

Package ‘jaccard’

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Type Package

Title Testing Similarity Between Binary Datasets using
Jaccard/Tanimoto Coefficients

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Description Calculate statistical significance of Jaccard/Tanimoto similarity
coefficients.

License GPL-2

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jaccard	<i>Compute a Jaccard/Tanimoto similarity coefficient</i>
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Description

Compute a Jaccard/Tanimoto similarity coefficient

Usage

```
jaccard(x, y, center = FALSE, px = NULL, py = NULL)
```

Arguments

x	a binary vector (e.g., fingerprint)
y	a binary vector (e.g., fingerprint)
center	whether to center the Jaccard/Tanimoto coefficient by its expectation
px	probability of successes in x (optional)
py	probability of successes in y (optional)

Value

jaccard.test.bootstrap returns an expected value.

Examples

```
set.seed(1234)
x = rbinom(100,1,.5)
y = rbinom(100,1,.5)
jaccard(x,y)
```

jaccard.ev	<i>Compute an expected Jaccard/Tanimoto similarity coefficient under independence</i>
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Description

Compute an expected Jaccard/Tanimoto similarity coefficient under independence

Usage

```
jaccard.ev(x, y, px = NULL, py = NULL)
```

Arguments

x	a binary vector (e.g., fingerprint)
y	a binary vector (e.g., fingerprint)
px	probability of successes in x (optional)
py	probability of successes in y (optional)

Value

jaccard.test.bootstrap returns an expected value.

Examples

```
set.seed(1234)
x = rbinom(100,1,.5)
y = rbinom(100,1,.5)
jaccard.ev(x,y)
```

jaccard.rahman

Compute p-value using the EC-BLAST method

Description

In the EC-BLAST paper, Rahman et al. (2014) provide the following description: The mean (μ) and s.d. (σ) of the similarity scores are used to define the z score, $z = (Tw - \mu)/\sigma$. For the purpose of calculating the P value, only hits with $T > 0$ are considered. The P value w is derived from the z score using an extreme value distribution $P = 1 - \exp\left(-e^{-z\pi/\sqrt{6}-\Gamma'(1)}\right)$, where the Euler-Mascheroni constant $\Gamma'(1) \approx 0.577215665$.

Usage

```
jaccard.rahman(j)
```

Arguments

j	a numeric vector of observed Jaccard coefficients (uncentered)
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Value

jaccard.rahman returns a numeric vector of p-values

References

Rahman, Cuesta, Furnham, Holliday, and Thornton (2014) EC-BLAST: a tool to automatically search and compare enzyme reactions. Nature Methods, 11(2) <https://www.nature.com/articles/nmeth.2803>

`jaccard.test`*Test for Jaccard/Tanimoto similarity coefficients*

Description

Compute statistical significance of Jaccard/Tanimoto similarity coefficients between binary vectors, using four different methods.

Usage

```
jaccard.test(x, y, method = "mca", px = NULL, py = NULL, verbose = TRUE, ...)
```

Arguments

<code>x</code>	a binary vector (e.g., fingerprint)
<code>y</code>	a binary vector (e.g., fingerprint)
<code>method</code>	a method to compute a p-value ("mca", "bootstrap", "asymptotic", or "exact")
<code>px</code>	probability of successes in x (optional)
<code>py</code>	probability of successes in y (optional)
<code>verbose</code>	whether to print progress messages
<code>...</code>	optional arguments for specific computational methods

Details

There exist four methods to compute p-values of Jaccard/Tanimoto similarity coefficients: `mca`, `bootstrap`, `asymptotic`, and `exact`. This is simply a wrapper function for corresponding four functions in this package: [jaccard.test.mca](#), [jaccard.test.bootstrap](#), [jaccard.test.asymptotic](#), and [jaccard.test.exact](#).

We recommend using either `mca` or `bootstrap` methods, since the `exact` solution is slow for a moderately large vector and `asymptotic` approximation may be inaccurate depending on the input vector size. The `bootstrap` method uses resampling with replacement binary vectors to compute a p-value (see optional arguments). The `mca` method uses the measure concentration algorithm that estimates the multinomial distribution with a known error bound (specified by an optional argument `accuracy`).

Value

`jaccard.test` returns a list mainly consisting of

<code>statistics</code>	centered Jaccard/Tanimoto similarity coefficient
<code>pvalue</code>	p-value
<code>expectation</code>	expectation

Optional arguments for method="bootstrap"

fix whether to fix (i.e., not resample) x and/or y
B a total bootstrap iteration
seed a seed for a random number generator

Optional arguments for method="mca"

accuracy an error bound on approximating a multinomial distribution
error.type an error type on approximating a multinomial distribution ("average", "upper", "lower")
seed a seed for the random number generator.

See Also

[jaccard.test.bootstrap](#) [jaccard.test.mca](#) [jaccard.test.exact](#) [jaccard.test.asymptotic](#)

Examples

```
set.seed(1234)
x = rbinom(100,1,.5)
y = rbinom(100,1,.5)
jaccard.test(x,y,method="bootstrap")
jaccard.test(x,y,method="mca")
jaccard.test(x,y,method="exact")
jaccard.test(x,y,method="asymptotic")
```

```
jaccard.test.asymptotic
```

Compute p-value using an asymptotic approximation

Description

Compute statistical significance of Jaccard/Tanimoto similarity coefficients.

Usage

```
jaccard.test.asymptotic(x, y, px = NULL, py = NULL, verbose = TRUE)
```

Arguments

x	a binary vector (e.g., fingerprint)
y	a binary vector (e.g., fingerprint)
px	probability of successes in x (optional)
py	probability of successes in y (optional)
verbose	whether to print progress messages

Value

jaccard.test.asymptotic returns a list consisting of

statistics	centered Jaccard/Tanimoto similarity coefficient
pvalue	p-value
expectation	expectation

Examples

```
set.seed(1234)
x = rbinom(100,1,.5)
y = rbinom(100,1,.5)
jaccard.test.asymptotic(x,y)
```

```
jaccard.test.bootstrap
```

Compute p-value using the bootstrap procedure

Description

Compute statistical significance of Jaccard/Tanimoto similarity coefficients.

Usage

```
jaccard.test.bootstrap(
  x,
  y,
  px = NULL,
  py = NULL,
  verbose = TRUE,
  fix = "x",
  B = 1000,
  seed = NULL
)
```

Arguments

x	a binary vector (e.g., fingerprint)
y	a binary vector (e.g., fingerprint)
px	probability of successes in x (optional)
py	probability of successes in y (optional)
verbose	whether to print progress messages
fix	whether to fix (i.e., not resample) x and/or y
B	a total bootstrap iteration
seed	a seed for a random number generator

Value

jaccard.test.bootstrap returns a list consisting of

statistics	centered Jaccard/Tanimoto similarity coefficient
pvalue	p-value
expectation	expectation

Examples

```
set.seed(1234)
x = rbinom(100,1,.5)
y = rbinom(100,1,.5)
jaccard.test.bootstrap(x,y,B=500)
```

jaccard.test.exact	<i>Compute p-value using the exact solution</i>
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Description

Compute statistical significance of Jaccard/Tanimoto similarity coefficients.

Usage

```
jaccard.test.exact(x, y, px = NULL, py = NULL, verbose = TRUE)
```

Arguments

x	a binary vector (e.g., fingerprint)
y	a binary vector (e.g., fingerprint)
px	probability of successes in x (optional)
py	probability of successes in y (optional)
verbose	whether to print progress messages

Value

jaccard.test.exact returns a list consisting of

statistics	centered Jaccard/Tanimoto similarity coefficient
pvalue	p-value
expectation	expectation

Examples

```
set.seed(1234)
x = rbinom(100,1,.5)
y = rbinom(100,1,.5)
jaccard.test.exact(x,y)
```

jaccard.test.mca

Compute p-value using the Measure Concentration Algorithm

Description

Compute statistical significance of Jaccard/Tanimoto similarity coefficients.

Usage

```
jaccard.test.mca(
  x,
  y,
  px = NULL,
  py = NULL,
  accuracy = 1e-05,
  error.type = "average",
  verbose = TRUE
)
```

Arguments

x	a binary vector (e.g., fingerprint)
y	a binary vector (e.g., fingerprint)
px	probability of successes in x (optional)
py	probability of successes in y (optional)
accuracy	an error bound on approximating a multinomial distribution
error.type	an error type on approximating a multinomial distribution ("average", "upper", "lower")
verbose	whether to print progress messages

Value

jaccard.test.mca returns a list consisting of

statistics	centered Jaccard/Tanimoto similarity coefficient
pvalue	p-value
expectation	expectation

Examples

```
set.seed(1234)
x = rbinom(100,1,.5)
y = rbinom(100,1,.5)
jaccard.test.mca(x,y,accuracy = 1e-05)
```

jaccard.test.pairwise *Pair-wise tests for Jaccard/Tanimoto similarity coefficients*

Description

Given a data matrix, it computes pair-wise Jaccard/Tanimoto similarity coefficients and p-values among rows (variables). Only for testing due to its use of a for-loop.

Usage

```
jaccard.test.pairwise(  
  dat,  
  method = "mca",  
  verbose = TRUE,  
  compute.qvalue = TRUE,  
  ...  
)
```

Arguments

dat	a data matrix
method	a method to compute a p-value ("mca", "bootstrap", "asymptotic", or "exact")
verbose	whether to print progress messages
compute.qvalue	whether to compute q-values
...	optional arguments for specific computational methods

Value

jaccard.test.pairwise returns a list of matrices

statistics	Jaccard/Tanimoto similarity coefficients
pvalues	p-values
qvalues	q-values

See Also

[jaccard.test](#)

`runJaccardApp`*Launch an interactive Shiny app on a local network*

Description

Launch an interactive Shiny app on a local network

Usage

```
runJaccardApp()
```

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