Package: xcore (via r-universe)

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Title xcore expression regulators inference

Version 1.9.0

Description xcore is an R package for transcription factor activity modeling based on known molecular signatures and user's gene expression data. Accompanying xcoredata package provides a collection of molecular signatures, constructed from publicly available ChiP-seq experiments. xcore use ridge regression to model changes in expression as a linear combination of molecular signatures and find their unknown activities. Obtained, estimates can be further tested for significance to select molecular signatures with the highest predicted effect on the observed expression changes.

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LazyData false
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Imports DelayedArray (>= 0.18.0), edgeR (>= 3.34.1), foreach (>= 1.5.1), GenomicRanges (>= 1.44.0), glmnet (>= 4.1.2), IRanges (>= 2.26.0), iterators (>= 1.0.13), magrittr (>= 2.0.1), Matrix (>= 1.3.4), methods (>= 4.1.1), MultiAssayExperiment (>= 1.18.0), stats, S4Vectors (>= 0.30.0), utils

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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.

```
data("rinderpest_mini", "remap_mini")
base_lvl <- "00hr"
design <- matrix(</pre>
  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(</pre>
  counts = rinderpest_mini,
  design = design,
  base_lvl = base_lvl)
mae <- addSignatures(mae, remap = remap_mini)</pre>
```

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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.

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design2factor

Transform design matrix to factor

Description

Transform design matrix to factor

Usage

```
design2factor(design)
```

Arguments

design

design matrix

Value

factor

Examples

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

```
estimateStat(x, y, u, s, method = "cv", nfold = 10, statistic = rsq, alpha = 0)
```

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Arguments

У

u

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)

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.

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 argu-

ments and return a numeric vector of the same length. See rsq, mse for exam-

ples.

alpha The elasticnet mixing parameter, with $0 \le \alpha \le 1$. 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

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

fisherMethod 7

Arguments

	mae	MultiAssayExperiment object.
	min	length one numeric between 0 and 1 defining minimum promoter coverage for the signature to pass filtering.
	max	length one numeric between 0 and 1 defining maximum promoter coverage for the signature to pass filtering.
	ref_experiment	string giving name of experiment to use for inferring total number of promoters.
omit_experiments		
		1

character giving names of experiments to exclude from filtering.

Value

MultiAssayExperiment object with selected experiments filtered.

Examples

```
data("rinderpest_mini", "remap_mini")
base_lvl <- "00hr"
design <- matrix(</pre>
  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(</pre>
  counts = rinderpest_mini,
  design = design,
  base_lvl = base_lvl)
mae <- addSignatures(mae, remap = remap_mini)</pre>
mae <- filterSignatures(mae)</pre>
```

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).

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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 $P[X \le x]$, 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

```
getCoverage(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.

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

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

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

getInteractionMatrix 9

```
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

а	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.

```
a <- GenomicRanges::GRanges(</pre>
  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(</pre>
  seqnames = c("chr4", "chr20"),
  ranges = IRanges::IRanges(
   start = c(173530229L, 63864270L),
    end = c(173530236L, 63864273L)),
  strand = c("-", "-"),
  name = c("HAND2", "GATA5"))
getInteractionMatrix(a, b)
```

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 ${\tt getVarianceWeightedAvgCoeff}$

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

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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	$Multi Assay Experiment\ object\ such\ as\ produced\ by\ prepare {\tt CountsForRegression}.$
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.
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 cv.glmnet by specifying nfolds 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 glmnet (Friedman, Hastie, and Tibshirani 2010).

If pvalues is set to 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 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

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.

pvalues 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.

zscore_avg Named list with elements corresponding to signatures specified in xnames. Each of these is a matrix holding replicate average Z-scores with columns corresponding to groups in the design.

coef_avg Named list with elements corresponding to signatures specified in xnames. Each of these is a matrix holding replicate averaged signatures activities with columns corresponding to groups in the design.

results Named list of a data. frames holding replicate average molecular signatures, overall molecular signatures Z-score and p-values calculated over groups using Stouffer's and Fisher's methods.

```
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)
mae <- filterSignatures(mae)
res <- modelGeneExpression(
    mae = mae,
    xnames = "remap",
    nfolds = 5)</pre>
```

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

Arguments

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 argument to internally used cv.glmnet function. Advised to be set to parallel 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.

```
modelGeneExpression_significance_testing_wraper
```

Statistical testing of ridge regression estimates wrapper for modelGeneExpression

Description

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

Usage

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

Arguments

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

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

```
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 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.

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

Value

MultiAssayExperiment object with two experiments:

U matrix giving expression values averaged over basal level samples

MultiAssayExperiment object.

Y matrix of expression values

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

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```
dimnames = list(colnames(rinderpest_mini), c("00hr", "12hr", "24hr")))
mae <- prepareCountsForRegression(
  counts = rinderpest_mini,
  design = design,
  base_lvl = base_lvl)</pre>
```

regressionData

Create MultiAssayExperiment object for expression modeling

Description

regressionData orgnize 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

```
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:

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.

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Examples

```
data("rinderpest_mini")
base_lvl <- "00hr"
design <- matrix(</pre>
  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(</pre>
  expr_mat = rinderpest_mini,
  design = design,
  base_lvl = base_lvl)
```

remap_mini

xcore example molecular signatures

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

```
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.

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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.

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Value

a data.frame with columns

coef beta's namesse 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

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```
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 23

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.

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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)</pre>
```

%>%

re-export magrittr pipe operator

Description

re-export magrittr pipe operator

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