Package 'doppelgangR'

October 15, 2023

Title Identify likely duplicate samples from genomic or meta-data **Version** 1.28.1

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).

Depends R (>= 3.5.0), Biobase, BiocParallel

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

Suggests BiocStyle, knitr, rmarkdown, curatedOvarianData, testthat

biocViews ImmunoOncology, RNASeq, Microarray, GeneExpression, QualityControl

License GPL (>=2.0) Encoding UTF-8

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

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

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doppelgangR-package

Identify likely duplicate samples from genomic or meta-data

Description

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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).

Author(s)

Levi Waldron, Markus Riester, Marcel Ramos

See Also

Useful links:

- https://github.com/lwaldron/doppelgangR
- Report bugs at https://github.com/lwaldron/doppelgangR/issues

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colFinder	Calculate pairwise similarities of colData between samples for a list containing two DataFrame

Description

This function acts as a wrapper to colData to handle cases of one DataFrame, a list of two identical DataFrame, or a list of two different DataFrame

Usage

```
colFinder(summex.list, ...)
```

Arguments

summex.list input: a list of DataFrame with two elements, or a DataFrame. 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.

... Extra arguments passed on to colFinder

Value

A matrix of similarities between the colData of pairs of samples.

Author(s)

Fabio Da Col, Marcel Ramos

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

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

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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

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

DoppelGang-class

DoppelGang S4 class

Description

S4 class containing results of doppelgangR() function.

Usage

```
## S4 method for signature 'DoppelGang'
summary(object)
## S4 method for signature 'DoppelGang'
show(object)
## S4 method for signature 'DoppelGang'
print(x)
```

Arguments

x, object A DoppelGang class object

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Objects from the Class

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

Author(s)

Levi Waldron and Markus Riester

See Also

```
plot, DoppelGang-method
```

doppelgangR

doppelgangR

Description

Identify samples with suspiciously high correlations and phenotype similarities

Usage

```
doppelgangR(
 esets,
  separator = ":",
 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),
 manual.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 ana-

lyzed.

separator a delimitor to use between dataset names and sample names corFinder.args a list of arguments to be passed to the corFinder function.

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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 multicore machine

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verbose

Print progress information

Value

Returns an object of S4-class "DoppelGang"

Author(s)

Levi Waldron, Markus Riester, Marcel Ramos

See Also

DoppelGang-class BiocParallelParam-class

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```
example("phenoFinder")
results2 <- doppelgangR(esets2, cache.dir = NULL)</pre>
results2
plot(results2)
summary(results2)
## Set phenoFinder.args=NULL to ignore similar phenotypes, and
## turn off ComBat batch correction:
## Not run:
results2 <- doppelgangR(testesets,</pre>
corFinder.args=list(use.ComBat=FALSE), phenoFinder.args=NULL,
    cache.dir=NULL)
summary(results2)
library(curatedOvarianData)
data(GSE32062.GPL6480_eset)
data(GSE32063_eset)
data(GSE12470_eset)
data(GSE17260_eset)
testesets <- list(JapaneseA = GSE32062.GPL6480_eset,
    JapaneseB = GSE32063_eset,
    Yoshihara2009 = GSE12470_eset,
    Yoshihara2010 = GSE17260_eset)
## standardize the sample ids to improve matching
## based on clinical annotation
testesets <- lapply(testesets, function(X) {</pre>
  X$alt_sample_name <-
    paste(X$sample_type, gsub("[^0-9]", "", X$alt_sample_name), sep = "_")
  pData(X) <-
    pData(X)[,!grepl("uncurated_author_metadata", colnames(pData(X)))]
  X[, 1:20] ##speed computations
})
(results1 <- doppelgangR(testesets, cache.dir = NULL))</pre>
plot(results1)
summary(results1)
## End(Not run)
```

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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)
rst(n = 1, location = 0, scale = 1, shape = 0, df = Inf, dp = NULL)

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,
    ...
)
```

Arguments

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

Value

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

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Details

Typical usages are

```
scale=1, shape=0, df=Inf, log=FALSE) dst(x, dp=, log=FALSE) pst(x,
location=0, scale=1, shape=0, df=Inf, ...) pst(x, dp=, log=FALSE) qst(p,
location=0, scale=1, shape=0, df=Inf, tol=1e-8, ...) qst(x, dp=, log=FALSE)
rst(n=1, location=0, scale=1, shape=0, df=Inf) rst(x, dp=, log=FALSE)
```

References

Azzalini, A. and Capitanio, A. (2003). Distributions generated by perturbation of symmetry with emphasis on a multivariate skew-t distribution. *J.Roy. Statist. Soc. B* **65**, 367–389.

See Also

```
st.mle
```

Examples

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

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

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

Arguments

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.
У	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.
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 taked 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 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 st.mle which is simply an interface to mst.mle.

The parameter 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 freq is not set, exact maximum likelihood estimation is performed.

likelihood estimation, use st.mle.grouped.

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Numerical search of the maximum likelihood estimates is performed in a suitable re-parameterization of the original parameters with aid of the selected optimizer (nlminb or optim) which is supplied with the derivatives of the log-likelihood function. Notice that, in case the optimizer is 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:

call a string containing the calling statement.

dp for mst.mle, this is a list containing the direct parameters beta, Omega, alpha.

Here, beta is a matrix of regression coefficients with dim(beta)=c(ncol(X), ncol(y)),

Omega is a covariance matrix of order ncol(y), alpha is a vector of shape parameters of length ncol(y). For st.mle, dp is a vector of length ncol(X)+3, containing c(beta, omega, alpha, df), where omega is the square root of Omega.

se a list containing the components beta, alpha, info. Here, beta and alpha are

the standard errors for the corresponding point estimates; info is the observed

information matrix for the working parameter, as explained below.

algorithm the list returned by the chose optimizer, either nlminb or optim, plus an item

with the name of the selected algorithm; see the documentation of either nlminb

or optim for explanation of the other components.

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 shape=0, the skew-t distribution reduces to the usual t distribution. When df=Inf the distribution reduces to the multivariate skew-normal one; see dmsn. See the reference below for additional information.

References

Azzalini, A. and Capitanio, A. (2003). Distributions generated by perturbation of symmetry with emphasis on a multivariate skew *t* distribution. The full version of the paper published in abriged form in *J.Roy. Statist. Soc. B* **65**, 367–389, is available at http://azzalini.stat.unipd.it/SN/se-ext.ps

See Also

dst

```
dat <- rt(100, df=5, ncp=100)
fit <- st.mle(y=dat)
fit</pre>
```

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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

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Examples

```
library(curatedOvarianData)
data(GSE32063_eset)
cormat <- cor(exprs(GSE32063_eset))
outlierFinder(cormat, bonf.prob = 0.05)</pre>
```

phenoDist	Calculate	distance	between	two	vectors,	rows	of	one	та-
	trix/datafr	ame, or ro	ws of two n	natric	es/datafrai	mes.			

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

```
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:</pre>
```

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```
graphics::boxplot(distmat)
## Not run:
  library(curatedOvarianData)
  data(GSE32063_eset)
  data(GSE17260_eset)
  pdat1 <- pData(GSE32063_eset)</pre>
  pdat2 <- pData(GSE17260_eset)</pre>
   ## Curation of the alternative sample identifiers makes duplicates stand out more:
  pdat1$alt_sample_name <-
     paste(pdat1$sample_type,
           gsub("[^0-9]", "", pdat1$alt_sample_name),
           sep = "_")
  pdat2$alt_sample_name <-
     paste(pdat2$sample_type,
           gsub("[^0-9]", "", pdat2$alt_sample_name),
           sep = "_")
 ## Removal of columns that cannot possibly match also helps duplicated patients to stand out
     pdat1[,!grep1("uncurated_author_metadata", colnames(pdat1))]
  pdat2 <-
    pdat2[,!grepl("uncurated_author_metadata", colnames(pdat2))]
   ## Use phenoDist() to calculate a weighted distance matrix
  distmat <- phenoDist(as.matrix(pdat1), as.matrix(pdat2))</pre>
  ## Note outliers with identical clinical data, these are probably the same patients:
  graphics::boxplot(distmat)
## End(Not run)
```

phenoFinder

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.

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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

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.

Usage

```
## S4 method for signature 'DoppelGang,ANY'
plot(x, skip.no.doppels = FALSE, plot.pair = NULL, ...)
```

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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

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

Author(s)

Levi Waldron

```
library(curatedOvarianData)
data(TCGA_eset)
data(GSE26712_eset)
## Remove some TCGA samples to speed computation:
keep.tcga <-
c("TCGA.13.2060", "TCGA.24.2290", "TCGA.25.2392", "TCGA.25.2404",
"TCGA.59.2349", "TCGA.09.2044", "TCGA.24.2262", "TCGA.24.2293",
"TCGA.25.2393", "TCGA.25.2408", "TCGA.59.2350", "TCGA.09.2045"
"TCGA.24.2267", "TCGA.59.2351", "TCGA.09.2048", "TCGA.24.2271", "TCGA.24.2298", "TCGA.25.2398", "TCGA.59.2354", "TCGA.09.2050",
"TCGA.24.2281", "TCGA.09.2051", "TCGA.29.2428", "TCGA.09.2055", "TCGA.24.2289", "TCGA.29.2414", "TCGA.59.2352", "TCGA.36.2532",
"TCGA.36.2529", "TCGA.36.2551", "TCGA.42.2590", "TCGA.13.2071",
"TCGA.29.2432", "TCGA.36.2537", "TCGA.36.2547", "TCGA.04.1369",
"TCGA.42.2591", "TCGA.23.2641", "TCGA.29.2434", "TCGA.36.2538",
"TCGA.36.2548", "TCGA.04.1516", "TCGA.42.2593", "TCGA.36.2549",
"TCGA.04.1644", "TCGA.13.2057", "TCGA.23.2647", "TCGA.36.2530",
"TCGA.36.2552", "TCGA.42.2587", "TCGA.13.2061", "TCGA.42.2588",
"TCGA.36.2544", "TCGA.42.2589", "TCGA.13.2066", "TCGA.61.2613",
"TCGA.61.2614", "TCGA.24.1852", "TCGA.29.1704", "TCGA.13.1819"
keep.tcga <- unique(c(keep.tcga, sampleNames(TCGA_eset)[1:200]))</pre>
testesets <- list(Bonome08=GSE26712_eset, TCGA=TCGA_eset[, keep.tcga])</pre>
results1 <- doppelgangR(testesets,</pre>
    corFinder.args=list(use.ComBat=FALSE), phenoFinder.args=NULL,
    cache.dir=NULL)
plot(results1)
```

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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

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

18 vectorHammingDist

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.

Usage

```
vectorHammingDist(x, y, k, 1)
```

Arguments

X	a matrix
У	a matrix with the same number of columns as \boldsymbol{x}
k	row in x to test for differences
1	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

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

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, 1)
```

Arguments

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

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

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

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