

Package ‘pRoloc’

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Type Package

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Description This package implements pattern recognition
techniques on quantitative mass spectrometry data to infer protein sub-cellular localisation.

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LinkingTo Rcpp, RcppArmadillo

License GPL-2

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R topics documented:

addLegend	2
addMarkers	3
chi2-methods	4
empPvalues	5
exprsToRatios-methods	6
GenRegRes-class	6
getMarkers	8
getPredictions	9

getStockcol	9
knnClassification	11
knnOptimisation	12
ksvmClassification	13
ksvmOptimisation	14
lopims	15
makeNaData	17
markerSet	18
minClassScore	19
minMarkers	20
MLearn-methods	21
nbClassification	21
nbOptimisation	22
nnetClassification	23
nnetOptimisation	24
perTurboClassification	25
perTurboOptimisation	27
phenoDisco	28
plot2D	29
plotDist	31
plsdaClassification	32
plsdaOptimisation	33
rfClassification	34
rfOptimisation	35
svmClassification	36
svmOptimisation	37
testMarkers	38
undocumented	39

Index**40**

<i>addLegend</i>	<i>Adds a legend</i>
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Description

Adds a legend to a [plot2D](#) figure.

Usage

```
addLegend(object, fcol = "markers", where = "other", col,
          ...)
```

Arguments

object	An instance of class MSnSet
fcol	Feature meta-data label (fData column name) defining the groups to be differentiated using different colours. Default is <code>markers</code> .
where	One of "other", "bottomleft", "bottomright", "topleft" or "topright" defining the location of the legend. "other" opens a new graphics device, while the other locations are passed to <code>legend</code> .
col	A character defining point colours.
...	Additional parameters passed to <code>legend</code> .

Value

Invisibly returns NULL

Author(s)

Laurent Gatto

addMarkers*Adds markers to the data*

Description

The function adds a 'markers' feature variable. These markers are read from a comma separated values (csv) spreadsheet file. This markers file is expected to have 2 columns (others are ignored) where the first is the name of the marker features and the second the group label. It is essential to assure that `featureNames(object)` and marker names (first column) match, i.e. the same feature identifiers and case fold are used.

Usage

```
addMarkers(object, markerfile, verbose = TRUE)
```

Arguments

object	An instance of class MSnSet.
markerfile	A character with the name the markers' csv file.
verbose	A logical indicating if number of markers and marker table should be printed to the console.

Value

A new instance of class MSnSet with an additional `markers` feature variable.

Author(s)

Laurent Gatto

Description

In the original protein correlation profiling (PCP), Andersen et al. use the peptide normalised profiles along gradient fractions and compared them with the reference profiles (or set of profiles) by computing Chi^2 values, $\frac{\sum(x_i - x_p)^2}{x_p}$, where x_i is the normalised value of the peptide in fraction i and x_p is the value of the marker (from Wiese et al., 2007). The protein Chi^2 is then computed as the median of the peptide Chi^2 values. Peptides and proteins with similar profiles to the markers will have small Chi^2 values.

The chi2 methods implement this idea and compute such Chi^2 values for sets of proteins.

Methods

```
signature(x = "matrix", y = "matrix", method = "character", fun = "NULL", na.rm = "logical")
Compute nrow(x) times nrow(y)  $\text{Chi}^2$  values, for each x, y feature pair. Method is one of
"Andersen2003" or "Wiese2007"; the former (default) computed the  $\text{Chi}^2$  as sum(y-x)^2/length(x),
while the latter uses sum((y-x)^2/x). na.rm defines if missing values (NA and NaN) should be
removed prior to summation. fun defines how to summarise the  $\text{Chi}^2$  values; default, NULL,
does not combine the  $\text{Chi}^2$  values.

signature(x = "matrix", y = "numeric", method = "character", na.rm = "logical")
Computes nrow(x)  $\text{Chi}^2$  values, for all the  $(x_i, y)$  pairs. See above for the other arguments.

signature(x = "numeric", y = "matrix", method = "character", na.rm = "logical")
Computes nrow(y)  $\text{Chi}^2$  values, for all the  $(x, y_i)$  pairs. See above for the other arguments.

signature(x = "numeric", y = "numeric", method = "character", na.rm = "logical")
Computes the  $\text{Chi}^2$  value for the  $(x, y)$  pairs. See above for the other arguments.
```

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

References

- Andersen, J. S., Wilkinson, C. J., Mayor, T., Mortensen, P. et al., Proteomic characterization of the human centrosome by protein correlation profiling. *Nature* 2003, 426, 570 - 574.
- Wiese, S., Gronemeyer, T., Ofman, R., Kunze, M. et al., Proteomics characterization of mouse kidney peroxisomes by tandem mass spectrometry and protein correlation profiling. *Mol. Cell. Proteomics* 2007, 6, 2045 - 2057.

See Also

[empPvalues](#)

Examples

```
mrk <- rnorm(6)
prot <- matrix(rnorm(60), ncol = 6)
chi2(mrk, prot, method = "Andersen2003")
chi2(mrk, prot, method = "Wiese2007")

pepmark <- matrix(rnorm(18), ncol = 6)
pepprot <- matrix(rnorm(60), ncol = 6)
chi2(pepmark, pepprot)
chi2(pepmark, pepprot, fun = sum)
```

empPvalues

Estimate empirical p-values for Chi^2 protein correlations.

Description

Andersen et al. (2003) used a fixed Chi^2 threshold of 0.05 to identify organelle-specific candidates. This function computes empirical p-values by permutation the markers relative intensities and computed null Chi^2 values.

Usage

```
empPvalues(marker, corMatrix, n = 100, ...)
```

Arguments

marker	A numerics with markers relative intensities.
corMatrix	A matrix of nrow(corMatrix) protein relative intensities to be compares against the marker.
n	The number of iterations.
...	Additional parameters to be passed to chi2.

Value

A numeric of length nrow(corMatrix).

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

References

Andersen, J. S., Wilkinson, C. J., Mayor, T., Mortensen, P. et al., Proteomic characterization of the human centrosome by protein correlation profiling. Nature 2003, 426, 570 - 574.

See Also

[chi2](#) for Chi^2 calculation.

Examples

```
set.seed(1)
mrk <- rnorm(6, 5, 1)
prot <- rbind(matrix(rnorm(120, 5, 1), ncol = 6),
               mrk + rnorm(6))
mrk <- mrk/sum(mrk)
prot <- prot/rowSums(prot)
empPvalues(mrk, prot)
```

exprsToRatios-methods *Calculate all ratio pairs*

Description

Calculations all possible ratios for the assayData columns in an "[MSnSet](#)".

Methods

`signature(object = "MSnSet", log = "logical")` If `log` is FALSE (default) the ratios for all the assayData columns are computed; otherwise, log ratios (differences) are calculated.

Examples

```
library("pRolocdata")
data(dunkley2006)
x <- dunkley2006[, 1:3]
head(exprs(x))
r <- exprsToRatios(x)
head(exprs(r))
pData(r)
```

GenRegRes-class *Class "GenRegRes"*

Description

Regularisation framework container.

Objects from the Class

Object of this class are created with the respective regularisation function: `knnRegularisation`, `svmRegularisation`, `plsdaRegularisation`, ...

Slots

algorithm: Object of class "character" storing the machine learning algorithm name.

hyperparameters: Object of class "list" with the respective algorithm hyper-parameters tested.

design: Object of class "numeric" describing the cross-validation design, the test data size and the number of replications.

log: Object of class "list" with warnings thrown during the hyper-parameters regularisation.

seed: Object of class "integer" with the random number generation seed.

results: Object of class "matrix" of dimensions times (see **design**) by number of hyperparameters + 1 storing the macro F1 values for the respective best hyper-parameters for each replication.

f1Matrices: Object of class "list" with respective times cross-validation F1 matrices.

cmMatrices: Object of class "list" with respective times contingency matrices.

testPartitions: Object of class "list" with respective times test partitions.

datasize: Object of class "list" with details about the respective inner and outer training and testing data sizes.

Methods

getF1Scores signature(object = "GenRegRes"): ...

f1Count signature(object = "GenRegRes", t = "numeric"): Constructs a table of all possible parameter combination and count how many have an F1 scores greater or equal than t. When t is missing (default), the best F1 score is used. This method is useful in conjunction with **plot**.

getRegularisedParams signature(object = "GenRegRes"): ...

getRegularizedParams signature(object = "GenRegRes"): ...

getSeed signature(object = "GenRegRes"): ...

getWarnings signature(object = "GenRegRes"): ...

levelPlot signature(object = "GenRegRes"): ...

plot signature(x = "GenRegRes", y = "missing"): ...

show signature(object = "GenRegRes"): ...

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

Examples

```
showClass("GenRegRes")
```

getMarkers*Returns the organelle markers in an 'MSnSet'***Description**

Convenience accessor to the organelle markers in an 'MSnSet'. This function returns the organelle markers of an MSnSet instance. As a side effect, it prints out a marker table.

Usage

```
getMarkers(object, fcol = "markers", names = TRUE,
          verbose = TRUE)
```

Arguments

<code>object</code>	An instance of class " MSnSet ".
<code>fcol</code>	The name of the markers column in the <code>featureData</code> slot. Default is <code>markers</code> .
<code>names</code>	A logical indicating if the markers vector should be named.
<code>verbose</code>	If <code>TRUE</code> , a marker table is printed and the markers are returned invisibly. If <code>FALSE</code> , the markers are returned.

Value

A character of length `ncol(object)`.

Author(s)

Laurent Gatto

See Also

[testMarkers](#) and [minMarkers](#)

Examples

```
library("pRolocdata")
data(dunkley2006)
mymarkers <- getMarkers(dunkley2006)
```

getPredictions	<i>Returns the predictions in an 'MSnSet'</i>
----------------	---

Description

Convenience accessor to the predicted feature localisation in an 'MSnSet'. This function returns the predictions of an MSnSet instance. As a side effect, it prints out a prediction table.

Usage

```
getPredictions(object, fcol, scol, t = 0, verbose = TRUE)
```

Arguments

object	An instance of class "MSnSet".
fcol	The name of the prediction column in the featureData slot.
scol	The name of the prediction score column in the featureData slot. If missing, created by pasting '.scores' after fcol. If NULL, ignored.
t	The score threshold. Predictions with score < t are set to 'unknown'. Default is 0.
verbose	If TRUE, a prediction table is printed and the predictions are returned invisibly. If FALSE, the predictions are returned.

Value

A character of length ncol(object).

Author(s)

Laurent Gatto

getStockcol	<i>Manage default colours and point characters</i>
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Description

These functions allow to get/set the default colours and point character that are used when plotting organelle clusters and unknown features. These values are parametrised at the session level.

Usage

```
getStockcol()
setStockcol(cols)
getStockpch()
setStockpch(pchs)
getUnknowncol()
setUnknowncol(col)
getUnknownpch()
setUnknownpch(pch)
```

Arguments

<code>cols</code>	A vector of colour characters or NULL, which sets the colours to the default values.
<code>pchs</code>	A vector of numeric or NULL, which sets the point characters to the default values.
<code>col</code>	A colour character or NULL, which sets the colour to #E7E7E7 (grey91), the default colour for unknown features.
<code>pch</code>	A numeric vector of length 1 or NULL, which sets the point character to 21, the default.

Value

- A character vector.
Invisibly returns `cols`.
- A numeric vector.
Invisibly returns `pchs`.
- A character vector or length 1.
Invisibly returns `col`.
- A numeric vector of length 1.
Invisibly returns `pch`.

Author(s)

Laurent Gatto

Examples

```
## defaults for clusters
getStockcol()
getStockpch()
## unknown features
getUnknownpch()
getUnknowncol()
## an example
library(pRoloedata)
data(dunkley2006)
par(mfrow = c(2, 1))
plot2D(dunkley2006, fcol = "markers", main = Default colours)
setUnknowncol("black")
plot2D(dunkley2006, fcol = "markers", main = setUnknowncol("black"))
getUnknowncol()
setUnknowncol(NULL)
getUnknowncol()
```

knnClassification *knn classification*

Description

Classification using for the k-nearest neighbours algorithm.

Usage

```
knnClassification(object, assessRes,
                  scores = c("prediction", "all", "none"), k,
                  fcol = "markers", ...)
```

Arguments

object	An instance of class " MSnSet ".
assessRes	An instance of class " GenRegRes ", as generated by knnOptimisation .
scores	One of "prediction", "all" or "none" to report the score for the predicted class only, for all cluster or none.
k	If <code>assessRes</code> is missing, a <code>k</code> must be provided.
fcol	The feature meta-data containing marker definitions. Default is <code>markers</code> .
...	Additional parameters passed to knn from package <code>class</code> .

Value

An instance of class "[MSnSet](#)" with `knn` and `knn.scores` feature variables storing the classification results and scores respectively.

Author(s)

Laurent Gatto

Examples

```
library(pRolocdata)
data(dunkley2006)
## reducing parameter search space and iterations
params <- knnOptimisation(dunkley2006, k = c(3, 10), times = 3)
params
plot(params)
f1Count(params)
levelPlot(params)
getParams(params)
res <- knnClassification(dunkley2006, params)
getPredictions(res, fcol = "knn")
getPredictions(res, fcol = "knn", t = 0.75)
plot2D(res, fcol = "knn")
```

knnOptimisation *knn parameter optimisation*

Description

Classification parameter optimisation for the k-nearest neighbours algorithm.

Usage

```
knnOptimisation(object, fcol = "markers",
  k = seq(3, 15, 2), times = 100, test.size = 0.2,
  xval = 5, fun = mean, seed, verbose = TRUE, ...)
```

Arguments

<code>object</code>	An instance of class " MSnSet ".
<code>fcol</code>	The feature meta-data containing marker definitions. Default is <code>markers</code> .
<code>k</code>	The hyper-parameter. Default values are <code>seq(3, 15, 2)</code> .
<code>times</code>	The number of times internal cross-validation is performed. Default is 100.
<code>test.size</code>	The size of test data. Default is 0.2 (20 percent).
<code>xval</code>	The n-cross validation. Default is 5.
<code>fun</code>	The function used to summarise the <code>xval</code> macro F1 matrices.
<code>seed</code>	The optional random number generator seed.
<code>verbose</code>	A logical defining whether a progress bar is displayed.
<code>...</code>	Additional parameters passed to <code>knn</code> from package <code>class</code> .

Value

An instance of class "[GenRegRes](#)".

Author(s)

Laurent Gatto

See Also

[knnClassification](#) and example therein.

`ksvmClassification` *ksvm classification*

Description

Classification using the support vector machine algorithm.

Usage

```
ksvmClassification(object, assessRes,
                    scores = c("prediction", "all", "none"), cost,
                    fcol = "markers", ...)
```

Arguments

<code>object</code>	An instance of class " MSnSet ".
<code>assessRes</code>	An instance of class " GenRegRes ", as generated by ksvmOptimisation .
<code>scores</code>	One of "prediction", "all" or "none" to report the score for the predicted class only, for all cluster or none.
<code>cost</code>	If <code>assessRes</code> is missing, a cost must be provided.
<code>fcol</code>	The feature meta-data containing marker definitions. Default is <code>markers</code> .
<code>...</code>	Additional parameters passed to <code>ksvm</code> from package <code>kernlab</code> .

Value

An instance of class "[MSnSet](#)" with `ksvm` and `ksvm.scores` feature variables storing the classification results and scores respectively.

Author(s)

Laurent Gatto

Examples

```
library(pRoloLocdata)
data(dunkley2006)
## reducing parameter search space and iterations
params <- ksvmOptimisation(dunkley2006, cost = 2^seq(-1,4,5), times = 3)
params
plot(params)
f1Count(params)
levelPlot(params)
getParams(params)
res <- ksvmClassification(dunkley2006, params)
getPredictions(res, fcol = "ksvm")
getPredictions(res, fcol = "ksvm", t = 0.75)
plot2D(res, fcol = "ksvm")
```

ksvmOptimisation *ksvm parameter optimisation*

Description

Classification parameter optimisation for the support vector machine algorithm.

Usage

```
ksvmOptimisation(object, fcol = "markers",
                  cost = 2^(-4:4), times = 100, test.size = 0.2,
                  xval = 5, fun = mean, seed, verbose = TRUE, ...)
```

Arguments

<code>object</code>	An instance of class " MSnSet ".
<code>fcol</code>	The feature meta-data containing marker definitions. Default is <code>markers</code> .
<code>cost</code>	The hyper-parameter. Default values are $2^{-4:4}$.
<code>times</code>	The number of times internal cross-validation is performed. Default is 100.
<code>test.size</code>	The size of test data. Default is 0.2 (20 percent).
<code>xval</code>	The n-cross validation. Default is 5.
<code>fun</code>	The function used to summarise the <code>xval</code> macro F1 matrices.
<code>seed</code>	The optional random number generator seed.
<code>verbose</code>	A logical defining whether a progress bar is displayed.
<code>...</code>	Additional parameters passed to <code>ksvm</code> from package <code>kernlab</code> .

Value

An instance of class "[GenRegRes](#)".

Author(s)

Laurent Gatto

See Also

[ksvmClassification](#) and example therein.

lopims

A complete LOPIMS pipeline

Description

The function processes MSe data using the [synergise](#) function of the [synapter](#) package and combines resulting [Synapter](#) instances into one "MSnSet" and organelle marker data is added as a feature-level annotation variable.

Usage

```
lopims(hdmsedir = "HDMSE", msedir = "MSE",
       pep3ddir = "pep3D", fastafile, markerfile,
       mfdr = 0.025, ...)
```

Arguments

hdmsedir	A character identifying the directory containing the HDMSe final peptide files. Default is HDMSe.
msedir	A character identifying the directory containing the MSe final peptide files. Default is MSe.
pep3ddir	A character identifying the directory containing the MSe pep 3D files. Default is pep3D.
fastafile	A character identifying the protein fasta database. Default is to use the fasta file in the current directory. If several such files exist, the function reports an error.
markerfile	A character identifying the marker file (see details for format). Default is to use a csv file starting with marker in the current directory. If several such files exist, the function reports an error.
mfdr	The master FDR value. Default is 0.025.
...	Additional paramters passed to synergise .

Details

The LOPIMS pipeline is composed of 5 steps:

1. The HDMSe final peptide files are used to compute false discovery rates upon all possible combinations of HDMSe final peptides files and the best combination smaller or equal to `mfdr` is chosen. See [estimateMasterFdr](#) for details. The corresponding master run is then created as described in [makeMaster](#).
2. Each MSE/pep3D pair is processed using the HDMSe master file using [synergise](#).
3. The respective peptide-level synergise output objects are converted and combined into a single "[MSnSet](#)" instance.
4. Protein-level quantitation is inferred as follows. For each protein, a reference sample/fraction is chosen based on the number of missing values (NA). If several samples have a same minimal number of NAs, ties are broken using the sum of counts. The peptide that do not display any missing values for each (frac_i, frac_ref) pair are summed and the ratio is reported (see `pRloc:::refNormMeanOfNonNAPepSum` for details).
5. The markers defined in the `markerfile` are collated as feature meta-data in the `markers` variable. See [addMarkers](#) for details.

Intermediate synergise reports as well as resulting objects are stored in a `LOPIMS_pipeline` directory. For details, please refer to the synapter vignette and reference papers.

Value

An instance of class "[MSnSet](#)" with protein level quantitation and respective organelle markers.

Author(s)

Laurent Gatto

References

Improving qualitative and quantitative performance for MSE-based label free proteomics. N.J. Bond, P.V. Shliaha, K.S. Lilley and L. Gatto, Journal of Proteome Research, 2013 (in press).

The Effects of Travelling Wave Ion Mobility Separation on Data Independent Acquisition in Proteomics Studies, P.V. Shliaha, N.J. Bond, L. Gatto and K.S. Lilley, Journal of Proteome Research, 2013 (in press).

MSnbbase-an R/Bioconductor package for isobaric tagged mass spectrometry data visualization, processing and quantitation. L. Gatto and KS. Lilley. Bioinformatics. 2012 Jan 15;28(2):288-9. doi: 10.1093/bioinformatics/btr645. Epub 2011 Nov 22. PubMed PMID: 22113085.

makeNaData*Create a data with missing values*

Description

These functions take an instance of class "[MSnSet](#)" and sets randomly selected values to NA.

Usage

```
makeNaData(object, nNA, pNA, exclude)  
makeNaData2(object, nRows, nNAs, exclude)  
whichNA(x)
```

Arguments

object	An instance of class MSnSet.
nNA	The absolute number of missing values to be assigned.
pNA	The proportion of missing values to be assignmed.
exclude	A vector to be used to subset object, defining rows that should not be used to set NAs.
nRows	The number of rows for each set.
nNAs	The number of missing values for each set.
x	A matrix or an instance of class MSnSet.

Details

`makeNaData` randomly selects a number `nNA` (or a proportion `pNA`) of cells in the expression matrix to be set to NA.

`makeNaData2` will select `length(nRows)` sets of rows from `object`, each with `nRows[i]` rows respectively. The first set will be assigned `nNAs[1]` missing values, the second `nNAs[2]`, ... As opposed to `makeNaData`, this permits to control the number of NAs per rows.

The `whichNA` can be used to extract the indices of the missing values, as illustrated in the example.

Value

An instance of class MSnSet, as `object`, but with the appropriate number/proportion of missing values. The returned object has an additional feature meta-data columns, `nNA`

Author(s)

Laurent Gatto

Examples

```

## Example 1
library(pRoloocdata)
data(dunkley2006)
sum(is.na(dunkley2006))
dunkleyNA <- makeNaData(dunkley2006, nNA = 150)
processingData(dunkleyNA)
sum(is.na(dunkleyNA))
table(fData(dunkleyNA)$nNA)
naIdx <- whichNA(dunkleyNA)
head(naIdx)
## Example 2
dunkleyNA <- makeNaData(dunkley2006, nNA = 150, exclude = 1:10)
processingData(dunkleyNA)
table(fData(dunkleyNA)$nNA[1:10])
table(fData(dunkleyNA)$nNA)
## Example 3
nr <- rep(10, 5)
na <- 1:5
x <- makeNaData2(dunkley2006[1:100, 1:5],
                  nRows = nr,
                  nNAs = na)
processingData(x)
(res <- table(fData(x)$nNA))
stopifnot(as.numeric(names(res)[-1]) == na)
stopifnot(res[-1] == nr)
## Example 2
nr2 <- c(5, 12, 11, 8)
na2 <- c(3, 8, 1, 4)
x2 <- makeNaData2(dunkley2006[1:100, 1:10],
                   nRows = nr2,
                   nNAs = na2)
processingData(x2)
(res2 <- table(fData(x2)$nNA))
stopifnot(as.numeric(names(res2)[-1]) == sort(na2))
stopifnot(res2[-1] == nr2[order(na2)])
## Example 5
nr3 <- c(5, 12, 11, 8)
na3 <- c(3, 8, 1, 3)
x3 <- makeNaData2(dunkley2006[1:100, 1:10],
                   nRows = nr3,
                   nNAs = na3)
processingData(x3)
(res3 <- table(fData(x3)$nNA))

```

markerSet

Extract marker subset

Description

This function extracts the marker proteins into a new MSnSet.

Usage

```
markerSet(object, fcol = "markers")
```

Arguments

object	An instance of class <code>MSnSet</code>
fcol	The name of the feature data column, that will be used to separate the markers from the proteins of unknown localisation (with <code>fData(object)[, fcol] == "unknown"</code>). Default is to use "markers".

Value

An new `MSnSet` with marker proteins only.

Author(s)

Laurent Gatto

Examples

```
library("pRolocdata")
data(dunkley2006)
mrk <- markerSet(dunkley2006)
dim(dunkley2006)
dim(mrk)
table(fData(dunkley2006)$markers)
table(fData(mrk)$markers)
```

`minClassScore`

Updates classes based on prediction scores

Description

This functions updates the classification results in an "`MSnSet`" based on a prediction score threshold `t`. All features with a score < `t` are set to 'unknown'. Note that the original levels are preserved while 'unknown' is added.

Usage

```
minClassScore(object, fcol, scol, t = 0)
```

Arguments

object	An instance of class " <code>MSnSet</code> ".
fcol	The name of the markers column in the <code>featureData</code> slot.
scol	The name of the prediction score column in the <code>featureData</code> slot. If missing, created by pasting '.scores' after <code>fcol</code> .
t	The score threshold. Predictions with score < <code>t</code> are set to 'unknown'. Default is 0.

Value

The original object with a modified fData(object)[, fcol] feature variable.

Author(s)

Laurent Gatto

Examples

```
library(pRolocdata)
data(dunkley2006)
## random scores
fData(dunkley2006)$assigned.scores <- runif(nrow(dunkley2006))
getPredictions(dunkley2006, fcol = "assigned")
getPredictions(dunkley2006, fcol = "assigned", t = 0.5)
x <- minClassScore(dunkley2006, fcol = "assigned", t = 0.5)
getPredictions(x, fcol = "assigned")
all.equal(getPredictions(dunkley2006, fcol = "assigned", t = 0.5),
          getPredictions(x, fcol = "assigned"))
```

minMarkers

Creates a reduced marker variable

Description

This function updates an MSnSet instances and sets markers class to unknown if there are less than n instances.

Usage

```
minMarkers(object, n = 10, fcol = "markers")
```

Arguments

- | | |
|--------|---|
| object | An instance of class " MSnSet ". |
| n | Minumum of marker instances per class. |
| fcol | The name of the markers column in the featureData slot. Default is <code>markers</code> . |

Value

An instance of class "[MSnSet](#)" with a new feature variables, named after the original fcol variable and the n value.

Author(s)

Laurent Gatto

Examples

```
library(pRolocdata)
data(dunkley2006)
d2 <- minMarkers(dunkley2006, 20)
getMarkers(dunkley2006)
getMarkers(d2, fcol = "markers20")
```

Description

This method implements MLInterfaces' MLean method for instances of the class "[MSnSet](#)".

Methods

```
signature(formula = "formula", data = "MSnSet", .method = "learnerSchema", trainInd = "numeric")
  The learning problem is stated with the formula and applies the .method schema on the
  MSnSet data input using the trainInd numeric indices as train data.

signature(formula = "formula", data = "MSnSet", .method = "learnerSchema", trainInd = "xvalSpec")
  In this case, an instance of xvalSpec is used for cross-validation.

signature(formula = "formula", data = "MSnSet", .method = "clusteringSchema", trainInd = "missing")
  Hierarchical (hclustI), k-means (kmeansI) and partitioning around medoids (pamI) cluster-
  ing algorithms using MLInterface's MLearn interface.
```

See Also

The MLInterfaces package documentation, in particular [MLearn](#).

Description

Classification using the naive Bayes algorithm.

Usage

```
nbClassification(object, assessRes,
  scores = c("prediction", "all", "none"), laplace,
  fcol = "markers", ...)
```

Arguments

<code>object</code>	An instance of class " MSnSet ".
<code>assessRes</code>	An instance of class " GenRegRes ", as generated by nbOptimisation .
<code>scores</code>	One of "prediction", "all" or "none" to report the score for the predicted class only, for all cluster or none.
<code>laplace</code>	If <code>assessRes</code> is missing, a <code>laplace</code> must be provided.
<code>fcol</code>	The feature meta-data containing marker definitions. Default is <code>markers</code> .
...	Additional parameters passed to naiveBayes from package e1071.

Value

An instance of class "[MSnSet](#)" with `nb` and `nb.scores` feature variables storing the classification results and scores respectively.

Author(s)

Laurent Gatto

Examples

```
library(pRolocdata)
data(dunkley2006)
## reducing parameter search space and iterations
params <- nbOptimisation(dunkley2006, laplace = c(0, 5), times = 3)
params
plot(params)
f1Count(params)
levelPlot(params)
getParams(params)
res <- nbClassification(dunkley2006, params)
getPredictions(res, fcol = "naiveBayes")
getPredictions(res, fcol = "naiveBayes", t = 1)
plot2D(res, fcol = "naiveBayes")
```

[nbOptimisation](#)

nb parameter optimisation

Description

Classification algorithm parameter for the naive Bayes algorithm.

Usage

```
nbOptimisation(object, fcol = "markers",
               laplace = seq(0, 5, 0.5), times = 100, test.size = 0.2,
               xval = 5, fun = mean, seed, verbose = TRUE, ...)
```

Arguments

object	An instance of class " MSnSet ".
fcol	The feature meta-data containing marker definitions. Default is <code>markers</code> .
laplace	The hyper-parameter. Default values are <code>seq(0, 5, 0.5)</code> .
times	The number of times internal cross-validation is performed. Default is 100.
test.size	The size of test data. Default is 0.2 (20 percent).
xval	The n-cross validation. Default is 5.
fun	The function used to summarise the xval macro F1 matrices.
seed	The optional random number generator seed.
verbose	A logical defining whether a progress bar is displayed.
...	Additional parameters passed to naiveBayes from package e1071.

Value

An instance of class "[GenRegRes](#)".

Author(s)

Laurent Gatto

See Also

[nbClassification](#) and example therein.

nnetClassification *nnet classification*

Description

Classification using the artificial neural network algorithm.

Usage

```
nnetClassification(object, assessRes,
  scores = c("prediction", "all", "none"), decay, size,
  fcol = "markers", ...)
```

Arguments

object	An instance of class " MSnSet ".
assessRes	An instance of class " GenRegRes ", as generated by nnetOptimisation .
scores	One of "prediction", "all" or "none" to report the score for the predicted class only, for all cluster or none.
decay	If assessRes is missing, a decay must be provided.
size	If assessRes is missing, a size must be provided.
fcol	The feature meta-data containing marker definitions. Default is <code>markers</code> .
...	Additional parameters passed to nnet from package <code>nnet</code> .

Value

An instance of class "[MSnSet](#)" with `nnet` and `nnet.scores` feature variables storing the classification results and scores respectively.

Author(s)

Laurent Gatto

Examples

```
library(pRolocdata)
data(dunkley2006)
## reducing parameter search space and iterations
params <- nnetOptimisation(dunkley2006, decay = 10^(c(-1, -5)), size = c(5, 10), times = 3)
params
plot(params)
f1Count(params)
levelPlot(params)
getParams(params)
res <- nnetClassification(dunkley2006, params)
getPredictions(res, fcol = "nnet")
getPredictions(res, fcol = "nnet", t = 0.75)
plot2D(res, fcol = "nnet")
```

nnetOptimisation *nnet parameter optimisation*

Description

Classification parameter optimisation for artificial neural network algorithm.

Usage

```
nnetOptimisation(object, fcol = "markers",
                 decay = c(0, 10^(-1:-5)), size = seq(1, 10, 2),
                 times = 100, test.size = 0.2, xval = 5, fun = mean,
                 seed, verbose = TRUE, ...)
```

Arguments

object	An instance of class " MSnSet ".
fcol	The feature meta-data containing marker definitions. Default is <code>markers</code> .
decay	The hyper-parameter. Default values are <code>c(0, 10^{(-1:-5)})</code> .
size	The hyper-parameter. Default values are <code>seq(1, 10, 2)</code> .
times	The number of times internal cross-validation is performed. Default is 100.
test.size	The size of test data. Default is 0.2 (20 percent).
xval	The n-cross validation. Default is 5.
fun	The function used to summarise the xval macro F1 matrices.
seed	The optional random number generator seed.
verbose	A logical defining whether a progress bar is displayed.
...	Additional parameters passed to <code>nnet</code> from package <code>nnet</code> .

Value

An instance of class "[GenRegRes](#)".

Author(s)

Laurent Gatto

See Also

[nnetClassification](#) and example therein.

`perTurboClassification`

perTurbo classification

Description

Classification using the PerTurbo algorithm.

Usage

```
perTurboClassification(object, assessRes,
  scores = c("prediction", "all", "none"), pRegul, sigma,
  inv, reg, fcol = "markers")
```

Arguments

<code>object</code>	An instance of class " MSnSet ".
<code>assessRes</code>	An instance of class " GenRegRes ", as generated by svmRegularisation .
<code>scores</code>	One of "prediction", "all" or "none" to report the score for the predicted class only, for all cluster or none.
<code>pRegul</code>	If <code>assessRes</code> is missing, a <code>pRegul</code> must be provided. See perTurboOptimisation for details.
<code>sigma</code>	If <code>assessRes</code> is missing, a <code>sigma</code> must be provided. See perTurboOptimisation for details.
<code>inv</code>	The type of algorithm used to invert the matrix. Values are : "Inversion Cholesky" (chol2inv), "Moore Penrose" (ginv), "solve" (solve), "svd" (svd). Default value is "Inversion Cholesky".
<code>reg</code>	The type of regularisation of matrix. Values are "none", "trunc" or "tikhonov". Default value is "tikhonov".
<code>fcol</code>	The feature meta-data containing marker definitions. Default is <code>markers</code> .

Value

An instance of class "[MSnSet](#)" with `perTurbo` and `perTurbo.scores` feature variables storing the classification results and scores respectively.

Author(s)

Thomas Burger and Samuel Wieczorek

References

N. Courty, T. Burger, J. Laurent. "PerTurbo: a new classification algorithm based on the spectrum perturbations of the Laplace-Beltrami operator", The European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (ECML-PKDD 2011), D. Gunopulos et al. (Eds.): ECML PKDD 2011, Part I, LNAI 6911, pp. 359 - 374, Athens, Greece, September 2011.

Examples

```
library(pRocLocdata)
data(dunkley2006)
## reducing parameter search space
params <- perTurboOptimisation(dunkley2006,
                                pRegul = 2^seq(-2,2,2),
                                sigma = 10^seq(-1, 1, 1),
                                inv = "Inversion Cholesky",
                                reg = "tikhonov",
                                times = 3)
params
plot(params)
f1Count(params)
levelPlot(params)
```

```
getParams(params)
res <- perTurboClassification(dunkley2006, params)
getPredictions(res, fcol = "perTurbo")
getPredictions(res, fcol = "perTurbo", t = 0.75)
plot2D(res, fcol = "perTurbo")
```

perTurboOptimisation *PerTurbo parameter optimisation*

Description

Classification parameter optimisation for the PerTurbo algorithm

Usage

```
perTurboOptimisation(object, fcol = "markers",
                      pRegul = 10^(seq(from = -1, to = 0, by = 0.2)),
                      sigma = 10^(seq(from = -1, to = 1, by = 0.5)),
                      inv = c("Inversion Cholesky", "Moore Penrose", "solve", "svd"),
                      reg = c("tikhonov", "none", "trunc"), times = 1,
                      test.size = 0.2, xval = 5, fun = mean, seed,
                      verbose = TRUE)
```

Arguments

<code>object</code>	An instance of class " MSnSet ".
<code>fcol</code>	The feature meta-data containing marker definitions. Default is <code>markers</code> .
<code>inv</code>	The type of algorithm used to invert the matrix. Values are : "Inversion Cholesky" (chol2inv), "Moore Penrose" (ginv), "solve" (solve), "svd" (svd). Default value is "Inversion Cholesky".
<code>reg</code>	The type of regularisation of matrix. Values are "none", "trunc" or "tikhonov". Default value is "tikhonov".
<code>pRegul</code>	The hyper-parameter for the regularisation (values are in]0,1]). If <code>reg == "trunc"</code> , <code>pRegul</code> is for the percentage of eigen values in matrix. If <code>reg == "tikhonov"</code> , then ' <code>pRegul</code> ' is the parameter for the tikhonov regularisation. Available configurations are : "Inversion Cholesky" - ("tikhonov" / "none"), "Moore Penrose" - ("tikhonov" / "none"), "solve" - ("tikhonov" / "none"), "svd" - ("tikhonov" / "none" / "trunc").
<code>sigma</code>	The hyper-parameter.
<code>times</code>	The number of times internal cross-validation is performed. Default is 100.
<code>test.size</code>	The size of test data. Default is 0.2 (20 percent).
<code>xval</code>	The n-cross validation. Default is 5.
<code>fun</code>	The function used to summarise the <code>times</code> macro F1 matrices.
<code>seed</code>	The optional random number generator seed.
<code>verbose</code>	A logical defining whether a progress bar is displayed.

Value

An instance of class "[GenRegRes](#)".

Author(s)

Thomas Burger and Samuel Wieczorek

See Also

[perTurboClassification](#) and example therein.

phenoDisco

Runs the phenoDisco algorithm.

Description

`phenoDisco` is a semi-supervised iterative approach to detect new protein clusters.

Usage

```
phenoDisco(object, fcol = "markers", times = 100,
           GS = 10, allIter = FALSE, p = 0.05, seed,
           verbose = TRUE)
```

Arguments

<code>object</code>	An instance of class <code>MSnSet</code> .
<code>fcol</code>	A character indicating the organellar markers column name in feature metadata. Default is <code>markers</code> .
<code>times</code>	Number of runs of tracking. Default is 100.
<code>GS</code>	Group size, i.e how many proteins make a group. Default is 10 (the minimum group size is 4).
<code>allIter</code>	<code>logical</code> , defining if predictions for all iterations should be saved. Default is <code>FALSE</code> .
<code>p</code>	Significance level for outlier detection. Default is 0.05.
<code>seed</code>	An optional numeric of length 1 specifying the random number generator seed to be used.
<code>verbose</code>	Logical, indicating if messages are to be printed out during execution of the algorithm.

Details

The algorithm performs a phenotype discovery analysis as described in Breckels et al. Using this approach one can identify putative subcellular groupings in organelle proteomics experiments for more comprehensive validation in an unbiased fashion. The method is based on the work of Yin et al. and used iterated rounds of Gaussian Mixture Modelling using the Expectation Maximisation algorithm combined with a non-parametric outlier detection test to identify new phenotype clusters.

One requires 2 or more classes to be labelled in the data and at a very minimum of 6 markers per class to run the algorithm. The function will check and remove feature with missing values using the [filterNA](#) method.

Important: Prior to version 1.1.2 the row order in the output was different from the row order in the input. This has now been fixed and row ordering is now the same in both input and output objects.

Value

An instance of class MSnSet containg the phenoDisco predictions.

Author(s)

Lisa M. Breckels <lms79@cam.ac.uk>

References

Yin Z, Zhou X, Bakal C, Li F, Sun Y, Perrimon N, Wong ST. Using iterative cluster merging with improved gap statistics to perform online phenotype discovery in the context of high-throughput RNAi screens. *BMC Bioinformatics*. 2008 Jun 5;9:264. PubMed PMID: 18534020; PubMed Central PMCID: PMC2443381.

Breckels LM, Gatto L, Christoforou A, Groen AJ, Lilley KS and Trotter MWB. The Effect of Organelle Discovery upon Sub-Cellular Protein Localisation. *J Proteomics*. In Press.

Examples

```
## Not run:  
library(pRoloedata)  
data(tan2009r1)  
pdres <- phenoDisco(tan2009r1, fcol = "PLSDA")  
getPredictions(pdres, fcol = "pd", scol = NULL)  
plot2D(pdres, fcol = "pd")  
  
## End(Not run)
```

plot2D

Plot organelle assignment data and results.

Description

Generate 2 dimensional or feature distribution plots to illustrate localistation clusters. In plot2D, rows containing NA values are removed prior to dimention reduction.

Usage

```
plot2D(object, fcol = "markers", fpch,
       unknown = "unknown", dims = 1:2, alpha, score = 1,
       outliers = TRUE, method = c("PCA", "MDS"),
       axsSwitch = FALSE, mirrorX = FALSE, mirrorY = FALSE,
       col, pch, cex, index = FALSE, idx.cex = 0.75,
       identify = FALSE, plot = TRUE, ...)
```

Arguments

<code>object</code>	An instance of class <code>MSnSet</code> .
<code>fcol</code>	Feature meta-data label (fData column name) defining the groups to be differentiated using different colours. Default is <code>markers</code> . Use <code>NULL</code> to suppress any colouring.
<code>fpch</code>	Feature meta-data label (fData column name) defining the groups to be differentiated using different point symbols.
<code>unknown</code>	A character (default is <code>"unknown"</code>) defining how proteins of unknown localisation are labelled.
<code>dims</code>	A numeric of length 2 defining the dimensions to be plotted, i.e the PC/MDS axes.
<code>alpha</code>	A numeric defining the alpha channel (transparency) of the points, where $0 \leq \alpha \leq 1$, 0 being completely transparent and opaque.
<code>score</code>	A numeric specifying the minimum organelle assignment score to consider features to be assigned an organelle. (not yet implemented).
<code>outliers</code>	A logical specifying whether outliers should be plotted or ignored (default is <code>TRUE</code> , i.e. all points are plotted). Useful when the presence of outliers masks the structure of the rest of the data. Outliers are defined by the 2.5 and 97.5 percentiles.
<code>method</code>	One of <code>PCA</code> (default) or <code>MDS</code> , defining if dimensionality reduction is done using principal component analysis (see <code>prcomp</code>) or classical multidimensional scaling (see <code>cmdscale</code>).
<code>axsSwitch</code>	A logical indicating whether the axes should be switched.
<code>mirrorX</code>	A logical indicating whether the x axis should be mirrored?
<code>mirrorY</code>	A logical indicating whether the y axis should be mirrored?
<code>col</code>	A character of appropriate length defining colours.
<code>pch</code>	A character of appropriate length defining point character.
<code>cex</code>	Character expansion.
<code>index</code>	A logical (default is <code>FALSE</code>), indicating if the feature indices should be plotted on top of the symbols.
<code>idx.cex</code>	A numeric specifying the character expansion (default is 0.75) for the feature indices. Only relevant when <code>index</code> is <code>TRUE</code> .
<code>identify</code>	A logical (default is <code>TRUE</code>) defining if user interaction will be expected to identify individual data points on the plot. See also <code>identify</code> .

plot	A logical defining if the figure should be plotted. Useful when retrieving data only. Default is TRUE.
...	Additional parameters passed to plot and points.

Value

Used for its side effects of generating a plot. Invisibly returns the 2d data.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

See Also

[addLegend](#) to add a legend to plot2D figures and [plotDist](#) for alternative graphical representation of quantitative organelle proteomics data.

Examples

```
library("pRoloLocData")
data(dunkley2006)
plot2D(dunkley2006, fcol = NULL)
plot2D(dunkley2006, fcol = NULL, method = "MDS")
plot2D(dunkley2006, fcol = "markers")
addLegend(dunkley2006,
          fcol = "markers",
          where = "topright",
          cex = 0.5, bty = "n", ncol = 3)
title(main = "plot2D example")
```

plotDist

Plots the distribution of features across fractions

Description

Produces a line plot showing the feature abundances across the fractions.

Usage

```
plotDist(object, markers, mcol = "steelblue",
         pcol = "grey90", alpha = 0.3, fractions, ...)
```

Arguments

<code>object</code>	An instance of class MSnSet.
<code>markers</code>	A character, numeric or logical of appropriate length and or content used to subset object and define the organelle markers.
<code>mcol</code>	A character define the colour of the marker features. Default is "steelblue".
<code>pcol</code>	A character define the colour of the non-markers features. Default is "grey90".
<code>alpha</code>	A numeric defining the alpha channel (transparency) of the points, where 0 <= alpha <= 1, 0 and 1 being completely transparent and opaque.
<code>fractions</code>	An optional character defining the phenoData variable to be used to label the fraction along the x axis. If missing, the phenoData variables are searched for a match to fraction. If no match is found, the fractions are labelled as numericals.
<code>...</code>	Additional parameters passed to <code>plot</code> .

Value

Used for its side effect of producing a feature distribution plot. Invisibly returns NULL.

Author(s)

Laurent Gatto

Examples

```
library("pRolocdata")
data(tan2009r1)
j <- which(fData(tan2009r1)$markers == "mitochondrion")
i <- which(fData(tan2009r1)$PLSDA == "mitochondrion")
plotDist(tan2009r1[i, ],
         markers = featureNames(tan2009r1)[j],
         main = "Mitochondrion")
```

`plsdaClassification` *plsda classification*

Description

Classification using the partial least square discriminant analysis algorithm.

Usage

```
plsdaClassification(object, assessRes,
                    scores = c("prediction", "all", "none"), ncomp,
                    fcol = "markers", ...)
```

Arguments

object	An instance of class " MSnSet ".
assessRes	An instance of class " GenRegRes ", as generated by plsdaOptimisation .
scores	One of "prediction", "all" or "none" to report the score for the predicted class only, for all cluster or none.
ncomp	If assessRes is missing, a ncomp must be provided.
fcol	The feature meta-data containing marker definitions. Default is <code>markers</code> .
...	Additional parameters passed to plsda from package <code>caret</code> .

Value

An instance of class "[MSnSet](#)" with `plsda` and `plsda.scores` feature variables storing the classification results and scores respectively.

Author(s)

Laurent Gatto

Examples

```
## Not run:
## not running this one for time considerations
library(pRolocdata)
data(dunkley2006)
## reducing parameter search space and iterations
params <- plsdaOptimisation(dunkley2006, ncomp = c(3, 10), times = 2)
params
plot(params)
f1Count(params)
levelPlot(params)
getParams(params)
res <- plsdaClassification(dunkley2006, params)
getPredictions(res, fcol = "plsda")
getPredictions(res, fcol = "plsda", t = 0.9)
plot2D(res, fcol = "plsda")

## End(Not run)
```

plsdaOptimisation *plsda parameter optimisation*

Description

Classification parameter optimisation for the partial least square discriminant analysis algorithm.

Usage

```
plsdaOptimisation(object, fcol = "markers", ncomp = 2:6,
  times = 100, test.size = 0.2, xval = 5, fun = mean,
  seed, verbose = TRUE, ...)
```

Arguments

object	An instance of class " MSnSet ".
fcol	The feature meta-data containing marker definitions. Default is <code>markers</code> .
ncomp	The hyper-parameter. Default values are <code>2:6</code> .
times	The number of times internal cross-validation is performed. Default is <code>100</code> .
test.size	The size of test data. Default is <code>0.2</code> (20 percent).
xval	The n-cross validation. Default is <code>5</code> .
fun	The function used to summarise the <code>xval</code> macro F1 matrices.
seed	The optional random number generator seed.
verbose	A logical defining whether a progress bar is displayed.
...	Additional parameters passed to <code>plsda</code> from package <code>caret</code> .

Value

An instance of class "[GenRegRes](#)".

Author(s)

Laurent Gatto

See Also

[plsdaClassification](#) and example therein.

`rfClassification` *rf classification*

Description

Classification using the random forest algorithm.

Usage

```
rfClassification(object, assessRes,
  scores = c("prediction", "all", "none"), mtry,
  fcol = "markers", ...)
```

Arguments

object	An instance of class " MSnSet ".
assessRes	An instance of class " GenRegRes ", as generated by rfOptimisation .
scores	One of "prediction", "all" or "none" to report the score for the predicted class only, for all cluster or none.
mtry	If assessRes is missing, a mtry must be provided.
fcol	The feature meta-data containing marker definitions. Default is <code>markers</code> .
...	Additional parameters passed to randomForest from package <code>randomForest</code> .

Value

An instance of class "[MSnSet](#)" with `rf` and `rf.scores` feature variables storing the classification results and scores respectively.

Author(s)

Laurent Gatto

Examples

```
library(pRolocdata)
data(dunkley2006)
## reducing parameter search space and iterations
params <- rfOptimisation(dunkley2006, mtry = c(2, 5, 10), times = 3)
params
plot(params)
f1Count(params)
levelPlot(params)
getParams(params)
res <- rfClassification(dunkley2006, params)
getPredictions(res, fcol = "rf")
getPredictions(res, fcol = "rf", t = 0.75)
plot2D(res, fcol = "rf")
```

Description

Classification parameter optimisation for the random forest algorithm.

Usage

```
rfOptimisation(object, fcol = "markers", mtry = NULL,
times = 100, test.size = 0.2, xval = 5, fun = mean,
seed, verbose = TRUE, ...)
```

Arguments

<code>object</code>	An instance of class " MSnSet ".
<code>fcol</code>	The feature meta-data containing marker definitions. Default is <code>markers</code> .
<code>mtry</code>	The hyper-parameter. Default value is <code>NULL</code> .
<code>times</code>	The number of times internal cross-validation is performed. Default is 100.
<code>test.size</code>	The size of test data. Default is 0.2 (20 percent).
<code>xval</code>	The n-cross validation. Default is 5.
<code>fun</code>	The function used to summarise the <code>xval</code> macro F1 matrices.
<code>seed</code>	The optional random number generator seed.
<code>verbose</code>	A logical defining whether a progress bar is displayed.
<code>...</code>	Additional parameters passed to <code>randomForest</code> from package <code>randomForest</code> .

Value

An instance of class "[GenRegRes](#)".

Author(s)

Laurent Gatto

See Also

[rfClassification](#) and example therein.

`svmClassification` *ksvm classification*

Description

Classification using the support vector machine algorithm.

Usage

```
svmClassification(object, assessRes,
  scores = c("prediction", "all", "none"), cost, sigma,
  fcol = "markers", ...)
```

Arguments

object	An instance of class " MSnSet ".
assessRes	An instance of class " GenRegRes ", as generated by svmOptimisation .
scores	One of "prediction", "all" or "none" to report the score for the predicted class only, for all cluster or none.
cost	If assessRes is missing, a cost must be provided.
sigma	If assessRes is missing, a sigma must be provided.
fcol	The feature meta-data containing marker definitions. Default is <code>markers</code> .
...	Additional parameters passed to svm from package e1071.

Value

An instance of class "[MSnSet](#)" with `svm` and `svm.scores` feature variables storing the classification results and scores respectively.

Author(s)

Laurent Gatto

Examples

```
library(pRolocdata)
data(dunkley2006)
## reducing parameter search space and iterations
params <- svmOptimisation(dunkley2006, cost = 2^seq(-2,2,2), sigma = 10^seq(-1, 1, 1), times = 3)
params
plot(params)
f1Count(params)
levelPlot(params)
getParams(params)
res <- svmClassification(dunkley2006, params)
getPredictions(res, fcol = "svm")
getPredictions(res, fcol = "svm", t = 0.75)
plot2D(res, fcol = "svm")
```

svmOptimisation *svm parameter optimisation*

Description

Classification parameter optimisation for the support vector machine algorithm.

Usage

```
svmOptimisation(object, fcol = "markers",
                cost = 2^(-4:4), sigma = 10^(-2:3), times = 100,
                test.size = 0.2, xval = 5, fun = mean, seed,
                verbose = TRUE, ...)
```

Arguments

<code>object</code>	An instance of class " MSnSet ".
<code>fcol</code>	The feature meta-data containing marker definitions. Default is <code>markers</code> .
<code>cost</code>	The hyper-parameter. Default values are $2^{-4:4}$.
<code>sigma</code>	The hyper-parameter. Default values are $10^{(-2:3)}$.
<code>times</code>	The number of times internal cross-validation is performed. Default is 100.
<code>test.size</code>	The size of test data. Default is 0.2 (20 percent).
<code>xval</code>	The n-cross validation. Default is 5.
<code>fun</code>	The function used to summarise the <code>xval</code> macro F1 matrices.
<code>seed</code>	The optional random number generator seed.
<code>verbose</code>	A logical defining whether a progress bar is displayed.
<code>...</code>	Additional parameters passed to svm from package e1071.

Value

An instance of class "[GenRegRes](#)".

Author(s)

Laurent Gatto

See Also

[svmClassification](#) and example therein.

`testMarkers`

Tests marker class sizes

Description

Tests if the marker class sizes are large enough for the parameter optimisation scheme, i.e. the size is greater than `xval + n`, where the default `xval` is 5 and `n` is 2. If the test is unsuccessful, a warning is thrown.

Usage

```
testMarkers(object, xval = 5, n = 2, fcol = "markers")
```

Arguments

<code>object</code>	An instance of class " MSnSet ".
<code>xval</code>	The number cross-validation partitions. See the <code>xval</code> argument in the parameter optimisation function(s). Default is 5.
<code>n</code>	Number of additional examples.
<code>fcol</code>	The name of the prediction column in the <code>featureData</code> slot. Default is "markers".

Details

In case the test indicates that a class contains too few examples, it is advised to either add some or, if not possible, to remove the class altogether (see [minMarkers](#)) as the parameter optimisation is likely to fail or, at least, produce unreliable results for that class.

Value

If successfull, the test invisibly returns NULL. Else, it invisibly returns the names of the classes that have too few examples.

Author(s)

Laurent Gatto

See Also

[getMarkers](#) and [minMarkers](#)

Examples

```
library("pRolocdata")
data(dunkley2006)
getMarkers(dunkley2006)
testMarkers(dunkley2006)
toosmall <- testMarkers(dunkley2006, xval = 15)
toosmall
```

undocumented

Undocumented/unexported entries

Description

This is just a dummy entry for methods from unexported classes that generate warnings during package checking.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

Index

*Topic **classes**
 GenRegRes-class, 6

*Topic **methods**
 chi2-methods, 4
 exprsToRatios-methods, 6
 MLearn-methods, 21

addLegend, 2, 31
addMarkers, 3, 16

chi2, 5
chi2(chi2-methods), 4
chi2,matrix,matrix-method
 (chi2-methods), 4
chi2,matrix,numeric-method
 (chi2-methods), 4
chi2,numeric,matrix-method
 (chi2-methods), 4
chi2,numeric,numeric-method
 (chi2-methods), 4
chi2-methods, 4
chol2inv, 26, 27
class:GenRegRes (GenRegRes-class), 6
cmdscale, 30

empPvalues, 4, 5
estimateMasterFdr, 16
exprsToRatios (exprsToRatios-methods), 6
exprsToRatios,MSnSet-method
 (exprsToRatios-methods), 6
exprsToRatios-methods, 6

f1Count (GenRegRes-class), 6
f1Count,GenRegRes-method
 (GenRegRes-class), 6
filterNA, 29

GenRegRes, 11, 13, 14, 22–26, 28, 33–38
GenRegRes (GenRegRes-class), 6
GenRegRes-class, 6
getF1Scores (GenRegRes-class), 6

getF1Scores,GenRegRes-method
 (GenRegRes-class), 6
getMarkers, 8, 39
getParams (GenRegRes-class), 6
getParams,ClustRegRes-method
 (undocumented), 39
getParams,GenRegRes-method
 (GenRegRes-class), 6
getPredictions, 9
getRegularisedParams (GenRegRes-class),
 6
getRegularisedParams,GenRegRes-method
 (GenRegRes-class), 6
getRegularizedParams (GenRegRes-class),
 6
getRegularizedParams,GenRegRes-method
 (GenRegRes-class), 6
getSeed (GenRegRes-class), 6
getSeed,GenRegRes-method
 (GenRegRes-class), 6
getStockcol, 9
getStockpch (getStockcol), 9
getUnknowncol (getStockcol), 9
getUnknownpch (getStockcol), 9
getWarnings (GenRegRes-class), 6
getWarnings,GenRegRes-method
 (GenRegRes-class), 6
ginv, 26, 27

identify, 30

knn, 11, 12
knnClassification, 11, 13
knnOptimisation, 11, 12
knnOptimization (knnOptimisation), 12
knnPrediction (knnClassification), 11
knnRegularisation, 6
knnRegularisation (knnOptimisation), 12
ksvm, 13, 14
ksvmClassification, 13, 15

ksvmOptimisation, 13, 14
ksvmOptimization (ksvmOptimisation), 14
ksvmPrediction (ksvmClassification), 13
ksvmRegularisation (ksvmOptimisation),
 14

legend, 3
levelPlot (GenRegRes-class), 6
levelPlot, ClustRegRes-method
 (undocumented), 39
levelPlot, GenRegRes-method
 (GenRegRes-class), 6
lopims, 15

makeMaster, 16
makeNaData, 17
makeNaData2 (makeNaData), 17
markerSet, 18
minClassScore, 19
minMarkers, 8, 20, 39
MLearn, 21
MLearn, formula, MSnSet, clusteringSchema, missing-method
 (MLearn-methods), 21
MLearn, formula, MSnSet, learnerSchema, numeric-method
 (MLearn-methods), 21
MLearn, formula, MSnSet, learnerSchema, xvalSpec-method
 (MLearn-methods), 21

MLearn-methods, 21
MLearnMSnSet (MLearn-methods), 21
MSnSet, 6, 8, 9, 11–17, 19–27, 33–38
MSnSetMLean (MLearn-methods), 21

naiveBayes, 22, 23
nbClassification, 21, 23
nbOptimisation, 22, 22
nbOptimization (nbOptimisation), 22
nbPrediction (nbClassification), 21
nbRegularisation (nbOptimisation), 22
nnet, 24, 25
nnetClassification, 23, 25
nnetOptimisation, 24, 24
nnetOptimization (nnetOptimisation), 24
nnetPrediction (nnetClassification), 23
nnetRegularisation (nnetOptimisation),
 24

perTurboClassification, 25, 28
perTurboOptimisation, 26, 27
perTurboOptimization
 (perTurboOptimisation), 27

phenoDisco, 28
plot, 32
plot, ClustRegRes, missing-method
 (undocumented), 39
plot, GenRegRes, missing-method
 (GenRegRes-class), 6
plot2D, 2, 29
plotDist, 31, 31
plsda, 33, 34
plsdaClassification, 32, 34
plsdaOptimisation, 33, 33
plsdaOptimization (plsdaOptimisation),
 33
plsdaPrediction (plsdaClassification),
 32
plsdaRegularisation, 6
plsdaRegularisation
 (plsdaOptimisation), 33
prcomp, 30

randomForest, 35, 36
rfClassification, 34, 36
rfOptimisation, 35, 35
rfOptimization (rfOptimisation), 35
rfPrediction (rfClassification), 34
rfRegularisation (rfOptimisation), 35

setStockcol (getStockcol), 9
setStockpch (getStockcol), 9
setUnknowncol (getStockcol), 9
setUnknownpch (getStockcol), 9
show, ClustRegRes-method (undocumented),
 39
show, GenRegRes-method
 (GenRegRes-class), 6
solve, 26, 27
svd, 26, 27
svm, 37, 38
svmClassification, 36, 38
svmOptimisation, 37, 37
svmOptimization (svmOptimisation), 37
svmPrediction (svmClassification), 36
svmRegularisation, 6, 26
svmRegularisation (svmOptimisation), 37
Synapter, 15
synapter, 15
synergise, 15, 16

testMarkers, 8, 38

undocumented, [39](#)

`whichNA` (`makeNaData`), [17](#)

`xvalSpec`, [21](#)