Package ‘eummd’

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Title Efficient Univariate Maximum Mean Discrepancy
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Description Computes maximum mean discrepancy two-sample test for univariate data using the Laplacian kernel, as described in Bodenham and Kawahara (2023) <doi:10.1007/s11222-023-10271-x>. The p-value is computed using permutations. Also includes implementation for computing the robust median difference statistic ‘Q_n’ from Croux and Rousseeuw (1992) <doi:10.1007/978-3-662-26811-7_58> based on Johnson and Mizoguchi (1978) <doi:10.1137/0207013>.

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energydist

Naive computation for Energy Distance

Description
Computes energy distance, and possibly a p-value. Suitable for multivariate data. Naive approach, quadratic in number of observations.

Usage
energydist(X, Y, pval = TRUE, numperm = 200, seednum = 0)

Arguments
- **X**: Matrix (or vector) of observations in first sample.
- **Y**: Matrix (or vector) of observations in second sample.
- **pval**: Boolean for whether to compute p-value or not.
- **numperm**: Number of permutations. Default is 200.
- **seednum**: Seed number for generating permutations. Default is 0, which means seed is set randomly. For values larger than 0, results will be reproducible.

Details
First checks number of columns (dimension) are equal. Suppose matrix X has n rows and d columns, and matrix Y has m rows; checks that Y has d columns (if not, then throws error). Then flattens matrices to vectors (or, if d = 1, they are already vectors. Then calls C++ method. If the first sample has n d-dimensional samples and the second sample has m d-dimensional samples, then the algorithm computes the statistic in $O((n + m)^2)$ time.

Random seed is set for std::mt19937 and std::shuffle in C++.

Value
A list with the following elements:
- **pval**: The p-value of the test, if it is computed (pval=TRUE).
- **stat**: The statistic of the test, which is always computed.

References
**Examples**

```r
X <- matrix(c(1:12), ncol=2, byrow=TRUE)
Y <- matrix(c(13:20), ncol=2, byrow=TRUE)
energydistList <- energydist(X=X, Y=Y, pval=FALSE)

# computing p-value
energydistList <- energydist(X=X, Y=Y)

# computing p-value
# using 1000 permutations and seed 1 for reproducibility.
energydistList <- energydist(X=X, Y=Y, numperm=1000, seednum=1)
```

**euMMD: Efficient Univariate Maximum Mean Discrepancy**

**Description**

Computes the maximum mean discrepancy statistic with the Laplacian kernel. Suitable only for univariate data. Computing the statistic alone for $n$ observations is $O(n \log n)$, and computing the p-value for $L$ permutations is $O(n \log n + Ln)$.

**Usage**

```r
eummd(x, y, beta = -0.1, pval = TRUE, numperm = 200, seednum = 0)
```

**Arguments**

- **x**: Univariate vector of observations in first sample.
- **y**: Univariate vector of observations in second sample.
- **beta**: kernel parameter. Must be positive; if not, computes median heuristic in quadratic time. Default value is $-0.1$, which will force median heuristic to be used.
- **pval**: Boolean for whether to compute p-value or not.
- **numperm**: Number of permutations. Default is 200.
- **seednum**: Seed number for generating permutations. Default is 0, which means seed is set randomly. For values larger than 0, results will be reproducible.

**Details**

If the total number of observations in both samples is $n$, first sort combined sample in $O(n \log n)$ before remaining steps are linear in $n$.

If beta is not a positive value, median difference is computed as follows:

$$m = \text{median}\{||x_i - x_j||_1; \ i > j, \ i = 1, 2, \ldots, n + m, \text{ and } j = 1, 2, \ldots, i - 1\}.$$
where $\|x_i - x_j\|_1$ is the 1-norm, and so if the data are univariate then

$$\|x_i - x_j\|_1 = |x_i - x_j|.$$

and finally median heuristic is $\beta = 1/m$. This can be computed in $O(n \log n)$ time using the algorithms of Johnson and Mizoguchi (1978) and Croux and Rousseeuw (1992); see `mediandiff` for references.

The Laplacian kernel $k$ is defined as

$$k(x, y) = \exp[-\beta \|x - y\|_1].$$

The random seed is set for `std::mt19937` and `std::shuffle` in C++.

**Value**

A list with the following elements:

- `pval` The p-value of the test, if it is computed (`pval=TRUE`). Otherwise, it is set to `NA`.
- `stat` The statistic of the test, which is always computed.
- `beta` The kernel parameter used in the test. If `beta` was not initialised or negative, this will be the median heuristic value.

**References**


**See Also**

`mediandiff`

**Examples**

```r
x <- c(7.1, 1.2, 4.3, 0.4)
y <- c(5.5, 2.6, 8.7)
#setting the kernel parameter to be 0.1; setting seed=1 for reproducibility
mmd_list <- eummd(x, y, beta=0.1, seednum=1)

#now using median heuristic (default)
mmd_list <- eummd(x, y, seednum=1)

#now not computing the p-value, only the statistic
mmd_list <- eummd(x, y, pval=FALSE, seednum=1)
```
meammd

MEA-MMD: Multivariate Efficient Approximate Maximum Mean Discrepancy

Description

Computes maximum mean discrepancy statistics with Laplacian or Gaussian kernel. Suitable for multivariate data. Naive approach, quadratic in number of observations.

Usage

```r
meammd(
  X,  # Matrix (or vector) of observations in first sample.
  Y,  # Matrix (or vector) of observations in second sample.
  beta = -0.1,  # kernel parameter. Must be positive; if not, computes median heuristic in quadratic time for each projection. Default value is -0.1, which will force median heuristic to be used.
  pval = TRUE,  # Boolean for whether to compute p-value or not.
  type = c("proj", "dist"),  # The type of projection used. Either "proj" for random projections (default) or "dist" for interpoint distances.
  numproj = 20,  # Number of projections (only used if type="proj"). Default is 20.
  nmethod = c(2, 1),  # Norm used for interpoint distances, if type="dist". Needs to be either 2 (for two-norm, default) or 1 (for one-norm).
  distpval = c("Hommel", "Fisher"),  # The p-value combination procedure if type="dist". Options are "Hommel" (default) or "Fisher". The Hommel method is preferred since the Type I error does not seem to be controlled if the Fisher method is used.
  numperm = 200,  # Number of permutations.
  seednum = 0  # Seed for random number generator.
)
```

Arguments

- **X**: Matrix (or vector) of observations in first sample.
- **Y**: Matrix (or vector) of observations in second sample.
- **beta**: kernel parameter. Must be positive; if not, computes median heuristic in quadratic time for each projection. Default value is -0.1, which will force median heuristic to be used.
- **pval**: Boolean for whether to compute p-value or not.
- **type**: The type of projection used. Either "proj" for random projections (default) or "dist" for interpoint distances.
- **numproj**: Number of projections (only used if type="proj"). Default is 20.
- **nmethod**: Norm used for interpoint distances, if type="dist". Needs to be either 2 (for two-norm, default) or 1 (for one-norm).
- **distpval**: The p-value combination procedure if type="dist". Options are "Hommel" (default) or "Fisher". The Hommel method is preferred since the Type I error does not seem to be controlled if the Fisher method is used.
numperm  Number of permutations. Default is 200.
seednum  Seed number for generating permutations. Default is 0, which means seed is set randomly. For values larger than 0, results will be reproducible.

Value
A list with the following elements:
pval  The p-value of the test, if it is computed (pval=TRUE). Otherwise, it is set to NA.
stat  The statistic of the test, which is only returned when type="proj", otherwise it is set to NA.

References

Examples
X <- matrix(c(1:12), ncol=2, byrow=TRUE)
Y <- matrix(c(13:20), ncol=2, byrow=TRUE)
# using the random projections method
mmdList <- meanmmd(X=X, Y=Y, pval=TRUE, type="proj", numproj=50)

# using the method were distances are computed to the various points
mmdList <- meanmmd(X=X, Y=Y, pval=TRUE, type="dist")

mediandiff

 mediandiff

Compute the median difference between pairs of values

Description
Compute the median of all differences between distinct pairs in vectors or matrices.

Usage
mediandiff(X, Y = NULL, kernel = c("Laplacian", "Gaussian"), fast = FALSE)

Arguments
X  Numeric vector or matrix of length n.
Y  Numeric vector or matrix of length m, or NULL.
kernel  String, either "Laplacian" or "Gaussian".
fast  Boolean; if TRUE will run O(N log N) algorithm, where N = n + m, but if FALSE (default) will run naive O(N^2 log N) algorithm.
mediandiff

Details
The median difference is defined as follows:

Z is the combined X and Y values into a single vector or matrix. Number of columns is the dimension, and these need to be equal for X and Y. Then, if the Laplacian kernel is used,

\[ m = \text{median}\{||x_i - x_j||; \, i > j, \, i = 1, 2, \ldots, n + m, \, \text{and} \, j = 1, 2, \ldots, i - 1\}, \]

where \( ||z_i - z_j||_1 \) is the 1-norm, and so if the data are d-dimensional then

\[ ||z_i - z_j||_1 = \sum_{k=1}^{d} |z_{i,k} - z_{j,k}|. \]

If the Gaussian kernel is specified, then the square of the two-norm is used.
The median heuristic is defined as \( \beta = 1/m \).

Naive method will compute all distinct pairs, of which there are \( N(N + 1)/2 \) differences. These are then sorted using a \( O(N \log N) \) algorithm, so overall \( O(N^2 \log N) \).
The fast method is \( O(N \log N) \) is from Croux and Rousseeuw (1992), which is based on Johnson and Mizoguchi (1978).

Value
A scalar, the median of all pairwise differences.

References

See Also
medianheuristic

Examples

```r
X <- c(7.1, 1.2, 4.3, 0.4)
Y <- c(5.5, 2.6, 8.7)
#using fast method, Laplacian kernel, loglinear in number of observations
md <- mediandiff(X, Y, fast=TRUE)

#using fast method, Gaussian kernel, loglinear in number of observations
md <- mediandiff(X, Y, fast=TRUE, kernel="Gaussian")

#using naive method (default), with Laplacian kernel
md <- mediandiff(X, Y)
```
medianheuristic  

*Compute the median heuristic*

**Description**
Computes the inverse of the median difference of all distinct pairs in vectors or matrices.

**Usage**

```
medianheuristic(X, Y = NULL, kernel = c("Laplacian", "Gaussian"), fast = FALSE)
```

**Arguments**

- **X**  
  Numeric vector or matrix of length n.
- **Y**  
  Numeric vector or matrix of length m, or NULL.
- **kernel**  
  String, either "Laplacian" or "Gaussian".
- **fast**  
  Boolean; if TRUE will run $O(N \log N)$ algorithm, where $N = n + m$, but if FALSE will run naive $O(N^2 \log(N))$ algorithm.

**Details**
Computes median of differences $md$ using mediandiff and then returns $1 / md$. See mediandiff for details.

**Value**
A scalar, the inverse of the median of all pairwise differences.

**See Also**
mediandiff

**Examples**
```
X <- c(7.1, 1.2, 4.3, 0.4)
Y <- c(5.5, 2.6, 8.7)
mh <- medianheuristic(X, Y, kernel="Laplacian", fast=TRUE)

#using fast method, Gaussian kernel, loglinear in number of observations
mh <- medianheuristic(X, Y, fast=TRUE, kernel="Gaussian")

#using naive method (default), with Laplacian kernel
mh <- medianheuristic(X, Y)
```
Naive computation for Maximum Mean Discrepancy

Description
Computes maximum mean discrepancy statistics with Laplacian or Gaussian kernel. Suitable for multivariate data. Naive approach, quadratic in number of observations.

Usage
```r
mmd(
  X,
  Y,
  beta = -0.1,
  pval = TRUE,
  kernel = c("Laplacian", "Gaussian"),
  numperm = 200,
  seednum = 0
)
```

Arguments
- **X**: Matrix (or vector) of observations in first sample.
- **Y**: Matrix (or vector) of observations in second sample.
- **beta**: Kernel parameter. Must be positive; if not, computes median heuristic in quadratic time. Default value is \(-0.1\), which will force median heuristic to be used.
- **pval**: Boolean for whether to compute p-value or not.
- **kernel**: String, either "Laplacian" or "Gaussian". Default is "Laplacian".
- **numperm**: Number of permutations. Default is 200.
- **seednum**: Seed number for generating permutations. Default is 0, which means seed is set randomly. For values larger than 0, results will be reproducible.

Details
First checks number of columns (dimension) are equal. Suppose matrix \(X\) has \(n\) rows and \(d\) columns, and matrix \(Y\) has \(m\) rows; checks that \(Y\) has \(d\) columns (if not, then throws error). Then flattens matrices to vectors (or, if \(d = 1\), they are already vectors). Then calls C++ method. If the first sample has \(n\) \(d\)-dimensional samples and the second sample has \(m\) \(d\)-dimensional samples, then the algorithm computes the statistic in \(O((n + m)^2)\) time.

Median difference is as follows:

\[
m = \text{median}\{ \|x_i - x_j\|_1; \ i > j, \ i = 1, 2, \ldots, n + m, \ \text{and} \ j = 1, 2, \ldots, i - 1 \},
\]

where \(\|x_i - x_j\|_1\) is the 1-norm, and so if the data are \(d\)-dimensional then
\[ \|x_i - x_j\|_1 = \sum_{k=1}^{d} |x_{i,k} - x_{j,k}|, \]
and finally median heuristic is \( \beta = 1/m \). This can be computed in \( O((n + m)^2) \) time.

The Laplacian kernel \( k \) is defined as
\[ k(x, y) = \exp(-\beta \|x_i - x_j\|_1). \]

Random seed is set for \( \text{std::mt19937} \) and \( \text{std::shuffle} \) in C++.

**Value**

A list with the following elements:

- `pval` The p-value of the test, if it is computed (\( \text{pval=TRUE} \)).
- `stat` The statistic of the test, which is always computed.
- `beta` The kernel parameter used in the test. If `beta` was not initialised or negative, this will be the median heuristic value.

**References**


**Examples**

```r
X <- matrix(c(1:12), ncol=2, byrow=TRUE)
Y <- matrix(c(13:20), ncol=2, byrow=TRUE)
mmdList <- mmd(X=X, Y=Y, beta=0.1, pval=FALSE)
# using median heuristic
mmdList <- mmd(X=X, Y=Y, pval=FALSE)
# using median heuristic and computing p-value
mmdList <- mmd(X=X, Y=Y)
# using median heuristic and computing p-value
# using 1000 permutations and seed 1 for reproducibility.
mmdList <- mmd(X=X, Y=Y, numperm=1000, seednum=1)
```
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