

Package ‘pRoloc’

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Type Package

Title A unifying bioinformatics framework for spatial proteomics

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Description The pRoloc package implements machine learning and
visualisation methods for the analysis and interrogation
of quantitative mass spectrometry data to reliably infer
protein sub-cellular localisation.

Depends R (>= 2.15), MSnbase (>= 1.19.20), MLInterfaces (>= 1.37.1),
methods, Rcpp (>= 0.10.3), BiocParallel

Imports Biobase, mclust (>= 4.3), caret, e1071, sampling, class,
kernlab, Rtsne (>= 0.13), lattice, nnet, randomForest, proxy,
FNN, hexbin, BiocGenerics, stats, dendextend, RColorBrewer,
scales, MASS, knitr, mvtnorm, gtools, plyr, ggplot2, biomaRt,
utils, grDevices, graphics

Suggests testthat, rmarkdown, pRolocdata (>= 1.9.4), roxygen2,
synapter, xtable, rgl, BiocStyle (>= 2.5.19), hpar (>= 1.15.3),
dplyr, GO.db, AnnotationDbi

LinkingTo Rcpp, RcppArmadillo

License GPL-2

VignetteBuilder knitr

Video <https://www.youtube.com/playlist?list=PLvIXxpatSLA2loV5Srs2VBpJIYUIVJ4ow>

URL <https://github.com/lgatto/pRoloc>

BugReports <https://github.com/lgatto/pRoloc/issues>

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machinelearning-framework-theta.R machinelearning-utils.R
machinelearning-functions-knn.R
machinelearning-functions-ksvm.R machinelearning-functions-nb.R
machinelearning-functions-nnet.R
machinelearning-functions-PerTurbo.R

machinelearning-functions-plsda.R
 machinelearning-functions-rf.R machinelearning-functions-svm.R
 machinelearning-functions-knntl.R belief.R distances.R
 markers.R pRolocmarkers.R chi2.R MLInterfaces.R
 clustering-framework.R MSnSet.R clustering-kmeans.R
 perTurbo-algorithm.R phenodisco.R plotting.R plotting2.R
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 annotation.R goenv.R go.R makeGoSet.R vis.R MartInterface.R
 dynamics.R zzz.R goannotations.R clusterdist-functions.R
 clusterdist-framework.R qsep.R

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addGoAnnotations	<i>Add GO annotations</i>
------------------	---------------------------

Description

Adds GO annotations to the feature data

Usage

```
addGoAnnotations(object, params, evidence, useID = FALSE,
  fcol = "GOAnnotations", ...)
```

Arguments

object	An instance of class MSnSet.
params	An instance of class AnnotationParams. If missing, getAnnotationParams will be used.
evidence	GO evidence filtering.
useID	Logical. Should GO term names or identifiers be used? If TRUE, identifiers will be used. If FALSE GO term names will be used.
fcol	Character. Name of the matrix of annotations to be added to the fData default is GOAnnotations
...	Other arguments passed to makeGoSet

Value

An updated MSnSet with new feature data column called GOAnnotations containing a matrix of GO annotations

Author(s)

Lisa M Breckels

Examples

```
library(pRolocdata)
data(dunkley2006)
par <- setAnnotationParams(inputs =
  c("Arabidopsis thaliana genes",
    "Gene stable ID"))
## add protein sets/annotation information
xx <- addGoAnnotations(dunkley2006, par)
dim(fData(xx)$GOAnnotations)

## filter sets
xx <- filterMinMarkers(xx, n = 50)
dim(fData(xx)$GOAnnotations)
xx <- filterMaxMarkers(xx, p = .25)
dim(fData(xx)$GOAnnotations)

## Subset for specific protein sets
sub <- subsetMarkers(xx, keep = c("vacuole"))

## Order protein sets
res <- orderGoAnnotations(xx, k = 1:3, p = 1/3, verbose = FALSE)
if (interactive()) {
  pRolocVis(res, fcol = "GOAnnotations")
}
```

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

Description

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

Usage

```
addLegend(object, fcol = "markers", where = c("bottomleft", "bottom",  
"bottomright", "left", "topleft", "top", "topright", "right", "center",  
"other"), col, bty = "n", ...)
```

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 markers.
where	One of "bottomleft" (default), "bottomright", "topleft", "topright" or "other" defining the location of the legend. "other" opens a new graphics device, while the other locations are passed to legend .
col	A character defining point colours.
bty	Box type, as in legend . Default is set to "n".
...	Additional parameters passed to legend .

Details

The function has been updated in version 1.3.6 to recycle the default colours when more organelle classes are provided. See [plot2D](#) for details.

Value

Invisibly returns NULL

Author(s)

Laurent Gatto

addMarkers	<i>Adds markers to the data</i>
------------	---------------------------------

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. Alternatively, a markers named vector as provided by the [pRolocmarkers](#) function can also be used.

Usage

```
addMarkers(object, markers, mcol = "markers", fcol, verbose = TRUE)
```

Arguments

object	An instance of class MSnSet.
markers	A character with the name the markers' csv file or a named character of markers as provided by pRolocmarkers .
mcol	A character of length 1 defining the feature variable label for the newly added markers. Default is "markers".
fcol	An optional feature variable to be used to match against the markers. If missing, the feature names are used.
verbose	A logical indicating if number of markers and marker table should be printed to the console.

Details

It is essential to assure that `featureNames(object)` (or `fcol`, see below) and marker names (first column) match, i.e. the same feature identifiers and case fold are used.

Value

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

Author(s)

Laurent Gatto

See Also

See [pRolocmarkers](#) for a list of spatial markers and [markers](#) for details about markers encoding.

Examples

```
library("pRolocdata")
data(dunkley2006)
atha <- pRolocmarkers("atha")
try(addMarkers(dunkley2006, atha)) ## markers already exists
fData(dunkley2006)$markers.org <- fData(dunkley2006)$markers
fData(dunkley2006)$markers <- NULL
marked <- addMarkers(dunkley2006, atha)
fvarLabels(marked)
## if 'makers' already exists
marked <- addMarkers(marked, atha, mcol = "markers2")
fvarLabels(marked)
stopifnot(all.equal(fData(marked)$markers, fData(marked)$markers2))
plot2D(marked)
addLegend(marked, where = "topleft", cex = .7)
```

 AnnotationParams-class

 Class "AnnotationParams"

Description

Class to store annotation parameters to automatically query a Biomart server, retrieve relevant annotation for a set of features of interest using, for example [getGOFromFeatures](#) and [makeGoSet](#).

Objects from the Class

Objects can be created and set with the `setAnnotationParams` function. Object are created by calling without any arguments `setAnnotationParams()`, which will open an interactive interface. Depending on the value of `"many.graphics"` option, a graphical or a text-based menu will open (the text interface can be forced by setting the `graphics` argument to `FALSE`: `setAnnotationParams(graphics = FALSE)`). The menu will allow to select the species of interest first and the type of features (ENSEMBL gene identifier, Entrez id, ...) second.

The species that are available are those for which ENSEMBL data is available in Biomart and have a set of attributes of interest available. The compatible identifiers for downstream queries are then automatically filtered and displayed for user selection.

It is also possible to pass a parameter inputs, a character vector of length 2 containing a pattern uniquely matching the species of interest (in position 1) and a patterns uniquely matching the feature types (in position 2). If the matches are not unique, an error will be thrown.

A new instance of the `AnnotationParams` will be created to enable easy and automatic query of the `Mart` instance. The instance is invisibly returned and stored in a global variable in the **pRoloc** package's private environment for automatic retrieval. If a variable containing an `AnnotationParams` instance is already available, it can be set globally by passing it as argument to the `setAnnotationParams` function. Globally set `AnnotationParams` instances can be accessed with the `getAnnotationParams` function.

See the `pRoloc-theta` vignette for details.

Slots

mart: Object of class "Mart" from the **biomaRt** package.

martname: Object of class "character" with the name of the `mart` instance.

dataset: Object of class "character" with the data set of the `mart` instance.

filter: Object of class "character" with the filter to be used when querying the `mart` instance.

date: Object of class "character" indicating when the current instance was created.

biomaRtVersion: Object of class "character" with the **biomaRt** version used to create the `AnnotationParams` instance.

__classVersion__: Object of class "Versions" with the version of the `AnnotationParams` class of the current instance.

Methods

show `signature(object = "AnnotationParams")`: to display objects.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

See Also

[getGOFromFeatures](#), [makeGoSet](#) and the pRoloc-theta vignette.

Examples

```
data(andy2011params)
andy2011params
data(dunkley2006params)
dunkley2006params

try(setAnnotationParams(inputs = c("nomatch1", "nomatch2")))
setAnnotationParams(inputs = c("Homo sapiens",
                               "UniProtKB/Swiss-Prot ID"))
getAnnotationParams()
```

checkFeatureNamesOverlap

Check feature names overlap

Description

Checks the marker and unknown feature overlap of two MSnSet instances.

Usage

```
checkFeatureNamesOverlap(x, y, fcolx = "markers", fcoly, verbose = TRUE)
```

Arguments

x	An MSnSet instance.
y	An MSnSet instance.
fcolx	The feature variable to separate unknown (fData(y)\$coly == "unknown") from the marker features in the x object.
fcoly	As fcolx, for the y object. If missing, the value of fcolx is used.
verbose	If TRUE (default), the overlap is printed out on the console.

Value

Invisibly returns a named list of common markers, unique x markers, unique y markers in, common unknowns, unique x unknowns and unique y unknowns.

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)` Chi^2 values, for each x, y feature pair. Method is one of "Andersen2003" or "Wiese2007"; the former (default) computed the Chi^2 as $\sum(y-x)^2/\text{length}(x)$, 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 Chi^2 values; default, NULL, does not combine the Chi^2 values.

`signature(x = "matrix", y = "numeric", method = "character", na.rm = "logical")`

Computes `nrow(x)` 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)` 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 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)
```

`classWeights`*Calculate class weights*

Description

Calculates class weights to be used for parameter optimisation and classification such as [svmOptimisation](#) or [svmClassification](#) - see the *pRoloc tutorial* vignette for an example. The weights are calculated for all non-*unknown* classes the inverse of the number of observations.

Usage

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

Arguments

<code>object</code>	An instance of class MSnSet
<code>fcol</code>	The name of the features to be weighted

Value

A table of class weights

Author(s)

Laurent Gatto

Examples

```
library("pRolocdata")
data(hyperLOPIT2015)
classWeights(hyperLOPIT2015)
data(dunkley2006)
classWeights(dunkley2006)
```

clustDist

*Pairwise Distance Computation for Protein Information Sets***Description**

This function computes the mean (normalised) pairwise distances for pre-defined sets of proteins.

Usage

```
clustDist(object, k = 1:5, fcol = "GOAnnotations", n = 5,
          verbose = TRUE, seed)
```

Arguments

object	An instance of class "MSnSet".
k	The number of clusters to try fitting to the protein set. Default is k = 1:5.
fcol	The feature meta-data containing matrix of protein sets/ marker definitions. Default is GOAnnotations.
n	The minimum number of proteins per set. If protein sets contain less than n instances they will be ignored. Default is 5.
verbose	A logical defining whether a progress bar is displayed.
seed	An optional seed for the random number generator.

Details

The input to the function is a MSnSet dataset containing a matrix appended to the feature data slot identifying the membership of protein instances to a pre-defined set(s) e.g. a specific Gene Ontology term etc.

For each protein set, the clustDist function (i) extracts all instances belonging to the set, (ii) using the kmeans algorithm fits and tests k = c(1:5) (default) cluster components to each set, (iii) calculates the mean pairwise distance for each k tested.

Note: currently distances are calculated in Euclidean space, but other distance metrics will be supported in the future).

The output is a list of ClustDist objects, one per information cluster. The ClustDist class summarises the algorithm information such as the number of k's tested for the kmeans, and mean and normalised pairwise Euclidean distances per number of component clusters tested. See ?ClustDist for more details.

Value

An instance of "ClustDistList" containing a "ClustDist" instance for every protein set, which summarises the algorithm information such as the number of k's tested for the kmeans, and mean and normalised pairwise Euclidean distances per number of component clusters tested.

Author(s)

Lisa Breckels

See Also

For class definitions see "[ClustDistList](#)" and "[ClustDist](#)".

Examples

```
library(pRolocdata)
data(dunkley2006)
par <- setAnnotationParams(inputs =
                           c("Arabidopsis thaliana genes",
                              "Gene stable ID"))
## add protein sets/annotation information
xx <- addGoAnnotations(dunkley2006, par)
## filter
xx <- filterMinMarkers(xx, n = 50)
xx <- filterMaxMarkers(xx, p = .25)
## get distances for protein sets
dd <- clustDist(xx)
## plot clusters for first 'ClustDist' object
## in the 'ClustDistList'
plot(dd[[1]], xx)
## plot distances for all protein sets
plot(dd)
## Extract normalised distances
## Normalise by n^1/3
minDist <- getNormDist(dd, p = 1/3)
## Get new order according to lowest distance
o <- order(minDist)
## Re-order GOAnnotations
fData(xx)$GOAnnotations <- fData(xx)$GOAnnotations[, o]
if (interactive()) {
  pRolocVis(xx, fcol = "GOAnnotations")
}
```

ClustDist-class	<i>Class "ClustDist"</i>
-----------------	--------------------------

Description

The ClustDist summaries algorithm information, from running the clustDist function, such as the number of k's tested for the kmeans, and mean and normalised pairwise (Euclidean) distances per number of component clusters tested.

Objects from the Class

Object of this class are created with the clustDist function.

Slots

k: Object of class "numeric" storing the number of k clusters tested.
dist: Object of class "list" storing the list of distance matrices.
term: Object of class "character" describing GO term name.
id: Object of class "character" describing the GO term ID.

nrow: Object of class "numeric" showing the number of instances in the set

clustsz: Object of class "list" describing the number of instances for each cluster for each k tested

components: Object of class "vector" storing the class membership of each protein for each k tested.

fcol: Object of class "character" showing the feature column name in the corresponding MSnSet where the protein set information is stored.

Methods

plot Plots the kmeans clustering results.

show Shows the object.

Author(s)

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

Examples

```
showClass("ClustDist")

library('pRolocdata')
data(dunkley2006)
par <- setAnnotationParams(inputs =
  c("Arabidopsis thaliana genes",
    "Gene stable ID"))

## add protein set/annotation information
xx <- addGoAnnotations(dunkley2006, par)

## filter
xx <- filterMinMarkers(xx, n = 50)
xx <- filterMaxMarkers(xx, p = .25)

## get distances for protein sets
dd <- clustDist(xx)

## plot clusters for first 'ClustDist' object
## in the 'ClustDistList'
plot(dd[[1]], xx)

## plot distances for all protein sets
plot(dd)
```

ClustDistList-class *Storing multiple ClustDist instances*

Description

A class for storing lists of [ClustDist](#) instances.

Objects from the Class

Object of this class are created with the `clustDist` function.

Slots

`x`: Object of class `list` containing valid `ClustDist` instances.

`log`: Object of class `list` containing an object creation log, containing among other elements the call that generated the object.

`.__classVersion__`: The version of the instance. For development purposes only.

Methods

`"["` Extracts a single `ClustDist` at position.

`"["` Extracts one or more `ClustDists` as `ClustDistList`.

`length` Returns the number of `ClustDists`.

`names` Returns the names of `ClustDists`, if available. The replacement method is also available.

`show` Display the object by printing a short summary.

`lapply(x, FUN, ...)` Apply function `FUN` to each element of the input `x`. If the application of `FUN` returns a `ClustDist`, then the return value is a `ClustDistList`, otherwise a `list`.

`plot` Plots a boxplot of the distance results per protein set.

Author(s)

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

Examples

```
library('pRolocdata')
data(dunkley2006)
par <- setAnnotationParams(inputs =
                           c("Arabidopsis thaliana genes",
                             "Gene stable ID"))

## add protein set/annotation information
xx <- addGoAnnotations(dunkley2006, par)

## filter
xx <- filterMinMarkers(xx, n = 50)
xx <- filterMaxMarkers(xx, p = .25)

## get distances for protein sets
dd <- clustDist(xx)

## plot distances for all protein sets
plot(dd)

names(dd)

## Extract first 4 ClustDist objects of the ClustDistList
dd[1:4]

## Extract 1st ClustDist object
dd[[1]]
```

`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

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

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)
```

 fDataToUnknown *Update a feature variable*

Description

This function replaces a string or regular expression in a feature variable using the [sub](#) function.

Usage

```
fDataToUnknown(object, fcol = "markers", from = "^$", to = "unknown", ...)
```

Arguments

object	An instance of class MSnSet.
fcol	Feature variable to be modified. Default is "markers". If NULL, all feature variables will be updated.
from	A character defining the string or regular expression of the pattern to be replaced. Default is the empty string, i.e. the regular expression "^\$". See sub for details. If NA, then NA values are replaced by to.
to	A replacement for matched pattern. Default is "unknown". See sub for details.
...	Additional arguments passed to sub .

Value

An updated MSnSet.

Author(s)

Laurent Gatto

Examples

```
library("pRolocdata")
data(dunkley2006)
getMarkers(dunkley2006, "markers")
dunkley2006 <- fDataToUnknown(dunkley2006,
                             from = "unknown", to = "unassigned")
getMarkers(dunkley2006, "markers")
```

filterBinMSnSet	<i>Filter a binary MSnSet</i>
-----------------	-------------------------------

Description

Removes columns or rows that have a certain proportion or absolute number of 0 values.

Usage

```
filterBinMSnSet(object, MARGIN = 2, t, q, verbose = TRUE)
```

Arguments

object	An MSnSet
MARGIN	1 or 2. Default is 2.
t	Rows/columns that have t or less 1s, it will be filtered out. When t and q are missing, default is to use t = 1.
q	If a row has a higher quantile than defined by q, it will be filtered out.
verbose	A logical defining of a message is to be printed. Default is TRUE.

Value

A filtered MSnSet.

Author(s)

Laurent Gatto

See Also

[zerosInBinMSnSet](#), [filterZeroCols](#), [filterZeroRows](#).

Examples

```

set.seed(1)
m <- matrix(sample(0:1, 25, replace=TRUE), 5)
m[1, ] <- 0
m[, 1] <- 0
rownames(m) <- colnames(m) <- letters[1:5]
fd <- data.frame(row.names = letters[1:5])
x <- MSnSet(exprs = m, fData = fd, pData = fd)
exprs(x)
## Remove columns with no 1s
exprs(filterBinMSnSet(x, MARGIN = 2, t = 0))
## Remove columns with one 1 or less
exprs(filterBinMSnSet(x, MARGIN = 2, t = 1))
## Remove columns with two 1s or less
exprs(filterBinMSnSet(x, MARGIN = 2, t = 2))
## Remove columns with three 1s
exprs(filterBinMSnSet(x, MARGIN = 2, t = 3))
## Remove columns that have half or less of 1s
exprs(filterBinMSnSet(x, MARGIN = 2, q = 0.5))

```

filterMaxMarkers	<i>Removes class/annotation information from a matrix of candidate markers that appear in the fData.</i>
------------------	--

Description

Removes annotation information that contain more that a certain number/percentage of proteins

Usage

```

filterMaxMarkers(object, n, p = 0.2, fcol = "GOAnnotations",
  verbose = TRUE)

```

Arguments

object	An instance of class MSnSet.
n	Maximum number of proteins allowed per class/information term.
p	Maximum percentage of proteins per column. Default is 0.2 i.e. remove columns that have information for greater than 20 of the total number of proteins in the dataset (note: this is useful for example, if information is GO terms, for removing very general and uninformative terms).
fcol	The name of the matrix of marker information. Default is GOAnnotations.
verbose	Number of marker candidates retained after filtering.

Value

An updated MSnSet

See Also

addGoAnnotations and example therein.

filterMinMarkers	<i>Removes class/annotation information from a matrix of candidate markers that appear in the fData.</i>
------------------	--

Description

Removes annotation information that contain less that a certain number/percentage of proteins

Usage

```
filterMinMarkers(object, n = 10, p, fcol = "GOAnnotations",
  verbose = TRUE)
```

Arguments

object	An instance of class MSnSet.
n	Minimum number of proteins allowed per column. Default is 10.
p	Minimum percentage of proteins per column.
fcol	The name of the matrix of marker information. Default is GOAnnotations.
verbose	Number of marker candidates retained after filtering.

Value

An updated MSnSet.

Author(s)

Lisa M Breckels

See Also

addGoAnnotations and example therein.

filterZeroCols	<i>Remove 0 columns/rows</i>
----------------	------------------------------

Description

Removes all assay data columns/rows that are composed of only 0, i.e. have a colSum/rowSum of 0.

Usage

```
filterZeroCols(object, verbose = TRUE)
```

```
filterZeroRows(object, verbose = TRUE)
```

Arguments

object	A MSnSet object.
verbose	Print a message with the number of filtered out columns/row (if any).

Value

An MSnSet.

Author(s)

Laurent Gatto

Examples

```
library("pRolocdata")
data(andy2011goCC)
any(colSums(exprs(andy2011goCC)) == 0)
exprs(andy2011goCC)[, 1:5] <- 0
ncol(andy2011goCC)
ncol(filterZeroCols(andy2011goCC))
```

GenRegRes-class

Class "GenRegRes" and "ThetaRegRes"

Description

Regularisation framework containers.

Objects from the Class

Object of this class are created with the respective regularisation function: [knnOptimisation](#), [svmOptimisation](#), [plsdaOptimisation](#), [knnt1Optimisation](#), ...

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.

Only in ThetaRegRes:

predictions: A list of predictions for the optimisation iterations.

otherWeights: Alternative best theta weights: a vector per iterations, NULL if no other best weights were found.

Methods

getF1Scores Returns a matrix of F1 scores for the optimisation parameters.

f1Count signature(object = "GenRegRes", t = "numeric") and signature(object = "ThetaRegRes", 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 conjunctin with plot.

getParams Returns the *best* parameters. It is however strongly recommended to inspect the optimisation results. For a ThetaRegRes optimisation result, the method to chose the best parameters can be "median" (default) or "mean" (the median or mean of the best weights is chosen), "max" (the first weights with the highest macro-F1 score, considering that multiple max scoring combinations are possible) or "count" (the observed weight that get the maximum number of observations, see f1Count). The favourP argument can be used to prioritise weights that favour the primary data (i.e. heigh weights). See favourPrimary below.

getSeed Returns the seed used for the optimisation run.

getWarnings signature(object = "GenRegRes"): Returns a vector of recorded warnings.

levelPlot signature(object = "GenRegRes"): Plots a heatmap of of the optimisation results. Only for "GenRegRes" instances.

plot Plots the optisisation results.

show Shows the object.

Other functions

Only for ThetaRegRes:

combineThetaRegRes(object) Takes a list of ThetaRegRes instances to be combined and returns a new ThetaRegRes instance.

favourPrimary(primary, auxiliary, object, verbose = TRUE) Takes the primary and auxiliary data sources (two MSnSet instances) and a ThetaRegRes object and returns and updated ThetaRegRes instance containing best parameters/weights (see the getParams function) favouring the primary data when multiple best theta weights are available.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

Examples

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

getGOFromFeatures *Retrieve GO terms for feature names*

Description

The function pulls the gene ontology (GO) terms for a set of feature names.

Usage

```
getGOFromFeatures(id, namespace = "cellular_component", evidence = NULL,
  params = NULL, verbose = FALSE, nmax = 500)
```

Arguments

id	An character with feature names to be pulled from biomart. If and MSnSet is provided, then featureNames(id) is used.
namespace	The GO namespace. One of biological_process, cellular_component (default) or molecular_function.
evidence	The GO evidence code. See showGOEvidenceCodes for details. If NULL (default), no filtering based on the evidence code is performed.
params	An instance of class " AnnotationParams ".
verbose	A logical defining verbosity of the function. Default is FALSE.
nmax	As described in https://support.bioconductor.org/p/86358/ , the Biomart result can be unreliable for large queries. This argument splits the input in chunks of length nmax (default is 500). If set to NULL, the query is performed in full.

Value

A data.frame with relevant GO terms.

Author(s)

Laurent Gatto

Examples

```
library(pRolocdata)
data(dunkley2006)
data(dunkley2006params)
dunkley2006params
fn <- featureNames(dunkley2006)[1:5]
getGOFromFeatures(fn, params = dunkley2006params)
```

getMarkerClasses	<i>Returns the organelle classes in an 'MSnSet'</i>
------------------	---

Description

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

Usage

```
getMarkerClasses(object, fcol = "markers", ...)
```

Arguments

object	An instance of class "MSnSet".
fcol	The name of the markers column in the featureData slot. Default is markers.
...	Additional parameters passed to sort from the base package.

Value

A character vector of the organelle classes in the data.

Author(s)

Lisa Breckels and Laurent Gatto

See Also

[getMarkers](#) to extract the marker proteins. See [markers](#) for details about spatial markers storage and encoding.

Examples

```
library("pRolocdata")
data(dunkley2006)
organelles <- getMarkerClasses(dunkley2006)
## same if markers encoded as a matrix
dunkley2006 <- mrkVecToMat(dunkley2006, mfcol = "Markers")
organelles2 <- getMarkerClasses(dunkley2006, fcol = "Markers")
stopifnot(all.equal(organelles, organelles2))
```

getMarkers

Get 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 print out a marker table.

Usage

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

Arguments

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

Value

A character (matrix) of length $(ncol) \times ncol(object)$, depending on the vector or matrix encoding of the markers.

Author(s)

Laurent Gatto

See Also

See [getMarkerClasses](#) to get the classes only. See [markers](#) for details about spatial markers storage and encoding.

Examples

```
library("pRolocdata")
data(dunkley2006)
## marker vectors
myVmarkers <- getMarkers(dunkley2006)
head(myVmarkers)
## marker matrix
dunkley2006 <- mrkVecToMat(dunkley2006, mfcoll = "Markers")
myMmarkers <- getMarkers(dunkley2006, fcoll = "Markers")
head(myMmarkers)
```

getNormDist

Extract Distances from a "ClustDistList" object

Description

This function computes and outputs normalised distances from a "[ClustDistList](#)" object.

Usage

```
getNormDist(object, p = 1/3)
```

Arguments

object	An instance of class " ClustDistList ".
p	The normalisation factor. Default is 1/3.

Value

An numeric of normalised distances, one per protein set in the [ClustDistList](#).

Author(s)

Lisa Breckels

See Also

["ClustDistList"](#), ["ClustDist"](#), and examples in [clustDist](#).

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, mcol = "markers", 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.
mcol	The feature meta data column containing the labelled training data.
t	The score threshold. Predictions with score < t are set to 'unknown'. Default is 0. It is also possible to define thresholds for each prediction class, in which case, t is a named numeric with names exactly matching the unique prediction class names.
verbose	If TRUE, a prediction table is printed and the predictions are returned invisibly. If FALSE, the predictions are returned.

Value

An instance of class "MSnSet" with fcol.pred feature variable storing the prediction results according to the chosen threshold.

Author(s)

Laurent Gatto and Lisa Breckels

See Also

[orgQuants](#) for calculating organelle-specific thresholds.

Examples

```
library("pRolocdata")
data(dunkley2006)
res <- svmClassification(dunkley2006, fcol = "pd.markers",
                        sigma = 0.1, cost = 0.5)
fData(res)$svm[500:510]
fData(res)$svm.scores[500:510]
getPredictions(res, fcol = "svm", t = 0) ## all predictions
getPredictions(res, fcol = "svm", t = .9) ## single threshold
## 50% top predictions per class
```

```
ts <- orgQuants(res, fcol = "svm", t = .5)
getPredictions(res, fcol = "svm", t = ts)
```

goIdToTerm	<i>Convert GO ids to/from terms</i>
------------	-------------------------------------

Description

Converts GO identifiers to/from GO terms, either explicitly or by checking if (any items in) the input contains "GO:".

Usage

```
goIdToTerm(x, names = TRUE, keepNA = TRUE)
goTermToId(x, names = TRUE, keepNA = TRUE)
flipGoTermId(x, names = TRUE, keepNA = TRUE)
prettyGoTermId(x)
```

Arguments

x	A character of GO ids or terms.
names	Should a named character be returned? Default is TRUE.
keepNA	Should any GO term/id names that are missing or obsolete be replaced with a NA? Default is TRUE. If FALSE then the GO term/id names is kept.

Value

A character of GO terms (ids) if x were ids (terms).

Author(s)

Laurent Gatto

Examples

```
goIdToTerm("GO:0000001")
goIdToTerm("GO:0000001", names = FALSE)
goIdToTerm(c("GO:0000001", "novalid"))
goIdToTerm(c("GO:0000001", "GO:0000002", "notvalid"))
goTermToId("mitochondrion inheritance")
goTermToId("mitochondrion inheritance", name = FALSE)
goTermToId(c("mitochondrion inheritance", "notvalid"))
prettyGoTermId("mitochondrion inheritance")
prettyGoTermId("GO:0000001")
flipGoTermId("mitochondrion inheritance")
flipGoTermId("GO:0000001")
flipGoTermId("GO:0000001", names = FALSE)
```

highlightOnPlot	<i>Highlight features of interest on a spatial proteomics plot</i>
-----------------	--

Description

Highlights a set of features of interest given as a `FeaturesOfInterest` instance on a PCA plot produced by `codeplot2D` or `plot3D`. If none of the features of interest are found in the `MSnset`'s `featureNames`, an warning is thrown.

Usage

```
highlightOnPlot(object, foi, labels, args = list(), ...)
```

```
highlightOnPlot3D(object, foi, labels, args = list(), radius = 0.1 * 3, ...)
```

Arguments

object	The main dataset described as an <code>MSnSet</code> or a matrix with the coordinates of the features on the PCA plot produced (and invisibly returned) by <code>plot2D</code> .
foi	An instance of <code>FeaturesOfInterest</code> , or, alternatively, a character of feature names.
labels	A character of length 1 with a feature variable name to be used to label the features of interest. This is only valid if <code>object</code> is an <code>MSnSet</code> . Alternatively, if <code>TRUE</code> , then <code>featureNames(object)</code> (or <code>colnames(object)</code> , if <code>object</code> is a matrix) are used. Default is missing, which does not add any labels.
args	A named list of arguments to be passed to <code>plot2D</code> if the PCA coordinates are to be calculated. Ignored if the PCA coordinates are passed directly, i.e. <code>object</code> is a matrix.
...	Additional parameters passed to <code>points</code> or <code>text</code> (when <code>labels</code> is <code>TRUE</code>) when adding to <code>plot2D</code> , or <code>spheres3d</code> or <code>text3d</code> when adding the <code>plot3D</code>
radius	Radius of the spheres to be added to the visualisation produced by <code>plot3D</code> . Default is 0.3 (i.e. <code>plot3D</code> 's <code>radius1 * 3</code>), to emphasise the features with regard to unknown (<code>radius1 = 0.1</code>) and marker (<code>radius1 * 2</code>) features.

Value

NULL; used for its side effects.

Author(s)

Laurent Gatto

Examples

```
library("pRolocdata")
data("tan2009r1")
x <- FeaturesOfInterest(description = "A test set of features of interest",
                        fnames = featureNames(tan2009r1)[1:10],
                        object = tan2009r1)

## using FeaturesOfInterest or feature names
```

```

par(mfrow = c(2, 1))
plot2D(tan2009r1)
highlightOnPlot(tan2009r1, x)
plot2D(tan2009r1)
highlightOnPlot(tan2009r1, featureNames(tan2009r1)[1:10])

.pca <- plot2D(tan2009r1)
head(.pca)
highlightOnPlot(.pca, x, col = "red")
highlightOnPlot(tan2009r1, x, col = "red", cex = 1.5)
highlightOnPlot(tan2009r1, x, labels = TRUE)

.pca <- plot2D(tan2009r1, dims = c(1, 3))
highlightOnPlot(.pca, x, pch = "+", dims = c(1, 3))
highlightOnPlot(tan2009r1, x, args = list(dims = c(1, 3)))

.pca2 <- plot2D(tan2009r1, mirrorX = TRUE, dims = c(1, 3))
## previous pca matrix, need to mirror X axis
highlightOnPlot(.pca, x, pch = "+", args = list(mirrorX = TRUE))
## new pca matrix, with X mirrors (and 1st and 3rd PCs)
highlightOnPlot(.pca2, x, col = "red")

plot2D(tan2009r1)
highlightOnPlot(tan2009r1, x)
highlightOnPlot(tan2009r1, x, labels = TRUE, pos = 3)
highlightOnPlot(tan2009r1, x, labels = "Flybase.Symbol", pos = 1)

## in 3 dimensions
plot3D(tan2009r1, radius1 = 0.05)
highlightOnPlot3D(tan2009r1, x, labels = TRUE)
highlightOnPlot3D(tan2009r1, x)

```

knnClassification	<i>knn classification</i>
-------------------	---------------------------

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 classes or none.
k	If assessRes is missing, a k must be provided.
fcol	The feature meta-data containing marker definitions. Default is markers.
...	Additional parameters passed to knn from package class.

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(pRocdata)
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 " <code>MSnSet</code> ".
<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 class.

Details

Note that when performance scores precision, recall and (macro) F1 are calculated, any NA values are replaced by 0. This decision is motivated by the fact that any class that would have either a NA precision or recall would result in an NA F1 score and, eventually, a NA macro F1 (i.e. mean(F1)). Replacing NAs by 0s leads to F1 values of 0 and a reduced yet defined final macro F1 score.

Value

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

Author(s)

Laurent Gatto

See Also

[knnClassification](#) and example therein.

knnt1Classification *knn transfer learning classification*

Description

Classification using a variation of the KNN implementation of Wu and Dietterich's transfer learning schema

Usage

```
knnt1Classification(primary, auxiliary, fcol = "markers", bestTheta, k,
  scores = c("prediction", "all", "none"), seed)
```

Arguments

primary	An instance of class " MSnSet ".
auxiliary	An instance of class " MSnSet ".
fcol	The feature meta-data containing marker definitions. Default is markers.
bestTheta	Best theta vector as output from knnt1Optimisation , see knnt1Optimisation for details
k	Numeric vector of length 2, containing the best k parameters to use for the primary and auxiliary datasets. If k is not specified it will be calculated internally.
scores	One of "prediction", "all" or "none" to report the score for the predicted class only, for all classes or none.
seed	The optional random number generator seed.

Value

A character vector of the classifications for the unknowns

Author(s)

Lisa Breckels

See Also

[knnt1Optimisation](#)

Examples

```
library(pRolocdata)
data(andy2011)
data(andy2011goCC)
## reducing calculation time of k by pre-running knnOptimisation
x <- c(andy2011, andy2011goCC)
k <- lapply(x, function(z)
  knnOptimisation(z, times=5,
                  fcol = "markers.orig",
                  verbose = FALSE))
k <- sapply(k, function(z) getParams(z))
k
## reducing parameter search with theta = 1,
## weights of only 1 or 0 will be considered
opt <- knnt1Optimisation(andy2011, andy2011goCC,
                        fcol = "markers.orig",
                        times = 2,
                        by = 1, k = k)

opt
th <- getParams(opt)
plot(opt)
res <- knnt1Classification(andy2011, andy2011goCC,
                          fcol = "markers.orig", th, k)

res
```

knnt1Optimisation *theta parameter optimisation*

Description

Classification parameter optimisation for the KNN implementation of Wu and Dietterich's transfer learning schema

Usage

```
knnt1Optimisation(primary, auxiliary, fcol = "markers", k, times = 50,
                  test.size = 0.2, xval = 5, by = 0.5, length.out, th, xfolds,
                  BPPARAM = BiocParallel::bpparam(), method = "Breckels", log = FALSE,
                  seed)
```


Arguments

primary	An instance of class "MSnSet".
auxiliary	An instance of class "MSnSet".
fcol	The feature meta-data containing marker definitions. Default is markers.
k	Numeric vector of length 2, containing the best k parameters to use for the primary (k[1]) and auxiliary (k[2]) datasets. See knnOptimisation for generating best k.
times	The number of times cross-validation is performed. Default is 50.
test.size	The size of test (validation) data. Default is 0.2 (20 percent).
xval	The number of rounds of cross-validation to perform.
by	The increment for theta, must be one of c(1, 0.5, 0.25, 0.2, 0.15, 0.1, 0.05)
length.out	Alternative to using by parameter. Specifies the desired length of the sequence of theta to test.
th	A matrix of theta values to test for each class as generated from the function thetas , the number of columns should be equal to the number of classes contained in fcol. Note: columns will be ordered according to getMarkerClasses(primary, fcol). This argument is only valid if the default method 'Breckels' is used.
xfolds	Option to pass specific folds for the cross validation.
BPPARAM	Required for parallelisation. If not specified selects a default BiocParallelParam, from global options or, if that fails, the most recently registered() back-end.
method	The k-NN transfer learning method to use. The default is 'Breckels' as described in the Breckels et al (2016). If 'Wu' is specified then the original method implemented Wu and Dietterich (2004) is implemented.
log	A logical defining whether logging should be enabled. Default is FALSE. Note that logging produces considerably bigger objects.
seed	The optional random number generator seed.

Details

knnt1Optimisation implements a variation of Wu and Dietterich's transfer learning schema: P. Wu and T. G. Dietterich. Improving SVM accuracy by training on auxiliary data sources. In Proceedings of the Twenty-First International Conference on Machine Learning, pages 871 - 878. Morgan Kaufmann, 2004. A grid search for the best theta is performed.

Value

A list of containing the theta combinations tested, associated macro F1 score and accuracy for each combination over each round (specified by times).

Author(s)

Lisa Breckels

References

Breckels LM, Holden S, Wonjar D, Mulvey CM, Christoforou A, Groen AJ, Kohlbacher O, Lilley KS, Gatto L. Learning from heterogeneous data sources: an application in spatial proteomics. bioRxiv. doi: <http://dx.doi.org/10.1101/022152>

Wu P, Dietterich TG. Improving SVM Accuracy by Training on Auxiliary Data Sources. Proceedings of the 21st International Conference on Machine Learning (ICML); 2004.

See Also

[knnt1Classification](#) 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

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

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(pRocdata)
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

object	An instance of class " MSnSet ".
fcol	The feature meta-data containing marker definitions. Default is markers.
cost	The hyper-parameter. Default values are $2^{-4:4}$.
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 ksvm from package kernlab.

Details

Note that when performance scores precision, recall and (macro) F1 are calculated, any NA values are replaced by 0. This decision is motivated by the fact that any class that would have either a NA precision or recall would result in an NA F1 score and, eventually, a NA macro F1 (i.e. mean(F1)). Replacing NAs by 0s leads to F1 values of 0 and a reduced yet defined final macro F1 score.

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](#). (function [lopims1](#))
2. Each MSe/pep3D pair is processed using the HDMSe master file using [synergise](#). (function [lopims2](#))
3. The respective peptide-level synergise output objects are converted and combined into a single "MSnSet" instance. (function [lopims3](#))
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 peptides that do not display any missing values for each (frac_i, frac_ref) pair are summed and the ratio is reported (see [pRoloc:::refNormMeanOfNonNAPepSum](#) for details). (function [lopims4](#))

- The markers defined in the markerfile are collated as feature meta-data in the markers variable. See [addMarkers](#) for details. (function lopims5)

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;12(6):2340-53. PMID: 23510225.

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;12(6):2323-39. PMID: 23514362.

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

makeGoSet	<i>Creates a GO feature MSnSet</i>
-----------	------------------------------------

Description

Creates a new "[MSnSet](#)" instance populated with a GO term binary matrix based on an original object.

Usage

```
makeGoSet(object, params, namespace = "cellular_component", evidence = NULL)
```

Arguments

object	An instance of class " MSnSet " or a character of feature names.
params	An instance of class " AnnotationParams ", compatible with <code>featureNames(object)</code> 's format.
namespace	The ontology name space. One or several of "biological_process", "cellular_component" or "molecular_function".
evidence	GO evidence filtering.

Value

A new "[MSnSet](#)" with the GO terms for the respective features in the original object.

Author(s)

Laurent Gatto

Examples

```
library("pRolocdata")
data(dunkley2006)
data(dunkley2006params)
goset <- makeGoSet(dunkley2006[1:10, ],
                  dunkley2006params)

goset
exprs(goset)[1:10, 1:5]
image(goset)
```

markerMSnSet

Extract marker/unknown subsets

Description

These function extract the marker or unknown proteins into a new MSnSet.

Usage

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

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

Arguments

object	An instance of class MSnSet
fcol	The name of the feature data column, that will be used to separate the markers from the proteins of unknown localisation. When the markers are encoded as vectors, features of unknown localisation are defined as <code>fData(object)[, fcol] == "unknown"</code> . For matrix-encoded markers, unlabelled proteins are defined as <code>rowSums(fData(object)[, fcol]) == 0</code> . Default is "markers".

Value

An new MSnSet with marker/unknown proteins only.

Author(s)

Laurent Gatto

See Also

[sampleMSnSet](#) [testMSnSet](#) and [markers](#) for markers encoding.

Examples

```

library("pRolocdata")
data(dunkley2006)
mrk <- markerMSnSet(dunkley2006)
unk <- unknownMSnSet(dunkley2006)
dim(dunkley2006)
dim(mrk)
dim(unk)
table(fData(dunkley2006)$markers)
table(fData(mrk)$markers)
table(fData(unk)$markers)
## matrix-encoded markers
dunkley2006 <- mrkVecToMat(dunkley2006)
dim(markerMSnSet(dunkley2006, "Markers"))
stopifnot(all.equal(featureNames(markerMSnSet(dunkley2006, "Markers")),
                    featureNames(markerMSnSet(dunkley2006, "markers"))))
dim(unknownMSnSet(dunkley2006, "Markers"))
stopifnot(all.equal(featureNames(unknownMSnSet(dunkley2006, "Markers")),
                    featureNames(unknownMSnSet(dunkley2006, "markers"))))

```

MartInstance-class	<i>Class "MartInstance"</i>
--------------------	-----------------------------

Description

Internal infrastructure to query/handle several individual mart instance. See `MartInterface.R` for details.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

minMarkers	<i>Creates a reduced marker variable</i>
------------	--

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 <code>"MSnSet"</code> .
n	Minimum of marker instances per class.
fcol	The name of the markers column in the featureData slot. Default is markers.

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

See Also

[getPredictions](#) to filter based on classification scores.

Examples

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

MLearn-methods

The MLearn interface for machine learning

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`) clustering algorithms using MLInterface's MLean interface.

See Also

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

`move2Ds`*Displays a spatial proteomics animation*

Description

Given two MSnSet instances of one MSnSetList with at least two items, this function produces an animation that shows the transition from the first data to the second.

Usage

```
move2Ds(object, pcol, fcol = "markers", n = 25, hl)
```

Arguments

<code>object</code>	An <code>linkS4class{MSnSet}</code> or a <code>MSnSetList</code> . In the latter case, only the two first elements of the list will be used for plotting and the others will be silently ignored.
<code>pcol</code>	If <code>object</code> is an <code>MSnSet</code> , a factor or the name of a phenotype variable (<code>phenoData</code> slot) defining how to split the single <code>MSnSet</code> into two or more data sets. Ignored if <code>object</code> is a MSnSetList .
<code>fcol</code>	Feature meta-data label (<code>fData</code> 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>n</code>	Number of frames, Default is 25.
<code>hl</code>	An optional instance of class <code>linkS4class{FeaturesOfInterest}</code> to track features of interest.

Value

Used for its side effect of producing a short animation.

Author(s)

Laurent Gatto

See Also

[plot2Ds](#) to a single figure with the two datasets.

Examples

```
library("pRolocdata")
data(dunkley2006)

## Create a relevant MSnSetList using the dunkley2006 data
xx <- split(dunkley2006, "replicate")
xx1 <- xx[[1]]
xx2 <- xx[[2]]
fData(xx1)$markers[374] <- "Golgi"
fData(xx2)$markers[412] <- "unknown"
xx@x[[1]] <- xx1
```

```

xx@x[[2]] <- xx2

## The features we want to track
foi <- FeaturesOfInterest(description = "test",
                          fnames = featureNames(xx[[1]])[c(374, 412)])

## (1) visualise each experiment separately
par(mfrow = c(2, 1))
plot2D(xx[[1]], main = "condition A")
highlightOnPlot(xx[[1]], foi)
plot2D(xx[[2]], mirrorY = TRUE, main = "condition B")
highlightOnPlot(xx[[2]], foi, args = list(mirrorY = TRUE))

## (2) plot both data on the same plot
par(mfrow = c(1, 1))
tmp <- plot2Ds(xx)
highlightOnPlot(data1(tmp), foi, lwd = 2)
highlightOnPlot(data2(tmp), foi, pch = 5, lwd = 2)

## (3) create an animation
move2Ds(xx, pcol = "replicate")
move2Ds(xx, pcol = "replicate", hl = foi)

```

mrkConsProfiles

Marker consensus profiles

Description

A function to calculate average marker profiles.

Usage

```
mrkConsProfiles(object, fcol = "markers", method = mean)
```

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 markers.
method	A function to average marker profiles. Default is mean.

Value

A matrix of dimensions *number of clusters* (exluding unknowns) by *number of fractions*.

Author(s)

Laurent Gatto and Lisa M. Breckels

See Also

The [mrkHClust](#) function to produce a hierarchical cluster.

Examples

```
library("pRolocdata")
data(dunkley2006)
mrkConsProfiles(dunkley2006)
mrkConsProfiles(dunkley2006, method = median)
mm <- mrkConsProfiles(dunkley2006)
## Reorder fractions
o <- order(dunkley2006$fraction)
## Plot mean organelle profiles using the
## default pRoloc colour palette.
matplot(t(mm[, o]), type = "l",
        xlab = "Fractions", ylab = "Relative intensity",
        main = "Mean organelle profiles",
        col = getStockcol(), lwd = 2, lty = 1)
## Add a legend
addLegend(markerMSnSet(dunkley2006), where = "topleft")
```

mrkHClust

Draw a dendrogram of subcellular clusters

Description

This function calculates an average protein profile for each marker class (proteins of unknown localisation are ignored) and then generates a dendrogram representing the relation between marker classes. The colours used for the dendrogram labels are taken from the default colours (see [getStockcol](#)) so as to match the colours with other spatial proteomics visualisations such as [plot2D](#).

Usage

```
mrkHClust(object, fcol = "markers", distargs, hclustargs, plot = TRUE, ...)
```

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 markers.
distargs	A list of arguments to be passed to the dist function.
hclustargs	A list of arguments to be passed to the hclust function.
plot	A logical defining whether the dendrogram should be plotted. Default is TRUE.
...	Additional parameters passed when plotting the dendrogram .

Value

Invisibly returns a matrix of average occupancy profiles for all marker classes defined in fcol.

Author(s)

Laurent Gatto

Examples

```
library("pRolocdata")
data(dunkley2006)
mrkHClust(dunkley2006)
```

mrkVecToMat

Create a marker vector or matrix.

Description

Functions producing a new vector (matrix) marker vector set from an existing matrix (vector) marker set.

Usage

```
mrkVecToMat(object, vfcoll = "markers", mfcoll = "Markers")
mrkMatToVec(object, mfcoll = "Markers", vfcoll = "markers")
mrkMatAndVec(object, vfcoll = "markers", mfcoll = "Markers")
showMrkMat(object, mfcoll = "Markers")
isMrkMat(object, fcoll = "Markers")
isMrkVec(object, fcoll = "markers")
mrkEncoding(object, fcoll = "markers")
```

Arguments

object	An MSnSet object
vfcoll	The name of the <i>vector</i> marker feature variable. Default is "markers".
mfcoll	The name of the <i>matrix</i> marker feature variable. Default is "Markers".
fcoll	A marker feature variable name.

Details

Sub-cellular markers can be encoded in two different ways. Sets of spatial markers can be represented as character *vectors* (character or factor, to be accurate), stored as feature metadata, and proteins of unknown or uncertain localisation (unlabelled, to be classified) are marked with the "unknown" character. While very handy, this encoding suffers from some drawbacks, in particular the difficulty to label proteins that reside in multiple (possible or actual) localisations. The markers vector feature data is typically named markers. A new *matrix* encoding is also supported. Each spatial compartment is defined in a column in a binary markers matrix and the resident proteins are encoded with 1s. The markers matrix feature data is typically named Markers. If proteins are assigned unique localisations only (i.e. no multi-localisation) or their localisation is unknown (unlabelled), then both encodings are equivalent. When the markers are encoded as vectors, features of unknown localisation are defined as `fData(object)[, fcoll] == "unknown"`. For matrix-encoded markers, unlabelled proteins are defined as `rowSums(fData(object)[, fcoll]) == 0`.

The `mrkMatToVec` and `mrkVecToMat` functions enable the conversion from matrix (vector) to vector (matrix). The `mrkMatAndVec` function generates the missing encoding from the existing one. If the destination encoding already exists, or, more accurately, if the feature variable of the destination encoding exists, an error is thrown. During the conversion from matrix to vector, if multiple possible label exists, they are dropped, i.e. they are converted to "unknown". Function `isMrkVec` and `isMrkMat` can be used to test if a marker set is encoded as a vector or a matrix. `mrkEncoding` returns either "vector" or "matrix" depending on the nature of the markers.

Value

An updated `MSnSet` with a new vector (matrix) marker set.

Author(s)

Laurent Gatto and Lisa Breckels

See Also

Other functions that operate on markers are [getMarkers](#), [getMarkerClasses](#) and [markerMSnSet](#). To add markers to an existing `MSnSet`, see the [addMarkers](#) function and [pRolocmarkers](#), for a list of suggested markers.

Examples

```
library("pRolocdata")
data(dunkley2006)
dunk <- mrkVecToMat(dunkley2006)
head(fData(dunk)$Markers)
fData(dunk)$markers <- NULL
dunk <- mrkMatToVec(dunk)
stopifnot(all.equal(fData(dunkley2006)$markers,
                    fData(dunk)$markers))
```

<code>nbClassification</code>	<i>nb classification</i>
-------------------------------	--------------------------

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 " <code>MSnSet</code> ".
<code>assessRes</code>	An instance of class " <code>GenRegRes</code> ", as generated by nbOptimisation .
<code>scores</code>	One of "prediction", "all" or "none" to report the score for the predicted class only, for all classes or none.
<code>laplace</code>	If <code>assessRes</code> is missing, a <code>laplace</code> must be provided.

fcol The feature meta-data containing marker definitions. Default is markers.
 ... 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 paramter 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 markers.
 laplace The hyper-parameter. Default values are seq(0, 5, 0.5).
 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.

Details

Note that when performance scores precision, recall and (macro) F1 are calculated, any NA values are replaced by 0. This decision is motivated by the fact that any class that would have either a NA precision or recall would result in an NA F1 score and, eventually, a NA macro F1 (i.e. mean(F1)). Replacing NAs by 0s leads to F1 values of 0 and a reduced yet defined final macro F1 score.

Value

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

Author(s)

Laurent Gatto

See Also

[nbClassification](#) and example therein.

nndist-methods

Nearest neighbour distances

Description

Methods computing the nearest neighbour indices and distances for *matrix* and *MSnSet* instances.

Methods

`signature(object = "matrix", k = "numeric", dist = "character", ...)` Calculates indices and distances to the *k* (default is 3) nearest neighbours of each feature (row) in the input *matrix* object. The distance *dist* can be either of "euclidean" or "mahalanobis". Additional parameters can be passed to the internal function `FNN::get.knn`. Output is a matrix with $2 * k$ columns and `nrow(object)` rows.

`signature(object = "MSnSet", k = "numeric", dist = "character", ...)` As above, but for an *MSnSet* input. The indices and distances to the *k* nearest neighbours are added to the object's feature metadata.

`signature(object = "matrix", query = "matrix", k = "numeric", ...)` If two *matrix* instances are provided as input, the *k* (default is 3) indices and distances of the nearest neighbours of *query* in *object* are returned as a matrix of dimensions $2 * k$ by `nrow(query)`. Additional parameters are passed to `FNN::get.knnx`. Only euclidean distance is available.

Examples

```
library("pRolocdata")
data(dunkley2006)

## Using a matrix as input
m <- exprs(dunkley2006)
m[1:4, 1:3]
head(nndist(m, k = 5))
tail(nndist(m[1:100, ], k = 2, dist = "mahalanobis"))
```

```
## Same as above for MSnSet
d <- nndist(dunkley2006, k = 5)
head(fData(d))

d <- nndist(dunkley2006[1:100, ], k = 2, dist = "mahalanobis")
tail(fData(d))

## Using a query
nndist(m[1:100, ], m[101:110, ], k = 2)
```

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 <code>nnetOptimisation</code> .
scores	One of "prediction", "all" or "none" to report the score for the predicted class only, for all classes 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 markers.
...	Additional parameters passed to <code>nnet</code> 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 markers.
decay	The hyper-parameter. Default values are $c(0, 10^{(-1:-5)})$.
size	The hyper-parameter. Default values are $seq(1, 10, 2)$.
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 nnet from package nnet .

Details

Note that when performance scores precision, recall and (macro) F1 are calculated, any NA values are replaced by 0. This decision is motivated by the fact that any class that would have either a NA precision or recall would result in an NA F1 score and, eventually, a NA macro F1 (i.e. $mean(F1)$). Replacing NAs by 0s leads to F1 values of 0 and a reduced yet defined final macro F1 score.

Value

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

Author(s)

Laurent Gatto

See Also

[nnetClassification](#) and example therein.

orderGoAnnotations *Orders annotation information*

Description

For a given matrix of annotation information, this function returns the information ordered according to the best fit with the data.

Usage

```
orderGoAnnotations(object, fcol = "GOAnnotations", k = 1:5, n = 5,  
  p = 1/3, verbose = TRUE, seed)
```

Arguments

object	An instance of class MSnSet.
fcol	The name of the annotations matrix. Default is GOAnnotations.
k	The number of clusters to test. Default is k = 1:5
n	The minimum number of proteins per component cluster.
p	The normalisation factor, per k tested
verbose	A logical indicating if a progress bar should be displayed. Default is TRUE.
seed	An optional random number generation seed.

Details

As there are typically many protein/annotation sets that may fit the data we order protein sets by best fit i.e. cluster tightness, by computing the mean normalised Euclidean distance for all instances per protein set.

For each protein set i.e. proteins that have been labelled with a specified term/information criteria, we find the best k cluster components for the set (the default is to test k = 1:5) according to the minimum mean normalised pairwise Euclidean distance over all component clusters. (Note: when testing k if any components are found to have less than n proteins these components are not included and k is reduced by 1).

Each component cluster is normalised by N^p (where N is the total number of proteins per component, and p is the power). Hueristically, $p = 1/3$ and normalising by $N^{1/3}$ has been found the optimum normalisation factor.

Candidates in the matrix are ordered according to lowest mean normalised pairwise Euclidean distance as we expect high density, tight clusters to have the smallest mean normalised distance.

This function is a wrapper for running `clustDist`, `getNormDist`, see the "Annotating spatial proteomics data" vignette for more details.

Value

An updated MSnSet containing the newly ordered fcol matrix.

Author(s)

Lisa M Breckels

See Also

`addGoAnnotations` and example therein.

orgQuants

Returns organelle-specific quantile scores

Description

This function produces organelle-specific quantiles corresponding to the given classification scores.

Usage

```
orgQuants(object, fcol, scol, mcol = "markers", t, 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.
mcol	The name of the column containing the training data in the featureData slot. Default is markers.
t	The quantile threshold.
verbose	If TRUE, the calculated thresholds are printed.

Value

A named vector of organelle thresholds.

Author(s)

Lisa Breckels

See Also

[getPredictions](#) to get organelle predictions based on calculated thresholds.

Examples

```
library("pRolocdata")
data(dunkley2006)
res <- svmClassification(dunkley2006, fcol = "pd.markers",
                        sigma = 0.1, cost = 0.5)
## 50% top predictions per class
ts <- orgQuants(res, fcol = "svm", t = .5)
getPredictions(res, fcol = "svm", t = ts)
```

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

object	An instance of class "MSnSet".
assessRes	An instance of class "GenRegRes", as generated by svmRegularisation .
scores	One of "prediction", "all" or "none" to report the score for the predicted class only, for all classes or none.
pRegul	If assessRes is missing, a pRegul must be provided. See perTurboOptimisation for details.
sigma	If assessRes is missing, a sigma must be provided. See perTurboOptimisation for details.
inv	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".
reg	The type of regularisation of matrix. Values are "none", "trunc" or "tikhonov". Default value is "tikhonov".
fcol	The feature meta-data containing marker definitions. Default is markers.

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 Wiczorek

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(pRolocdata)
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

object	An instance of class " <i>MSnSet</i> ".
fcol	The feature meta-data containing marker definitions. Default is markers.
pRegul	The hyper-parameter for the regularisation (values are in]0,1]). If reg == "trunc", pRegul is for the percentage of eigen values in matrix. If reg == "tikhonov", then 'pRegul' 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").
sigma	The hyper-parameter.
inv	The type of algorithm used to invert the matrix. Values are : "Inversion Cholesky" (<i>chol2inv</i>), "Moore Penrose" (<i>ginv</i>), "solve" (<i>solve</i>), "svd" (<i>svd</i>). Default value is "Inversion Cholesky".
reg	The type of regularisation of matrix. Values are "none", "trunc" or "tikhonov". Default value is "tikhonov".

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 times macro F1 matrices.
seed	The optional random number generator seed.
verbose	A logical defining whether a progress bar is displayed.

Details

Note that when performance scores precision, recall and (macro) F1 are calculated, any NA values are replaced by 0. This decision is motivated by the fact that any class that would have either a NA precision or recall would result in an NA F1 score and, eventually, a NA macro F1 (i.e. mean(F1)). Replacing NAs by 0s leads to F1 values of 0 and a reduced yet defined final macro F1 score.

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, ndims = 2,
  modelNames = mclust.options("emModelNames"), G = 1:9, BPPARAM, tmpfile,
  seed, verbose = TRUE, dimred = c("PCA", "t-SNE"), ...)
```

Arguments

object	An instance of class MSnSet.
fcol	A character indicating the organellar markers column name in feature meta-data. Default is markers.
times	Number of runs of tracking. Default is 100.
GS	Group size, i.e how many proteins make a group. Default is 10 (the minimum group size is 4).
allIter	logical, defining if predictions for all iterations should be saved. Default is FALSE.

p	Significance level for outlier detection. Default is 0.05.
ndims	Number of principal components to use as input for the discovery analysis. Default is 2. Added in version 1.3.9.
modelName	A vector of characters indicating the models to be fitted in the EM phase of clustering using Mclust. The help file for <code>mclustModelNames</code> describes the available models. Default model names are <code>c("EII", "VII", "EEI", "VEI", "EVI", "VVI", "EEE", "EEV", "EEV", "VEV", "VVV")</code> , i.e. only ellipsoidal models.
G	An integer vector specifying the numbers of mixture components (clusters) for which the BIC is to be calculated. The default is <code>G=1:9</code> (as in Mclust).
BPPARAM	Support for parallel processing using the BiocParallel infrastructure. When missing (default), the default registered BiocParallelParam parameters are used. Alternatively, one can pass a valid BiocParallelParam parameter instance: <code>SnowParam</code> , <code>MulticoreParam</code> , <code>DoparParam</code> , ... see the BiocParallel package for details. To revert to the original serial implementation, use <code>NULL</code> .
tmpfile	An optional character to save a temporary MSnSet after each iteration. Ignored if missing. This is useful for long runs to track phenotypes and possibly kill the run when convergence is observed. If the run completes, the temporary file is deleted before returning the final result.
seed	An optional numeric of length 1 specifying the random number generator seed to be used. Only relevant when executed in serialised mode with <code>BPPARAM = NULL</code> . See <code>BPPARAM</code> for details.
verbose	Logical, indicating if messages are to be printed out during execution of the algorithm.
dimred	A character defining which of Principal Component Analysis ("PCA") or t-Distributed Stochastic Neighbour Embedding ("t-SNE") should be used to reduce dimensions prior to running phenoDisco novelty detection.
...	Additional arguments passed to the dimensionality reduction method. For both PCA and t-SNE, the data is scaled and centred by default, and these parameters (scale and centre for PCA, and <code>pca_scale</code> and <code>pca_center</code> for t-SNE can't be set). When using t-SNE however, it is important to tune the perplexity and max iterations parameters. See the <i>Dimensionality reduction</i> section in the pRoloc vignette for details.

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 features with missing values using the `filterNA` method.

A parallel implementation, relying on the BiocParallel package, has been added in version 1.3.9. See the `BPPARAM` argument for details.

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` containing 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.

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*. 2013 Aug 2;88:129-40. doi: 10.1016/j.jprot.2013.02.019. Epub 2013 Mar 21. PubMed PMID: 23523639.

Examples

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

## to pre-process the data with t-SNE instead of PCA
pdres <- phenoDisco(tan2009r1, fcol = "PLSDA", dimred = "t-SNE")

## End(Not run)
```

plot2D

Plot organelle assignment data and results.

Description

Generate 2 or 3 dimensional feature distribution plots to illustrate localisation clusters. Rows/features containing NA values are removed prior to dimension reduction. `plot3D` relies on the `rgl` package, that will be loaded automatically.

Usage

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

## S4 method for signature 'MSnSet'
plot3D(object, fcol = "markers", dims = c(1, 2, 3),
  radius1 = 0.1, radius2 = radius1 * 2, plot = TRUE, ...)
```


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 markers. Use NULL to suppress any colouring.
fpch	Feature meta-data label (fData column name) defining the groups to be differentiated using different point symbols.
unknown	A character (default is "unknown") defining how proteins of unknown/unlabelled localisation are labelled.
dims	A numeric of length 2 (or 3 for plot3D) defining the dimensions to be plotted. Defaults are c(1,2) and c(1, 2, 3). Always 1:2 for MDS.
score	A numeric specifying the minimum organelle assignment score to consider features to be assigned an organelle. (not yet implemented).
method	<p>A character describe how to transform the data or what to plot. One of "PCA" (default), "MDS", "kpca", "t-SNE" or "lda", defining what dimensionality reduction is applied: principal component analysis (see prcomp), classical multi-dimensional scaling (see cmdscale), kernel PCA (see kpca), t-SNE (see Rtsne) or linear discriminant analysis (see lda). The last method uses fcol to defined the sub-cellular clusters so that the ration between within ad between cluster variance is maximised. All the other methods are unsupervised and make use fcol only to annotate the plot. Prior to t-SNE, duplicated features are removed and a message informs the user if such filtering is needed.</p> <p>"scree" can also be used to produce a scree plot. "hexbin" applies PCA to the data and uses bivariate binning into hexagonal cells from hexbin to emphasise cluster density.</p> <p>If none is used, the data is plotted as is, i.e. without any transformation. In this case, object can either be an MSnSet or a matrix (as invisibly returned by plot2D). This enables to re-generate the figure without computing the dimensionality reduction over and over again, which can be time consuming for certain methods. If object is a matrix, an MSnSet containing the feature meta-data must be provided in methargs (see below for details).</p> <p>Available methods are listed in plot2Dmethods.</p>
methargs	A list of arguments to be passed when method is called. If missing, the data will be scaled and centred prior to PCA and t-SNE (i.e. Rtsne's arguments pca_center and pca_scale are set to TRUE). If method = "none" and object is a matrix, then the first and only argument of methargs must be an MSnSet with matching features with object.
axsSwitch	A logical indicating whether the axes should be switched.
mirrorX	A logical indicating whether the x axis should be mirrored?
mirrorY	A logical indicating whether the y axis should be mirrored?
col	A character of appropriate length defining colours.
pch	A character of appropriate length defining point character.
cex	Character expansion.
index	A logical (default is FALSE, indicating of the feature indices should be plotted on top of the symbols.
idx.cex	A numeric specifying the character expansion (default is 0.75) for the feature indices. Only relevant when index is TRUE.

addLegend	A character indicating where to add the legend. See addLegend for details. If missing (default), no legend is added.
identify	A logical (default is TRUE) defining if user interaction will be expected to identify individual data points on the plot. See also identify .
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.
radius1	A numeric specifying the radius of feature of unknown localisation. Default is 0.1, which is specified on the data scale. See plot3d for details.
radius2	A numeric specifying the radius of marker feature. Default is radius * 2.

Details

- Note that plot2D has been update in version 1.3.6 to support more organelle classes than colours defined in [getStockcol](#). In such cases, the default colours are recycled using the default plotting characters defined in [getStockpch](#). See the example for an illustration. The alpha argument is also depreciated in version 1.3.6. Use [setStockcol](#) to set colours with transparency instead. See example below.
- Version 1.11.3: to plot data as is, i.e. without any transformation, method can be set to "none" (as opposed to passing pre-computed values to method as a matrix, in previous versions). If object is an MSnSet, the untransformed values in the assay data will be plotted. If object is a matrix with coordinates, then a matching MSnSet must be passed to methargs.

Value

Used for its side effects of generating a plot. Invisibly returns the 2 or 3 dimensions that are plotted.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

See Also

[addLegend](#) to add a legend to plot2D figures (the legend is added by default on plot3D) and [plotDist](#) for alternative graphical representation of quantitative organelle proteomics data. [plot2Ds](#) to overlay 2 data sets on the same PCA plot.

Examples

```
library("pRolocdata")
data(dunkley2006)
plot2D(dunkley2006, fcol = NULL)
plot2D(dunkley2006, fcol = NULL, col = "black")
plot2D(dunkley2006, fcol = "markers")
addLegend(dunkley2006,
          fcol = "markers",
          where = "topright",
          cex = 0.5, bty = "n", ncol = 3)
title(main = "plot2D example")
## available methods
plot2Dmethods
plot2D(dunkley2006, fcol = NULL, method = "kpca", col = "black")
plot2D(dunkley2006, fcol = NULL, method = "kpca", col = "black",
```

```

        methargs = list(kpar = list(sigma = 1)))
plot2D(dunkley2006, method = "lda")
plot2D(dunkley2006, method = "hexbin")
## Using transparent colours
setStockcol(paste0(getStockcol(), "80"))
plot2D(dunkley2006, fcol = "markers")
## New behaviour in 1.3.6 when not enough colours
setStockcol(c("blue", "red", "green"))
getStockcol() ## only 3 colours to be recycled
getMarkers(dunkley2006)
plot2D(dunkley2006)
## reset colours
setStockcol(NULL)
plot2D(dunkley2006, method = "none") ## plotting along 2 first fractions
plot2D(dunkley2006, dims = c(3, 5), method = "none") ## plotting along fractions 3 and 5
## pre-calculate PC1 and PC2 coordinates
pca <- plot2D(dunkley2006, plot=FALSE)
head(pca)
plot2D(pca, method = "none", methargs = list(dunkley2006))

## plotting in 3 dimensions
plot3D(dunkley2006)
plot3D(dunkley2006, radius2 = 0.3)
plot3D(dunkley2006, dims = c(2, 4, 6))

```

plot2Ds

Draw 2 data sets on one PCA plot

Description

Takes 2 `linkS4class{MSnSet}` instances as input to plot the two data sets on the same PCA plot. The second data points are projected on the PC1 and PC2 dimensions calculated for the first data set.

Usage

```

plot2Ds(object, pcol, fcol = "markers", cex.x = 1, cex.y = 1,
        pch.x = 21, pch.y = 23, col, mirrorX = FALSE, mirrorY = FALSE,
        plot = TRUE, ...)

```

Arguments

<code>object</code>	An MSnSet or a <code>MSnSetList</code> . In the latter case, only the two first elements of the list will be used for plotting and the others will be silently ignored.
<code>pcol</code>	If <code>object</code> is an <code>MSnSet</code> , a factor or the name of a phenotype variable (<code>phenoData</code> slot) defining how to split the single <code>MSnSet</code> into two or more data sets. Ignored if <code>object</code> is a MSnSetList .
<code>fcol</code>	Feature meta-data label (<code>fData</code> 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>cex.x</code>	Character expansion for the first data set. Default is 1.
<code>cex.y</code>	Character expansion for the second data set. Default is 1.

pch.x	Plotting character for the first data set. Default is 21.
pch.y	Plotting character for the second data set. Default is 23.
col	A vector of colours to highlight the different classes defined by fcol. If missing (default), default colours are used (see getStockcol).
mirrorX	A logical indicating whether the x axis should be mirrored?
mirrorY	A logical indicating whether the y axis should be mirrored?
plot	If TRUE (default), a plot is produced.
...	Additional parameters passed to plot and points.

Value

Used for its side effects of producing a plot. Invisibly returns an object of class plot2Ds, which is a list with the PCA analyses results (see [prcomp](#)) of the first data set and the new coordinates of the second data sets, as used to produce the plot and the respective point colours. Each of these elements can be accessed with data1, data2, col1 and code2 respectively.

Author(s)

Laurent Gatto

See Also

See [plot2D](#) to plot a single data set and [move2Ds](#) for an animation.

Examples

```
library("pRolocdata")
data(tan2009r1)
data(tan2009r2)
msnl <- MSnSetList(list(tan2009r1, tan2009r2))
plot2Ds(msnl)
## tweaking the parameters
plot2Ds(list(tan2009r1, tan2009r2),
         fcol = NULL, cex.x = 1.5)
## input is 1 MSnSet containing 2 data sets
data(dunkley2006)
plot2Ds(dunkley2006, pcol = "replicate")
## no plot, just the data
res <- plot2Ds(dunkley2006, pcol = "replicate",
              plot = FALSE)

res
head(data1(res))
head(col1(res))
```

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 = getUnknowncol(),
  alpha = 0.3, type = "b", lty = 1, fractions = sampleNames(object),
  ylab = "Intensity", xlab = "Fractions", ylim, ...)
```

Arguments

object	An instance of class MSnSet.
markers	A character, numeric or logical of appropriate length and or content used to subset object and define the organelle markers.
mcol	A character define the colour of the marker features. Default is "steelblue".
pcol	A character define the colour of the non-markers features. Default is the colour used for features of unknown localisation, as returned by getUnknowncol .
alpha	A numeric defining the alpha channel (transparency) of the points, where $0 \leq \alpha \leq 1$, 0 and 1 being completely transparent and opaque.
type	Character string defining the type of lines. For example "p" for points, "l" for lines, "b" for both. See plot for all possible types.
lty	Vector of line types for the marker profiles. Default is 1 (solid). See par for details.
fractions	A character defining the phenoData variable to be used to label the fraction along the x axis. Default is to use sampleNames(object) .
ylab	y-axis label. Default is "Intensity".
xlab	x-axis label. Default is "Fractions".
ylim	A numeric vector of length 2, giving the y coordinates range.
...	Additional parameters passed to plot .

Value

Used for its side effect of producing a feature distribution plot. Invisibly returns the data matrix.

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])
plotDist(tan2009r1[i, ], markers = featureNames(tan2009r1)[j],
  fractions = "Fractions")
```

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 classes or none.
ncomp	If assessRes is missing, a ncomp must be provided.
fcol	The feature meta-data containing marker definitions. Default is markers.
...	Additional parameters passed to plsda from package caret .

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 running this one for time considerations  
library(pRocdata)  
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")
```

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 markers.
ncomp	The hyper-parameter. Default values are 2:6.
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 plsda from package caret .

Details

Note that when performance scores precision, recall and (macro) F1 are calculated, any NA values are replaced by 0. This decision is motivated by the fact that any class that would have either a NA precision or recall would result in an NA F1 score and, eventually, a NA macro F1 (i.e. mean(F1)). Replacing NAs by 0s leads to F1 values of 0 and a reduced yet defined final macro F1 score.

Value

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

Author(s)

Laurent Gatto

See Also

[plsdaClassification](#) and example therein.

pRolocmarkers

Organelle markers

Description

This function retrieves a list of organelle markers or, if no species is provided, prints a description of available marker sets. The markers can be added to an MSnSet using the [addMarkers](#) function.

Usage

```
pRolocmarkers(species)
```

Arguments

`species` The species of interest.

Details

The markers have been contributed by various members of the Cambridge Centre for Proteomics, in particular Dr Dan Nightingale for yeast, Dr Andy Christoforou and Dr Claire Mulvey for human, Dr Arnoud Groen for Arabidopsis and Dr Claire Mulvey for mouse. In addition, original (curated) markers from the pRolocdata datasets have been extracted (see pRolocdata for details and references). Curation involved verification of publicly available subcellular localisation annotation based on the curators knowledge of the organelles/proteins considered and tracing the original statement in the literature.

These markers are provided as a starting point to generate reliable sets of organelle markers but still need to be verified against any new data in the light of the quantitative data and the study conditions.

Value

Prints a description of the available marker lists if `species` is missing or a named character with organelle markers.

Author(s)

Laurent Gatto

See Also

[addMarkers](#) to add markers to an MSnSet and [markers](#) for more information about marker encoding.

Examples

```
pRolocmarkers()  
table(pRolocmarkers("atha"))  
table(pRolocmarkers("hsap"))
```


QSep-class

*Quantify resolution of a spatial proteomics experiment***Description**

The QSep infrastructure provide a way to quantify the resolution of a spatial proteomics experiment, i.e. to quantify how well annotated sub-cellular clusters are separated from each other.

The QSep function calculates all between and within cluster average distances. These distances are then divided column-wise by the respective within cluster average distance. For example, for a dataset with only 2 spatial clusters, we would obtain

$$\begin{array}{cc} & \begin{array}{c} c_1 \\ c_2 \end{array} \\ \begin{array}{c} c_1 \\ c_2 \end{array} & \begin{array}{cc} d_{11} & d_{12} \\ d_{21} & d_{22} \end{array} \end{array}$$

Normalised distance represent the ratio of between to within average distances, i.e. how much bigger the average distance between cluster c_i and c_j is compared to the average distance within cluster c_i .

$$\begin{array}{cc} & \begin{array}{c} c_1 \\ c_2 \end{array} \\ \begin{array}{c} c_1 \\ c_2 \end{array} & \begin{array}{cc} 1 & \frac{d_{12}}{d_{22}} \\ \frac{d_{21}}{d_{11}} & 1 \end{array} \end{array}$$

Note that the normalised distance matrix is not symmetric anymore and the normalised distance ratios are proportional to the tightness of the reference cluster (along the columns).

Objects from the Class

Objects can be created by calls using the constructor QSep (see below).

Slots

x: Object of class "matrix" containing the pairwise distance matrix, accessible with `qseq(. , norm = FALSE)`.

xnorm: Object of class "matrix" containing the normalised pairwise distance matrix, accessible with `qsep(. , norm = TRUE)` or `qsep(.)`.

object: Object of class "character" with the variable name of `MSnSet` object that was used to generate the QSep object.

__classVersion__: Object of class "Versions" storing the class version of the object.

Extends

Class "`Versioned`", directly.

Methods and functions

QSeq signature(object = "MSnSet", fcol = "character"): constructor for QSep objects. The `fcol` argument defines the name of the feature variable that annotates the sub-cellular clusters. Non-marker proteins, that are marked as "unknown" are automatically removed prior to distance calculation.

qssep signature(object = "QSep", norm = "logical"): accessor for the normalised (when norm is TRUE, which is default) and raw (when norm is FALSE) pairwise distance matrices.

names signature(object = "QSep"): method to retrieve the names of the sub-cellular clusters originally defined in QSep's fcol argument. A replacement method names(.) <- is also available.

summary signature(object = "QSep", ..., verbose = "logical"): Invisible return all between cluster average distances and prints (when verbose is TRUE, default) a summary of those.

levelPlot signature(object = "QSep", norm = "logical", ...): plots an annotated heatmap of all normalised pairwise distances. norm (default is TRUE) defines whether normalised distances should be plotted. Additional arguments ... are passed to the `levelplot`.

plot signature(object = "QSep", norm = "logical", ...): produces a boxplot of all normalised pairwise distances. The red points represent the within average distance and black points between average distances. norm (default is TRUE) defines whether normalised distances should be plotted.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

Examples

```
## Test data from Christoforou et al. 2016
library("pRolocdata")
data(hyperLOPIT2015)

## Create the object and get a summary
hlq <- QSep(hyperLOPIT2015)
hlq
summary(hlq)

## mean distance matrix
qssep(hlq, norm = FALSE)

## normalised average distance matrix
qssep(hlq)

## Update the organelle cluster names for better
## rendering on the plots
names(hlq) <- sub("/", "\n", names(hlq))
names(hlq) <- sub(" - ", "\n", names(hlq))
names(hlq)

## Heatmap of the normalised intensities
levelPlot(hlq)

## Boxplot of the normalised intensities
par(mar = c(3, 10, 2, 1))
plot(hlq)

## Boxplot of all between cluster average distances
x <- summary(hlq, verbose = FALSE)
boxplot(x)
```

rfClassification	<i>rf classification</i>
------------------	--------------------------

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 <code>"MSnSet"</code> .
assessRes	An instance of class <code>"GenRegRes"</code> , as generated by <code>rfOptimisation</code> .
scores	One of <code>"prediction"</code> , <code>"all"</code> or <code>"none"</code> to report the score for the predicted class only, for all classes or none.
mtry	If <code>assessRes</code> is missing, a <code>mtry</code> must be provided.
fcol	The feature meta-data containing marker definitions. Default is <code>markers</code> .
...	Additional parameters passed to <code>randomForest</code> 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)  
getParam(params)  
res <- rfClassification(dunkley2006, params)  
getPredictions(res, fcol = "rf")  
getPredictions(res, fcol = "rf", t = 0.75)  
plot2D(res, fcol = "rf")
```

rfOptimisation

svm parameter optimisation

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

object	An instance of class " MSnSet ".
fcol	The feature meta-data containing marker definitions. Default is markers.
mtry	The hyper-parameter. Default value is NULL.
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 randomForest from package randomForest.

Details

Note that when performance scores precision, recall and (macro) F1 are calculated, any NA values are replaced by 0. This decision is motivated by the fact that any class that would have either a NA precision or recall would result in an NA F1 score and, eventually, a NA macro F1 (i.e. mean(F1)). Replacing NAs by 0s leads to F1 values of 0 and a reduced yet defined final macro F1 score.

Value

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

Author(s)

Laurent Gatto

See Also

[rfClassification](#) and example therein.

sampleMSnSet	<i>Extract a stratified sample of an MSnSet</i>
--------------	---

Description

This function extracts a stratified sample of an MSnSet.

Usage

```
sampleMSnSet(object, fcol = "markers", size = 0.2, seed)
```

Arguments

object	An instance of class MSnSet
fcol	The feature meta-data column name containing the marker (vector or matrix) definitions on which the MSnSet will be stratified. Default is markers.
size	The size of the stratified sample to be extracted. Default is 0.2 (20 percent).
seed	The optional random number generator seed.

Value

A stratified sample (according to the defined fcol) which is an instance of class "[MSnSet](#)".

Author(s)

Lisa Breckels

See Also

[testMSnSet](#) [unknownMSnSet](#) [markerMSnSet](#). See [markers](#) for details about markers encoding.

Examples

```
library(pRolocdata)
data(tan2009r1)
dim(tan2009r1)
smp <- sampleMSnSet(tan2009r1, fcol = "markers")
dim(smp)
getMarkers(tan2009r1)
getMarkers(smp)
```

setLisacol	<i>Manage default colours and point characters</i>
------------	--

Description

These functions allow to get/set the colours and point character that are used when plotting organelle clusters and unknown features. These values are parametrised at the session level. Two palettes are available: the default palette (previously *Lisa's colours*) containing 30 colours and the old (original) palette, containing 13 colours.

Usage

```

setLisacol()

getLisacol()

getOldcol()

setOldcol()

getStockcol()

setStockcol(cols)

getStockpch()

setStockpch(pchs)

getUnknowncol()

setUnknowncol(col)

getUnknownpch()

setUnknownpch(pch)

```

Arguments

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

Value

The set functions set (and invisibly returns) colours. The get functions returns a character vector of colours. For the pch functions, numerics rather than characters.

Author(s)

Laurent Gatto

Examples

```
## defaults for clusters
getStockcol()
getStockpch()
## unknown features
getUnknownpch()
getUnknowncol()
## an example
library(pRocdata)
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()
getStockcol()
getOldcol()
```

showGOEvidenceCodes *GO Evidence Codes*

Description

This function prints a textual description of the Gene Ontology evidence codes.

Usage

```
showGOEvidenceCodes()

getGOEvidenceCodes()
```

Value

These functions are used for their side effects of printing evidence codes and their description.

Author(s)

Laurent Gatto

Examples

```
showGOEvidenceCodes()
getGOEvidenceCodes()
```

SpatProtVis-class *Class* SpatProtVis

Description

A class for spatial proteomics visualisation, that upon instantiation, pre-computes all defined visualisations. Objects can be created with the SpatProtVis constructor and visualised with the plot method.

The class is essentially a wrapper around several calls to `plot2D` that stores the dimensionality reduction outputs, and is likely to be updated in the future.

Usage

```
SpatProtVis(x, methods, dims, methargs, ...)
```

Arguments

x	An instance of class <code>MsnSet</code> to visualise.
methods	Dimensionality reduction methods to be used to visualise the data. Must be contained in <code>plot2Dmethods</code> (except "scree"). See <code>plot2D</code> for details.
dims	A list of numerics defining dimensions used for plotting. Default are 1 and 2. If provided, the length of this list must be identical to the length of methods.
methargs	A list of additional arguments to be passed for each visualisation method. If provided, the length of this list must be identical to the length of methods.
...	Additional arguments. Currently ignored.

Slots

`vismats`: A "list" of matrices containing the feature projections in 2 dimensions.

`data`: The original spatial proteomics data stored as an "MsnSet".

`methargs`: A "list" of additional plotting arguments.

`objname`: A "character" defining how to name the dataset. By default, this is set using the variable name used at object creation.

Methods

`plot`: Generates the figures for the respective methods and additional arguments defined in the constructor. If used in an interactive session, the user is prompted to press 'Return' before new figures are displayed.

`show`: A simple textual summary of the object.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

See Also

The data for the individual visualisations is created by `plot2D`.

Examples

```

library("pRolocdata")
data(dunkley2006)
## Default parameters for a set of methods
## (in the interest of time, don't use t-SNE)
m <- c("PCA", "MDS", "kpca")
vis <- SpatProtVis(dunkley2006, methods = m)
vis
plot(vis)
plot(vis, legend = "topleft")

## Setting method arguments
margs <- c(list(kpar = list(sigma = 0.1)),
           list(kpar = list(sigma = 1.0)),
           list(kpar = list(sigma = 10)),
           list(kpar = list(sigma = 100)))
vis <- SpatProtVis(dunkley2006,
                  methods = rep("kpca", 4),
                  methargs = margs)
par(mfrow = c(2, 2))
plot(vis)

## Multiple PCA plots but different PCs
dims <- list(c(1, 2), c(3, 4))
vis <- SpatProtVis(dunkley2006, methods = c("PCA", "PCA"), dims = dims)
plot(vis)

```

subsetMarkers

Subsets markers

Description

Subsets a matrix of markers by specific terms

Usage

```
subsetMarkers(object, fcol = "GOAnnotations", keep)
```

Arguments

object	An instance of class MSnSet.
fcol	The name of the markers matrix. Default is GOAnnotations.
keep	Integer or character vector specifying the columns to keep in the markers matrix, as defined by fcol.

Value

An updated MSnSet

Author(s)

Lisa M Breckels

See Also

addGoAnnotations and example therein.

svmClassification *svm 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 classes 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 markers.
...	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^(-3:2), 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 markers.
cost	The hyper-parameter. Default values are $2^{-4:4}$.
sigma	The hyper-parameter. Default values are $10^{-2:3}$.
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 svm from package e1071 .

Details

Note that when performance scores precision, recall and (macro) F1 are calculated, any NA values are replaced by 0. This decision is motivated by the fact that any class that would have either a NA precision or recall would result in an NA F1 score and, eventually, a NA macro F1 (i.e. $\text{mean}(F1)$). Replacing NAs by 0s leads to F1 values of 0 and a reduced yet defined final macro F1 score.

Value

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

Author(s)

Laurent Gatto

See Also

[svmClassification](#) and example therein.

testMarkers	<i>Tests marker class sizes</i>
-------------	---------------------------------

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", error = FALSE)
```

Arguments

object	An instance of class "MSnSet".
xval	The number cross-validation partitions. See the <code>xval</code> argument in the parameter optimisation function(s). Default is 5.
n	Number of additional examples.
fcol	The name of the prediction column in the featureData slot. Default is "markers".
error	A logical specifying if an error should be thrown, instead of a warning.

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 successful, 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
try(testMarkers(dunkley2006, xval = 15, error = TRUE))
```

testMSnSet	<i>Create a stratified 'test' MSnSet</i>
------------	--

Description

This function creates a stratified 'test' MSnSet which can be used for algorithmic development. A "MSnSet" containing only the marker proteins, as defined in fcol, is returned with a new feature data column appended called test in which a stratified subset of these markers has been relabelled as 'unknowns'.

Usage

```
testMSnSet(object, fcol = "markers", size = 0.2, seed)
```

Arguments

object	An instance of class "MSnSet"
fcol	The feature meta-data column name containing the marker definitions on which the data will be stratified. Default is markers.
size	The size of the data set to be extracted. Default is 0.2 (20 percent).
seed	The optional random number generator seed.

Value

An instance of class "MSnSet" which contains only the proteins that have a labelled localisation i.e. the marker proteins, as defined in fcol and a new column in the feature data slot called test which has part of the labels relabelled as "unknown" class (the number of proteins renamed as "unknown" is according to the parameter size).

Author(s)

Lisa Breckels

See Also

[sampleMSnSet](#) [unknownMSnSet](#) [markerMSnSet](#)

Examples

```
library(pRolocdata)
data(tan2009r1)
sample <- testMSnSet(tan2009r1)
getMarkers(sample, "test")
all(dim(sample) == dim(markerMSnSet(tan2009r1)))
```

thetas	<i>Draw matrix of thetas to test</i>
--------	--------------------------------------

Description

The possible weights to be considered is a sequence from 0 (favour auxiliary data) to 1 (favour primary data). Each possible combination of weights for `nclass` classes must be tested. The `thetas` function produces a weight matrix for `nclass` columns (one for each class) with all possible weight combinations (number of rows).

Usage

```
thetas(nclass, by = 0.5, length.out, verbose = TRUE)
```

Arguments

<code>nclass</code>	Number of marker classes
<code>by</code>	The increment of the weights. One of 1, 0.5, 0.25, 2, 0.1 or 0.05.
<code>length.out</code>	The desired length of the weight sequence.
<code>verbose</code>	A logical indicating if the weight sequences should be printed out. Default is TRUE.

Value

A matrix with all possible theta weight combinations.

Author(s)

Lisa Breckels

Examples

```
dim(thetas(4, by = 0.5))
dim(thetas(4, by = 0.2))
dim(thetas(5, by = 0.2))
dim(thetas(5, length.out = 5))
dim(thetas(6, by = 0.2))
```

undocumented	<i>Undocumented/unexported entries</i>
--------------	--

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>

zerosInBinMSnSet	<i>Compute the number of non-zero values in each marker classes</i>
------------------	---

Description

The function assumes that its input is a binary MSnSet and computes, for each marker class, the number of non-zero expression profiles. The function is meant to be used to produce heatmaps (see the example) and visualise binary (such as GO) MSnSet objects and assess their utility: all zero features/classes will not be informative at all (and can be filtered out with [filterBinMSnSet](#)) while features/classes with many annotations (GO terms) are likely not be be informative either.

Usage

```
zerosInBinMSnSet(object, fcol = "markers", as.matrix = TRUE,  
  percent = TRUE)
```

Arguments

object	An instance of class MSnSet with binary data.
fcol	A character defining the feature data variable to be used as markers. Default is "markers".
as.matrix	If TRUE (default) the data is formatted and returned as a matrix. Otherwise, a list is returned.
percent	If TRUE, percentages are returned. Otherwise, absolute values.

Value

A matrix or a list indicating the number of non-zero value per marker class.

Author(s)

Laurent Gatto

See Also

[filterBinMSnSet](#)

Examples

```
library(pRocdata)  
data(hyperLOPIT2015goCC)  
zerosInBinMSnSet(hyperLOPIT2015goCC)  
zerosInBinMSnSet(hyperLOPIT2015goCC, percent = FALSE)  
pal <- colorRampPalette(c("white", "blue"))  
library(lattice)  
levelplot(zerosInBinMSnSet(hyperLOPIT2015goCC),  
  xlab = "Number of non-0s",  
  ylab = "Marker class",  
  col.regions = pal(140))
```

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