesKernel),
                             predictParams = predictParams,
                             resubstituteParams = resubstituteParams)
```

NSCpredictInterface   *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'
NSCpredictInterface(trained, test, ...)
   ## S4 method for signature 'pamrtrained,DataFrame'
NSCpredictInterface(trained, test, classes = NULL, ..., returnType = c("class", "score", "both"), verbo
   ## S4 method for signature 'pamrtrained,MultiAssayExperiment'
NSCpredictInterface(trained, test, targets = names(test), ...)
```

Arguments

trained	An object of class pamrtrained.
test	An object of the same class as measurements with no samples in common with measurements used in the training stage and the same number of features as it. Also, if a DataFrame, the class column must be absent.
classes	Either NULL or a character vector of length 1, specifying the column name to remove.
targets	If test is a MultiAssayExperiment, the names of the data tables to be used. "clinical" is also a valid value and specifies that numeric variables from the clinical data table will be used.
...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method or optional settings that are passed to pamr.predict.
returnType	Default: "class". Either "class", "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	Default: 3. 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. It selects the highest threshold that gives the minimum error rate in the training data.

Value

Either a factor vector of predicted classes, a matrix of scores for each class, or a table of both the class labels and class scores, depending on the setting of returnType.

Author(s)

Dario Strbenac

See Also

pamr.predict for the function that was interfaced to.

Examples

```
if(require(pamr))
{
  # Samples in one class with differential expression to other class.
  genesMatrix <- sapply(1:25, function(geneColumn) c(rnorm(100, 9, 1)))
  genesMatrix <- cbind(genesMatrix, sapply(1:25, function(geneColumn)
                              c(rnorm(75, 9, 1), rnorm(25, 14, 1))))
  classes <- factor(rep(c("Poor", "Good"), each = 25))

  fit <- NSCtrainInterface(genesMatrix[, c(1:20, 26:45)], classes[c(1:20, 26:45)])
  NSCpredictInterface(fit, genesMatrix[, c(21:25, 46:50)])
}
```

NSCselectionInterface *Interface for* pamr.listgenes *Function from* pamr *CRAN Package*

Description

Restructures variables from ClassifyR framework to be compatible with [pamr.listgenes](#) definition.

Usage

```
   ## S4 method for signature 'matrix'
NSCselectionInterface(measurements, classes, ...)
   ## S4 method for signature 'DataFrame'
NSCselectionInterface(measurements, classes, datasetName,
                trained, ..., selectionName = "Shrunken Centroids", verbose = 3)
   ## S4 method for signature 'MultiAssayExperiment'
NSCselectionInterface(measurements, targets = names(measurements), ...)
```

Arguments

measurements	Either a [matrix](#), [DataFrame](#) or [MultiAssayExperiment](#) containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	Either a vector of class labels of class [factor](#) of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
targets	If measurements is a MultiAssayExperiment, the names of the data tables to be used. "clinical" is also a valid value and specifies that numeric variables from the clinical data table will be used.
datasetName	A name for the data set used. Stored in the result.
trained	The output of [NSCtrainInterface](#), which is identical to the output of [pamr.listgenes](#).
...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method or extra arguments passed to [pamr.listgenes](#).

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

verbose   Default: 3. 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
`NSCtrainInterface` 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.

Examples

```
if(require(pamr))
{
  # Genes 76 to 100 have differential expression.
  genesMatrix <- sapply(1:25, function(geneColumn) c(rnorm(100, 9, 1)))
  genesMatrix <- cbind(genesMatrix, sapply(1:25, function(geneColumn)
                               c(rnorm(75, 9, 1), rnorm(25, 14, 1))))
  rownames(genesMatrix) <- paste("Gene", 1:nrow(genesMatrix))
  classes <- factor(rep(c("Poor", "Good"), each = 25))

  trained <- NSCtrainInterface(genesMatrix, classes)
  selected <- NSCselectionInterface(genesMatrix, classes, "Example", trained)

  selected@chosenFeatures
}
```

NSCtrainInterface   *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'
NSCtrainInterface(measurements, classes, ...)
   ## S4 method for signature 'DataFrame'
NSCtrainInterface(measurements, classes, ..., verbose = 3)
   ## S4 method for signature 'MultiAssayExperiment'
NSCtrainInterface(measurements, targets = names(measurements), ...)
```

Arguments

measurements	Either a `matrix`, `DataFrame` or `MultiAssayExperiment` containing the training data. For a `matrix`, the rows are features, and the columns are samples.
classes	Either a vector of class labels of class `factor` of the same length as the number of samples in `measurements` or if the measurements are of class `DataFrame` a character vector of length 1 containing the column name in `measurement` is also permitted. Not used if `measurements` is a `MultiAssayExperiment` object.
targets	If `measurements` is a `MultiAssayExperiment`, the names of the data tables to be used. `"clinical"` is also a valid value and specifies that numeric variables from the clinical data table will be used.
...	Variables not used by the `matrix` nor the `MultiAssayExperiment` method which are passed into and used by the `DataFrame` method or extra arguments passed to `pamr.train`.
verbose	Default: 3. 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.

Examples

```
if(require(pamr))
{
  # Samples in one class with differential expression to other class.
  genesMatrix <- sapply(1:25, function(geneColumn) c(rnorm(100, 9, 1)))
  genesMatrix <- cbind(genesMatrix, sapply(1:25, function(geneColumn)
```

```
                                  c(rnorm(75, 9, 1), rnorm(25, 14, 1))))
    classes <- factor(rep(c("Poor", "Good"), each = 25))

    NSCtrainInterface(genesMatrix, classes)
  }
```

---

pairsDifferencesSelection

Selection of Pairs of Features that are Different Between Classes

---

Description

Ranks pre-specified pairs of features by the largest difference of the sum of measurement differences over all samples within a class and chooses the pairs of features which have the best resubstitution performance.

Usage

```
  ## S4 method for signature 'matrix'
pairsDifferencesSelection(measurements, classes, featurePairs = NULL, ...)
  ## S4 method for signature 'DataFrame'
pairsDifferencesSelection(measurements, classes, featurePairs = NULL,
                    datasetName, trainParams, predictParams, resubstituteParams,
                    selectionName = "Pairs Differences", verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
pairsDifferencesSelection(measurements, target = names(measurements)[1], featurePairs = NULL, ...)
```

Arguments

measurements	Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	Either a vector of class labels of class [factor]() of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
featurePairs	An S4 object of type [Pairs]() containing feature identifiers to calculate the sum of differences within each class for.
target	If measurements is a MultiAssayExperiment, the name of the data table to be used.
...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method.
datasetName	A name for the data set 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   Default: 3. 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

Instead of considering whether one feature in a pair of features is consistently lower or higher than the other in the pair, this method takes the sum of differences across all samples within a class, to prevent ties in the ranking of pairs of features.

Value

An object of class `SelectResult` or a list of such objects, if the classifier which was used for determining the specified performance metric made a number of prediction varieties.

Author(s)

Dario Strbenac

References

Simple decision rules for classifying human cancers from gene expression profiles, Aik C Tan, Daniel Q Naiman, Lei Xu, Raimond L. Winslow and Donald Geman, 2005, *Bioinformatics*, Volume 21 Issue 20, https://academic.oup.com/bioinformatics/article/21/20/3896/203010.

See Also

`kTSPclassifier` for a classifier which makes use of the pairs of selected features in classification.

Examples

```
featurePairs <- Pairs(c('A', 'A'), c('B', 'C'))

# Difference in differences for features A and C between classes.
measurements <- matrix(c(9.9, 10.5, 10.1, 10.9, 11.0, 6.6, 7.7, 7.0, 8.1, 6.5,
                         8.5, 10.5, 12.5, 10.5, 9.5, 8.5, 10.5, 12.5, 10.5, 9.5,
                         6.6, 7.7, 7.0, 8.1, 6.5, 11.2, 11.0, 11.1, 11.4, 12.0,
                         8.1, 10.6, 7.4, 7.1, 10.4, 6.1, 7.3, 2.7, 11.0, 9.1,
                         round(rnorm(60, 8, 1), 1)), ncol = 10, byrow = TRUE)
classes <- factor(rep(c("Good", "Poor"), each = 5))

rownames(measurements) <- LETTERS[1:10]
colnames(measurements) <- names(classes) <- paste("Patient", 1:10)

# The features are pairs and there are only two in this example.
resubstituteParams <- ResubstituteParams(nFeatures = 1:2,
                              performanceType = "balanced error", better = "lower")
```

```
    predictParams <- PredictParams(NULL)
    pairsDifferencesSelection(measurements, classes, featurePairs = featurePairs,
                              datasetName = "Example",
                              trainParams = TrainParams(kTSPclassifier),
                              predictParams = predictParams,
                              resubstituteParams = resubstituteParams)
```

---

pamrtrained   *Trained pamr Object*

Description

Enables S4 method dispatching on it.

Author(s)

Dario Strbenac

---

performancePlot   *Plot Performance Measures for Various Classifications*

Description

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

Usage

```
    ## S4 method for signature 'list'
performancePlot(results, aggregate = character(),
            xVariable = c("classificationName", "datasetName", "selectionName",
                          "validation"),
                performanceName = NULL,
            boxFillColouring = c("classificationName", "datasetName", "selectionName",
                                 "validation", "None"),
                boxFillColours = NULL,
            boxLineColouring = c("classificationName", "datasetName", "selectionName",
                                 "validation", "None"),
                boxLineColours = NULL,
            rowVariable = c("None", "validation", "datasetName", "classificationName",
                           "selectionName"),
            columnVariable = c("datasetName", "classificationName", "validation",
                              "selectionName", "None"),
              yLimits = c(0, 1), fontSizes = c(24, 16, 12, 12), title = NULL,
              xLabel = "Analysis", yLabel = performanceName,
              margin = grid::unit(c(0, 0, 0, 0), "lines"), rotate90 = FALSE,
              showLegend = TRUE, plot = TRUE)
```

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 particularly 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

Examples

```
predicted <- list(data.frame(sample = sample(LETTERS[1:10], 20, replace = TRUE),
                             class = factor(rep(c("Healthy", "Cancer"), each = 10))),
                  data.frame(sample = sample(LETTERS[1:10], 20, replace = TRUE),
                             class = factor(rep(c("Healthy", "Cancer"), each = 10))),
                  data.frame(sample = sample(LETTERS[1:10], 20, replace = TRUE),
                             class = factor(rep(c("Healthy", "Cancer"), each = 10))),
                  data.frame(sample = sample(LETTERS[1:10], 20, replace = TRUE),
                             class = factor(rep(c("Healthy", "Cancer"), each = 10))))
actual <- factor(rep(c("Healthy", "Cancer"), each = 5))
result1 <- ClassifyResult("Example", "Differential Expression", "t-test",
                          LETTERS[1:10], LETTERS[10:1], 100, list(1:100, c(1:9, 11:101)),
                            list(c(1:3), c(2, 5, 6), c(1:4), c(5:8), 1:5),
                            list(function(oracle){}), predicted, actual,
                            validation = list("permuteFold", 2, 2))
result1 <- calcCVperformance(result1, "macro F1")

predicted <- list(data.frame(sample = sample(LETTERS[1:10], 20, replace = TRUE),
                             class = factor(rep(c("Healthy", "Cancer"), each = 10))),
                  data.frame(sample = sample(LETTERS[1:10], 20, replace = TRUE),
                             class = factor(rep(c("Healthy", "Cancer"), each = 10))),
                  data.frame(sample = sample(LETTERS[1:10], 20, replace = TRUE),
                             class = factor(rep(c("Healthy", "Cancer"), each = 10))),
                  data.frame(sample = sample(LETTERS[1:10], 20, replace = TRUE),
                             class = factor(rep(c("Healthy", "Cancer"), each = 10))))
result2 <- ClassifyResult("Example", "Differential Variability", "Bartlett Test",
                          LETTERS[1:10], LETTERS[10:1], 100, list(1:100, c(1:5, 11:105)),
                            list(c(1:3), c(4:6), c(1, 6, 7, 9), c(5:8), c(1, 5, 10)),
                            list(function(oracle){}), predicted, actual,
                            validation = list("permuteFold", 2, 2))
result2 <- calcCVperformance(result2, "macro F1")

performancePlot(list(result1, result2), performanceName = "Macro F1 Score",
                title = "Comparison", boxLineColouring = "None", columnVariable = "None")
```

---

plotFeatureClasses	*Plot Density, Scatterplot, Parallel Plot or Bar Chart for Features By Class*

Description

Allows the visualisation of measurements in the data set. If `targets` is of type [Pairs](#), then a parallel plot is automatically drawn. If it's a single categorical variable, then a bar chart is automatically drawn.

Usage

```
   ## S4 method for signature 'matrix'
plotFeatureClasses(measurements, classes, targets, ...)
   ## S4 method for signature 'DataFrame'
plotFeatureClasses(measurements, classes, targets, groupBy = NULL,
                 groupingName = NULL, whichNumericFeaturePlots = c("both", "density", "stripchart"),
                    measurementLimits = NULL, lineWidth = 1, dotBinWidth = 1,
                     xAxisLabel = NULL, yAxisLabels = c("Density", "Classes"),
                    showXtickLabels = TRUE, showYtickLabels = TRUE,
                    xLabelPositions = "auto", yLabelPositions = "auto",
                    fontSizes = c(24, 16, 12, 12, 12),
              colours = c("#3F48CC", "#880015"), showDatasetName = TRUE, plot = TRUE)
   ## S4 method for signature 'MultiAssayExperiment'
plotFeatureClasses(measurements, targets, groupBy = NULL, groupingName = NULL,
                    showDatasetName = TRUE, ...)
```

Arguments

measurements	A [matrix](), [DataFrame]() or a [MultiAssayExperiment]() object containing the data. For a matrix, the rows are for features and the columns are for samples. A column with name "class" must be present in the DataFrame stored in the colData slot.
classes	Either a vector of class labels of class [factor]() or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
targets	If measurements is a matrix or DataFrame, then a vector of numeric or character indicies or the feature identifiers corresponding to the feature(s) to be plotted. If measurements is a MultiAssayExperiment, then a DataFrame of 2 columns must be specified. The first column contains the names of the tables and the second contains the names of the variables, thus each row unambiguously specifies a variable to be plotted.
groupBy	If measurements is a DataFrame, then a character vector of length 1, which contains the name of a categorical feature, may be specified. If measurements is a MultiAssayExperiment, then a character vector of length 2, which contains the name of a data table as the first element and the name of a categorical feature as the second element, may be specified. Additionally, the value "clinical" may be used to refer to the column annotation stored in the colData slot of the of the MultiAssayExperiment object. A density plot will have additional lines of different line types for each category. A strip chart plot will have a separate strip chart created for each category and the charts will be drawn in a single column on the graphics device. A parallel plot and bar chart plot will similarly be laid out.
groupingName	A label for the grouping variable to be used in plots.
...	Unused variables by the three top-level methods passed to the internal method which generates the plot(s).

whichNumericFeaturePlots

If the feature is a single feature and has numeric measurements, this option specifies which types of plot(s) to draw. The default value is "both", which draws a density plot and also a stip chart below the density plot. Other options are "density" for drawing only a density plot and "stripchart" for drawing only a strip chart.

measurementLimits

The minimum and maximum expression values to plot. Default: NULL. By default, the limits are automatically computed from the data values.

lineWidth   Numeric value that alters the line thickness for density plots. Default: 1.

dotBinWidth   Numeric value that alters the diameter of dots in the strip chart. Default: 1.

xAxisLabel   The axis label for the plot's horizontal axis. Default: NULL.

yAxisLabels   A character vector of length 1 or 2. If the feature's measurements are numeric an whichNumericFeaturePlots has the value "both", the first value is the y-axis label for the density plot and the second value is the y-axis label for the strip chart. Otherwise, if the feature's measurements are numeric and only one plot is drawn, then a character vector of length 1 specifies the y-axis label for that particular plot. Ignored if the feature's measurements are categorical.

showXtickLabels

Logical. Default: TRUE. If set to FALSE, the x-axis labels are hidden.

showYtickLabels

Logical. Default: TRUE. If set to 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. The length of this vector must be as long as the distinct number of classes in the data set.

showDatasetName

Logical. Default: TRUE. If TRUE and the data is in a MultiAssayExperiment object, the the name of the table in which the feature is stored in is added to the plot title.

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

Value

Plots are created on the current graphics device and a list of plot objects is invisibly returned. The classes of the plot object are determined based on the type of data plotted and the number of plots per feature generated. If the plotted variable is discrete or if the variable is numeric and one plot

type was specified, the list element is an object of class ggplot. Otherwise, if the variable is numeric and both the density and stripchart plot types were made, the list element is an object of class TableGrob.

Settling lineWidth and dotBinWidth to the same value doesn't result in the density plot and the strip chart having elements of the same size. Some manual experimentation is required to get similarly sized plot elements.

Author(s)

Dario Strbenac

Examples

```
# First 25 samples and first 5 genes are mixtures of two normals. Last 25 samples are
# one normal.
genesMatrix <- sapply(1:15, function(geneColumn) c(rnorm(5, 5, 1)))
genesMatrix <- cbind(genesMatrix, sapply(1:10, function(geneColumn) c(rnorm(5, 15, 1))))
genesMatrix <- cbind(genesMatrix, sapply(1:25, function(geneColumn) c(rnorm(5, 9, 2))))
genesMatrix <- rbind(genesMatrix, sapply(1:50, function(geneColumn) rnorm(95, 9, 3)))
rownames(genesMatrix) <- paste("Gene", 1:100)
colnames(genesMatrix) <- paste("Sample", 1:50)
classes <- factor(rep(c("Poor", "Good"), each = 25), levels = c("Good", "Poor"))
plotFeatureClasses(genesMatrix, classes, targets = "Gene 4",
                   xAxisLabel = bquote(log[2]*'(expression)'), dotBinWidth = 0.5)


infectionResults <- c(rep(c("No", "Yes"), c(20, 5)), rep(c("No", "Yes"), c(5, 20)))
genders <- factor(rep(c("Male", "Female"), each = 10, length.out = 50))
clinicalData <- DataFrame(Gender = genders, Sugar = runif(50, 4, 10),
                          Infection = factor(infectionResults, levels = c("No", "Yes")),
                          row.names = colnames(genesMatrix))
plotFeatureClasses(clinicalData, classes, targets = "Infection")
plotFeatureClasses(clinicalData, classes, targets = "Infection", groupBy = "Gender")

dataContainer <- MultiAssayExperiment(list(RNA = genesMatrix),
                                      colData = cbind(clinicalData, class = classes))
targetFeatures <- DataFrame(table = "RNA", feature = "Gene 50")
plotFeatureClasses(dataContainer, targets = targetFeatures,
                   groupBy = c("clinical", "Gender"),
                   xAxisLabel = bquote(log[2]*'(expression)'))
```

PredictParams	*Parameters for Classifier Prediction*

Description

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

The function specified must return either a factor vector of class predictions, or a numeric vector of scores for the second class, according to the levels of the class vector of the input data set, or a data frame which has two columns named class and score.

Constructor

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

PredictParams(predictor, intermediate = character(0),...) Creates a PredictParams object which stores the function which will do the class prediction, if required, and parameters that the function will use. If the training function also makes predictions, this must be set to NULL.

predictor Either NULL or a function to make predictions with. If it is a function, then the first argument must accept the classifier made in the training step. The second argument must accept a DataFrame of new data.

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

... Other arguments that predictor may use.

Author(s)

Dario Strbenac

Examples

```
predictParams <- PredictParams(predictor = DLDApredictInterface)
# For prediction by trained object created by DLDA training function.
PredictParams(predictor = NULL)
# For when the training function also does prediction and directly returns the
# predictions.
```

---

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

```
  ## S4 method for signature 'matrix'
previousSelection(measurements, ...)
  ## S4 method for signature 'DataFrame'
previousSelection(measurements, classes, datasetName,
                  classifyResult, minimumOverlapPercent = 80,
                   selectionName = "Previous Selection", .iteration, verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
previousSelection(measurements, ...)
```

Arguments

measurements	Either a [matrix](#), [DataFrame](#) or [MultiAssayExperiment](#) containing the training data. For a matrix, the rows are features, and the columns are samples.
classes	Do not specify this variable. It is ignored and only used to create consistency of formal parameters with other feature selection methods.
...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method.
datasetName	A name for the data set 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 data set, then the selection stops with an error.
selectionName	A name to identify this selection method by. Stored in the result.
.iteration	Do not specify this variable. It is set by [runTests](#) if this function is being repeatedly called by runTests.
verbose	Default: 3. 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

Examples

```
#if(require(sparsediscrim))
#{
  # Genes 76 to 100 have differential expression.
  genesMatrix <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))
  genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample)
                                  c(rnorm(75, 9, 2), rnorm(25, 14, 2))))
  colnames(genesMatrix) <- paste("Sample", 1:50)
  rownames(genesMatrix) <- paste("Gene", 1:100)
  classes <- factor(rep(c("Poor", "Good"), each = 25))
  resubstitute <- ResubstituteParams(nFeatures = seq(10, 100, 10),
                      performanceType = "error", better = "lower")
  result <- runTests(genesMatrix, classes, datasetName = "Example",
                     classificationName = "Differential Expression",
                     permutations = 2, fold = 2,
                     params = list(SelectParams(), TrainParams(), PredictParams()))
  features(result)

  # Genes 50 to 74 have differential expression in new data set.
  newDataset <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))
  newDataset <- cbind(newDataset, rbind(sapply(1:25, function(sample) rnorm(49, 9, 2)),
```

```
                                    sapply(1:25, function(sample) rnorm(25, 14, 2)),
                                    sapply(1:25, function(sample) rnorm(26, 9, 2))))

    rownames(newDataset) <- rownames(genesMatrix)
    colnames(newDataset) <- colnames(genesMatrix)

    newerResult <- runTests(newDataset, classes, datasetName = "Latest Data Set",
                            classificationName = "Differential Expression",
                            permutations = 2, fold = 2,
                     params = list(SelectParams(previousSelection,
                                      intermediate = ".iteration",
                                      classifyResult = result),
                     TrainParams(), PredictParams()))

    # However, only genes 76 to 100 are chosen, because the feature selections are
    # carried over from the first cross-validated classification.
    features(newerResult)
  #}
```

---

previousTrained   *Automated Usage of Previously Created Classifiers*

Description

Uses the trained classifier of the same cross-validation iteration of a previous classification for the current classification task.

Usage

```
   ## S4 method for signature 'ClassifyResult'
previousTrained(classifyResult, .iteration, verbose = 3)
```

Arguments

classifyResult   A [ClassifyResult](#) object which stores the models fitted previously.

.iteration   Do not specify this variable. It is set by [runTests](#) if this function is being repeatedly called by runTests.

verbose   Default: 3. 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

A trained classifier from a previously completed classification task.

Author(s)

Dario Strbenac

Examples

```
#if(require(sparsediscrim))
#{
  # Genes 76 to 100 have differential expression.
  genesMatrix <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))
  genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample)
                                c(rnorm(75, 9, 2), rnorm(25, 14, 2))))
  colnames(genesMatrix) <- paste("Sample", 1:50)
  rownames(genesMatrix) <- paste("Gene", 1:100)
  classes <- factor(rep(c("Poor", "Good"), each = 25))
  resubstitute <- ResubstituteParams(nFeatures = seq(10, 100, 10),
                      performanceType = "error", better = "lower")
  result <- runTests(genesMatrix, classes, datasetName = "Example",
                     classificationName = "Differential Expression",
                     permutations = 2, fold = 2,
                     params = list(SelectParams(), TrainParams(), PredictParams()))
  models(result)

  # Genes 50 to 74 have differential expression in new data set.
  newDataset <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))
  newDataset <- cbind(newDataset, rbind(sapply(1:25, function(sample) rnorm(49, 9, 2)),
                                      sapply(1:25, function(sample) rnorm(25, 14, 2)),
                                      sapply(1:25, function(sample) rnorm(26, 9, 2))))

  rownames(newDataset) <- rownames(genesMatrix)
  colnames(newDataset) <- colnames(genesMatrix)

  newerResult <- runTests(newDataset, classes, datasetName = "Latest Data Set",
                          classificationName = "Differential Expression",
                          permutations = 2, fold = 2,
                          params = list(SelectParams(previousSelection,
                                                     intermediate = ".iteration",
                                                     classifyResult = result),
                                        TrainParams(previousTrained,
                                                    intermediate = ".iteration",
                                                    classifyResult = result),
                                        PredictParams()))

  models(newerResult)
#}
```

---

randomForest   *Trained randomForest Object*

Description

Enables S4 method dispatching on it.

Author(s)

Dario Strbenac

---

randomForestInterface   *An Interface for randomForest Package's randomForest Function*

Description

A random forest classifier builds multiple decision trees and uses the predictions of the trees to determine a single prediction for each test sample.

Usage

```
  ## S4 method for signature 'matrix'
randomForestTrainInterface(measurements, classes, ...)
  ## S4 method for signature 'DataFrame'
randomForestTrainInterface(measurements, classes, ..., verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
randomForestTrainInterface(measurements, targets = names(measurements), ...)
  ## S4 method for signature 'randomForest,matrix'
randomForestPredictInterface(forest, test, ...)
  ## S4 method for signature 'randomForest,DataFrame'
randomForestPredictInterface(forest, test, ...,
                             returnType = c("class", "score", "both"), verbose = 3)
  ## S4 method for signature 'randomForest,MultiAssayExperiment'
randomForestPredictInterface(forest, test, targets = names(test), ...)
```

Arguments

measurements	Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training data. For a `matrix`, the rows are features, and the columns are samples.
classes	Either a vector of class labels of class [factor]() of the same length as the number of samples in `measurements` or if the measurements are of class DataFrame a character vector of length 1 containing the column name in `measurement` is also permitted. Not used if `measurements` is a MultiAssayExperiment object.
forest	A trained random forest classifier, as created by randomForestTrainInterface, which has the same form as the output of [randomForest]().
test	An object of the same class as `measurements` with no samples in common with `measurements` and the same number of features as it.
targets	If `measurements` is a MultiAssayExperiment, the names of the data tables to be used. `"clinical"` is also a valid value and specifies that integer variables from the clinical data table will be used.
...	Variables not used by the `matrix` nor the `MultiAssayExperiment` method which are passed into and used by the `DataFrame` method (e.g. `verbose`) or options which are accepted by the [randomForest]() or [predict.randomForest]() functions.

returnType	Default: ″class″. Either ″class″, ″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	Default: 3. 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 measurements is an object of class MultiAssayExperiment, the factor of sample classes must be stored in the DataFrame accessible by the colData function with column name ″class″.

Value

For randomForestTrainInterface, the trained random forest. For randomForestPredictInterface, either a factor vector of predicted classes, a matrix of scores for each class, or a table of both the class labels and class scores, depending on the setting of returnType.

Author(s)

Dario Strbenac

Examples

```
if(require(randomForest))
{
  # Genes 76 to 100 have differential expression.
  genesMatrix <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))
  genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample)
                                    c(rnorm(75, 9, 2), rnorm(25, 14, 2))))
  classes <- factor(rep(c(″Poor″, ″Good″), each = 25))
  colnames(genesMatrix) <- paste(″Sample″, 1:ncol(genesMatrix), sep = '')
  rownames(genesMatrix) <- paste(″Gene″, 1:nrow(genesMatrix), sep = '')
  trainingSamples <- c(1:20, 26:45)
  testingSamples <- c(21:25, 46:50)

  trained <- randomForestTrainInterface(genesMatrix[, trainingSamples],
                                        classes[trainingSamples])
  predicted <- randomForestPredictInterface(trained, genesMatrix[, testingSamples])
}
```

---

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", "selectionName"),
          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",
                         "selectionName"),
        columnVariable = c("classificationName", "datasetName", "validation",
                              "selectionName", "None"),
        yMax = 100, fontSizes = c(24, 16, 12, 12, 12, 16),
       title = if(comparison[1] == "within") "Feature Ranking Stability" else
                  "Feature Ranking Commonality",
        xLabelPositions = seq(10, 100, 10),
       yLabel = if(is.null(referenceLevel)) "Average Common Features (%)" else
          paste("Average Common Features with", referenceLevel, "(%)"),
          margin = grid::unit(c(1, 1, 1, 1), "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.
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, selection algorithm and data set. 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 data set, 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 data set. If comparison is *"datasetName"*, then the feature rankings are compared across different data sets, for each level of *"classificationName"*, *"selectionName"* and *"validation"*. The result will inform how stable the feature rankings are between different data sets, for every classification algorithm and every data set. 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.

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),
                        class = rep(c("Healthy", "Cancer"), each = 50))
actual <- factor(rep(c("Healthy", "Cancer"), each = 5))
features <- sapply(1:100, function(index) paste(sample(LETTERS, 3), collapse = ''))
rankList <- list(list(features[1:100], features[c(5:1, 6:100)]),
             list(features[c(1:9, 11, 10, 12:100)], features[c(1:50, 60:51, 61:100)]))
result1 <- ClassifyResult("Example", "Differential Expression",
                          "Example Selection", LETTERS[1:10], features,
                          100, 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(function(oracle){}),
                          list(predicted), actual, list("permuteFold", 2, 2))

predicted[, "class"] <- sample(predicted[, "class"])
rankList <- list(list(features[1:100], features[c(sample(20), 21:100)]),
             list(features[c(1:9, 11, 10, 12:100)], features[c(1:50, 60:51, 61:100)]))
result2 <- ClassifyResult("Example", "Differential Variability",
                          "Example Selection",
                          LETTERS[1:10], features, 100, 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(function(oracle){}),
                        list(predicted), actual, validation = list("permuteFold", 2, 2))

rankingPlot(list(result1, result2), pointTypeVariable = "classificationName")

oneRanking <- features[c(10, 8, 1, 2, 3, 4, 7, 9, 5, 6)]
otherRanking <- features[c(8, 2, 3, 4, 1, 10, 6, 9, 7, 5)]
oneResult <- SelectResult("Example", "One Method", 10, list(oneRanking), list(oneRanking[1:5]))
otherResult <- SelectResult("Example", "Another Method", 10, 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)
```

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 10, 20, 30, 40, 50, 60, 70, 80, 90, 100. The performance measure used is the balanced error rate.

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 rate for.

    performanceType One of the eleven types of performance metrics which can be calculated by calcCVperformance.

    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 the classifier.

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

Author(s)

Dario Strbenac

Examples

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

ROCplot   *Plot Receiver Operating Curve Graphs for Classification Results*

Description

Creates one ROC plot or multiple ROC plots for a list of ClassifyR objects. One plot is created if the data set has two classes and multiple plots are created if the data set has three or more classes.

Usage

```
   ## S4 method for signature 'list'
ROCplot(results, nBins = sapply(results, totalPredictions),
       comparisonVariable = c("classificationName", "datasetName", "selectionName",
        "validation", "None"), lineColours = NULL,
       lineWidth = 1, fontSizes = c(24, 16, 12, 12, 12), labelPositions = seq(0.0, 1.0, 0.2),
        plotTitle = "ROC", legendTitle = NULL, xLabel = "False Positive Rate",
        yLabel = "True Positive Rate", plot = TRUE, showAUC = TRUE)
```

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.
comparisonVariable	
	If the data set has two classes, then the slot name with factor levels to be used for colouring the lines. Possible values are "datasetName", "classificationName", and "validation". If "None", then all lines drawn will be black. Otherwise, it specifies the variable used for plot facetting.
lineColours	A vector of colours for different levels of the line colouring parameter. If NULL, a default colour palette is used.
lineWidth	A single number controlling the thickness of lines drawn.
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

The scores stored in the results should be higher if the sample is more likely to be from the class which the score is associated with. The score for each class must be in a column which has a column name equal to the class name.

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

Examples

```
predicted <- list(data.frame(sample = LETTERS[c(1, 8, 15, 3, 11, 20, 19, 18)],
                             Healthy = c(0.89, 0.68, 0.53, 0.76, 0.13, 0.20, 0.60, 0.25),
                             Cancer = c(0.11, 0.32, 0.47, 0.24, 0.87, 0.80, 0.40, 0.75)),
                   data.frame(sample = LETTERS[c(11, 18, 15, 4, 6, 10, 11, 12)],
                             Healthy = c(0.45, 0.56, 0.33, 0.56, 0.33, 0.20, 0.60, 0.40),
                             Cancer = c(0.55, 0.44, 0.67, 0.44, 0.67, 0.80, 0.40, 0.60)))
actual <- factor(c(rep("Healthy", 10), rep("Cancer", 10)), levels = c("Healthy", "Cancer"))
result1 <- ClassifyResult("Example", "Differential Expression", "t-test",
                          LETTERS[1:20], LETTERS[10:1], 100,
                    list(1:100, c(1:9, 11:101)), list(sample(10, 10), sample(10, 10)),
                          list(function(oracle){}), predicted, actual,
                          list("permuteFold", 2, 2))

predicted[[1]][c(2, 6), "Healthy"] <- c(0.40, 0.60)
predicted[[1]][c(2, 6), "Cancer"] <- c(0.60, 0.40)
result2 <- ClassifyResult("Example", "Differential Variability", "Bartlett Test",
                          LETTERS[1:20], LETTERS[10:1], 100, list(1:100, c(1:5, 11:105)),
                          list(sample(10, 10), sample(10, 10)), list(function(oracle){}),
                              predicted, actual, validation = list("permuteFold", 2, 2))
ROCplot(list(result1, result2), comparisonVariable = "classificationName",
        plotTitle = "Cancer ROC")
```

---

runTest   *Perform a Single Classification*

Description

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

Usage

```
  ## S4 method for signature 'matrix'
runTest(measurements, classes, ...)
  ## S4 method for signature 'DataFrame'
runTest(measurements, classes, featureSets = NULL, metaFeatures = NULL,
          minimumOverlapPercent = 80, datasetName, classificationName,
        training, testing, params = list(SelectParams(), TrainParams(), PredictParams()),
        verbose = 1, .iteration = NULL)
  ## S4 method for signature 'MultiAssayExperiment'
runTest(measurements, targets = names(measurements), ...)
  ## S4 method for signature 'MultiAssayExperiment'
runTestEasyHard(measurements, easyDatasetID = "clinical", hardDatasetID = names(measurements)[1],
            featureSets = NULL, metaFeatures = NULL, minimumOverlapPercent = 80,
          datasetName = NULL, classificationName = "Easy-Hard Classifier", training, testing, ..., v
```

Arguments

measurements   Either a [matrix](), [DataFrame]() or [MultiAssayExperiment]() containing the training
                data. For a matrix, the rows are features, and the columns are samples. The
                sample identifiers must be present as column names of the matrix or the row
                names of the DataFrame.

classes   Either a vector of class labels of class [factor]() of the same length as the number
                of samples in measurements or if the measurements are of class DataFrame a
                character vector of length 1 containing the column name in measurement is also
                permitted. Not used if measurements is a MultiAssayExperiment object.

featureSets   An object of type [FeatureSetCollection]() which defines sets of features or sets
                of edges.

metaFeatures   Either NULL or a DataFrame which has meta-features of the numeric data of
                interest.

minimumOverlapPercent

                If featureSets stores sets of features, the minimum overlap of feature IDs with
                measurements for a feature set to be retained in the analysis. If featureSets
                stores sets of network edges, the minimum percentage of edges with both vertex
                IDs found in measurements that a set has to have to be retained in the analysis.

targets   If measurements is a MultiAssayExperiment, the names of the data tables to
                be used. "clinical" is also a valid value and specifies that numeric variables
                from the clinical data table will be used.

...   For runTest, variables not used by the matrix nor the MultiAssayExperiment
                method which are passed into and used by the DataFrame method. For runTestEasyHard,
                easyClassifierParams and hardClassifierParams to be passed to [easyHardClassifierTrain]().

datasetName   A name associated with the data set 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.
easyDatasetID	The name of a data set in measurements or "clinical" to indicate the patient information in the column data be used.
hardDatasetID	The name of a data set in measurements different to the value of easyDatasetID to be used for classifying the samples not classified by the easy classifier.
verbose	Default: 1. A number between 0 and 3 for the amount of progress messages to give. A higher number will produce more messages as more lower-level functions print 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 enables a number of different cross-validation schemes to be applied and uses this function to perform each iteration. datasetName and classificationName need to be provided.

Value

If called directly by the user rather than being used internally by runTests, a SelectResult object.

Author(s)

Dario Strbenac

Examples

```
#if(require(sparsediscrim))
#{
  data(asthma)
  resubstituteParams <- ResubstituteParams(nFeatures = seq(5, 25, 5),
                                           performanceType = "balanced error",
                                           better = "lower")
  runTest(measurements, classes,
          datasetName = "Asthma", classificationName = "Different Means",
          params = list(SelectParams(limmaSelection, "Moderated t Statistic",
                                     resubstituteParams = resubstituteParams),
                        TrainParams(DLDAtrainInterface),
                        PredictParams(DLDApredictInterface)
                        ),
          training = (1:ncol(measurements)) %% 2 == 0,
          testing = (1:ncol(measurements)) %% 2 != 0)
#}

genesMatrix <- matrix(c(rnorm(90, 9, 1),
                        9.5, 9.4, 5.2, 5.3, 5.4, 9.4, 9.6, 9.9, 9.1, 9.8),
    ncol = 10, byrow = TRUE)
```

```
colnames(genesMatrix) <- paste("Sample", 1:10)
rownames(genesMatrix) <- paste("Gene", 1:10)
genders <- factor(c("Male", "Male", "Female", "Female", "Female",
                    "Female", "Female", "Female", "Female", "Female"))

# Scenario: Male gender can predict the hard-to-classify Sample 1 and Sample 2.
clinical <- DataFrame(age = c(31, 34, 32, 39, 33, 38, 34, 37, 35, 36),
                      gender = genders,
                      class = factor(rep(c("Poor", "Good"), each = 5)),
        row.names = colnames(genesMatrix))
dataset <- MultiAssayExperiment(ExperimentList(RNA = genesMatrix), clinical)

selParams <- SelectParams(featureSelection = differentMeansSelection, selectionName = "Difference in Means",
                  resubstituteParams = ResubstituteParams(1:10, "balanced error", "lower"))
easyHardCV <- runTestEasyHard(dataset, datasetName = "Test Data", classificationName = "Easy-Hard", training = 1:
                        easyClassifierParams = list(minCardinality = 2, minPurity = 0.9),
                    hardClassifierParams = list(selParams, TrainParams(), PredictParams())
                            )
```

---

runTests   *Reproducibly Run Various Kinds of Cross-Validation*

Description

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

Usage

```
  ## S4 method for signature 'matrix'
runTests(measurements, classes, ...)
  ## S4 method for signature 'DataFrame'
runTests(measurements, classes, featureSets = NULL, metaFeatures = NULL,
        minimumOverlapPercent = 80, datasetName, classificationName,
        validation = c("permute", "leaveOut", "fold"),
        permutePartition = c("fold", "split"),
        permutations = 100, percent = 25, folds = 5, leave = 2,
        seed, parallelParams = bpparam(),
       params = list(SelectParams(), TrainParams(), PredictParams()), verbose = 1)
  ## S4 method for signature 'MultiAssayExperiment'
runTests(measurements, targets = names(measurements), ...)
  ## S4 method for signature 'MultiAssayExperiment'
runTestsEasyHard(measurements, easyDatasetID = "clinical", hardDatasetID = names(measurements)[1],
            featureSets = NULL, metaFeatures = NULL, minimumOverlapPercent = 80,
              datasetName = NULL, classificationName = "Easy-Hard Classifier",
                  validation = c("permute", "leaveOut", "fold"),
                  permutePartition = c("fold", "split"),
                  permutations = 100, percent = 25, folds = 5, leave = 2,
                  seed, parallelParams = bpparam(), ..., verbose = 1)
```

Arguments

measurements	Either a [matrix](#), [DataFrame](#) or [MultiAssayExperiment](#) containing the training data. For a matrix, the rows are features, and the columns are samples. The sample identifiers must be present as column names of the matrix or the row names of the DataFrame.
classes	Either a vector of class labels of class [factor](#) of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
featureSets	An object of type [FeatureSetCollection](#) which defines sets of features or sets of edges.
metaFeatures	Either NULL or a DataFrame which has meta-features of the numeric data of interest.
minimumOverlapPercent	
	If featureSets stores sets of features, the minimum overlap of feature IDs with measurements for a feature set to be retained in the analysis. If featureSets stores sets of network edges, the minimum percentage of edges with both vertex IDs found in measurements that a set has to have to be retained in the analysis.
targets	If measurements is a MultiAssayExperiment, the names of the data tables to be used. "clinical" is also a valid value and specifies that numeric variables from the clinical data table will be used.
...	For runTests, variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method. For runTestsEasyHard, easyClassifierParams and hardClassifierParams to be passed to [easyHardClassifierTrain](#)
datasetName	A name associated with the data set used.
classificationName	
	A name associated with the classification.
validation	Default: "permute". "permute" for repeated permuting. "leaveOut" for leaving all possible combinations of k samples as test samples. "fold" for folding of the data set (no resampling).
permutePartition	
	Default: "fold". Either "fold" or "split". Only applicable if validation is "permute". 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.
permutations	Default: 100. Relevant when permuting is used. The number of times to do reordering of the samples before splitting or folding them.
percent	Default: 25. Used when permutation with the split method is chosen. The percentage of samples to be in the test set.
folds	Default: 5. Relevant when repeated permutations are done and permutePartition is set to "fold" or when validation is set to "fold". The number of folds to break the data set into. Each fold is used once as the test set.
leave	Default: 2. Relevant when leave-k-out cross-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.

easyDatasetID   The name of a data set in measurements or "clinical" to indicate the patient
                information in the column data be used.

hardDatasetID   The name of a data set in measurements different to the value of easyDatasetID
                to be used for classifying the samples not classified by the easy classifier.

verbose   Default: 1. A number between 0 and 3 for the amount of progress messages to
                give. A higher number will produce more messages as more lower-level func-
                tions print 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

Examples

```
#if(require(sparsediscrim))
#{
  data(asthma)

  resubstituteParams <- ResubstituteParams(nFeatures = seq(5, 25, 5),
                                    performanceType = "balanced error",
                                    better = "lower")
  runTests(measurements, classes, datasetName = "Asthma",
          classificationName = "Different Means", permutations = 5,
          params = list(SelectParams(differentMeansSelection, "t Statistic",
                                    resubstituteParams = resubstituteParams),
                      TrainParams(DLDAtrainInterface),
                      PredictParams(DLDApredictInterface)
                      )
          )
#}

genesMatrix <- matrix(c(rnorm(90, 9, 1),
                      9.5, 9.4, 5.2, 5.3, 5.4, 9.4, 9.6, 9.9, 9.1, 9.8),
    ncol = 10, byrow = TRUE)

colnames(genesMatrix) <- paste("Sample", 1:10)
rownames(genesMatrix) <- paste("Gene", 1:10)
genders <- factor(c("Male", "Male", "Female", "Female", "Female",
                  "Female", "Female", "Female", "Female", "Female"))
```

```
        # Scenario: Male gender can predict the hard-to-classify Sample 1 and Sample 2.
        clinical <- DataFrame(age = c(31, 34, 32, 39, 33, 38, 34, 37, 35, 36),
                              gender = genders,
                              class = factor(rep(c("Poor", "Good"), each = 5)),
               row.names = colnames(genesMatrix))
        dataset <- MultiAssayExperiment(ExperimentList(RNA = genesMatrix), clinical)
        selParams <- SelectParams(featureSelection = differentMeansSelection, selectionName = "Difference in Means",
                        resubstituteParams = ResubstituteParams(1:10, "balanced error", "lower"))
        easyHardCV <- runTestsEasyHard(dataset, datasetName = "Test Data", classificationName = "Easy-Hard",
                              easyClassifierParams = list(minCardinality = 2, minPurity = 0.9),
                           hardClassifierParams = list(selParams, TrainParams(), PredictParams()),
                                     validation = "leaveOut", leave = 1)
```

---

samplesMetricMap   *Plot a Grid of Sample Error Rates or Accuracies*

Description

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

Usage

```
   ## S4 method for signature 'list'
samplesMetricMap(results,
              comparison = c("classificationName", "datasetName", "selectionName",
                              "validation"),
           metric = c("error", "accuracy"), featureValues = NULL, featureName = NULL,
              metricColours = list(c("#3F48CC", "#6F75D8", "#9FA3E5", "#CFD1F2", "#FFFFFF"),
                            c("#880015", "#A53F4F", "#C37F8A", "#E1BFC4", "#FFFFFF")),
              classColours = c("#3F48CC", "#880015"), groupColours = c("darkgreen", "yellow2"),
                    fontSizes = c(24, 16, 12, 12, 12),
                 mapHeight = 4, title = "Error Comparison", showLegends = TRUE,
                 xAxisLabel = "Sample Name", showXtickLabels = TRUE,
                 yAxisLabel = "Analysis", showYtickLabels = TRUE,
                 legendSize = grid::unit(1, "lines"), plot = TRUE)
   ## S4 method for signature 'matrix'
samplesMetricMap(results, classes,
                    metric = c("error", "accuracy"),
                    featureValues = NULL, featureName = NULL,
              metricColours = list(c("#3F48CC", "#6F75D8", "#9FA3E5", "#CFD1F2", "#FFFFFF"),
                            c("#880015", "#A53F4F", "#C37F8A", "#E1BFC4", "#FFFFFF")),
              classColours = c("#3F48CC", "#880015"), groupColours = c("darkgreen", "yellow2"),
                    fontSizes = c(24, 16, 12, 12, 12),
                 mapHeight = 4, title = "Error Comparison", showLegends = TRUE,
                 xAxisLabel = "Sample Name", showXtickLabels = TRUE,
                 yAxisLabel = "Analysis", showYtickLabels = TRUE,
                 legendSize = grid::unit(1, "lines"), plot = TRUE)
```

Arguments

results	A list of [ClassifyResult](#) objects. Could also be a matrix, for backwards compatibility.
classes	If results is a matrix, this is a factor vector of the same length as the number of columns that results has.
comparison	The aspect of the experimental design to compare.
metric	The sample-wise metric to plot.
featureValues	If not NULL, can be a named factor or named numeric vector specifying some variable of interest to plot underneath the class bar.
featureName	A label describing the information in featureValues. It must be specified if featureValues is.
metricColours	A vector of colours for metric levels.
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.
groupColours	A vector of colours for group levels. Only useful if groups is not NULL.
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 metricColours determines how many bins the metric values 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

Examples

```
predicted <- data.frame(sample = LETTERS[sample(10, 100, replace = TRUE)],
                        class = rep(c("Healthy", "Cancer"), each = 50))
actual <- factor(rep(c("Healthy", "Cancer"), each = 5), levels = c("Healthy", "Cancer"))
features <- sapply(1:100, function(index) paste(sample(LETTERS, 3), collapse = ''))
result1 <- ClassifyResult("Example", "Differential Expression", "t-test",
                    LETTERS[1:10], features, 100, list(1:100), list(sample(10, 10)),
                            list(function(oracle){}), list(predicted), actual,
                            list("permuteFold", 100, 5))
predicted[, "class"] <- sample(predicted[, "class"])
result2 <- ClassifyResult("Example", "Differential Variability", "Bartlett Test",
                    LETTERS[1:10], features, 100, list(1:100), list(sample(10, 10)),
                            list(function(oracle){}), list(predicted), actual,
                            validation = list("leave", 2))
result1 <- calcCVperformance(result1, "sample error")
result2 <- calcCVperformance(result2, "sample error")
groups <- factor(rep(c("Male", "Female"), length.out = 10))
names(groups) <- LETTERS[1:10]
cholesterol <- c(4.0, 5.5, 3.9, 4.9, 5.7, 7.1, 7.9, 8.0, 8.5, 7.2)
names(cholesterol) <- LETTERS[1:10]

wholePlot <- samplesMetricMap(list(Gene = result1, Protein = result2))
wholePlot <- samplesMetricMap(list(Gene = result1, Protein = result2),
                                featureValues = groups, featureName = "Gender")
wholePlot <- samplesMetricMap(list(Gene = result1, Protein = result2),
                                featureValues = cholesterol, featureName = "Cholesterol")
```

---

selectionPlot	*Plot Pair-wise Overlap or Selection Size Distribution of Selected 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 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", "selectionName"),
                referenceLevel = NULL,
          xVariable = c("classificationName", "datasetName", "validation", "selectionName"),
              boxFillColouring = c("classificationName", "size", "datasetName",
                                   "validation", "selectionName", "None"),
              boxFillColours = NULL,
              boxFillBinBoundaries = NULL, setSizeBinBoundaries = NULL,
              boxLineColouring = c("validation", "classificationName",
                                   "datasetName", "selectionName", "None"),
              boxLineColours = NULL,
              rowVariable = c("None", "validation", "datasetName",
                              "classificationName", "selectionName"),
              columnVariable = c("datasetName", "classificationName",
                                 "validation", "selectionName", "None"),
            yMax = 100, fontSizes = c(24, 16, 12, 16),
          title = if(comparison[1] == "within") "Feature Selection Stability"
                  else if(comparison == "size") "Feature Selection Size" else
                    "Feature Selection Commonality",
            xLabel = "Analysis",
        yLabel = if(is.null(referenceLevel) && comparison != "size") "Common Features (%)"
                    else if(comparison == "size") "Set Size" else
                    paste("Common Features with", referenceLevel, "(%)"),
            margin = grid::unit(c(1, 1, 1, 1), "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.

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, selection algorithm and data set. 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 data set, 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 data set. If comparison is "datasetName", then the feature selections are compared across different data sets, for each level of "classificationName", "selectionName", and "validation". The result will inform how stable the feature selections are between different data sets, for every classification algorithm and every data set. 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](cut).

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),
                        class = rep(c("Healthy", "Cancer"), each = 50))
actual <- factor(rep(c("Healthy", "Cancer"), each = 5))
features <- sapply(1:100, function(index) paste(sample(LETTERS, 3), collapse = ''))
rankList <- list(list(features[1:100], features[c(5:1, 6:100)]),
              list(features[c(1:9, 11, 10, 12:100)], features[c(1:50, 60:51, 61:100)]))
result1 <- ClassifyResult("Example", "Differential Expression",
                          "Example Selection", LETTERS[1:10], features,
                          100, 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(function(oracle){}),
                          list(predicted), actual, list("permuteFold", 2, 2))

predicted[, "class"] <- sample(predicted[, "class"])
rankList <- list(list(features[1:100], features[c(sample(20), 21:100)]),
              list(features[c(1:9, 11, 10, 12:100)], features[c(1:50, 60:51, 61:100)]))
result2 <- ClassifyResult("Example", "Differential Variability",
                          "Example Selection",
                          LETTERS[1:10], features, 100, 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(function(oracle){}),
                       list(predicted), actual, validation = list("permuteFold", 2, 2))

selectionPlot(list(result1, result2), xVariable = "classificationName",
              xLabel = "Analysis", columnVariable = "None", rowVariable = "None",
              boxFillColouring = "classificationName")

selectionPlot(list(result1, result2), comparison = "size",
              xVariable = "classificationName", xLabel = "Analysis",
              columnVariable = "None", rowVariable = "None",
              boxFillColouring = "size", boxFillBinBoundaries = seq(0, 100, 10),
              setSizeBinBoundaries = seq(0, 25, 5), boxLineColouring = "None")

oneRanking <- features[c(10, 8, 1, 2, 3, 4, 7, 9, 5, 6)]
otherRanking <- features[c(8, 2, 3, 4, 1, 10, 6, 9, 7, 5)]
oneResult <- SelectResult("Example", "One Method", 10, list(oneRanking), list(oneRanking[1:5]))
otherResult <- SelectResult("Example", "Another Method", 10, list(otherRanking), list(otherRanking[1:2]))

selectionPlot(list(oneResult, otherResult), comparison = "selectionName",
              xVariable = "selectionName", xLabel = "Selection Method",
              columnVariable = "None", rowVariable = "None",
```

```
                    boxFillColouring = "selectionName", boxLineColouring = "None")
```

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 either an ordinary t-test or ANOVA (depending on the number of classes) and tries the top 10 to top 100 features in increments of 10, and picks the number of features with the best resubstitution balanced 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), subsetToSelections = TRUE, ...)

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 [DataFrame](#) 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.

subsetToSelections Whether to subset the data table(s), after feature 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

Examples

```
#if(require(sparsediscrim))
#{
  SelectParams(differentMeansSelection, "t-test",
               trainParams = TrainParams(), predictParams = PredictParams(),
               resubstituteParams = ResubstituteParams())
```

```
    # For pamr shrinkage selection.
    SelectParams(NSCselectionInterface, datasetName = "Cancer",
                 intermediate = "trained", subsetToSelections = FALSE)
#}
```

SelectResult   *Container for Storing Feature Selection Results*

Description

Contains a list of ranked names of features, from most discriminative to least discriminative, and a list of features selected for use in classification. The names will be in a data frame if the input data set is a [MultiAssayExperiment](), with the first column containing the name of the data table the feature is from and the second column containing the name of the feature. Each vector or data frame element in the list corresponds to a particular iteration of classifier training. Nested lists will be present if the permutation and folding cross-validation scheme was used. This class is not intended to be created by the user, but could be used in another software package.

Constructor

  SelectResult(datasetName,selectionName,totalFeatures,rankedFeatures,chosenFeatures)

datasetName A name associated with the data set used.

selectionName A name associated with the classification.

totalFeatures The total number of features in the data set.

rankedFeatures Identifiers of all features or meta-features if meta-features were used by the classifier, from most to least discriminative.

chosenFeatures Identifiers of features or meta-features if meta-features were used by the classifier 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("Asthma", "Moderated t-test", 50, list(1:50), list(1:10))
```

---

subtractFromLocation   *Subtract Numeric Feature Measurements from a Location*

Description

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

Usage

```
   ## S4 method for signature 'matrix'
subtractFromLocation(measurements, training, location = c("mean", "median"),
                       absolute = TRUE, verbose = 3)
   ## S4 method for signature 'DataFrame'
subtractFromLocation(measurements, training, location = c("mean", "median"),
                       absolute = TRUE, verbose = 3)
   ## S4 method for signature 'MultiAssayExperiment'
subtractFromLocation(measurements, training, targets = names(measurements),
                       location = c("mean", "median"), absolute = TRUE, verbose = 3)
```

Arguments

measurements	A `matrix`, `DataFrame` or a `MultiAssayExperiment` object containing the data. For a matrix, the rows are for features and the columns are for samples.
training	A vector specifying which samples are in the training set.
location	Character. Either "mean" or "median".
absolute	Logical. Default: TRUE. If TRUE, then absolute values of the differences are returned. Otherwise, they are signed.
targets	If `measurements` is a `MultiAssayExperiment`, the names of the data tables to be used. `"clinical"` is also a valid value and specifies that numeric variables from the clinical data table will be used.
verbose	Default: 3. A progress message is shown if this value is 3.

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

The same class of variable as the input variable `measurements` is, with the numeric features subtracted from the calculated location.

Author(s)

Dario Strbenac

Examples

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

---

svm   *Trained svm Object*

Description

Enables S4 method dispatching on it.

Author(s)

Dario Strbenac

SVMinterface   *An Interface for e1071 Package's Support Vector Machine Classifier.*

Description

SVMtrainInterface generates a trained SVM classifier and SVMpredictInterface uses it to make
predictions on a test data set.

Usage

```
  ## S4 method for signature 'matrix'
SVMtrainInterface(measurements, classes, ...)
  ## S4 method for signature 'DataFrame'
SVMtrainInterface(measurements, classes, ..., verbose = 3)
  ## S4 method for signature 'MultiAssayExperiment'
SVMtrainInterface(measurements, targets = names(measurements), ...)
  ## S4 method for signature 'svm,matrix'
SVMpredictInterface(model, test, ...)
  ## S4 method for signature 'svm,DataFrame'
SVMpredictInterface(model, test, classes = NULL, returnType = c("class", "score", "both"), verbose = 3)
  ## S4 method for signature 'svm,MultiAssayExperiment'
SVMpredictInterface(model, test, targets = names(test), ...)
```

Arguments

measurements	Either a [matrix](#), [DataFrame](#) or [MultiAssayExperiment](#) containing the training data. For a matrix, the rows are features, and the columns are samples. If of type [DataFrame](#), the data set is subset to only those features of type integer.
classes	Either a vector of class labels of class [factor](#) of the same length as the number of samples in measurements or if the measurements are of class DataFrame a character vector of length 1 containing the column name in measurement is also permitted. Not used if measurements is a MultiAssayExperiment object.
returnType	Default: "class". Either "class", "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.
test	An object of the same class as measurements with no samples in common with measurements and the same number of features as it. Also, if a DataFrame, the class column must be absent.
targets	If measurements is a MultiAssayExperiment, the names of the data tables to be used. "clinical" is also a valid value and specifies that numeric variables from the clinical data table will be used.
model	A fitted model as returned by SVMtrainInterface.
...	Variables not used by the matrix nor the MultiAssayExperiment method which are passed into and used by the DataFrame method (e.g. verbose) or options that are used by the [svm](#) function.
verbose	Default: 3. 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 measurements is an object of class MultiAssayExperiment, the factor of sample classes must be stored in the DataFrame accessible by the colData function with column name "class".

Value

For SVMtrainInterface, a trained SVM classifier of type svm. For SVMpredictInterface, either a factor vector of predicted classes, a vector of secores for the second class, or a table of both the class labels and second class scores, depending on the setting of returnType.

Author(s)

Dario Strbenac

Examples

```
if(require(e1071))
{
  # Genes 76 to 100 have differential expression.
  genesMatrix <- sapply(1:25, function(sample) c(rnorm(100, 9, 2)))
  genesMatrix <- cbind(genesMatrix, sapply(1:25, function(sample)
```

```
                                         c(rnorm(75, 9, 2), rnorm(25, 14, 2))))
    classes <- factor(rep(c("Poor", "Good"), each = 25))
    colnames(genesMatrix) <- paste("Sample", 1:ncol(genesMatrix))
    rownames(genesMatrix) <- paste("Gene", 1:nrow(genesMatrix))
    trainingSamples <- c(1:20, 26:45)
    testingSamples <- c(21:25, 46:50)

    classifier <- SVMtrainInterface(genesMatrix[, trainingSamples],
                                    classes[trainingSamples], kernel = "linear")
    SVMpredictInterface(classifier, genesMatrix[, testingSamples])
}
```

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, intermediate = character(0), getFeatures = NULL, ...)

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 [DataFrame](#) object. The second argument must be a vector of classes. If the function also makes predictions and the value of the predictor setting of PredictParams is therefore NULL, the third argument must be a DataFrame of test data. The function must also accept a parameter named verbose. The function's return value can be either a trained classifier if the function only does training or a vector or data frame of class predictions if it also does prediction with the test set samples.

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

getFeatures A function may be specified that extracts the selected features from the trained model. This is relevant if using a classifier that does feature selection within training (e.g. random forest). The function must return a list of two vectors. The first vector contains the ranked features (or empty if the training algorithm doesn't produce rankings) and the second vector contains the selected features.

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

Author(s)

Dario Strbenac

Examples

```
#if(require(sparsediscrim))
  trainParams <- TrainParams(DLDAtrainInterface)
```

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 TransformParams 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 a DataFrame 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

Examples

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

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