Package ‘doppelgangR’

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Depends R (>= 3.3), Biobase, BiocParallel

Suggests BiocStyle, knitr, rmarkdown, curatedOvarianData, ROCR, pROC, RUnit, simulatorZ, proxy

Imports sva, impute, digest, mnormt, methods, grDevices, graphics, stats, utils

Author Levi Waldron, Markus Riester, Marcel Ramos

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License GPL (>=2.0)

Title Identify likely duplicate samples from genomic or meta-data

Description The main function is doppelgangR(), which takes as minimal input a list of ExpressionSet object, and searches all list pairs for duplicated samples. The search is based on the genomic data (exprs(eset)), phenotype/clinical data (pData(eset)), and ‘‘smoking guns’’ - supposedly unique identifiers found in pData(eset).

URL https://github.com/lwaldron/doppelgangR

BugReports https://github.com/lwaldron/doppelgangR/issues

VignetteBuilder knitr

biocViews RNASeq, Microarray, GeneExpression, QualityControl

NeedsCompilation no

R topics documented:

doppelgangR-package .......................................................... 2
corFinder ............................................................................ 3
DoppelGang-class ................................................................. 4
doppelgangR ................................................................. 5
dst ................................................................................... 6
mst.mle ................................................................................. 8
outlierFinder ........................................................................ 10
phenoDist ........................................................................... 11
phenoFinder ......................................................................... 12
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The DESCRIPTION file:

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Maintainer: Levi Waldron <lwaldron.research@gmail.com>
Depends: R (>= 3.3), Biobase, BiocParallel
Suggests: BiocStyle, knitr, rmarkdown, curatedOvarianData, ROCR, pROC, RUnit, simulatorZ, proxy
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Index of help topics:

- DoppelGang-class
- corFinder
- doppelgangR
- doppelgangR-package
- dst

DoppelGang S4 class
Calculate pair-wise correlations between samples using the expr() slots of a list of two ExpressionSets.
doppelgangR
doppelgangR-package
 Identify likely duplicate samples from genomic or meta-data
dst
Skew-t Distribution
corFinder

mst.mle Maximum likelihood estimation for a (multivariate) skew-t distribution
outlierFinder Identifies outliers in a similarity matrix.
phenoDist Calculate distance between two vectors, rows of one matrix/dataframe, or rows of two matrices/dataframes.
phenoFinder Calculate pairwise similarities of phenoData between samples for a list containing two ExpressionSets
plot-methods Histograms of all pairwise sample correlations, showing identified doppelgangers.
print-methods Print a DoppelGang object
show-methods Show a DoppelGang object
smokingGunFinder Find doppelgangers based on “smoking gun” phenotypes - those that should be unique to each patient.
summary-methods Summarizes a DoppelGang object
vectorHammingDist Calculate Hamming Distance between two vectors, using pairwise complete observations.
vectorWeightedDist Calculate a weighted distance between two vectors, using pairwise complete observations.

Author(s)
Levi Waldron, Markus Riester, Marcel Ramos
Maintainer: Levi Waldron <lwaldron.research@gmail.com>

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corFinder

Calculate pair-wise correlations between samples using the expr() slots of a list of two ExpressionSets.

Description
This function acts as a wrapper around ComBat (sva package) and cor(), to calculate pairwise correlations within one or between two ExpressionSets.

Usage

```r
corFinder(eset.pair, separator = ":", use.ComBat = TRUE, ...)
```

Arguments

- **eset.pair**: a list of ExpressionSets, with two elements. If the two elements are identical, return the correlation matrix for pairs of samples in the first element. If not identical, return pairs between the two elements.
- **separator**: Separator between dataset name and sample name. Dataset names are added to sample names to keep track of dataset of origin.
- **use.ComBat**: Use the sva::ComBat function for batch correction of the expr() data between the two datasets.
- **...**: Extra arguments passed to the cor() function.
Value

Returns a matrix of sample-wise Pearson Correlations.

Author(s)

Levi Waldron, Markus Riester, Marcel Ramos

Examples

```r
example("phenoFinder")
corFinder(esets2)
```

---

DoppelGang-class

**DoppelGang S4 class**

Description

S4 class containing results of doppelgangR() function.

Objects from the Class

Objects can be created by calls of the form `new(DoppelGang ...)`

Slots

- `fullresults`: Object of class "list"
- `summaryresults`: Object of class "data.frame"
- `inputargs`: "list" object containing input arguments to doppelgangR() function.

Methods

- `plot` signature(x = "DoppelGang"): See ?plot,DoppelGang-method
- `summary` signature(object = "DoppelGang"): produces a data.frame of potential doppel-gangers, with similarity measures and available phenoData for both of each potential doppel-ganger pair. Can be saved as a csv table and inspected carefully in a spreadsheet.
- `print` signature(x = "DoppelGang"): ...
- `show` signature(object = "DoppelGang"): ...

Author(s)

Levi Waldron and Markus Riester

See Also

`plot,DoppelGang-method`
**Description**

Identify samples with suspiciously high correlations and phenotype similarities

**Usage**

```r
doppelgangR(esets, separator = "\n", corFinder.args = list(separator = separator,
  use.ComBat = TRUE, method = "pearson"),
  phenofinder.args = list(separator = separator,
  vectorDistFun = vectorWeightedDist),
  outlierFinder.expr.args = list(bonf.prob = 0.5,
  transFun = atanh, tail = "upper"),
  outlierFinder.pheno.args = list(normal.upper.thresh = 0.99,
  bonf.prob = NULL, tail = "upper"),
  smokingGunFinder.args = list(transFun = I),
  impute.knn.args = list(k = 10, rowmax = 0.5, colmax = 0.8,
  maxp = 1500, rng.seed = 362436069),
  automatic.smokingguns = NULL,
  automatic.smokingguns = FALSE, within.datasets.only = FALSE,
  intermediate.pruning = FALSE, cache.dir = "cache", BPPARAM = bpparam(),
  verbose = TRUE)
```

**Arguments**

- `esets` a list of ExpressionSets, containing the numeric and phenotypic data to be analyzed.
- `separator` a delimiter to use between dataset names and sample names
- `corFinder.args` a list of arguments to be passed to the corFinder function.
- `phenofinder.args` a list of arguments to be passed to the phenoFinder function. If NULL, samples with similar phenotypes will not be searched for.
- `outlierFinder.expr.args` a list of arguments to be passed to outlierFinder when called for expression data
- `outlierFinder.pheno.args` a list of arguments to be passed to outlierFinder when called for phenotype data
- `smokingGunFinder.args` a list of arguments to be passed to smokingGunFinder
- `impute.knn.args` a list of arguments to be passed to impute::impute.knn. Set to NULL to do no knn imputation.
- `manual.smokingguns` a character vector of phenoData columns that, if identical, will be considered evidence of duplication
- `automatic.smokingguns` automatically look for "smoking guns." If TRUE, look for phenotype variables that are unique to each patient in dataset 1, also unique to each patient in dataset 2, but contain exact matches between datasets 1 and 2.
- `within.datasets.only` If TRUE, only search within each dataset for doppelgangers.
intermediate.pruning

The default setting FALSE will result in output with no missing values, but uses extra memory because all results from the expression, phenotype, and smoking gun doppelganger searches must be saved until the end. Setting this to TRUE will save memory for very large searches, but distance metrics will only be available if that value was identified as a doppelganger (for example, phenotype doppelgangers will have missing values for the expression and smoking gun similarity).

cache.dir

The name of a directory in which to cache or look up results to save re-calculating correlations. Set to NULL for no caching.

BPPARAM

Argument for BiocParallel::bplapply(), by default will use all cores of a multi-core machine

verbose

Print progress information

Value

Returns an object of S4-class "DoppelGang". See ?DoppelGang-class.

Author(s)

Levi Waldron, Markus Riester, Marcel Ramos

See Also

?BiocParallel::BiocParallelParam-class

Examples

echant("phenoFinder")

results2 <- doppelgangR(esets2, cache.dir = NULL)
results2
plot(results2)
summary(results2)
## Set phenoFinder.args=NULL to ignore similar phenotypes, and
## turn off ComBat batch correction:
## results2 <- doppelgangR(testesets, corfinder.args=list(use.ComBat=FALSE), phenoFinder.args=NULL, cache
## summary(results2)

dst

Skew-t Distribution

Description

Density function, distribution function and random number generation for the skew-t (ST) distribution. Functions copied from sn CRAN library v0.4.18 for argument name compatibility with st.mle function from the same version.

Usage

dst(x, location = 0, scale = 1, shape = 0, df = Inf, dp = NULL, log = FALSE)
pst(x, location = 0, scale = 1, shape = 0, df = Inf, dp = NULL, ...)
qst(p, location = 0, scale = 1, shape = 0, df = Inf, tol = 1e-06, dp = NULL, ...)
rst(n = 1, location = 0, scale = 1, shape = 0, df = Inf, dp = NULL)
Arguments

- \texttt{x}: vector of quantiles. Missing values (NAs) are allowed.
- \texttt{p}: vector of probabilities
- \texttt{location}: vector of location parameters.
- \texttt{scale}: vector of (positive) scale parameters.
- \texttt{shape}: vector of shape parameters. With \texttt{pst} and \texttt{qst}, it must be of length 1.
- \texttt{df}: degrees of freedom (scalar); default is \texttt{df=Inf} which corresponds to the skew-normal distribution.
- \texttt{dp}: a vector of length 4, whose elements represent location, scale (positive), shape and \texttt{df}, respectively. If \texttt{dp} is specified, the individual parameters cannot be set.
- \texttt{n}: sample size.
- \texttt{log}: logical; if TRUE, densities are given as log-densities.
- \texttt{tol}: a scalar value which regulates the accuracy of the result of \texttt{qsn}.
- \texttt{...}: additional parameters passed to \texttt{integrate}.

Value

Density (\texttt{dst}), probability (\texttt{pst}), quantiles (\texttt{qst}) and random sample (\texttt{rst}) from the skew-t distribution with given location, scale, shape and \texttt{df} parameters.

Details

Typical usages are

- \texttt{dst(x, location=0, scale=1, shape=0, df=Inf, log=FALSE)}
- \texttt{dst(x, dp=, log=FALSE)}
- \texttt{pst(x, location=0, scale=1, shape=0, df=Inf, \ldots)}
- \texttt{pst(x, dp=, log=FALSE)}
- \texttt{qst(p, location=0, scale=1, shape=0, df=Inf, tol=1e-8, \ldots)}
- \texttt{qst(x, dp=, log=FALSE)}
- \texttt{rst(n=1, location=0, scale=1, shape=0, df=Inf)}
- \texttt{rst(x, dp=, log=FALSE)}

Background

The family of skew-t distributions is an extension of the Student’s \textit{t} family, via the introduction of a shape parameter which regulates skewness; when \texttt{shape=0}, the skew-\textit{t} distribution reduces to the usual Student’s \textit{t} distribution. When \texttt{df=Inf}, it reduces to the skew-normal distribution. A multivariate version of the distribution exists. See the reference below for additional information.

References


See Also

\texttt{st.mle}
Examples

```r
pdf <- dst(seq(-4, 4, by=0.1), shape=3, df=5)
rnd <- rst(100, 5, 2, -5, 8)
q <- qst(c(0.25, 0.5, 0.75), shape=3, df=5)
stopifnot(identical(all.equal(pst(q, shape=3, df=5), c(0.25, 0.5, 0.75)), TRUE))
```

mst.mle  
*Maximum likelihood estimation for a (multivariate) skew-t distribution*

Description

Fits a skew-t (ST) or multivariate skew-t (MST) distribution to data, or fits a linear regression model with (multivariate) skew-t errors, using maximum likelihood estimation. Functions copied from sn CRAN library v0.4.18 because they were later deprecated in that library.

Usage

```r
mst.mle(X, y, freq, start, fixed.df=NA, trace=FALSE,
        algorithm = c("nlminb", "Nelder-Mead", "BFGS", "CG", "SANN"),
        control=list())
```

```r
st.mle(X, y, freq, start, fixed.df=NA, trace=FALSE,
       algorithm = c("nlminb", "Nelder-Mead", "BFGS", "CG", "SANN"),
       control=list())
```

Arguments

- **y**  
  a matrix (for mst.mle) or a vector (for st.mle). If y is a matrix, rows refer to observations, and columns to components of the multivariate distribution.

- **X**  
  a matrix of covariate values. If missing, a one-column matrix of 1’s is created; otherwise, it must have the same number of rows of y. If X is supplied, then it must include a column of 1’s.

- **freq**  
  a vector of weights. If missing, a vector of 1’s is created; otherwise it must have length equal to the number of rows of y.

- **start**  
  for mst.mle, a list containing the components beta, Omega, alpha, df of the type described below; for st.mle, a vector whose components contain analogous ingredients as before, with the exception that the scale parameter is the square root of Omega. In both cases, the dp component of the returned list from a previous call has the required format and it can be used as a new start. If the start parameter is missing, initial values are selected by the function.

- **fixed.df**  
  a scalar value containing the degrees of freedom (df), if these must be taken as fixed, or NA (default value) if df is a parameter to be estimated.

- **trace**  
  logical value which controls printing of the algorithm convergence. If trace=TRUE, details are printed. Default value is FALSE.

- **algorithm**  
  a character string which selects the numerical optimization procedure used to maximize the loglikelihood function. If this string is set equal to "nlminb", then this function is called; in all other cases, optim is called, with method set equal to the given string. Default value is "nlminb".

- **control**  
  this parameter is passed to the chose optimizer, either nlminb or optim; see the documentation of this function for its usage.
Details

If y is a vector and it is supplied to \texttt{mst.mle}, then it is converted to a one-column matrix, and a
scalar skew-t distribution is fitted. This is also the mechanism used by \texttt{st.mle} which is simply an
interface to \texttt{mst.mle}.

The parameter \texttt{freq} is intended for use with grouped data, setting the values of y equal to the central
values of the cells; in this case the resulting estimate is an approximation to the exact maximum
likelihood estimate. If \texttt{freq} is not set, exact maximum likelihood estimation is performed.

Numerical search of the maximum likelihood estimates is performed in a suitable re-parameterization
of the original parameters with aid of the selected optimizer (\texttt{nlminb} or \texttt{optim}) which is supplied
with the derivatives of the log-likelihood function. Notice that, in case the optimizer is \texttt{optim}, the
gradient may or may not be used, depending on which specific method has been selected. On exit
from the optimizer, an inverse transformation of the parameters is performed. For a specific description
on the re-parametrization adopted, see Section 5.1 and Appendix B of Azzalini \\& Capitanio (2003).

Value

A list containing the following components:

\begin{itemize}
    \item \texttt{call} a string containing the calling statement.
    \item \texttt{dp} for \texttt{mst.mle}, this is a list containing the direct parameters \texttt{beta}, \texttt{Omega}, \texttt{alpha}.
        Here, \texttt{beta} is a matrix of regression coefficients with \texttt{dim(beta)=c(ncol(X),ncol(y))},
        \texttt{Omega} is a covariance matrix of order \texttt{ncol(y)}, \texttt{alpha} is a vector of shape pa-
        rameters of length \texttt{ncol(y)}. For \texttt{st.mle}, \texttt{dp} is a vector of length \texttt{ncol(X)+3},
        containing \texttt{c(beta, omega, alpha, df)}, where \texttt{omega} is the square root of
        \texttt{Omega}.
    \item \texttt{se} a list containing the components \texttt{beta}, \texttt{alpha}, \texttt{info}. Here, \texttt{beta} and \texttt{alpha} are
        the standard errors for the corresponding point estimates; \texttt{info} is the observed
        information matrix for the working parameter, as explained below.
    \item \texttt{algorithm} the list returned by the chose optimizer, either \texttt{nlminb} or \texttt{optim}, plus an item
        with the name of the selected algorithm; see the documentation of either \texttt{nlminb}
        or \texttt{optim} for explanation of the other components.
\end{itemize}

Background

The family of multivariate skew-t distributions is an extension of the multivariate Student’s t family,
via the introduction of a shape parameter which regulates skewness; when \texttt{shape}=0, the skew-t
distribution reduces to the usual t distribution. When \texttt{df}=Inf the distribution reduces to the multi-
variate skew-normal one; see \texttt{dmsn}. See the reference below for additional information.

References

emphasis on a multivariate skew \textit{t} distribution. The full version of the paper published in abridged
\texttt{se-ext.ps}

See Also

\texttt{dst}
outlierFinder

Identifies outliers in a similarity matrix.

Description
By default uses the Fisher z-transform for Pearson correlation (atanh), and identifies outliers as those above the quantile of a skew-t distribution with mean and standard deviation estimated from the z-transformed matrix. The quantile is calculated from the Bonferroni-corrected cumulative probability of the upper tail.

Usage
outlierFinder(similarity.mat, bonf.prob = 0.05, transFun = atanh, normal.upper.thresh = NULL, tail = "upper")

Arguments
similarity.mat  A matrix of similarities - larger values mean more similar.
bonf.prob  Bonferroni-corrected probability. A raw.prob is calculated by dividing this by the number of non-missing values in similarity.mat, and the rejection threshold is qnorm(1-raw.prob, mean, sd) where mean and sd are estimated from the transFun-transformed similarity.mat.
transFun  A function applied to the numeric values of similarity.mat, that should result in normally-distributed values.
normal.upper.thresh  Instead of specifying bonf.prob and transFun, an upper similarity threshold can be set, and values above this will be considered likely duplicates. If specified, this over-rides bonf.prob.
tail  "upper" to look for samples with very high similarity values, "lower" to look for very low values, or "both" to look for both.

Value
Returns either NULL or a dataframe with three columns: sample1, sample2, and similarity.

Author(s)
Levi Waldron, Markus Riester, Marcel Ramos

Examples
library(curatedOvarianData)
data(GSE32063_eset)
cormat <- cor(exprs(GSE32063_eset))
outlierFinder(cormat, bonf.prob = 0.05)

dat <- rt(100, df=5, ncp=100)
fit <- st.mle(y=dat)
fit
phenoDist

Calculate distance between two vectors, rows of one matrix/dataframe, or rows of two matrices/dataframes.

Description

This function does some simple looping to allow x and y to be various combinations of vectors and matrices/dataframes.

Usage

phenoDist(x, y = NULL, bins = 10, vectorDistFun = vectorWeightedDist, ...)

Arguments

x A vector, matrix or dataframe
y NULL, a vector, matrix, or dataframe. If x is a vector, y must also be specified.
bins discretize continuous fields in the specified number of bins
vectorDistFun A function of two vectors that returns the distance between those vectors.
... Extra arguments passed on to vectorDistFun

Value

a matrix of distances between pairs of rows of x (if y is unspecified), or between all pairs of rows between x and y (if both are provided).

Author(s)

Levi Waldron, Markus Riester, Marcel Ramos

Examples

e.example("phenoFinder")
pdat1 <- pData(esets2[[1]])
pdat2 <- pData(esets2[[2]])

## Use phenoDist() to calculate a weighted distance matrix
distmat <- phenoDist(as.matrix(pdat1), as.matrix(pdat2))
## Note outliers with identical clinical data, these are probably the same patients:
go.graphics::boxplot(distmat)
Calculate pairwise similarities of phenoData between samples for a list containing two ExpressionSets

Description
This function acts as a wrapper to phenoDist to handle cases of one ExpressionSet, a list of two identical ExpressionSets, or a list of two different ExpressionSets.

Usage
phenoFinder(eset.pair, separator = ":", ...)

Arguments
eset.pair input: a list of ExpressionSets with two elements, or an ExpressionSet. If the two elements are identical, return the correlation matrix for pairs of samples in the first element. If not identical, return pairs between the two elements.

separator a separator between dataset name (taken from the list names) and sample name (taken from sampleNames(eset), to keep track of which samples come from which dataset.

...
Extra arguments passed on to phenoDist

Value
A matrix of similarities between the phenotypes of pairs of samples.

Author(s)
Levi Waldron, Markus Riester, Marcel Ramos

Examples
library(curatedOvarianData)
data(GSE32063_eset)
data(GSE17260_eset)
esets2 <- list(JapaneseB=GSE32063_eset,
               Yoshihara2010=GSE17260_eset)
## standardize the sample ids to improve matching based on clinical annotation
esets2 <- lapply(esets2, function(X){
  X$alt_sample_name <- paste(X$sample_type, gsub("[^0-9]", ",", X$alt_sample_name), sep="-")
}
## Removal of columns that cannot possibly match also helps duplicated patients to stand out
pData(X) <- pData(X)[, !grepl("uncurated_author_metadata", colnames(pData(X)))]
X <- X[, 1:20] ##speed computations
return(X) })
## See first six samples in both rows and columns
phenoFinder(esets2)[1:6, 1:6]
**plot-methods**

**Histograms of all pairwise sample correlations, showing identified doppelgangers.**

**Description**

Identified doppelgangers are shown with a red vertical line overlaid on a histogram of pairwise sample correlations. One plot is made per pair of datasets.

**Arguments**

- `x` An object of class `DoppelGang`
- `skip.no.doppels` (default FALSE) If TRUE, do not plot histograms where no doppelgangers were identified.
- `plot.pair` An optional character vector of length two, providing the names of two datasets. If provided, only the comparison of these two datasets will be plotted.
- `...` Additional arguments passed on to `hist`.

**Value**

None

**Methods**

signature(x = "DoppelGang") Histograms of all pairwise sample correlations, showing identified doppelgangers.

**Author(s)**

Levi Waldron

**Examples**

```r
library(curatedOvarianData)
data(TCGA_eset)
data(GSE26712_eset)
## Remove some TCGA samples to speed computation:
```
smokingGunFinder

Find doppelgangers based on "smoking gun" phenotypes - those that should be unique to each patient.

Description

Checks all pairwise combinations of samples for values of the "smoking" gun phenotypes that are identical.

Usage

smokingGunFinder(eset.pair, smokingguns, transFun = I, separator = ":")
**Arguments**

- `eset.pair`  
  A list of ExpressionSets, with two elements. If the two elements are identical, the function will check for duplicate IDs within one element. If not identical, it will check for duplicate IDs between elements.

- `smokingguns`  
  Phenodata column names found in multiple elements of `eset.pair` that may contain "smoking guns" such as identifiers that should be unique to each sample.

- `transFun`  
  A function to apply to IDs before comparing. By default apply no transformation.

- `separator`  
  Separator between dataset name and sample name. Dataset names are added to sample names to keep track of dataset of origin.

**Value**

Returns an adjacency matrix for samples where matches have value 1, non-matches have value zero. Value for a sample against itself is NA.

**Author(s)**

Levi Waldron, Markus Riester, Marcel Ramos

**Examples**

```r
example("phenoFinder")
smokingGunFinder(esets2, "days_to_death")
```

---

**summary-methods**  
*Summarizes a DoppelGang object*

**Description**

Summarizes the @summaryresults slot of a DoppelGang object.

**Methods**

signature(object = "DoppelGang") Summarizes the @summaryresults slot of a DoppelGang object.

---

**vectorHammingDist**  
*Calculate Hamming Distance between two vectors, using pairwise complete observations.*

**Description**

Simple function to count the fraction of different elements (in the same position) between two vectors of the same length, after removing elements from both vectors corresponding to positions that are NA in either vector.
vectorWeightedDist

Calculate a weighted distance between two vectors, using pairwise complete observations.

Description

Simple function to count the fraction of different elements (in the same position) between two vectors of the same length, after removing elements from both vectors corresponding to positions that are NA in either vector. Distance is the probability for observing the matches and mismatches in two random patients.

Usage

vectorWeightedDist(x, y, k, l)

Arguments

x          a matrix
y          a matrix with the same number of columns as x
k          row in x to test for differences
l          row in y to test for differences

Value

Returns a numeric value, the Hamming Distance (the number of non-equal values between x and y).

Author(s)

Levi Waldron, Markus Riester, Marcel Ramos

Examples

(mat <- matrix(c(paste0("A", 1:5), paste0("A", 5:1)), nrow = 2, byrow = TRUE))
stopifnot(vectorHammingDist(mat, mat, 1, 2) == 0.8)
stopifnot(vectorHammingDist(mat, mat, 1, 1) == 0)
mat[1, 1] <- NA
stopifnot(vectorHammingDist(mat, mat, 1, 2) == 0.75)
stopifnot(vectorHammingDist(mat, mat, 1, 1) == 0)
mat[1, 3] <- NA
stopifnot(vectorHammingDist(mat, mat, 1, 2) == 1)
**vectorWeightedDist**

**Value**

Returns a numeric value, the log of the probability of observing the matches in x and y

**Author(s)**

Levi Waldron, Markus Riester, Marcel Ramos

**Examples**

```r
mymat1 <- matrix(rnorm(20), ncol = 5)
mymat1[1, 4] <- NA
mymat2 <- matrix(rnorm(20), ncol = 5)
vectorWeightedDist(mymat1, mymat2, 1, 2)
```
Index

* Topic **distribution**
  dst, 6
  mst.mle, 8

* Topic **methods**
  plot-methods, 13
  print-methods, 14
  show-methods, 14
  summary-methods, 15

* Topic **package**
  doppelgangR-package, 2

* Topic **regression**
  mst.mle, 8

corFinder, 3

DoppelGang, 13
DoppelGang (DoppelGang-class), 4
DoppelGang-class, 4
doppelgangR, 5
doppelgangR-package, 2
dst, 6, 9

hist, 13

mst.mle, 8

outlierFinder, 10

phenoDist, 11
phenoFinder, 12
plot,DoppelGang (plot-methods), 13
plot,DoppelGang,ANY-method (plot-methods), 13
plot,DoppelGang-method (plot-methods), 13
plot-methods, 13
plot.DoppelGang (plot-methods), 13
plot.doppelgangR (plot-methods), 13
print,DoppelGang-method (print-methods), 14
print-methods, 14
pst (dst), 6
qst (dst), 6
rst (dst), 6

show,DoppelGang-method (show-methods), 14
show-methods, 14
smokingGunFinder, 14
st.mle, 7
st.mle (mst.mle), 8
summary,DoppelGang-method (summary-methods), 15
summary-methods, 15

vectorHammingDist, 15
vectorWeightedDist, 16