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addSignatures  

**Add molecular signatures to MultiAssayExperiment**

---

**Description**

addSignatures extends mae by adding to it new experiments. Rows consistency is ensured by taking an intersection of rows after new experiments are added.

**Usage**

`addSignatures(mae, ..., intersect_rows = TRUE)`

**Arguments**

- `mae`  
  MultiAssayExperiment object.
- `...`  
  named experiments to be added to mae.
- `intersect_rows`  
  logical flag indicating if only common rows across experiments should be included. Only set to `FALSE` if you know what you are doing.

**Value**

MultiAssayExperiment object with new experiments added.

**Examples**

```r
data("rinderpest_mini", "remap_mini")
base_lvl <- "00hr"
design <- matrix(
  data = c(1, 0, 0,
           1, 0, 0,
           1, 0, 0,
           0, 1, 0,
           0, 1, 0,
           0, 1, 0,
           0, 0, 1,
           0, 0, 1,
           0, 0, 1),
  ncol = 3,
  nrow = 9,
  byrow = TRUE,
  dimnames = list(colnames(rinderpest_mini), c("00hr", "12hr", "24hr")))
mae <- prepareCountsForRegression(
  counts = rinderpest_mini,
  design = design,
  base_lvl = base_lvl)
mae <- addSignatures(mae, remap = remap_mini)
```
applyOverColumnGroups  Apply function over groups of columns

Description

Returns a array obtained by applying a function to rows of submatrices of the input matrix, where the submatrices are divided into specified groups of columns.

Usage

applyOverColumnGroups(mat, groups, f, ...)

Arguments

mat a matrix.
groups a vector giving columns grouping.
f function to be applied.
... optional arguments to f.

Value

a matrix of dimensions nrow(mat) x nlevels(groups).

applyOverDFList  Apply function over selected column in list of data frames

Description

applyOverDFList operates on a list of data frames where all data frames has the same size and columns. Column of interest is extracted from each data frame and column binded in groups, next fun is applied over rows. Final result is a matrix with result for each group on a separate column. Function is parallelized over groups.

Usage

applyOverDFList(list_of_df, col_name, fun, groups)

Arguments

list_of_df list of data.frames.
col_name string specifying column in data.frames to apply fun on.
fun function to apply, should take a single vector as a argument.
groups factor defining how elements of list_of_df should be grouped.

Value

matrix with nrow(list_of_df[[1]]) rows and nlevels(groups) columns.
design2factor

Transform design matrix to factor

Description
Transform design matrix to factor

Usage

\[ \text{design2factor}(\text{design}) \]

Arguments

- \text{design} \hspace{1em} \text{design matrix}

Value

\text{factor}

Examples

\begin{verbatim}
## Not run:
design <- matrix(data = c(1, 1, 0, 0, 0, 0, 1, 1),
nrow = 4,
ncol = 2,
dimnames = list(c(paste("sample", 1:4)), c("gr1", "gr2")))
design2factor(design)
## End(Not run)
\end{verbatim}

estimateStat

Estimate linear models goodness of fit statistic

Description
Estimate goodness of fit statistic of penalized linear regression models. Works with different goodness of fit statistic functions.

Usage

\[ \text{estimateStat}(x, y, u, s, \text{method} = \text{"cv"}, \text{nfold} = 10, \text{statistic} = \text{rsq}, \alpha = 0) \]
filterSignatures

Arguments

x input matrix, of dimension nobs x nvars; each row is an observation vector. Can be in sparse matrix format (inherit from class "sparseMatrix" as in package Matrix)

y response variable. Quantitative for family="gaussian", or family="poisson" (non-negative counts). For family="binomial" should be either a factor with two levels, or a two-column matrix of counts or proportions (the second column is treated as the target class; for a factor, the last level in alphabetical order is the target class). For family="multinomial", can be a nc>=2 level factor, or a matrix with nc columns of counts or proportions. For either "binomial" or "multinomial", if y is presented as a vector, it will be coerced into a factor. For family="cox", preferably a Surv object from the survival package: see Details section for more information. For family="mgaussian", y is a matrix of quantitative responses.

u offset vector as in glmnet. "U" experiment in mae.

s user supplied lambda.

method currently only cross-validation is implemented.

nfold number of fold to use in cross-validation.

statistic function computing goodness of fit statistic. Should accept y, x, offset arguments and return a numeric vector of the same length. See rsq, mse for examples.

alpha The elasticnet mixing parameter, with 0 ≤ α ≤ 1. The penalty is defined as 

\[(1 - \alpha)/2||\beta||^2_2 + \alpha||\beta||_1\]

alpha=1 is the lasso penalty, and alpha=0 the ridge penalty.

Value

numeric vector of statistic estimates.

---

filterSignatures Filter signatures by coverage

Description

Filter signatures overlapping low or high number of promoters. Useful to get rid of signatures that have very low variance.

Usage

```r
filterSignatures(
  mae,
  min = 0.05,
  max = 0.95,
  ref_experiment = "Y",
  omit_experiments = c("Y", "U")
)
```
**fisherMethod**

Combine p-values using Fisher method

**Description**

Fisher’s method is a meta-analysis technique used to combine the results from independent statistical tests with the same hypothesis ([Wikipedia article](https://en.wikipedia.org/wiki/Fisher%27s_method)).
Usage

```
fisherMethod(p.value, lower.tail = FALSE, log.p = TRUE)
```

Arguments

- `p.value`: a numeric vector of p-values to combine.
- `lower.tail`: logical; if TRUE (default), probabilities are \( P[X \leq x] \), otherwise, \( P[X > x] \).
- `log.p`: logical; if TRUE, probabilities p are given as \( \log(p) \).

Value

a number giving combined p-value.

---

**getCoverage**

Calculate regions coverage

Description

getCoverage calculates coverage of regions (rows in interaction matrix) by features (columns). It is possible to specify features grouping variable `gr` then coverage tells how many distinct groups the region overlap with.

Usage

```
gerCoverage(mat, gr)
```

Arguments

- `mat`: dgCMatrix interaction matrix such as produced by `getInteractionMatrix`.
- `gr`: factor specifying features groups. Must have length equal to number of columns in `mat`.

Value

Numeric vector.

Examples

data("remap_mini")
y <- colnames(remap_mini)

# simple coverage
gr <- seq_along(y) %>% as.factor()
gerCoverage(remap_mini, gr)

# per cell type coverage
gr <- sub(".*\.", "," , y) %>% as.factor()
gerCoverage(remap_mini, gr)
getInteractionMatrix

Compute interaction matrix

Description

getInteractionMatrix construct interaction matrix between two Granges objects. Names of object a became row names and names of b column names.

Usage

getInteractionMatrix(a, b, ext = 500, count = FALSE)

Arguments

a GRanges object.
b GRanges object.
ext Integer specifying number of base pairs the a coordinates should be extended in upstream and downstream directions.
count Logical indicating if matrix should hold number of overlaps between a and b or if FALSE presence / absence indicators.

Value

Sparse matrix of class dgCMatrix, with rows corresponding to a and columns to b. Each cell holds a number indicating how many times a and b overlapped.

Examples

```r
a <- GenomicRanges::GRanges(
  seqnames = c("chr20", "chr4"),
  ranges = IRanges::IRanges(
    start = c(62475984L, 173530220L),
    end = c(62476001L, 173530236L)),
  strand = c("-", ":"),
  name = c("hg19::chr20:61051039..61051057,-;hg_188273.1",
            "hg19::chr4:174451370..174451387,-;hg_54881.1"))
b <- GenomicRanges::GRanges(
  seqnames = c("chr4", "chr20"),
  ranges = IRanges::IRanges(
    start = c(173530229L, 63864270L),
    end = c(173530236L, 63864273L)),
  strand = c("-", ":"),
  name = c("HAND2", "GATA5"))
getInteractionMatrix(a, b)
```
getVarianceWeightedAvgCoeff

*Calculate variance weighted average coefficients matrix*

**Description**

Calculate variance weighted average coefficients matrix

**Usage**

`getVarianceWeightedAvgCoeff(pvalues, groups)`

**Arguments**

- `pvalues`: list of data.frames outputs from `ridgePvals`.
- `groups`: factor giving the grouping.

**Value**

variance weighted average coefficients matrix

---

isTRUEorFALSE

*Check if argument is a binary flag*

**Description**

Check if argument is a binary flag

**Usage**

`isTRUEorFALSE(x)`

**Arguments**

- `x`: object to test

**Value**

binary flag
**mae**

*Calculate Mean Absolute Error*

**Description**

Calculate Mean Absolute Error

**Usage**

`mae(y, yhat, ...)`

**Arguments**

- `y`: numeric vector of observed expression values.
- `yhat`: numeric vector of predicted expression values.
- `...`: not used.

**Value**

numeric vector

**maeSummary**

*Helper summarizing MAE object*

**Description**

Helper summarizing MAE object

**Usage**

`maeSummary(mae)`

**Arguments**

- `mae`: MultiAssayExperiment object.

**Value**

named list giving number of rows and columns, overall mean and standard deviation in mae’s experiments.
modelGeneExpression

Gene expression modeling pipeline

Description

modelGeneExpression uses parallelization if parallel backend is registered. For that reason we advise against passing parallel argument to internally called cv.glmnet routine.

Usage

modelGeneExpression(
  mae,
  yname = "Y",
  uname = "U",
  xnames,
  design = NULL,
  standardize = TRUE,
  parallel = FALSE,
  pvalues = TRUE,
  precalcmodels = NULL,
  ...
)

Arguments

mae MultiAssayExperiment object such as produced by prepareCountsForRegression.
yname string indicating experiment in mae to use as the expression input.
uname string indicating experiment in mae to use as the basal expression level.
xnames character indicating experiments in mae to use as molecular signatures.
design matrix giving the design matrix for the samples. Default (NULL) is to use design found in mae metadata. Columns corresponds to samples groups and rows to samples names. Only samples included in the design will be processed.
standardize logical flag indicating if the molecular signatures should be scaled. Advised to be set to TRUE.
parallel parallel argument to internally used cv.glmnet function. Advised to be set to FALSE as it might interfere with parallelization used in modelGeneExpression.
pvalues logical flag indicating if significance testing for the estimated molecular signatures activities should be performed.
p precalcmodels optional list of precomputed 'cv.glmnet' objects for each molecular signature and sample. The elements of this list should be matching the xnames vector. Each of those elements should be a named list holding 'cv.glmnet' objects for each sample. If provided those models will be used instead of running regression from scratch.
... arguments passed to glmnet::cv.glmnet.
Details

For speeding up the calculations consider lowering number of folds used in internally run \texttt{cv.glmnet} by specifying \texttt{n folds} argument. By default 10 fold cross validation is used.

The relationship between the expression (Y) and molecular signatures (X) is described using linear model formulation. The pipeline attempts to model the change in expression between basal expression level (u) and each sample, with the goal of finding the unknown molecular signatures activities. Linear models are fit using popular ridge regression implementation \texttt{glmnet} (Friedman, Hastie, and Tibshirani 2010).

If \texttt{pvalues} is set to \texttt{TRUE} the significance of the estimated molecular signatures activities is tested using methodology introduced by (Cule, Vineis, and De Iorio 2011) which original implementation can be found in \texttt{ridge-package}.

If replicates are available the signatures activities estimates and their standard error estimates can be combined. This is done by averaging signatures activities estimates and pooling their significance estimates using Stouffer’s method for the Z-scores and Fisher’s method for the p-values.

For detailed pipeline description we refer interested user to paper accompanying this package.

Value

Nested list with following elements

\begin{enumerate}
\item \textbf{regression\_models} Named list with elements corresponding to signatures specified in \texttt{xnames}. Each of these is a list holding \texttt{cv.glmnet} objects corresponding to each sample.
\item \textbf{pvalues} Named list with elements corresponding to signatures specified in \texttt{xnames}. Each of these is a list holding \texttt{data.frame} of signature’s p-values and test statistics estimated for each sample.
\item \textbf{zscore\_avg} Named list with elements corresponding to signatures specified in \texttt{xnames}. Each of these is a \texttt{matrix} holding replicate average Z-scores with columns corresponding to groups in the design.
\item \textbf{coef\_avg} Named list with elements corresponding to signatures specified in \texttt{xnames}. Each of these is a \texttt{matrix} holding replicate averaged signatures activities with columns corresponding to groups in the design.
\item \textbf{results} Named list of a \texttt{data.frame}s holding replicate average molecular signatures, overall molecular signatures Z-score and p-values calculated over groups using Stouffer’s and Fisher’s methods.
\end{enumerate}

Examples

```r
data("rinderpest_mini", "remap_mini")
base_lvl <- "00hr"
design <- matrix(
data = c(1, 0, 0,
1, 0, 0,
1, 0, 0,
0, 1, 0,
0, 1, 0,
0, 1, 0,
0, 0, 1,
0, 0, 1,)
```
modelGeneExpression_ridge_regression_wrapper

Ridge regression wrapper for modelGeneExpression

Description

Internal function used in modelGeneExpression. It runs ridge regression parallelly across signatures and samples as specified by experiment design.

Usage

modelGeneExpression_ridge_regression_wrapper(
  mae,
  yname,
  uname,
  xnames,
  groups,
  standardize,
  parallel,
  precalcmodels,
  ...
)

Arguments

mae MultiAssayExperiment object such as produced by prepareCountsForRegression.
yname string indicating experiment in mae to use as the expression input.
uname string indicating experiment in mae to use as the basal expression level.
xnames character indicating experiments in mae to use as molecular signatures.
groups factor representation of design matrix.
standardize  logical flag indicating if the molecular signatures should be scaled. Advised to be set to TRUE.

parallel  parallel argument to internally used `cv.glmnet` function. Advised to be set to FALSE as it might interfere with parallelization used in `modelGeneExpression`.

precalcmodels  optional list of precomputed `cv.glmnet` objects for each molecular signature and sample. The elements of this list should be matching the xnames vector. Each of those elements should be a named list holding `cv.glmnet` objects for each sample. If provided those models will be used instead of running regression from scratch.

... arguments passed to glmnet::cv.glmnet.

Value

Named list with elements corresponding to signatures specified in xnames. Each of these is a list holding `cv.glmnet` objects corresponding to each sample.

Usage

```r
modelGeneExpression_significance_testing_wraper(
  mae,
  yname,
  uname,
  xnames,
  groups,
  standardize,
  regression_models
)
```

Arguments

- **mae**: MultiAssayExperiment object such as produced by `prepareCountsForRegression`.
- **yname**: string indicating experiment in mae to use as the expression input.
- **uname**: string indicating experiment in mae to use as the basal expression level.
- **xnames**: character indicating experiments in mae to use as molecular signatures.
- **groups**: factor representation of design matrix.
prepareCountsForRegression

**standardize**

Logical flag indicating if the molecular signatures should be scaled. Advised to be set to TRUE.

**regression_models**

Named list with elements corresponding to signatures specified in `xnames`. Each of these is a list holding `cv.glmnet` objects corresponding to each sample. Usually returned by `modelGeneExpression_ridge_regression_wraper`.

**Value**

Named list with elements corresponding to signatures specified in `xnames`. Each of these is a list holding `data.frame` of signature’s p-values and test statistics estimated for each sample.

---

**mse**

*Calculate Mean Squared Error*

**Description**

Calculate Mean Squared Error

**Usage**

```
mse(y, yhat, ...)```

**Arguments**

- `y` numeric vector of observed expression values.
- `yhat` numeric vector of predicted expression values.
- `...` not used.

**Value**

numeric vector

---

prepareCountsForRegression

*Process count matrix for expression modeling*

**Description**

Expression counts are processed using edgeR following User’s Guide. Shortly, counts for each sample are filtered for lowly expressed promoters, normalized for the library size and transformed into counts per million (CPM). Optionally, CPM are log2 transformed with addition of pseudo count. Basal level expression is calculated by averaging base lvl samples expression values.
Usage

```r
prepareCountsForRegression(
    counts,
    design,
    base_lvl,
    log2 = TRUE,
    pseudo_count = 1L,
    drop_base_lvl = TRUE
)
```

Arguments

- `counts`: matrix of read counts.
- `design`: matrix giving the design matrix for the samples. Columns correspond to samples groups and rows to samples names.
- `base_lvl`: string indicating group in design corresponding to basal expression level. The reference samples to which expression change will be compared.
- `log2`: logical flag indicating if counts should be log2(counts per million) should be returned.
- `pseudo_count`: integer count to be added before taking log2.
- `drop_base_lvl`: logical flag indicating if `base_lvl` samples should be dropped from resulting MultiAssayExperiment object.

Value

MultiAssayExperiment object with two experiments:

- **U**: matrix giving expression values averaged over basal level samples
- **Y**: matrix of expression values

Design with `base_lvl` dropped is stored in metadata and directly available for `modelGeneExpression`.

Examples

```r
data("rinderpest_mini")
base_lvl <- "00hr"
design <- matrix(
    data = c(1, 0, 0,
             1, 0, 0,
             1, 0, 0,
             0, 1, 0,
             0, 1, 0,
             0, 1, 0,
             0, 0, 1,
             0, 0, 1,
             0, 0, 1),
    ncol = 3,
    nrow = 9,
    byrow = TRUE,
)```
```r
dimnames = list(colnames(rinderpest_mini), c("00hr", "12hr", "24hr"))
mae <- prepareCountsForRegression(
  counts = rinderpest_mini,
  design = design,
  base_lvl = base_lvl)
```

---

**regressionData**

Create MultiAssayExperiment object for expression modeling

**Description**

`regressionData` organize expression data and experiment design into MultiAssayExperiment object that can be further used in xcore framework. Additionally, function calculate basal expression level, for latter use in expression modeling, by averaging `base_lvl` samples expression values.

**Usage**

```r
regressionData(expr_mat, design, base_lvl, drop_base_lvl = TRUE)
```

**Arguments**

- `expr_mat`: matrix of expression values.
- `design`: matrix giving the design matrix for the samples. Columns corresponds to samples groups and rows to samples names.
- `base_lvl`: string indicating group in design corresponding to basal expression level. The reference samples to which expression change will be compared.
- `drop_base_lvl`: logical flag indicating if `base_lvl` samples should be dropped from resulting MultiAssayExperiment object.

**Details**

Note that `regressionData` does not apply any normalization or transformation to the input data! Use `prepareCountsForRegression` if you want to start with raw expression counts.

**Value**

MultiAssayExperiment object with two experiments:

- \( \mathbf{U} \) matrix giving expression values averaged over basal level samples
- \( \mathbf{Y} \) matrix of expression values

Design with `base_lvl` dropped is stored in metadata and directly available for `modelGeneExpression`.
Examples

```r
data("rinderpest_mini")
base_lvl <- "00hr"
design <- matrix(
data = c(1, 0, 0,
      1, 0, 0,
      1, 0, 0,
      0, 1, 0,
      0, 1, 0,
      0, 1, 0,
      0, 0, 1,
      0, 0, 1,
      0, 0, 1),
ncol = 3,
nrow = 9,
byrow = TRUE,
dimnames = list(colnames(rinderpest_mini), c("00hr", "12hr", "24hr")))
mae <- regressionData(
  expr_mat = rinderpest_mini,
  design = design,
  base_lvl = base_lvl)
```

Description

Molecular signatures data intended for use in xcore vignette and examples. It is build ReMap2020 molecular signatures constructed against FANTOM5 annotation, which can be found in xcoredata package. Here the data is only a subset limited to core promoters (promoters_f5_core) and randomly selected 600 signatures.

Usage

```r
data(remap_mini)
```

Format

A `dgCMatrix` with 14191 rows and 600 columns holding interaction matrix for subset of ReMap2020 molecular signatures against FANTOM5 annotation. Rows corresponds to FANTOM5 promoters and columns to signatures.
**repVarianceWeightedAvgZscore**

*Calculate replicate variance weighted averaged Z-scores*

**Description**

Replicate averaged Z-scores is calculated by dividing replicate average coefficient by replicate pooled standard error.

**Usage**

```
repVarianceWeightedAvgZscore(pvalues, groups)
```

**Arguments**

- `pvalues`: Data frame with 'se' (standard error) and 'coef' (coefficient) columns. Such as in pvalues output of modelGeneExpression.
- `groups`: Factor giving group membership for samples in pvalues.

**Value**

Numeric matrix of averaged Z-scores. Columns correspond to groups and rows to predictors.

---

**ridgePvals**

*Significance testing in linear ridge regression*

**Description**

Standard error estimation and significance testing for coefficients estimated in linear ridge regression. ridgePvals re-implement original method by (Cule et al. BMC Bioinformatics 2011.) found in ridge-package. This function is intended to use with cv.glmnet output.

**Usage**

```
ridgePvals(x, y, beta, lambda, standardizex = TRUE, svdX = NULL)
```

**Arguments**

- `x`: input matrix, same as used in cv.glmnet.
- `y`: response variable, same as used in cv.glmnet.
- `beta`: matrix of coefficients, estimated using cv.glmnet.
- `lambda`: lambda value for which beta was estimated.
- `standardizex`: logical flag for x variable standardization, should be set to same value as standarize flag in cv.glmnet.
- `svdX`: optional singular-value decomposition of x matrix. One can be obtained using link[base]{svd}. Passing this argument omits internal call to link[base]{svd}, this is useful when calling ridgePvals repeatedly using same x.
Value

a data.frame with columns

**coef** beta's names

**se** beta's standard errors

**tstat** beta's test statistic

**pval** beta's p-values

---

**rinderpest_mini**  
**xcore example expression data**

---

**Description**

Expression data intended for use in xcore vignette and examples. It is build from FANTOM5’s 293SLAM rinderpest infection time course dataset. Here the data is only a subset limited to core promoters (**promoters_f5_core**).

**Usage**

data(rinderpest_mini)

---

**Format**

A matrix with 14191 rows and 6 columns holding expression counts from CAGE-seq experiment. Rows corresponds to FANTOM5 promoters and columns to time points at which expression was measured 0 and 24 hours post infection.

---

**rsq**  
**Calculate $R^2$**

---

**Description**

Calculate $R^2$

**Usage**

rsq(y, yhat, offset)

**Arguments**

- **y**  
  numeric vector of observed expression values.

- **yhat**  
  numeric vector of predicted expression values.

- **offset**  
  numeric vector giving basal expression level.

**Value**

numeric vector
simplifyInteractionMatrix

Simplify Interaction Matrix

Description

Simplify Interaction Matrix

Usage

simplifyInteractionMatrix(mat, alpha = 0.5, colname = NA)

Arguments

mat
dgCMatrix interaction matrix such as produced by getInteractionMatrix.

alpha
Number between 0 and 1 specifying voting threshold. Eg. for 3 column matrix alpha 0.5 will give voting criteria >= 2.

colname
character giving new column name.

Value
dgCMatrix

stoufferZMethod

Combine Z-scores using Stouffer's method

Description

Stouffer's Z-score method is a meta-analysis technique used to combine the results from independent statistical tests with the same hypothesis. It is closely related to Fisher's method, but operates on Z-scores instead of p-values (Wikipedia article).

Usage

stoufferZMethod(z)

Arguments

z
a numeric vector of Z-score to combine.

Value

a number giving combined Z-score.
subsetWithMissing

Subset keeping missing

Description
Subset matrix keeping unmatched rows as NA.

Usage
subsetWithMissing(mat, rows)

Arguments
- mat: matrix
- rows: character

Value
a matrix

translateCounts

Translate counts matrix rownames

Description
translateCounts renames counts matrix rownames according to supplied dictionary. Function can handle many to one assignments by taking a sum or an average over counts rows. Other types of ambiguous assignments are not supported.

Usage
translateCounts(counts, dict)

Arguments
- counts: matrix of expression values.
- dict: named character vector mapping counts rownames to new values. Values of vector should correspond to new desired rownames, and its names to current rownames.

Value
matrix of expression values with new rownames.
Examples

counts <- matrix(
  data = c(5, 4, 3, 2),
  nrow = 2,
  dimnames = list(
    c("ENSG00000130700", "ENSG00000089225"),
    c("treatment", "control")
  )
)
dict <- c(ENSG00000130700 = "GATA5", ENSG00000089225 = "TBX5")
translateCounts(counts, dict)

%>%

re-export magrittr pipe operator

Description

re-export magrittr pipe operator
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