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Title Similarity and Distance Quantification Between Probability Functions

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Description Computes 46 optimized distance and similarity measures for comparing probability functions (Drost (2018) <[doi:10.21105/joss.00765](https://doi.org/10.21105/joss.00765)>). These comparisons between probability functions have their foundations in a broad range of scientific disciplines from mathematics to ecology. The aim of this package is to provide a core framework for clustering, classification, statistical inference, goodness-of-fit, non-parametric statistics, information theory, and machine learning tasks that are based on comparing univariate or multivariate probability functions.

Depends R (>= 3.1.2)

Imports Rcpp, KernSmooth, poorman

License GPL-2

LazyData false

LinkingTo Rcpp

URL <https://drostlab.github.io/philentropy/>,
<https://github.com/drostlab/philentropy>

Suggests testthat, knitr, rmarkdown, microbenchmark

VignetteBuilder knitr

BugReports <https://github.com/drostlab/philentropy/issues>

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Repository <https://drostlab.r-universe.dev>

RemoteUrl <https://github.com/drostlab/philentropy>

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additive_symm_chi_sq *Additive symmetric chi-squared distance (lowlevel function)*

Description

The lowlevel function for computing the *additive_symm_chi_sq* distance.

Usage

```
additive_symm_chi_sq(P, Q, testNA)
```

Arguments

<i>P</i>	a numeric vector storing the first distribution.
<i>Q</i>	a numeric vector storing the second distribution.
<i>testNA</i>	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
additive_symm_chi_sq(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

avg *AVG distance (lowlevel function)*

Description

The lowlevel function for computing the avg distance.

Usage

```
avg(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
avg(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

bhattacharyya *Bhattacharyya distance (lowlevel function)*

Description

The lowlevel function for computing the bhattacharyya distance.

Usage

```
bhattacharyya(P, Q, testNA, unit, epsilon)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
unit	type of log function. Option are
epsilon	epsilon a small value to address cases in the distance computation where division by zero occurs. In these cases, $x / 0$ or $0 / 0$ will be replaced by epsilon. The default is <code>epsilon = 0.00001</code> . However, we recommend to choose a custom epsilon value depending on the size of the input vectors, the expected similarity between compared probability density functions and whether or not many 0 values are present within the compared vectors. As a rough rule of thumb we suggest that when dealing with very large input vectors which are very similar and contain many 0 values, the epsilon value should be set even smaller (e.g. <code>epsilon = 0.000000001</code>), whereas when vector sizes are small or distributions very divergent then higher epsilon values may also be appropriate (e.g. <code>epsilon = 0.01</code>). Addressing this epsilon issue is important to avoid cases where distance metrics return negative values which are not defined and only occur due to the technical issues of computing $x / 0$ or $0 / 0$ cases.

Author(s)

Hajk-Georg Drost

Examples

```
bhattacharyya(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE,
  unit = "log2", epsilon = 0.00001)
```

binned.kernel.est *Kernel Density Estimation*

Description

This function implements an interface to the kernel density estimation functions provided by the **KernSmooth** package.

Usage

```
binned.kernel.est(
  data,
  kernel = "normal",
  bandwidth = NULL,
  canonical = FALSE,
  scalest = "minim",
  level = 2L,
```

```

    gridsize = 401L,
    range.data = range(data),
    truncate = TRUE
  )

```

Arguments

data	a numeric vector containing the sample on which the kernel density estimate is to be constructed.
kernel	character string specifying the smoothing kernel
bandwidth	the kernel bandwidth smoothing parameter.
canonical	a logical value indicating whether canonically scaled kernels should be used
scaletest	estimate of scale. <ul style="list-style-type: none"> • "stdev" - standard deviation is used. • "iqr" - inter-quartile range divided by 1.349 is used. • "minim" - minimum of "stdev" and "iqr" is used.
level	number of levels of functional estimation used in the plug-in rule.
gridsize	the number of equally-spaced points over which binning is performed to obtain kernel functional approximation.
range.data	vector containing the minimum and maximum values of data at which to compute the estimate. The default is the minimum and maximum data values.
truncate	logical value indicating whether data with x values outside the range specified by range.data should be ignored.

Author(s)

Hajk-Georg Drost

References

- Matt Wand (2015). KernSmooth: Functions for Kernel Smoothing Supporting Wand & Jones (1995). R package version 2.23-14.
- Henry Deng and Hadley Wickham (2011). Density estimation in R. <http://vita.had.co.nz/papers/density-estimation.pdf>.

canberra

Canberra distance (lowlevel function)

Description

The lowlevel function for computing the canberra distance.

Usage

```
canberra(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
canberra(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

CE *Shannon's Conditional-Entropy $H(X|Y)$*

Description

Compute Shannon's Conditional-Entropy based on the chain rule $H(X|Y) = H(X, Y) - H(Y)$ based on a given joint-probability vector $P(X, Y)$ and probability vector $P(Y)$.

Usage

```
CE(xy, y, unit = "log2")
```

Arguments

xy	a numeric joint-probability vector $P(X, Y)$ for which Shannon's Joint-Entropy $H(X, Y)$ shall be computed.
y	a numeric probability vector $P(Y)$ for which Shannon's Entropy $H(Y)$ (as part of the chain rule) shall be computed. It is important to note that this probability vector must be the probability distribution of random variable Y ($P(Y)$ for which $H(Y)$ is computed).
unit	a character string specifying the logarithm unit that shall be used to compute distances that depend on log computations.

Details

This function might be useful to fastly compute Shannon's Conditional-Entropy for any given joint-probability vector and probability vector.

Value

Shannon's Conditional-Entropy in bit.

Note

Note that the probability vector $P(Y)$ must be the probability distribution of random variable Y ($P(Y)$ for which $H(Y)$ is computed) and furthermore used for the chain rule computation of $H(X|Y) = H(X, Y) - H(Y)$.

Author(s)

Hajk-Georg Drost

References

Shannon, Claude E. 1948. "A Mathematical Theory of Communication". *Bell System Technical Journal* **27** (3): 379-423.

See Also

[H, JE](#)

Examples

```
CE(1:10/sum(1:10), 1:10/sum(1:10))
```

chebyshev

Chebyshev distance (lowlevel function)

Description

The lowlevel function for computing the chebyshev distance.

Usage

```
chebyshev(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
chebyshev(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

clark_sq	<i>Clark squared distance (lowlevel function)</i>
----------	---

Description

The lowlevel function for computing the clark_sq distance.

Usage

```
clark_sq(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
clark_sq(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

cosine_dist	<i>Cosine distance (lowlevel function)</i>
-------------	--

Description

The lowlevel function for computing the cosine_dist distance.

Usage

```
cosine_dist(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
cosine_dist(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

czekanowski	<i>Czekanowski distance (lowlevel function)</i>
-------------	---

Description

The lowlevel function for computing the czekanowski distance.

Usage

```
czekanowski(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
czekanowski(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

dice_dist	<i>Dice distance (lowlevel function)</i>
-----------	--

Description

The lowlevel function for computing the dice_dist distance.

Usage

```
dice_dist(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
dice_dist(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

dist.diversity	<i>Distance Diversity between Probability Density Functions</i>
----------------	---

Description

This function computes all distance values between two probability density functions that are available in [getDistMethods](#) and returns a vector storing the corresponding distance measures. This vector is *named distance diversity vector*.

Usage

```
dist.diversity(x, p, test.na = FALSE, unit = "log2")
```

Arguments

x	a numeric data.frame or matrix (storing probability vectors) or a numeric data.frame or matrix storing counts (if est.prob is specified).
p	power of the Minkowski distance.
test.na	a boolean value indicating whether input vectors should be tested for NA values. Faster computations if test.na = FALSE.
unit	a character string specifying the logarithm unit that should be used to compute distances that depend on log computations. Options are: <ul style="list-style-type: none"> • unit = "log" • unit = "log2" • unit = "log10"

Author(s)

Hajk-Georg Drost

Examples

```
dist.diversity(rbind(1:10/sum(1:10), 20:29/sum(20:29)), p = 2, unit = "log2")
```

`distance`*Distances and Similarities between Probability Density Functions*

Description

This functions computes the distance/dissimilarity between two probability density functions.

Usage

```
distance(  
  x,  
  method = "euclidean",  
  p = NULL,  
  test.na = TRUE,  
  unit = "log",  
  epsilon = 1e-05,  
  est.prob = NULL,  
  use.row.names = FALSE,  
  as.dist.obj = FALSE,  
  diag = FALSE,  
  upper = FALSE,  
  mute.message = FALSE  
)
```

Arguments

<code>x</code>	a numeric <code>data.frame</code> or matrix (storing probability vectors) or a numeric <code>data.frame</code> or matrix storing counts (if <code>est.prob</code> is specified).
<code>method</code>	a character string indicating whether the distance measure that should be computed.
<code>p</code>	power of the Minkowski distance.
<code>test.na</code>	a boolean value indicating whether input vectors should be tested for NA values. Faster computations if <code>test.na = FALSE</code> .
<code>unit</code>	a character string specifying the logarithm unit that should be used to compute distances that depend on log computations.
<code>epsilon</code>	a small value to address cases in the distance computation where division by zero occurs. In these cases, $x / 0$ or $0 / 0$ will be replaced by <code>epsilon</code> . The default is <code>epsilon = 0.00001</code> . However, we recommend to choose a custom <code>epsilon</code> value depending on the size of the input vectors, the expected similarity between compared probability density functions and whether or not many 0 values are present within the compared vectors. As a rough rule of thumb we suggest that when dealing with very large input vectors which are very similar and contain many 0 values, the <code>epsilon</code> value should be set even smaller (e.g. <code>epsilon = 0.00000001</code>), whereas when vector sizes are small or distributions very divergent then higher <code>epsilon</code> values may also be appropriate (e.g.

epsilon = 0.01). Addressing this epsilon issue is important to avoid cases where distance metrics return negative values which are not defined and only occur due to the technical issues of computing $x / 0$ or $0 / 0$ cases.

est.prob	method to estimate probabilities from input count vectors such as non-probability vectors. Default: est.prob = NULL. Options are: <ul style="list-style-type: none"> • est.prob = "empirical": The relative frequencies of each vector are computed internally. For example an input matrix <code>rbind(1:10, 11:20)</code> will be transformed to a probability vector <code>rbind(1:10 / sum(1:10), 11:20 / sum(11:20))</code>
use.row.names	a logical value indicating whether or not row names from the input matrix shall be used as rownames and colnames of the output distance matrix. Default value is use.row.names = FALSE.
as.dist.obj	shall the return value or matrix be an object of class <code>link[stats]{dist}</code> ? Default is as.dist.obj = FALSE.
diag	if as.dist.obj = TRUE, then this value indicates whether the diagonal of the distance matrix should be printed. Default
upper	if as.dist.obj = TRUE, then this value indicates whether the upper triangle of the distance matrix should be printed.
mute.message	a logical value indicating whether or not messages printed by distance shall be muted. Default is mute.message = FALSE.

Details

Here a distance is defined as a quantitative degree of how far two mathematical objects are apart from each other (Cha, 2007).

This function implements the following distance/similarity measures to quantify the distance between probability density functions:

- L_p Minkowski family
 - Euclidean : $d = \sqrt{\sum |P_i - Q_i|^2}$
 - Manhattan : $d = \sum |P_i - Q_i|$
 - Minkowski : $d = (\sum |P_i - Q_i|^p)^{1/p}$
 - Chebyshev : $d = \max |P_i - Q_i|$
- L₁ family
 - Sorensen : $d = \sum |P_i - Q_i| / \sum (P_i + Q_i)$
 - Gower : $d = 1/d * \sum |P_i - Q_i|$
 - Soergel : $d = \sum |P_i - Q_i| / \sum \max(P_i, Q_i)$
 - Kulczynski d : $d = \sum |P_i - Q_i| / \sum \min(P_i, Q_i)$
 - Canberra : $d = \sum |P_i - Q_i| / (P_i + Q_i)$
 - Lorentzian : $d = \sum \ln(1 + |P_i - Q_i|)$
- Intersection family
 - Intersection : $s = \sum \min(P_i, Q_i)$
 - Non-Intersection : $d = 1 - \sum \min(P_i, Q_i)$

- Wave Hedges : $d = \sum |P_i - Q_i| / \max(P_i, Q_i)$
- Czekanowski : $d = \sum |P_i - Q_i| / \sum |P_i + Q_i|$
- Motyka : $d = \sum \min(P_i, Q_i) / (P_i + Q_i)$
- Kulczynski s : $d = 1 / \sum |P_i - Q_i| / \sum \min(P_i, Q_i)$
- Tanimoto : $d = \sum (\max(P_i, Q_i) - \min(P_i, Q_i)) / \sum \max(P_i, Q_i)$; equivalent to Soergel
- Ruzicka : $s = \sum \min(P_i, Q_i) / \sum \max(P_i, Q_i)$; equivalent to 1 - Tanimoto = 1 - Soergel
- Inner Product family
 - Inner Product : $s = \sum P_i * Q_i$
 - Harmonic mean : $s = 2 * \sum (P_i * Q_i) / (P_i + Q_i)$
 - Cosine : $s = \sum (P_i * Q_i) / \sqrt{\sum P_i^2} * \sqrt{\sum Q_i^2}$
 - Kumar-Hassebrook (PCE) : $s = \sum (P_i * Q_i) / (\sum P_i^2 + \sum Q_i^2 - \sum (P_i * Q_i))$
 - Jaccard : $d = 1 - \sum (P_i * Q_i) / (\sum P_i^2 + \sum Q_i^2 - \sum (P_i * Q_i))$; equivalent to 1 - Kumar-Hassebrook
 - Dice : $d = \sum (P_i - Q_i)^2 / (\sum P_i^2 + \sum Q_i^2)$
- Squared-chord family
 - Fidelity : $s = \sum \sqrt{P_i * Q_i}$
 - Bhattacharyya : $d = -\ln \sum \sqrt{P_i * Q_i}$
 - Hellinger : $d = 2 * \sqrt{1 - \sum \sqrt{P_i * Q_i}}$
 - Matusita : $d = \sqrt{2 - 2 * \sum \sqrt{P_i * Q_i}}$
 - Squared-chord : $d = \sum (\sqrt{P_i} - \sqrt{Q_i})^2$
- Squared L_2 family (X^2 squared family)
 - Squared Euclidean : $d = \sum (P_i - Q_i)^2$
 - Pearson X^2 : $d = \sum ((P_i - Q_i)^2 / Q_i)$
 - Neyman X^2 : $d = \sum ((P_i - Q_i)^2 / P_i)$
 - Squared X^2 : $d = \sum ((P_i - Q_i)^2 / (P_i + Q_i))$
 - Probabilistic Symmetric X^2 : $d = 2 * \sum ((P_i - Q_i)^2 / (P_i + Q_i))$
 - Divergence : X^2 : $d = 2 * \sum ((P_i - Q_i)^2 / (P_i + Q_i)^2)$
 - Clark : $d = \sqrt{\sum (|P_i - Q_i| / (P_i + Q_i))^2}$
 - Additive Symmetric X^2 : $d = \sum (((P_i - Q_i)^2 * (P_i + Q_i)) / (P_i * Q_i))$
- Shannon's entropy family
 - Kullback-Leibler : $d = \sum P_i * \log(P_i / Q_i)$
 - Jeffreys : $d = \sum (P_i - Q_i) * \log(P_i / Q_i)$
 - K divergence : $d = \sum P_i * \log(2 * P_i / (P_i + Q_i))$
 - Topsoe : $d = \sum (P_i * \log(2 * P_i / (P_i + Q_i))) + (Q_i * \log(2 * Q_i / (P_i + Q_i)))$
 - Jensen-Shannon : $d = 0.5 * (\sum P_i * \log(2 * P_i / (P_i + Q_i)) + \sum Q_i * \log(2 * Q_i / (P_i + Q_i)))$
 - Jensen difference : $d = \sum ((P_i * \log(P_i) + Q_i * \log(Q_i)) / 2) - (P_i + Q_i) / 2 * \log((P_i + Q_i) / 2)$
- Combinations
 - Taneja : $d = \sum (P_i + Q_i) / 2 * \log((P_i + Q_i) / (2 * \sqrt{P_i * Q_i}))$
 - Kumar-Johnson : $d = \sum (P_i^2 - Q_i^2)^2 / 2 * (P_i * Q_i)^{1.5}$

$$- \text{Avg}(L_1, L_n) : d = \sum |P_i - Q_i| + \max |P_i - Q_i|/2$$

In cases where `x` specifies a count matrix, the argument `est.prob` can be selected to first estimate probability vectors from input count vectors and second compute the corresponding distance measure based on the estimated probability vectors.

The following probability estimation methods are implemented in this function:

- `est.prob = "empirical"` : relative frequencies of counts.

Value

The following results are returned depending on the dimension of `x`:

- in case `nrow(x) = 2` : a single distance value.
- in case `nrow(x) > 2` : a distance matrix storing distance values for all pairwise probability vector comparisons.

Note

According to the reference in some distance measure computations invalid computations can occur when dealing with 0 probabilities.

In these cases the convention is treated as follows:

- division by zero - case $0/0$: when the divisor and dividend become zero, $0/0$ is treated as 0 .
- division by zero - case $n/0$: when only the divisor becomes 0 , the corresponding 0 is replaced by a small $\epsilon = 0.00001$.
- log of zero - case $0 * \log(0)$: is treated as 0 .
- log of zero - case $\log(0)$: zero is replaced by a small $\epsilon = 0.00001$.

Author(s)

Hajk-Georg Drost

References

Sung-Hyuk Cha. (2007). *Comprehensive Survey on Distance/Similarity Measures between Probability Density Functions*. International Journal of Mathematical Models and Methods in Applied Sciences 4: 1.

See Also

[getDistMethods](#), [estimate.probability](#), [dist.diversity](#)

Examples

```
# Simple Examples

# receive a list of implemented probability distance measures
getDistMethods()
```

```

## compute the euclidean distance between two probability vectors
distance(rbind(1:10/sum(1:10), 20:29/sum(20:29)), method = "euclidean")

## compute the euclidean distance between all pairwise comparisons of probability vectors
ProbMatrix <- rbind(1:10/sum(1:10), 20:29/sum(20:29),30:39/sum(30:39))
distance(ProbMatrix, method = "euclidean")

# compute distance matrix without testing for NA values in the input matrix
distance(ProbMatrix, method = "euclidean", test.na = FALSE)

# alternatively use the colnames of the input data for the rownames and colnames
# of the output distance matrix
ProbMatrix <- rbind(1:10/sum(1:10), 20:29/sum(20:29),30:39/sum(30:39))
rownames(ProbMatrix) <- paste0("Example", 1:3)
distance(ProbMatrix, method = "euclidean", use.row.names = TRUE)

# Specialized Examples

CountMatrix <- rbind(1:10, 20:29, 30:39)

## estimate probabilities from a count matrix
distance(CountMatrix, method = "euclidean", est.prob = "empirical")

## compute the euclidean distance for count data
## NOTE: some distance measures are only defined for probability values,
distance(CountMatrix, method = "euclidean")

## compute the Kullback-Leibler Divergence with different logarithm bases:
### case: unit = log (Default)
distance(ProbMatrix, method = "kullback-leibler", unit = "log")

### case: unit = log2
distance(ProbMatrix, method = "kullback-leibler", unit = "log2")

### case: unit = log10
distance(ProbMatrix, method = "kullback-leibler", unit = "log10")

```

dist_many_many	<i>Distances and Similarities between Many Probability Density Functions</i>
----------------	--

Description

This functions computes the distance/dissimilarity between two sets of probability density functions.

Usage

```
dist_many_many(
```



```

dists1,
dists2,
method,
p = NA_real_,
testNA = TRUE,
unit = "log",
epsilon = 1e-05
)

```

Arguments

dists1	a numeric matrix storing distributions in its rows.
dists2	a numeric matrix storing distributions in its rows.
method	a character string indicating whether the distance measure that should be computed.
p	power of the Minkowski distance.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
unit	type of log function. Option are <ul style="list-style-type: none"> • unit = "log" • unit = "log2" • unit = "log10"
epsilon	epsilon a small value to address cases in the distance computation where division by zero occurs. In these cases, $x / 0$ or $0 / 0$ will be replaced by epsilon. The default is <code>epsilon = 0.00001</code> . However, we recommend to choose a custom epsilon value depending on the size of the input vectors, the expected similarity between compared probability density functions and whether or not many 0 values are present within the compared vectors. As a rough rule of thumb we suggest that when dealing with very large input vectors which are very similar and contain many 0 values, the epsilon value should be set even smaller (e.g. <code>epsilon = 0.00000001</code>), whereas when vector sizes are small or distributions very divergent then higher epsilon values may also be appropriate (e.g. <code>epsilon = 0.01</code>). Addressing this epsilon issue is important to avoid cases where distance metrics return negative values which are not defined and only occur due to the technical issues of computing $x / 0$ or $0 / 0$ cases.

Value

A matrix of distance values

Examples

```

set.seed(2020-08-20)
M1 <- t(replicate(10, sample(1:10, size = 10) / 55))
M2 <- t(replicate(10, sample(1:10, size = 10) / 55))
result <- dist_many_many(M1, M2, method = "euclidean", testNA = FALSE)

```

dist_one_many	<i>Distances and Similarities between One and Many Probability Density Functions</i>
---------------	--

Description

This functions computes the distance/dissimilarity between one probability density functions and a set of probability density functions.

Usage

```
dist_one_many(
  P,
  dists,
  method,
  p = NA_real_,
  testNA = TRUE,
  unit = "log",
  epsilon = 1e-05
)
```

Arguments

P	a numeric vector storing the first distribution.
dists	a numeric matrix storing distributions in its rows.
method	a character string indicating whether the distance measure that should be computed.
p	power of the Minkowski distance.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
unit	type of log function. Option are <ul style="list-style-type: none"> • unit = "log" • unit = "log2" • unit = "log10"
epsilon	epsilon a small value to address cases in the distance computation where division by zero occurs. In these cases, $x / 0$ or $0 / 0$ will be replaced by epsilon. The default is $\text{epsilon} = 0.00001$. However, we recommend to choose a custom epsilon value depending on the size of the input vectors, the expected similarity between compared probability density functions and whether or not many 0 values are present within the compared vectors. As a rough rule of thumb we suggest that when dealing with very large input vectors which are very similar and contain many 0 values, the epsilon value should be set even smaller (e.g. $\text{epsilon} = 0.000000001$), whereas when vector sizes are small or distributions very divergent then higher epsilon values may also be appropriate (e.g. $\text{epsilon} = 0.01$). Addressing this epsilon issue is important to avoid cases

where distance metrics return negative values which are not defined and only occur due to the technical issues of computing $x / 0$ or $0 / 0$ cases.

Value

A vector of distance values

Examples

```
set.seed(2020-08-20)
P <- 1:10 / sum(1:10)
M <- t(replicate(100, sample(1:10, size = 10) / 55))
dist_one_many(P, M, method = "euclidean", testNA = FALSE)
```

dist_one_one	<i>Distances and Similarities between Two Probability Density Functions</i>
--------------	---

Description

This functions computes the distance/dissimilarity between two probability density functions.

Usage

```
dist_one_one(
  P,
  Q,
  method,
  p = NA_real_,
  testNA = TRUE,
  unit = "log",
  epsilon = 1e-05
)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
method	a character string indicating whether the distance measure that should be computed.
p	power of the Minkowski distance.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
unit	type of log function. Option are <ul style="list-style-type: none"> • unit = "log" • unit = "log2" • unit = "log10"

epsilon epsilon a small value to address cases in the distance computation where division by zero occurs. In these cases, $x / 0$ or $0 / 0$ will be replaced by epsilon. The default is `epsilon = 0.00001`. However, we recommend to choose a custom epsilon value depending on the size of the input vectors, the expected similarity between compared probability density functions and whether or not many 0 values are present within the compared vectors. As a rough rule of thumb we suggest that when dealing with very large input vectors which are very similar and contain many 0 values, the epsilon value should be set even smaller (e.g. `epsilon = 0.000000001`), whereas when vector sizes are small or distributions very divergent then higher epsilon values may also be appropriate (e.g. `epsilon = 0.01`). Addressing this epsilon issue is important to avoid cases where distance metrics return negative values which are not defined and only occur due to the technical issues of computing $x / 0$ or $0 / 0$ cases.

Value

A single distance value

Examples

```
P <- 1:10 / sum(1:10)
Q <- 20:29 / sum(20:29)
dist_one_one(P, Q, method = "euclidean", testNA = FALSE)
```

divergence_sq	<i>Divergence squared distance (lowlevel function)</i>
---------------	--

Description

The lowlevel function for computing the `divergence_sq` distance.

Usage

```
divergence_sq(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
divergence_sq(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

estimate.probability *Estimate Probability Vectors From Count Vectors*

Description

This function takes a numeric count vector and returns estimated probabilities of the corresponding counts.

The following probability estimation methods are implemented in this function:

- method = "empirical" : generates the relative frequency of the data $x/\text{sum}(x)$.
-
-

Usage

```
estimate.probability(x, method = "empirical")
```

Arguments

x	a numeric vector storing count values.
method	a character string specifying the estimation method tht should be used to estimate probabilities from input counts.

Value

a numeric probability vector.

Author(s)

Hajk-Georg Drost

Examples

```
# generate a count vector
x <- runif(100)

# generate a probability vector from corresponding counts
# method = "empirical"
x.prob <- estimate.probability(x, method = "empirical")
```

euclidean	<i>Euclidean distance (lowlevel function)</i>
-----------	---

Description

The lowlevel function for computing the euclidean distance.

Usage

```
euclidean(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
euclidean(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

fidelity	<i>Fidelity distance (lowlevel function)</i>
----------	--

Description

The lowlevel function for computing the fidelity distance.

Usage

```
fidelity(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
fidelity(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

getDistMethods	<i>Get method names for distance</i>
----------------	--------------------------------------

Description

This function returns the names of the methods that can be applied to compute distances between probability density functions using the [distance](#) function.

Usage

```
getDistMethods()
```

Author(s)

Hajk-Georg Drost

Examples

```
getDistMethods()
```

gJSD	<i>Generalized Jensen-Shannon Divergence</i>
------	--

Description

This function computes the Generalized Jensen-Shannon Divergence of a probability matrix.

Usage

```
gJSD(x, unit = "log2", weights = NULL, est.prob = NULL)
```

Arguments

x	a probability matrix.
unit	a character string specifying the logarithm unit that shall be used to compute distances that depend on log computations.
weights	a numeric vector specifying the weights for each distribution in x. Default: weights = NULL; in this case all distributions are weighted equally (= uniform distribution of weights). In case users wish to specify non-uniform weights for e.g. 3 distributions, they can specify the argument weights = c(0.5, 0.25, 0.25). This notation denotes that vec1 is weighted by 0.5, vec2 is weighted by 0.25, and vec3 is weighted by 0.25 as well.
est.prob	method to estimate probabilities from input count vectors such as non-probability vectors. Default: est.prob = NULL. Options are: <ul style="list-style-type: none"> • est.prob = "empirical": The relative frequencies of each vector are computed internally. For example an input matrix rbind(1:10, 11:20) will be transformed to a probability vector rbind(1:10 / sum(1:10), 11:20 / sum(11:20))

Details

Function to compute the Generalized Jensen-Shannon Divergence

$$JSD_{\pi_1, \dots, \pi_n}(P_1, \dots, P_n) = H(\sum_{i=1}^n \pi_i * P_i) - \sum_{i=1}^n \pi_i * H(P_i)$$

where π_1, \dots, π_n denote the weights selected for the probability vectors P_1, \dots, P_n and $H(P_i)$ denotes the Shannon Entropy of probability vector P_i .

Value

The Jensen-Shannon divergence between all possible combinations of comparisons.

Author(s)

Hajk-Georg Drost

See Also

[KL](#), [H](#), [JSD](#), [CE](#), [JE](#)

Examples

```
# define input probability matrix
Prob <- rbind(1:10/sum(1:10), 20:29/sum(20:29), 30:39/sum(30:39))

# compute the Generalized JSD comparing the PS probability matrix
gJSD(Prob)

# Generalized Jensen-Shannon Divergence between three vectors using different log bases
gJSD(Prob, unit = "log2") # Default
gJSD(Prob, unit = "log")
gJSD(Prob, unit = "log10")
```



```
# Jensen-Shannon Divergence Divergence between count vectors P.count and Q.count
P.count <- 1:10
Q.count <- 20:29
R.count <- 30:39
x.count <- rbind(P.count, Q.count, R.count)
gJSD(x.count, est.prob = "empirical")
```

gower

Gower distance (lowlevel function)

Description

The lowlevel function for computing the gower distance.

Usage

```
gower(P, Q, testNA)
```

Arguments

P a numeric vector storing the first distribution.
 Q a numeric vector storing the second distribution.
 testNA a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
gower(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

H

Shannon's Entropy $H(X)$

Description

Compute the Shannon's Entropy $H(X) = - \sum P(X) * \log_2(P(X))$ based on a given probability vector $P(X)$.

Usage

```
H(x, unit = "log2")
```

Arguments

x	a numeric probability vector $P(X)$ for which Shannon's Entropy $H(X)$ shall be computed.
unit	a character string specifying the logarithm unit that shall be used to compute distances that depend on log computations.

Details

This function might be useful to fastly compute Shannon's Entropy for any given probability vector.

Value

a numeric value representing Shannon's Entropy in bit.

Author(s)

Hajk-Georg Drost

References

Shannon, Claude E. 1948. "A Mathematical Theory of Communication". *Bell System Technical Journal* **27** (3): 379-423.

See Also

[JE](#), [CE](#), [KL](#), [JSD](#), [gJSD](#)

Examples

```
H(1:10/sum(1:10))
```

harmonic_mean_dist *Harmonic mean distance (lowlevel function)*

Description

The lowlevel function for computing the harmonic_mean_dist distance.

Usage

```
harmonic_mean_dist(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
harmonic_mean_dist(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

hellinger	<i>Hellinger distance (lowlevel function)</i>
-----------	---

Description

The lowlevel function for computing the hellinger distance.

Usage

```
hellinger(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
hellinger(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

inner_product	<i>Inner product distance (lowlevel function)</i>
---------------	---

Description

The lowlevel function for computing the inner_product distance.

Usage

```
inner_product(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
inner_product(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

intersection_dist *Intersection distance (lowlevel function)*

Description

The lowlevel function for computing the intersection_dist distance.

Usage

```
intersection_dist(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
intersection_dist(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

jaccard	<i>Jaccard distance (lowlevel function)</i>
---------	---

Description

The lowlevel function for computing the jaccard distance.

Usage

```
jaccard(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
jaccard(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

JE	<i>Shannon's Joint-Entropy $H(X, Y)$</i>
----	---

Description

This function computes Shannon's Joint-Entropy $H(X, Y) = -\sum \sum P(X, Y) * \log_2(P(X, Y))$ based on a given joint-probability vector $P(X, Y)$.

Usage

```
JE(x, unit = "log2")
```

Arguments

x	a numeric joint-probability vector $P(X, Y)$ for which Shannon's Joint-Entropy $H(X, Y)$ shall be computed.
unit	a character string specifying the logarithm unit that shall be used to compute distances that depend on log computations.

Value

a numeric value representing Shannon's Joint-Entropy in bit.

Author(s)

Hajk-Georg Drost

References

Shannon, Claude E. 1948. "A Mathematical Theory of Communication". *Bell System Technical Journal* **27** (3): 379-423.

See Also

[H](#), [CE](#), [KL](#), [JSD](#), [gJSD](#), [distance](#)

Examples

```
JE(1:100/sum(1:100))
```

jeffreys

Jeffreys distance (lowlevel function)

Description

The lowlevel function for computing the jeffreys distance.

Usage

```
jeffreys(P, Q, testNA, unit, epsilon)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
unit	type of log function. Option are <ul style="list-style-type: none"> • unit = "log" • unit = "log2" • unit = "log10"

`epsilon` epsilon a small value to address cases in the distance computation where division by zero occurs. In these cases, $x / 0$ or $0 / 0$ will be replaced by `epsilon`. The default is `epsilon = 0.00001`. However, we recommend to choose a custom `epsilon` value depending on the size of the input vectors, the expected similarity between compared probability density functions and whether or not many 0 values are present within the compared vectors. As a rough rule of thumb we suggest that when dealing with very large input vectors which are very similar and contain many 0 values, the `epsilon` value should be set even smaller (e.g. `epsilon = 0.000000001`), whereas when vector sizes are small or distributions very divergent then higher `epsilon` values may also be appropriate (e.g. `epsilon = 0.01`). Addressing this `epsilon` issue is important to avoid cases where distance metrics return negative values which are not defined and only occur due to the technical issues of computing $x / 0$ or $0 / 0$ cases.

Author(s)

Hajk-Georg Drost

Examples

```
jeffreys(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE,
unit = "log2", epsilon = 0.00001)
```

`jensen_difference` *Jensen difference (lowlevel function)*

Description

The lowlevel function for computing the `jensen_difference` distance.

Usage

```
jensen_difference(P, Q, testNA, unit)
```

Arguments

<code>P</code>	a numeric vector storing the first distribution.
<code>Q</code>	a numeric vector storing the second distribution.
<code>testNA</code>	a logical value indicating whether or not distributions shall be checked for NA values.
<code>unit</code>	type of log function. Option are <ul style="list-style-type: none"> • <code>unit = "log"</code> • <code>unit = "log2"</code> • <code>unit = "log10"</code>

Author(s)

Hajk-Georg Drost

Examples

```
jensen_difference(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE, unit = "log2")
```

jensen_shannon	<i>Jensen-Shannon distance (lowlevel function)</i>
----------------	--

Description

The lowlevel function for computing the jensen_shannon distance.

Usage

```
jensen_shannon(P, Q, testNA, unit)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
unit	type of log function. Option are <ul style="list-style-type: none">• unit = "log"• unit = "log2"• unit = "log10"

Author(s)

Hajk-Georg Drost

Examples

```
jensen_shannon(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE, unit = "log2")
```


JSD

*Jensen-Shannon Divergence***Description**

This function computes a distance matrix or distance value based on the Jensen-Shannon Divergence with equal weights.

Usage

```
JSD(x, test.na = TRUE, unit = "log2", est.prob = NULL)
```

Arguments

<code>x</code>	a numeric data.frame or matrix (storing probability vectors) or a numeric data.frame or matrix storing counts (if <code>est.prob = TRUE</code>). See distance for details.
<code>test.na</code>	a boolean value specifying whether input vectors shall be tested for NA values.
<code>unit</code>	a character string specifying the logarithm unit that shall be used to compute distances that depend on log computations.
<code>est.prob</code>	method to estimate probabilities from input count vectors such as non-probability vectors. Default: <code>est.prob = NULL</code> . Options are: <ul style="list-style-type: none"> • <code>est.prob = "empirical"</code>: The relative frequencies of each vector are computed internally. For example an input matrix <code>rbind(1:10, 11:20)</code> will be transformed to a probability vector <code>rbind(1:10 / sum(1:10), 11:20 / sum(11:20))</code>

Details

Function to compute the Jensen-Shannon Divergence $JSD(P \parallel Q)$ between two probability distributions P and Q with equal weights $\pi_1 = \pi_2 = 1/2$.

The Jensen-Shannon Divergence $JSD(P \parallel Q)$ between two probability distributions P and Q is defined as:

$$JSD(P \parallel Q) = 0.5 * (KL(P \parallel R) + KL(Q \parallel R))$$

where $R = 0.5 * (P + Q)$ denotes the mid-point of the probability vectors P and Q , and $KL(P \parallel R)$, $KL(Q \parallel R)$ denote the Kullback-Leibler Divergence of P and R , as well as Q and R .

General properties of the Jensen-Shannon Divergence:

- 1) JSD is non-negative.
- 2) JSD is a symmetric measure $JSD(P \parallel Q) = JSD(Q \parallel P)$.
- 3) $JSD = 0$, if and only if $P = Q$.

Value

a distance value or matrix based on JSD computations.

Author(s)

Hajk-Georg Drost

References

Lin J. 1991. "Divergence Measures Based on the Shannon Entropy". IEEE Transactions on Information Theory. (33) 1: 145-151.

Endres M. and Schindelin J. E. 2003. "A new metric for probability distributions". IEEE Trans. on Info. Thy. (49) 3: 1858-1860.

See Also

[KL](#), [H](#), [CE](#), [gJSD](#), [distance](#)

Examples

```
# Jensen-Shannon Divergence between P and Q
P <- 1:10/sum(1:10)
Q <- 20:29/sum(20:29)
x <- rbind(P,Q)
JSD(x)

# Jensen-Shannon Divergence between P and Q using different log bases
JSD(x, unit = "log2") # Default
JSD(x, unit = "log")
JSD(x, unit = "log10")

# Jensen-Shannon Divergence Divergence between count vectors P.count and Q.count
P.count <- 1:10
Q.count <- 20:29
x.count <- rbind(P.count,Q.count)
JSD(x.count, est.prob = "empirical")

# Example: Distance Matrix using JSD-Distance

Prob <- rbind(1:10/sum(1:10), 20:29/sum(20:29), 30:39/sum(30:39))

# compute the KL matrix of a given probability matrix
JSDMatrix <- JSD(Prob)

# plot a heatmap of the corresponding JSD matrix
heatmap(JSDMatrix)
```

 KL *Kullback-Leibler Divergence*

Description

This function computes the Kullback-Leibler divergence of two probability distributions P and Q.

Usage

```
KL(x, test.na = TRUE, unit = "log2", est.prob = NULL, epsilon = 1e-05)
```

Arguments

x	a numeric data.frame or matrix (storing probability vectors) or a numeric data.frame or matrix storing counts (if est.prob = TRUE). See distance for details.
test.na	a boolean value indicating whether input vectors should be tested for NA values.
unit	a character string specifying the logarithm unit that shall be used to compute distances that depend on log computations.
est.prob	method to estimate probabilities from a count vector. Default: est.prob = NULL.
epsilon	a small value to address cases in the KL computation where division by zero occurs. In these cases, x / 0 or 0 / 0 will be replaced by epsilon. The default is epsilon = 0.00001. However, we recommend to choose a custom epsilon value depending on the size of the input vectors, the expected similarity between compared probability density functions and whether or not many 0 values are present within the compared vectors. As a rough rule of thumb we suggest that when dealing with very large input vectors which are very similar and contain many 0 values, the epsilon value should be set even smaller (e.g. epsilon = 0.000000001), whereas when vector sizes are small or distributions very divergent then higher epsilon values may also be appropriate (e.g. epsilon = 0.01). Addressing this epsilon issue is important to avoid cases where distance metrics return negative values which are not defined and only occur due to the technical issues of computing x / 0 or 0 / 0 cases.

Details

$$KL(P||Q) = \sum P(P) * \log_2(P(P)/P(Q)) = H(P, Q) - H(P)$$

where H(P,Q) denotes the joint entropy of the probability distributions P and Q and H(P) denotes the entropy of probability distribution P. In case P = Q then KL(P,Q) = 0 and in case P != Q then KL(P,Q) > 0.

The KL divergence is a non-symmetric measure of the directed divergence between two probability distributions P and Q. It only fulfills the *positivity* property of a *distance metric*.

Because of the relation $KL(P||Q) = H(P, Q) - H(P)$, the Kullback-Leibler divergence of two probability distributions P and Q is also named *Cross Entropy* of two probability distributions P and Q.

Value

The Kullback-Leibler divergence of probability vectors.

Author(s)

Hajk-Georg Drost

References

Cover Thomas M. and Thomas Joy A. 2006. Elements of Information Theory. *John Wiley & Sons*.

See Also

[H](#), [CE](#), [JSD](#), [gJSD](#), [distance](#)

Examples

```
# Kulback-Leibler Divergence between P and Q
P <- 1:10/sum(1:10)
Q <- 20:29/sum(20:29)
x <- rbind(P,Q)
KL(x)

# Kulback-Leibler Divergence between P and Q using different log bases
KL(x, unit = "log2") # Default
KL(x, unit = "log")
KL(x, unit = "log10")

# Kulback-Leibler Divergence between count vectors P.count and Q.count
P.count <- 1:10
Q.count <- 20:29
x.count <- rbind(P.count,Q.count)
KL(x, est.prob = "empirical")

# Example: Distance Matrix using KL-Distance

Prob <- rbind(1:10/sum(1:10), 20:29/sum(20:29), 30:39/sum(30:39))

# compute the KL matrix of a given probability matrix
KLMatrix <- KL(Prob)

# plot a heatmap of the corresponding KL matrix
heatmap(KLMatrix)
```

kulczynski_d	<i>Kulczynski_d distance (lowlevel function)</i>
--------------	--

Description

The lowlevel function for computing the kulczynski_d distance.

Usage

```
kulczynski_d(P, Q, testNA, epsilon)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
epsilon	epsilon a small value to address cases in the distance computation where division by zero occurs. In these cases, $x / 0$ or $0 / 0$ will be replaced by epsilon. The default is $\text{epsilon} = 0.00001$. However, we recommend to choose a custom epsilon value depending on the size of the input vectors, the expected similarity between compared probability density functions and whether or not many 0 values are present within the compared vectors. As a rough rule of thumb we suggest that when dealing with very large input vectors which are very similar and contain many 0 values, the epsilon value should be set even smaller (e.g. $\text{epsilon} = 0.00000001$), whereas when vector sizes are small or distributions very divergent then higher epsilon values may also be appropriate (e.g. $\text{epsilon} = 0.01$). Addressing this epsilon issue is important to avoid cases where distance metrics return negative values which are not defined and only occur due to the technical issues of computing $x / 0$ or $0 / 0$ cases.

Author(s)

Hajk-Georg Drost

Examples

```
kulczynski_d(P = 1:10/sum(1:10), Q = 20:29/sum(20:29),  
  testNA = FALSE, epsilon = 0.00001)
```

kullback_leibler_distance
kullback-Leibler distance (lowlevel function)

Description

The lowlevel function for computing the kullback_leibler_distance distance.

Usage

```
kullback_leibler_distance(P, Q, testNA, unit, epsilon)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
unit	type of log function. Option are <ul style="list-style-type: none">• unit = "log"• unit = "log2"• unit = "log10"
epsilon	epsilon a small value to address cases in the distance computation where division by zero occurs. In these cases, $x / 0$ or $0 / 0$ will be replaced by epsilon. The default is <code>epsilon = 0.00001</code> . However, we recommend to choose a custom epsilon value depending on the size of the input vectors, the expected similarity between compared probability density functions and whether or not many 0 values are present within the compared vectors. As a rough rule of thumb we suggest that when dealing with very large input vectors which are very similar and contain many 0 values, the epsilon value should be set even smaller (e.g. <code>epsilon = 0.000000001</code>), whereas when vector sizes are small or distributions very divergent then higher epsilon values may also be appropriate (e.g. <code>epsilon = 0.01</code>). Addressing this epsilon issue is important to avoid cases where distance metrics return negative values which are not defined and only occur due to the technical issues of computing $x / 0$ or $0 / 0$ cases.

Author(s)

Hajk-Georg Drost

Examples

```
kullback_leibler_distance(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE,  
unit = "log2", epsilon = 0.00001)
```

kumar_hassebrook	<i>Kumar hassebrook distance (lowlevel function)</i>
------------------	--

Description

The lowlevel function for computing the kumar_hassebrook distance.

Usage

```
kumar_hassebrook(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
kumar_hassebrook(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

kumar_johnson	<i>Kumar-Johnson distance (lowlevel function)</i>
---------------	---

Description

The lowlevel function for computing the kumar_johnson distance.

Usage

```
kumar_johnson(P, Q, testNA, epsilon)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
epsilon	epsilon a small value to address cases in the distance computation where division by zero occurs. In these cases, $x / 0$ or $0 / 0$ will be replaced by epsilon. The default is <code>epsilon = 0.00001</code> . However, we recommend to choose a custom epsilon value depending on the size of the input vectors, the expected similarity between compared probability density functions and whether or not many 0 values are present within the compared vectors. As a rough rule of thumb we suggest that when dealing with very large input vectors which are very similar and contain many 0 values, the epsilon value should be set even smaller (e.g. <code>epsilon = 0.000000001</code>), whereas when vector sizes are small or distributions very divergent then higher epsilon values may also be appropriate (e.g. <code>epsilon = 0.01</code>). Addressing this epsilon issue is important to avoid cases where distance metrics return negative values which are not defined and only occur due to the technical issues of computing $x / 0$ or $0 / 0$ cases.

Author(s)

Hajk-Georg Drost

Examples

```
kumar_johnson(P = 1:10/sum(1:10), Q = 20:29/sum(20:29),
  testNA = FALSE, epsilon = 0.00001)
```

k_divergence	<i>K-Divergence (lowlevel function)</i>
--------------	---

Description

The lowlevel function for computing the k_divergence distance.

Usage

```
k_divergence(P, Q, testNA, unit)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

unit type of log function. Option are

- unit = "log"
- unit = "log2"
- unit = "log10"

Author(s)

Hajk-Georg Drost

Examples

```
k_divergence(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE, unit = "log2")
```

lin.cor

*Linear Correlation***Description**

This function computed the linear correlation between two vectors or a correlation matrix for an input matrix.

The following methods to compute linear correlations are implemented in this function:

Usage

```
lin.cor(x, y = NULL, method = "pearson", test.na = FALSE)
```

Arguments

x a numeric vector, matrix, or data.frame.
y a numeric vector that should be correlated with x.
method the method to compute the linear correlation between x and y.
test.na a boolean value indicating whether input data should be checked for NA values.

Details

- method = "pearson" : Pearson's correlation coefficient (centred).
- method = "pearson2" : Pearson's uncentred correlation coefficient.
- method = "sq_pearson" . Squared Pearson's correlation coefficient.
- method = "kendall" : Kendall's correlation coefficient.
- method = "spearman" : Spearman's correlation coefficient.

Further Details:

- *Pearson's correlation coefficient (centred)* :

Author(s)

Hajk-Georg Drost

lorentzian	<i>Lorentzian distance (lowlevel function)</i>
------------	--

Description

The low-level function for computing the lorentzian distance.

Usage

```
lorentzian(P, Q, testNA, unit)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
unit	type of log function. Option are <ul style="list-style-type: none">• unit = "log"• unit = "log2"• unit = "log10"

Author(s)

Hajk-Georg Drost

Examples

```
lorentzian(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE, unit = "log2")
```

manhattan	<i>Manhattan distance (lowlevel function)</i>
-----------	---

Description

The lowlevel function for computing the manhattan distance.

Usage

```
manhattan(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
manhattan(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

matusita	<i>Matusita distance (lowlevel function)</i>
----------	--

Description

The lowlevel function for computing the matusita distance.

Usage

```
matusita(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
matusita(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

MI *Shannon's Mutual Information $I(X, Y)$*

Description

Compute Shannon's Mutual Information based on the identity $I(X, Y) = H(X) + H(Y) - H(X, Y)$ based on a given joint-probability vector $P(X, Y)$ and probability vectors $P(X)$ and $P(Y)$.

Usage

```
MI(x, y, xy, unit = "log2")
```

Arguments

x	a numeric probability vector $P(X)$.
y	a numeric probability vector $P(Y)$.
xy	a numeric joint-probability vector $P(X, Y)$.
unit	a character string specifying the logarithm unit that shall be used to compute distances that depend on log computations.

Details

This function might be useful to fastly compute Shannon's Mutual Information for any given joint-probability vector and probability vectors.

Value

Shannon's Mutual Information in bit.

Author(s)

Hajk-Georg Drost

References

Shannon, Claude E. 1948. "A Mathematical Theory of Communication". *Bell System Technical Journal* **27** (3): 379-423.

See Also

[H](#), [JE](#), [CE](#)

Examples

```
MI( x = 1:10/sum(1:10), y = 20:29/sum(20:29), xy = 1:10/sum(1:10) )
```

minkowski	<i>Minkowski distance (lowlevel function)</i>
-----------	---

Description

The lowlevel function for computing the minkowski distance.

Usage

```
minkowski(P, Q, n, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
n	index for the minkowski exponent.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
minkowski(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), n = 2, testNA = FALSE)
```

motyka	<i>Motyka distance (lowlevel function)</i>
--------	--

Description

The lowlevel function for computing the motyka distance.

Usage

```
motyka(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
motyka(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

neyman_chi_sq	<i>Neyman chi-squared distance (lowlevel function)</i>
---------------	--

Description

The lowlevel function for computing the neyman_chi_sq distance.

Usage

```
neyman_chi_sq(P, Q, testNA, epsilon)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
epsilon	epsilon a small value to address cases in the distance computation where division by zero occurs. In these cases, $x / 0$ or $0 / 0$ will be replaced by epsilon. The default is <code>epsilon = 0.00001</code> . However, we recommend to choose a custom epsilon value depending on the size of the input vectors, the expected similarity between compared probability density functions and whether or not many 0 values are present within the compared vectors. As a rough rule of thumb we suggest that when dealing with very large input vectors which are very similar and contain many 0 values, the epsilon value should be set even smaller (e.g. <code>epsilon = 0.000000001</code>), whereas when vector sizes are small or distributions very divergent then higher epsilon values may also be appropriate (e.g. <code>epsilon = 0.01</code>). Addressing this epsilon issue is important to avoid cases where distance metrics return negative values which are not defined and only occur due to the technical issues of computing $x / 0$ or $0 / 0$ cases.

Author(s)

Hajk-Georg Drost

Examples

```
neyman_chi_sq(P = 1:10/sum(1:10), Q = 20:29/sum(20:29),
  testNA = FALSE, epsilon = 0.00001)
```

pearson_chi_sq	<i>Pearson chi-squared distance (lowlevel function)</i>
----------------	---

Description

The lowlevel function for computing the pearson_chi_sq distance.

Usage

```
pearson_chi_sq(P, Q, testNA, epsilon)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
epsilon	epsilon a small value to address cases in the distance computation where division by zero occurs. In these cases, $x / 0$ or $0 / 0$ will be replaced by epsilon. The default is $\text{epsilon} = 0.00001$. However, we recommend to choose a custom epsilon value depending on the size of the input vectors, the expected similarity between compared probability density functions and whether or not many 0 values are present within the compared vectors. As a rough rule of thumb we suggest that when dealing with very large input vectors which are very similar and contain many 0 values, the epsilon value should be set even smaller (e.g. $\text{epsilon} = 0.000000001$), whereas when vector sizes are small or distributions very divergent then higher epsilon values may also be appropriate (e.g. $\text{epsilon} = 0.01$). Addressing this epsilon issue is important to avoid cases where distance metrics return negative values which are not defined and only occur due to the technical issues of computing $x / 0$ or $0 / 0$ cases.

Author(s)

Hajk-Georg Drost

Examples

```
pearson_chi_sq(P = 1:10/sum(1:10), Q = 20:29/sum(20:29),  
testNA = FALSE, epsilon = 0.00001)
```

prob_symm_chi_sq *Probability symmetric chi-squared distance (lowlevel function)*

Description

The lowlevel function for computing the prob_symm_chi_sq distance.

Usage

```
prob_symm_chi_sq(P, Q, testNA)
```

Arguments

P a numeric vector storing the first distribution.
Q a numeric vector storing the second distribution.
testNA a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
prob_symm_chi_sq(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

ruzicka *Ruzicka distance (lowlevel function)*

Description

The lowlevel function for computing the ruzicka distance.

Usage

```
ruzicka(P, Q, testNA)
```

Arguments

P a numeric vector storing the first distribution.
Q a numeric vector storing the second distribution.
testNA a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
ruzicka(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

`soergel`*Soergel distance (lowlevel function)*

Description

The lowlevel function for computing the soergel distance.

Usage

```
soergel(P, Q, testNA)
```

Arguments

P a numeric vector storing the first distribution.
Q a numeric vector storing the second distribution.
testNA a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
soergel(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

`sorensen`*Sorensen distance (lowlevel function)*

Description

The lowlevel function for computing the sorensen distance.

Usage

```
sorensen(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
sorensen(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

squared_chi_sq	<i>Squared chi-squared distance (lowlevel function)</i>
----------------	---

Description

The lowlevel function for computing the squared_chi_sq distance.

Usage

```
squared_chi_sq(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
squared_chi_sq(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

squared_chord	<i>Squared chord distance (lowlevel function)</i>
---------------	---

Description

The lowlevel function for computing the squared_chord distance.

Usage

```
squared_chord(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
squared_chord(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

squared_euclidean	<i>Squared euclidean distance (lowlevel function)</i>
-------------------	---

Description

The lowlevel function for computing the squared_euclidean distance.

Usage

```
squared_euclidean(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
squared_euclidean(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

 taneja

Taneja difference (lowlevel function)

Description

The lowlevel function for computing the taneja distance.

Usage

```
taneja(P, Q, testNA, unit, epsilon)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
unit	type of log function. Option are <ul style="list-style-type: none"> • unit = "log" • unit = "log2" • unit = "log10"
epsilon	epsilon a small value to address cases in the distance computation where division by zero occurs. In these cases, $x / 0$ or $0 / 0$ will be replaced by epsilon. The default is <code>epsilon = 0.00001</code> . However, we recommend to choose a custom epsilon value depending on the size of the input vectors, the expected similarity between compared probability density functions and whether or not many 0 values are present within the compared vectors. As a rough rule of thumb we suggest that when dealing with very large input vectors which are very similar and contain many 0 values, the epsilon value should be set even smaller (e.g. <code>epsilon = 0.000000001</code>), whereas when vector sizes are small or distributions very divergent then higher epsilon values may also be appropriate (e.g. <code>epsilon = 0.01</code>). Addressing this epsilon issue is important to avoid cases where distance metrics return negative values which are not defined and only occur due to the technical issues of computing $x / 0$ or $0 / 0$ cases.

Author(s)

Hajk-Georg Drost

Examples

```
taneja(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE,  
unit = "log2", epsilon = 0.00001)
```

tanimoto	<i>Tanimoto distance (lowlevel function)</i>
----------	--

Description

The lowlevel function for computing the tanimoto distance.

Usage

```
tanimoto(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
tanimoto(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

topsoe	<i>Topsoe distance (lowlevel function)</i>
--------	--

Description

The lowlevel function for computing the topsoe distance.

Usage

```
topsoe(P, Q, testNA, unit)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.
unit	type of log function. Option are <ul style="list-style-type: none">• unit = "log"• unit = "log2"• unit = "log10"

Author(s)

Hajk-Georg Drost

Examples

```
topsoe(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE, unit = "log2")
```

wave_hedges

Wave hedges distance (lowlevel function)

Description

The lowlevel function for computing the wave_hedges distance.

Usage

```
wave_hedges(P, Q, testNA)
```

Arguments

P	a numeric vector storing the first distribution.
Q	a numeric vector storing the second distribution.
testNA	a logical value indicating whether or not distributions shall be checked for NA values.

Author(s)

Hajk-Georg Drost

Examples

```
wave_hedges(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```

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