Package 'httrpathway'

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```
Type Package
Title Pathway Scoring and Concentration Response for high-throughput transcriptomics (HTTr) data
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Description
      This package generates pathway (signature) scores with associated concentration response
      modeling. This package contains functions to create input files (log2-
      fold change, or (12fc) matrices) and run concentration-
      response modeling of signature or gene/probe-level HTTr data.
Imports stats,
      stringr,
      grDevices,
      graphics,
      utils,
      methods,
      future.apply,
      future,
      moments,
      numDeriv,
      openxlsx,
      parallel,
      RColorBrewer,
      reshape2,
      data.table,
      e1071,
      mongolite,
      testthat,
      tcplfit2,
      stringi,
      matrixStats,
      tidyr,
      gplots,
      ggplot2
```

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auc

Area Under the Curve

Description

Compute AUC for an ROC curve.

Usage

```
auc(tpr, fpr)
```

Arguments

tpr Vector of true positive rates.

fpr Vector of false positive rates.

Details

Uses trapezoid rule numerical integration to approximate AUC. Will be more accurate with more fine-grained inputs.

Value

AUC

Examples

```
auc(c(0,.5,1), c(0,.5,1)) auc(c(0,1,1), c(0,.5,1))
```

buildFCMAT2

Transpose and filter the fold change matrix FCMAT1 in long format into a gene x sample format. Function returns FCMAT2 and CHEM_DICT as a list R object

Description

Transpose and filter the fold change matrix FCMAT1 in long format into a gene x sample format. Function returns FCMAT2 and CHEM_DICT as a list R object

Usage

```
buildFCMAT2(
  FCMAT1 = NULL,
  time = 24,
  media = "DMEM",
  output_dir = "../input/fcdata/",
  method = "gene",
  sample_type = "test sample",
  writing_to_disk = FALSE
)
```

Arguments

The input data structure that contains the data frame from the httrlib buildFC-

MAT1() function or provided by the user in the same format. FCMAT1 should be a long format table with rows denoting genes/probes and an 'l2fc' column which contains log2 fold-change data from DESeq2 or another method.

time The time in hours that the chemical dosing was run

media The name of the media used

output_dir The directory from which to read all of the raw files

method Either "gene" or "probe_id". Specifying "gene" will average probes that target

the same gene, whereas "probe_id" will keep all probes separate when making

the FCMAT2 table.

sample_type either "test sample" or "reference chemical" will determine what sample type

the FCMAT2/CHEM_DICT tables will include

writing_to_disk

dictates whether all results should be saved to disk (path is defined by output_dir

parameter)

Value

Global variables are created for the FC matrix (FCMAT2) and the chemical dictionary (CHEM_DICT) which translates from the sample key (sample_id_conc_time) to the individual components

list consisting of matrices FCMAT2 and CHEM_DICT

compareSignatureCutoffs

Generates a plot comparing two cutoff calculation methods

Description

Generates a plot comparing two cutoff calculation methods

```
compareSignatureCutoffs(empirical_cutoffs, cutoffs, nsig = NULL)
```

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Arguments

```
empirical_cutoffs
output from the exportSignatureCutoffs function
cutoffs
calculated cutoffs provided by cutoffCalc function
nsig
number of signatures to compare
```

Value

ggplot object which is the scatterplot comparing the two methods

cutoffCalc

Calculate the signature-wise cutoffs based on the analytical method which does not break any correlations between genes and compare with already defined signature_cr object (see exportSignatureCutoffs function)

Description

Calculate the signature-wise cutoffs based on the analytical method which does not break any correlations between genes and compare with already defined signature_cr object (see exportSignatureCutoffs function)

Usage

```
cutoffCalc(
  sigcatalog,
  sigset,
  pval = 0.05,
  seed = 12345,
  nlowconc = 2,
  mc.cores = 1,
  dtxsid.exclude = NULL,
  do.cov = T,
  do.compare = F,
  to.file = F,
  sigdbgenelist,
  FCMAT2,
  CHEM_DICT
)
```

Arguments

```
sigcatalog The name of the signature catalog to use sigset The signature set pval The p-value for the baseline distribution
```

seed Random seed

nlowconc Only include the nlowconc concentrations for each chemical when calcualting

the cutoff

mc.cores Number of cores to use when running parallel

dtxsid.exclude

dtxsids to exclude, default NULL

do.cov If TRUE, calculate the covariance matrix and store in a global

do.compare If TRUE, compare the cutoffs with those from the original method with no gene-

gene correlation

to.file If TRUE, and do.compare=TRUE, send a plot of the comparison to a file

sigdbgenelist

full path to the signatureDB_genelist.RDS file

FCMAT2 Sample by gene matrix of log2(fold change)'s. Rownames are sample keys and

colnames are genes.

CHEM_DICT Dataframe with one row per sample key and seven columns: sample_key, sam-

ple_id, conc, time, casrn, name, dtxsid.

Value

calculated cutoffs dataframe

cutoffCalc.inner.empirical

Inner function for the cutoff calculation based on the empirical distri-

butions

Description

Inner function for the cutoff calculation based on the empirical distributions

Usage

```
cutoffCalc.inner.empirical(signature, pval, SIGSCOREMAT)
```

Arguments

signature The name of the signature for which the cutoff is to be calculated

pval The p-value for the baseline distribution

SIGSCOREMAT The signature score matrix

Value

vector containing the signature, cutoff, sd (one standard deviation of the signature score matrix), bmed (median of the signature score matrix)

cutoffCalc.inner.fc 7

```
cutoffCalc.inner.fc
```

Inner function for the cutoff calculation based on the analytical method

Description

Inner function for the cutoff calculation based on the analytical method

Usage

```
cutoffCalc.inner.fc(parent, catalog, allgenes, pval)
```

Arguments

parent The name of the signature parent for which the cutoff is to be calculated

catalog The signature catalog

allgenes The list of all the genes in the data set
pval The p-value for the baseline distribution

Value

vector containing the parent (signature), cutoff, sd, bmed

```
cutoffCalcEmpirical
```

Calculate the signature-wise cutoffs based on the empirical distributions which does not break any correlations between genes

Description

Calculate the signature-wise cutoffs based on the empirical distributions which does not break any correlations between genes

```
cutoffCalcEmpirical(
  pval = 0.05,
  nlowconc = 2,
  mc.cores = 1,
  dtxsid.exclude = NULL,
  signaturescoremat,
  CHEM_DICT
)
```

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Arguments

pval The p-value for the baseline distribution

nlowconc Only include the lowest nlowconc concentrations for each chemical

mc.cores Number of cores to use when running parallel

dtxsid.exclude

dtxsids to exclude, default NULL

signaturescoremat

Dataframe with one row per chemical/conc/signature combination. Columns are: sample_id, dtxsid, casrn, name, time, conc, sigset, signature, size, signa-

ture_score

CHEM_DICT Dataframe with one row per sample key and seven columns: sample_key, sam-

ple_id, conc, time, casrn, name, dtxsid.

Value

signature-wise cutoffs dataframe

exportSignatureCutoffs

Export the signature-wise cutoffs

Description

Export the signature-wise cutoffs

Usage

```
exportSignatureCutoffs(signature_cr)
```

Arguments

signature_cr dataframe returned by the signatureConcResp function

geneConcResp Gene Concentration Response

Description

Wrapper that performs concentration response modeling for gene/probe log2 fold-change values

GSEA 9

Usage

```
geneConcResp(
  mc.cores = 20,
  to.file.path = NULL,
  pval = 0.05,
  aicc = F,
  fitmodels = c("cnst", "hill", "poly1", "poly2", "pow", "exp2", "exp3", "exp4", "exp4",
```

Arguments

mc.cores	Number of parallel cores to use.
to.file.path	when provided, path of RDS file where results are written to
pval	P-value cutoff between 0 and 1.
aicc	If aicc = T, corrected AIC is used instead of first order (regular) AIC.
fitmodels	Vector of models names to be used. Default is all of them.
genefile	An optional file $(.xlsx)$ that can be used to filter concentration-response modeling for a subset of genes of interest
FCMAT2	chem/conc by gene or chem/conc by probe. Uses two lowest concentration of each column to estimate noise cutoff (as opposed to signature CR).
CHEM_DICT	Dataframe with one row per sample key and seven columns: sample_key, sample_id, conc, time, casrn, name, dtxsid.

Details

Uses two lowest concentration of each column to estimate noise cutoff (as opposed to signature CR).

Value

dataframe of concentration response modeling results

GSEA	My Gene Set Enrichment Analysis

Description

Performs tweaked version of single sample GSEA.

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Usage

```
GSEA(
   X,
   geneSets,
   min.sz = 1,
   max.sz = Inf,
   alpha = 0.25,
   verbose = T,
   useranks = T
)
```

Arguments

X	Transposed FCMAT2; i.e a gene by sample matrix of l2fc's including rownames and colnames. Equivalent to expr in gsva.
geneSets	Named list of signature definitions. Each element is a vector of gene names. Each element name is a signature name. E quivalent to gset.idx.list in gsva.
min.sz	Minimum signature size (deprecated).
max.sz	Maximum signature size (deprecated)
alpha	Power of R to use. Higher alpha will upweight more extreme ranks relative to middle ranks.
verbose	verbose = T prints gene set length message.
useranks	useranks = T uses ranks as in ssGSEA, while useranks = F uses the bare fold changes instead.

Details

Based on the GSVA ssGSEA code. Main changes are: NAs are now handled correctly and rank is now centered on zero instead of beginning at one. Since signature sizes are undercounted here due to missing values, they are assessed more accurately in signatureScoreCoreGSEA and limits are enforced after scoring.

Value

Outputs signature by sample matrix of signature scores.

Examples

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myrndwalk

 $GSVA:::rndwalk\ but\ able\ to\ handle\ sum(Ralpha)=0$

Description

GSVA:::rndwalk but able to handle sum(Ralpha) = 0

Usage

```
myrndwalk(gSetIdx, geneRanking, j, R, alpha)
```

Arguments

```
gSetIdx gSetIdx
geneRanking geneRanking
j j
R R
alpha alpha
```

printCurrentFunction

Print the name of the current function

Description

Print the name of the current function

Usage

```
printCurrentFunction(comment.string = NA)
```

Arguments

```
comment.string
```

An optional string to be printed

Value

nothing

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R2

R Squared

Description

Calculate coefficient of determination.

Usage

```
R2(y, pred)
```

Arguments

```
y Vector of actual values.pred Vector of corresponding predicted values.
```

Details

Note that order matters: R2(x,y) != R2(y,x) in general.

Value

Coefficient of determination.

Examples

```
R2(c(1:10), c(1:10*.8))
R2(c(1:10*.8), c(1:10))
```

randomdata

Randomized Null Data

Description

Generate randomized null data based on actual data.

```
randomdata(
  nchem = 1000,
  seed = 12345,
  maxconc = 1e+06,
  nlowconc = 2,
  dtxsid.exclude = NULL,
  FCMAT2,
  CHEM_DICT,
```

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```
output_dir = "../data/",
writing_to_disk = FALSE
)
```

Arguments

nchem Number of null chemicals. Number of null samples is approximately eight times

this value.

seed Random seed.

maxconc Only use concentrations less than maxconc, default 1000000

nlowconc If not NULL, only include the lowest nlowconc concentrations for each chemical

dtxsid.exclude

dtxsids to exclude, default NULL

FCMAT2 Sample by gene matrix of log2(fold change)'s. Rownames are sample keys and

colnames are genes.

CHEM DICT Data frame with one row per sample key and seven columns: sample key, sam-

ple_id, conc, time, casrn, name, dtxsid.

output_dir full path to directory/file where the CHEM_DICT/FCMAT2 data frames should

be saved

writing_to_disk

boolean, TRUE if the resulting CHEM_DICT/FCMAT2 data frames are to be

saved to disk

Details

Randomization is performed by sampling the quantile function for each gene in the actual data. The null set will have roughly the same distribution of values for each gene in the actual data.

Value

list of the randomized FCMAT2 and CHEM_DICT data frame

RMSE Root-mean-square-error

Description

Computes root-mean-square-error between two vectors.

Usage

```
RMSE(x, y)
```

Arguments

x First vector.y Second vector.

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Value

RMSE

Examples

```
RMSE(1:3, c(1,3,5))
```

rowMean

Utility function used by cutoffCalc.inner.fc

Description

Utility function used by cutoffCalc.inner.fc

Usage

```
rowMean(x)
```

Arguments

x = matrix or data.frame

Value

vector of mean value of each row

```
runAllSignatureCR Run All Pathway Concentration Response (P-Value)
```

Description

Driver for signature scoring and concentration response (CR).

```
runAllSignatureCR(
  dataset,
  sigset,
  sigcatalog = "../inst/extdata/signatureDB_master_catalog_2022-05-16.xlsx",
  method,
  bmr_scale = 1.349,
  normfactor = 7500,
  minsigsize = 10,
  pval = 0.05,
  nlowconc = 2,
  mc.cores = 1,
```

signatureCatalogLoader 15

```
fitmodels = c("cnst", "hill", "poly1", "poly2", "pow", "exp2", "exp3", "exp4", "e
FCMAT2,
CHEM_DICT,
sigdbgenelist = "../inst/extdata/signatureDB_genelists.RDS"
)
```

Arguments

dataset	Name of data set.
sigset	Name of signature set.
sigcatalog	Name of the signature catalog
method	Pathway scoring method in c("fc", "gsva", "gsea")
bmr_scale	benchmark response (bmr) scaling factor. Default = 1.349
normfactor	Factor to scale the native units up by to get onto a reasonable plotting value (\sim -1 to 1)
minsigsize	Minimum signature size.
pval	P-value to use for noise estimation.
nlowconc	Only include the lowest nlowconc concentrations for each chemical
mc.cores	Vector with two values: number of cores to use for signature scoring and number of cores to use for CR. CR can usually handle the maximum number, but gsva scoring might require a smaller number to avoid memory overflow.
fitmodels	Vector of model names to run conc/resp with. "cnst" should always be chosen.
FCMAT2	Sample by gene matrix of log2(fold change)'s. Rownames are sample keys and colnames are genes.
CHEM_DICT	Dataframe with one row per sample key and seven columns: sample_key, sample_id, conc, time, casrn, name, dtxsid.
sigdbgenelis	
	full path to signature DB gene list file; default is repo version

Value

dataframe with signature concentration-response results

```
signatureCatalogLoader

Read in signature catalog
```

Description

Read in signature catalog

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Usage

```
signatureCatalogLoader(
  sigset = "wgcna",
  sigcatalog = "../inst/extdata/signatureDB_master_catalog_2022-05-16.xlsx",
  sigdbgenelist = "../inst/extdata/signatureDB_genelists.RDS"
)
```

Arguments

```
sigset Name of the signature set to use; derived from the sigcatalog sigcatalog full path to signature catalog xlsx file; default is repo version sigdbgenelist full path to signature DB gene list file; default is repo version
```

Value

the trimmed signature table

```
signatureConcResp Pathway Concentration Response (P-value)
```

Description

Performs signature concentration response using p-value based cutoffs.

```
signatureConcResp(
 dataset,
  sigset,
  sigcatalog = "../inst/extdata/signatureDB_master_catalog_2022-05-16.xlsx",
 method,
 bmr scale = 1.349,
 mc.cores = 1,
 pval = 0.05,
 nlowconc = 2,
 aicc = F,
 dtxsid.exclude = NULL,
 minsigsize = 10,
  fitmodels = c("cnst", "hill", "poly1", "poly2", "pow", "exp2", "exp3", "exp4", "e
  signaturescoremat,
  sigdbgenelist = "../inst/extdata/signatureDB_genelists.RDS",
  CHEM DICT
)
```

signatureScore 17

Arguments

sigset Name of the signature set.

sigcatalog Name of the signature catalog file

method Pathway scoring method in c("fc", "gsva", "gsea")

bmr_scale bmr scaling factor. Default = 1.349
mc.cores Number of cores to parallelize with.

pval Desired cutoff p-value.

nlowconc Only include the lowest nlowconc concentrations for each chemical

aicc = T uses corrected AIC to choose winning method; otherwise regular AIC

dtxsid.exclude

dtxsids to exclude, default NULL

minsigsize Minimum allowed signature size. Sample/signature combinations with less than

this number of non-missing 12fc's will be discarded.

fitmodels Vector of model names to use. Probably should include "cnst".

signaturescoremat

dataframe returned by the upstream signatureScoreMerge function

sigdbgenelist

full path to signature DB gene list file; default is repo version

CHEM_DICT Dataframe with one row per sample key and seven columns: sample_key, sam-

ple id, conc, time, casrn, name, dtxsid.

Details

dataset should have already been scored using signatureScore and signatureScoreMerge and the given sigset and method. This function prepares signatureScore output for CR processing, calls tcplfit2::concRespCore, and formats the output.

Value

dataframe with signature CR output.

signatureScore Signature Score

Description

Computes and saves signature scores.

18 signatureScore

Usage

```
signatureScore(
  FCMAT2,
  CHEM_DICT,
  sigset,
  sigcatalog = "../inst/extdata/signatureDB_master_catalog_2022-05-16.xlsx",
  method,
  normfactor = 7500,
  mc.cores = 1,
  minsigsize = 10,
  sigdbgenelist = "../inst/extdata/signatureDB_genelists.RDS"
)
```

Arguments

FCMAT2	Sample by gene matrix of log2(fold change)'s. Rownames are sample keys and colnames are genes.
CHEM_DICT	Dataframe with one row per sample key and seven columns: sample_key, sample_id, conc, time, casrn, name, dtxsid.
sigset	Name of signature set.
sigcatalog	full path to signature catalog xlsx file; default is repo version
method	Signature scoring method in c("fc", "gsva", "gsea")
normfactor	Value passed to the plotting code to scale the y values
mc.cores	Number of cores to use.
minsigsize	Minimum allowed signature size BEFORE accounting for missing values.
sigdbgenelis	t
	full path to signature DB gene list file; default is repo version

Details

signatureScore is a driver for various scoring methods. The three that are currently available are "gsva", "gsea", "fc". Beware running out of memory on large runs with gsva, Linux, and many cores – ensure your system has enough memory allocated depending on data size. Signature size is counted according to number of genes in the signature that are also in the column names of FCMAT2. However, each method performs a more rigorous size count internally that accounts for missing values and adds this to the output.

Value

Returns data frame of signature scores

signatureScoreCoreFC 19

```
signatureScoreCoreFC
```

Signature Score Core - FC

Description

Computes fold change signature scores.

Usage

```
signatureScoreCoreFC(
  fcmat,
  sigset,
  chem_dict,
  signature_data,
  ngenemax = NULL,
  verbose = F
)
```

Arguments

fcmat	Expects FCMAT2. Sample by gene matrix of log2(fold change)'s. Rownames are sample keys and colnames are genes.
sigset	Name of signature set.
chem_dict	Expects CHEM_DICT object. Dataframe with one row per sample key and seven columns: sample_key, sample_id, conc, time, casrn, name, dtxsid.
signature_data	
	Named list of gene name vectors. Each element is one signature, defined by the genes it contains.
ngenemax	If ngene is not NULL, then only the most extreme n genes of the signature will

be used for the "in" set

verbose If TRUE, write extra diagnostic output

Details

This fast implementation of fold change signature scores uses matrix multiplication. The score is simply: mean(fold change of genes in signature) - mean(fold change of genes outside signature).

Value

Dataframe with one row per chemical/conc/signature combination. Columns are: sample_id, dtxsid, casrn, name, time, conc, sigset, signature, size (signature size accounting for missing values), mean_fc_scaled_in, mean_fc_scaled_out, signature_score.

```
signatureScoreCoreGSEA
```

Signature Score Core - GSEA

Description

Computes signature scores for gsea.

Usage

```
signatureScoreCoreGSEA(
    sk.list,
    normfactor = 7500,
    sigset,
    fcmat,
    chem_dict,
    signature_data,
    mc.cores = 1,
    normalization = T,
    useranks = T
)
```

Arguments

sk.list Sample keys to use; should correspond to fcmat rownames.

normfactor = proceed on first 1/normfactor of GSEA data

sigset Name of signature set.

fcmat Expects FCMAT2. Sample by gene matrix of log2(fold change)'s. Rownames

are sample keys and colnames are genes.

seven columns: sample_key, sample_id, conc, time, casrn, name, dtxsid.

signature_data

Named list of gene name vectors. Each element is one signature, defined by the

genes it contains.

mc.cores Number of cores to use.

normalization

normalization = T normalizes final scores.

useranks useranks = T uses score ranks for weighting; otherwise, fold changes are used

for weights.

Details

This function is a parallelized wrapper for gsea, which does the actual scoring. gsea method uses ranks and normalizationby default. Normalization divides final scores by difference between max and min score. Without normalization, scores from individual samples have no impact on each other.

Value

Dataframe with one row per chemical/conc/signature combination. Columns are: sample_id, dtxsid, casrn, name, time, conc, sigset, signature, size, signature_score

```
signatureScoreCoreGSVA
```

Signature Score Core - GSVA

Description

Computes GSVA signature scores.

Usage

```
signatureScoreCoreGSVA(
   sk.list,
   sigset = "FILTERED",
   fcmat,
   chem_dict,
   signature_data,
   mc.cores = 1
)
```

Arguments

sk.list	Sample keys to use; should correspond to fcmat rownames.
sigset	Name of signature set.
fcmat	Expects FCMAT2. Sample by gene matrix of log2(fold change)'s. Rownames are sample keys and colnames are genes.
chem_dict	Expects CHEM_DICT object. Dataframe with one row per sample key and seven columns: sample_key, sample_id, conc, time, casrn, name, dtxsid.
signature_data	
	Named list of gene name vectors. Each element is one signature, defined by the genes it contains.
mc.cores	Number of cores to use. Parallelization is performed by gsva itself.

Details

This function is a wrapper for GSVA with Gaussian cumulative distribution function (cdf) kernels.

Value

Dataframe with one row per chemical/conc/signature combination. Columns are: sample_id, dtxsid, casrn, name, time, conc, sigset, signature, size, signature_score

TxT

```
signatureScoreMerge
```

Merge the up and down halves of the directional pathway data

Description

Merge the up and down halves of the directional pathway data

Usage

```
signatureScoreMerge(
   sigset,
   sigcatalog = "../inst/extdata/signatureDB_master_catalog_2022-05-16.xlsx",
   method,
   signaturescoremat,
   sigdbgenelist = "../inst/extdata/signatureDB_genelists.RDS"
)
```

Arguments

```
sigset Name of the signature set.

sigcatalog Name of the catalog file

method Pathway scoring method in c("fc", "gsva", "gsea")

signaturescoremat
dataframe returned by the upstream signatureScore function

sigdbgenelist
full path to signature DB gene list file; default is repo version
```

Value

signaturescoremat dataframe

TxT

Calculate several statistics on a 2 x 2 matrix

Description

Calculate several statistics on a 2 x 2 matrix

```
TxT(tp, fp, fn, tn, do.p = TRUE, rowname = NA)
```

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Arguments

tp	number of true positives
fp	number of false positives
fn	number of false negatives
tn	number of true negatives
do.p	if TRUE, calculate an exact p-value
rowname	if not NA, add a column to the output with this rowname

Value

Returns a list of the results with the following columns: TP (true positives), FP (false positives), FN (false negatives), TN (true negatives), Sens (sensitivity), Spec (specificity), BA (Balanced Accuracy), Acrcy (Accuracy), RelRsk Relative Risk, OR Odds Ratio, CI.OR.LWR (lower confidence interval of the Odds Ratio), CI.OR.UPR (upper confidence interval of the Odds Ratio), PPV (Positive Predictive Value), NPV (Negative Predictive Value), F1 (2TP/(2TP+FP+FN)), p.value (Chi-squared p-value)

WRMSE

Weighted Root-mean-square-error

Description

Computes root-mean-square error with weighted average.

Usage

```
WRMSE(x, y, w)
```

Arguments

x First vector of numbers.
 y Second vector of numbers.
 w Vector of weights.

Details

x,y,w should all be the same length. Order of x and y won't change output.

Value

Weighted RMSE.

Examples

```
WRMSE (1:3, c(1,3,5), 1:3)
```

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