Package 'philentropy'

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Type Package

Title Similarity and Distance Quantification Between Probability Functions

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Description Computes 46 optimized distance and similarity measures for comparing probability func-tions (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

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>

RoxygenNote 7.3.1

NeedsCompilation yes

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Contents

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

Author(s)

Hajk-Georg Drost

```
additive_symm_chi_sq(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```
The lowlevel function for computing the avg distance.

Usage

avg(P, Q, testNA)

Arguments

Author(s)

Hajk-Georg Drost

Examples

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

Description

The lowlevel function for computing the bhattacharyya distance.

Usage

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

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Arguments

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
\mathcal{L}
```
Arguments

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/](http://vita.had.co.nz/papers/density-estimation.pdf) [papers/density-estimation.pdf](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

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

Details

This function might be useful to fastly compute Shannon's Conditional-Entropy for any given jointprobability 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](#page-24-1), [JE](#page-28-1)

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

Author(s)

Hajk-Georg Drost

Examples

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

The lowlevel function for computing the clark_sq distance.

Usage

clark_sq(P, Q, testNA)

Arguments

Author(s)

Hajk-Georg Drost

Examples

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

cosine_dist *Cosine distance (lowlevel function)*

Description

The lowlevel function for computing the cosine_dist distance.

Usage

cosine_dist(P, Q, testNA)

Author(s)

Hajk-Georg Drost

Examples

```
cosine_dist(P = 1:10/\text{sum}(1:10), Q = 20:29/\text{sum}(20:29), testNA = FALSE)
```
czekanowski *Czekanowski distance (lowlevel function)*

Description

The lowlevel function for computing the czekanowski distance.

Usage

czekanowski(P, Q, testNA)

Arguments

Author(s)

Hajk-Georg Drost

Examples

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


Description

The lowlevel function for computing the dice_dist distance.

Usage

dice_dist(P, Q, testNA)

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Arguments

Author(s)

Hajk-Georg Drost

Examples

```
dice_dist(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```
dist.diversity *Distance Diversity between Probability Density Functions*

Description

This function computes all distance values between two probability density functions that are available in [getDistMethods](#page-22-1) 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

Author(s)

Hajk-Georg Drost

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


Details

Here a distance is defined as a quantitative degree of how far two mathematical objects are apart from eachother (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 : $d = (\sum |P_i Q_i|^p)^1/p$
	- \blacksquare Chebyshev : $d = max|P_i Q_i|$
- L_1 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
	- $\overline{}$ 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 $X^{\wedge}2 : d = \sum ((P_i Q_i)^2 / Q_i)$
	- Neyman $X^{\wedge}2 : d = \sum ((P_i Q_i)^2 / P_i)$
	- − Squared X^2 : $d = \sum ((P_i Q_i)^2 / (P_i + Q_i))$
	- Probabilistic Symmetric $X^{\wedge}2 : d = 2 * \sum ((P_i Q_i)^2/(P_i + Q_i))$
	- Divergence : $X^2 \cdot d = 2 * \sum ((P_i Q_i)^2 / (P_i + Q_i)^2)$
	- − 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 : $d = \sum (P_i^2 Q_i^2)^2 / 2 * (P_i * Q_i)^1.5$

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\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 corresponsning 0 is replaced by a small $\epsilon = 0.00001$.
- log of zero case $0 \times \log(0)$: 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](#page-22-1), [estimate.probability](#page-20-1), [dist.diversity](#page-10-1)

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 = log10distance(ProbMatrix, method = "kullback-leibler", unit = "log10")
```


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

Usage

dist_many_many(

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```
dists1,
  dists2,
  method,
  p = NA\_real_testNA = TRUE,
  unit = "log",
  epsilon = 1e-05
\mathcal{L}
```
Arguments

Value

A matrix of distance values

```
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)
```


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
)
```


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 \le -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 *Distances and Similarities between Two Probability Density Functions*

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
)
```


```
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 similar-
                  ity 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 simi-
                  lar 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 distri-
                  butions 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 \le -1:10 / sum(1:10)Q \le -20:29 / sum(20:29)
dist_one_one(P, Q, method = "euclidean", testNA = FALSE)
```
divergence_sq *Divergence squared distance (lowlevel function)*

Description

The lowlevel function for computing the divergence_sq distance.

Usage

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

Author(s)

Hajk-Georg Drost

```
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/sum(x).

Usage

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

Value

a numeric probability vector.

Author(s)

Hajk-Georg Drost

```
# generate a count vector
x \leftarrow runif(100)# generate a probability vector from corresponding counts
x.prob <- estimate.probability(x, method = 'empirical')
```


The lowlevel function for computing the euclidean distance.

Usage

euclidean(P, Q, testNA)

Arguments

Author(s)

Hajk-Georg Drost

Examples

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

fidelity *Fidelity distance (lowlevel function)*

Description

The lowlevel function for computing the fidelity distance.

Usage

fidelity(P, Q, testNA)

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Author(s)

Hajk-Georg Drost

Examples

fidelity(P = $1:10/\text{sum}(1:10)$, Q = $20:29/\text{sum}(20:29)$, testNA = FALSE)

getDistMethods *Get method names for* distance

Description

This function returns the names of the methods that can be applied to compute distances between probability density functions using the [distance](#page-11-1) function.

Usage

getDistMethods()

Author(s)

Hajk-Georg Drost

Examples

getDistMethods()

gJSD *Generalized Jensen-Shannon Divergence*

Description

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

Usage

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

Details

Function to compute the Generalized Jensen-Shannon Divergence

 $JSD_{\pi_1,...,\pi_n}(P_1,...,P_n) = H(\sum_{i=1}^n \pi_i * P_i) - \sum_{i=1}^n \pi_i * H(P_i)$ where $\pi_1, ..., \pi_n$ denote the weights selected for the probability vectors P₁,..., 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](#page-34-1), [H](#page-24-1), [JSD](#page-32-1), [CE](#page-6-1), [JE](#page-28-1)

```
# 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")
```
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```
# 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

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 $H(X) = -\sum P(X) * log2(P(X))$ based on a given probability vector $P(X)$.

Usage

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

Arguments

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](#page-28-1), [CE](#page-6-1), [KL](#page-34-1), [JSD](#page-32-1), [gJSD](#page-22-2)

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)
```


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Author(s)

Hajk-Georg Drost

Examples

```
harmonic_mean_dist(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)
```
hellinger *Hellinger distance (lowlevel function)*

Description

The lowlevel function for computing the hellinger distance.

Usage

hellinger(P, Q, testNA)

Arguments

Author(s)

Hajk-Georg Drost

Examples

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


Description

The lowlevel function for computing the inner_product distance.

Usage

inner_product(P, Q, testNA)

Arguments

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

Author(s)

Hajk-Georg Drost

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


The lowlevel function for computing the jaccard distance.

Usage

jaccard(P, Q, testNA)

Arguments

Author(s)

Hajk-Georg Drost

Examples

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

JE *Shannon's Joint-Entropy* H(X, Y)

Description

This funciton computes Shannon's Joint-Entropy $H(X,Y) = -\sum_{Y} \sum_{Y} P(X,Y) * log2(P(X,Y))$ based on a given joint-probability vector $P(X, Y)$.

Usage

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

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](#page-24-1), [CE](#page-6-1), [KL](#page-34-1), [JSD](#page-32-1), [gJSD](#page-22-2), [distance](#page-11-1)

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)


```
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 similar-
                  ity 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 simi-
                  lar 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 distri-
                  butions 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)
```


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 *Jensen-Shannon distance (lowlevel function)*

Description

The lowlevel function for computing the jensen_shannon distance.

Usage

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

Author(s)

Hajk-Georg Drost

Examples

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

This function computes a divergence matrix or divergence value based on the Jensen-Shannon Divergence with equal weights. Please be aware that when aiming to compute the Jensen-Shannon Distance (rather than Divergence), you will need to apply the link{sqrt} on the JSD() output.

Usage

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

Arguments

Details

Function to compute the Jensen-Shannon Divergence JSD(P || 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:

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

where $R = 0.5 * (P + Q)$ denotes the mid-point of the probability vectors P and Q, and KL(P || R), KL(Q || 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 divergence 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](#page-34-1), [H](#page-24-1), [CE](#page-6-1), [gJSD](#page-22-2), [distance](#page-11-1)

```
# Jensen-Shannon Divergence between P and Q
P \le -1:10/sum(1:10)Q <- 20:29/sum(20:29)
x \leftarrow \text{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 <-1:10Q.count <- 20:29
x.count <- rbind(P.count,Q.count)
JSD(x.count, est.prob = "empirical")
# Example: Divergence Matrix using JSD-Divergence
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)
```
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

Details

$$
KL(P||Q) = \sum P(P) * log2(P(P)/P(Q)) = H(P,Q) - H(P)
$$

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 $KL(PI|Q) = H(P,Q) - H(P)$, 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](#page-24-1), [CE](#page-6-1), [JSD](#page-32-1), [gJSD](#page-22-2), [distance](#page-11-1)

```
# Kulback-Leibler Divergence between P and Q
P \le -1:10/sum(1:10)Q <- 20:29/sum(20:29)
x \leftarrow \text{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)
```


The lowlevel function for computing the kulczynski_d distance.

Usage

kulczynski_d(P, Q, testNA, epsilon)

Arguments

Author(s)

Hajk-Georg Drost

```
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

Author(s)

Hajk-Georg Drost

```
kullback_leibler_distance(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE,
unit = "log2", epsilon = 0.00001)
```
kumar_hassebrook *Kumar hassebrook distance (lowlevel function)*

Description

The lowlevel function for computing the kumar_hassebrook distance.

Usage

kumar_hassebrook(P, Q, testNA)

Arguments

Author(s)

Hajk-Georg Drost

Examples

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

Description

The lowlevel function for computing the kumar_johnson distance.

Usage

kumar_johnson(P, Q, testNA, epsilon)

Arguments

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 *K-Divergence (lowlevel function)*

Description

The lowlevel function for computing the k_divergence distance.

Usage

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


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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

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

The low-level function for computing the lorentzian distance.

Usage

lorentzian(P, Q, testNA, unit)

Arguments

Author(s)

Hajk-Georg Drost

Examples

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

Description

The lowlevel function for computing the manhattan distance.

Usage

manhattan(P, Q, testNA)

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Arguments

Author(s)

Hajk-Georg Drost

Examples

manhattan(P = $1:10/\text{sum}(1:10)$, Q = $20:29/\text{sum}(20:29)$, testNA = FALSE)

matusita *Matusita distance (lowlevel function)*

Description

The lowlevel function for computing the matusita distance.

Usage

matusita(P, Q, testNA)

Arguments

Author(s)

Hajk-Georg Drost

```
matusita(P = 1:10/\text{sum}(1:10), Q = 20:29/\text{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

Details

This function might be useful to fastly compute Shannon's Mutual Information for any given jointprobability 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](#page-24-1), [JE](#page-28-1), [CE](#page-6-1)

Examples

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

The lowlevel function for computing the minkowski distance.

Usage

minkowski(P, Q, n, testNA)

Arguments

Author(s)

Hajk-Georg Drost

Examples

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

motyka *Motyka distance (lowlevel function)*

Description

The lowlevel function for computing the motyka distance.

Usage

motyka(P, Q, testNA)

Author(s)

Hajk-Georg Drost

Examples

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

Description

The lowlevel function for computing the neyman_chi_sq distance.

Usage

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

Author(s)

Hajk-Georg Drost

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


The lowlevel function for computing the pearson_chi_sq distance.

Usage

pearson_chi_sq(P, Q, testNA, epsilon)

Arguments

Author(s)

Hajk-Georg Drost

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


The lowlevel function for computing the prob_symm_chi_sq distance.

Usage

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

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)

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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

Author(s)

Hajk-Georg Drost

Examples

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

Description

The lowlevel function for computing the sorensen distance.

Usage

sorensen(P, Q, testNA)

Arguments

Author(s)

Hajk-Georg Drost

Examples

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

Description

The lowlevel function for computing the squared_chi_sq distance.

Usage

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

Author(s)

Hajk-Georg Drost

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


The lowlevel function for computing the squared_chord distance.

Usage

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

Author(s)

Hajk-Georg Drost

Examples

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

squared_euclidean *Squared euclidean distance (lowlevel function)*

Description

The lowlevel function for computing the squared_euclidean distance.

Usage

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


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

Author(s)

Hajk-Georg Drost

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Examples

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


tanimoto *Tanimoto distance (lowlevel function)*

Description

The lowlevel function for computing the tanimoto distance.

Usage

tanimoto(P, Q, testNA)

Arguments

Author(s)

Hajk-Georg Drost

Examples

 t animoto(P = 1:10/sum(1:10), Q = 20:29/sum(20:29), testNA = FALSE)

topsoe *Topsoe distance (lowlevel function)*

Description

The lowlevel function for computing the topsoe distance.

Usage

topsoe(P, Q, testNA, unit)

Arguments

Author(s)

Hajk-Georg Drost

Examples

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

Description

The lowlevel function for computing the wave_hedges distance.

Usage

wave_hedges(P, Q, testNA)

Arguments

Author(s)

Hajk-Georg Drost

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