

Package ‘BIDistances’

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Type Package

Title Bioinformatic Distances

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Description A selection of distances measures for bioinformatics data. Other important distance measures for bioinformatics data are selected from the R package 'parallelDist'. A special distance measure for the Gene Ontology is available.

Depends R (>= 3.5.0)

Imports Rcpp (>= 1.0.8), RcppParallel, parallelDist, parallel, DataVisualizations, diptest, e1071, vegan, methods, pracma, ggplot2

Suggests knitr, rmarkdown, remotes, sphet, transport, ineq

LinkingTo Rcpp, RcppArmadillo, RcppParallel

NeedsCompilation yes

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License GPL-3

LazyLoad yes

LazyData TRUE

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VignetteBuilder knitr

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Contents

CosinusDistance	2
Dist2All	3
DistanceDistributions	4
DistanceMatrix	5
fastPdist	7
fastPdistC	8
FractionalDistance	8
GiniDist	9
Hearingloss_N109	10
Hepta	10
jaccard	11
Mahalanobis	12
msmd	13
nearest	14
SharedNeighborDistance	14
Tfidf_dist	15
ToroidDist2All	16
TransformSimilarity2MetricDistance	17
twed	18
VariablePrecision	19
WassersteinDist	19
Index	21

CosinusDistance	<i>Cosine Distance</i>
-----------------	------------------------

Description

Calculates the cosine distance

Usage

CosinusDistance(Data)

Arguments

Data [1:n,1:d] matrix with n cases, d variables

Details

https://en.wikipedia.org/wiki/Cosine_similarity

Value

Distance [1:n,1:n] symmetric matrix, containing the distanes of the cases (rows) for the given data

Note

The cosine distance is calculated by calculating the cosine similarity $d(i, j) = \max s - s(i, j)$, where s is the cosine similarity and the d the cosine distance.

Author(s)

Michael Thrun

Examples

```
data(Hepta)
distMatrix = CosinusDistance(Hepta$Data)
```

Dist2All

Distances to all data points

Description

Calculates all distances from a given vector to the rows of a matrix.

Usage

```
Dist2All(X, Data, SelectFeatures, method = "euclidean", p=2, knn=1)
```

Arguments

X	A vector containing the data point to be compared to data.
Data	A matrix containing the data points to be compared with x.
SelectFeatures	A vector of the same length as x and the rows of data, containing TRUE for all columns of the data to be compared and any other value for columns to be discarded.
method	(Optional) String marking, which distance measure is to be used. Euclidean by default.
p	(Optional) Scalar, The pp-th root of the sum of the pp-th powers of the differences of the components. Default is 2
knn	(Optional) Scalar, gives the number of the indices of the k nearest neighbors returned. Default is 1

Value

List with

distToAll A vector containing the distances from x to all rows of data.

KNN Numeric vector, containing the indices of the k nearest neighbors (rows) to the given points

Note

This function is very inefficient for large Data.

Author(s)

Michael Thrun

Examples

```
data(Hepta)
Dist2All(Hepta$Data[1,],Hepta$Data)
```

DistanceDistributions *Distance Distribution*

Description

Calculates the distribution of the distances between the data points

Usage

```
DistanceDistributions(Data, DistanceMethods=c('bhattacharyya', 'bray',
                                             'canberra', 'chord',
                                             'divergence', 'euclidean',
                                             'minkowski', 'geodesic',
                                             'hellinger', 'kullback',
                                             'manhattan', 'maximum',
                                             'soergel', 'wave',
                                             'whittaker'),
                    CosineNonParallel = TRUE, CorrelationDist = TRUE,
                    Mahalanobis = FALSE, Podani = FALSE,
                    PlotIt = FALSE, PlotSampleSize = 5e3)
```

Arguments

Data	[1:n, 1:m] A matrix, containing data as rows.
DistanceMethods	Character vector stating all distance methods such as 'euclidean'.
CosineNonParallel	Boolean stating if cosine should be computed in parallel.
CorrelationDist	Boolean stating if CorrelationDist should be computed.
Mahalanobis	Boolean stating if Mahalanobis should be computed.
Podani	Boolean stating if Podani should be computed.
PlotIt	Boolean: TRUE => create plot. FALSE => no plot.
PlotSampleSize	Integer stating the number of samples for plotting.

Value

List with elements

DistanceMatrix [1:n, 1:n] numeric matrix containing the distance matrix

DistanceChoice [1:n, 1:n] numeric matrix containing the distance matrix

OrderedDistances

[1:n, 1:n] numeric matrix containing the distance matrix

ggobject ggplot object

Author(s)

Michael Thrun

Examples

```
iris=datasets::iris
if(requireNamespace("DataVisualizations",quietly=TRUE)){
  library(DataVisualizations)
  DistanceDistributions(as.matrix(iris[,1:4]), c("euclidean"), PlotIt = FALSE)
}
```

DistanceMatrix	<i>Pairwise distance between pairs of objects</i>
----------------	---

Description

computes the distance between objects in the data matrix, X, using the method specified by method

Usage

```
DistanceMatrix(X,method='euclidean',dim=2,outputisvector=FALSE)
```

Arguments

X	data matrix [1:n,1:d], n cases d variables
method	Optional, method specified by distance string: 'binary','canberra','cityblock','euclidean','sqEuclidean','maximum','cosine','chebychev','jaccard','kendallM','kendallD','mahalanobis','minkowski','manhattan','braycur','cosine','wasserstein','pearsonD','spearmanD','pearson'
dim	Optional: if method="minkowski", or wasserstein, choose scalar. For minkowski the ppth root of the sum of the ppth powers of the differences of the components. For wasserstein the order, default should be then 1
outputisvector	Optional: should the output be converted to a vector

Details

If possible uses implementation parallelized by the parallelDist package. Otherwise R implementations besides Euclidean for which a GPU implementation is provided.

'binary' (aka asymmetric binary): The vectors are regarded as binary bits, so non-zero elements are 'on' and zero elements are 'off'. The distance is the proportion of bits in which only one is on amongst those in which at least one is on.

'cityblock'==manhattan

'maximum': Maximum distance between two components of x and y (supremum norm)

'cosine' calculates a similarity matrix sim between all column vectors of a matrix x. This matrix might be a document-term matrix, so columns would be expected to be documents and rows to be terms. the distances is than defined with $D = \max(\text{sim}) - \text{sim}$

'jaccard' Jaccard index is computed as $2B/(1+B)$, where B is Bray-Curtis dissimilarity: the number of items which occur in both elements divided by the total number of items in the elements (Sneath, 1957). This measure is often also called: binary, asymmetric binary, etc.

'mahalanobis' the squared generalized Mahalanobis distance between all pairs of rows in a data frame with respect to a covariance matrix. The element of the i-th row and j-th column of the distance matrix is defined as $D_{ij}^2 = (\mathbf{x}_i - \mathbf{x}_j)' \mathbf{S}^{-1} (\mathbf{x}_i - \mathbf{x}_j)$

'minkowski': The p norm, the pth root of the sum of the pth powers of the differences of the components.

'manhattan': Absolute distance between the two vectors (1 norm aka L₁).

'chebychev'==max(abs(x-y)),

'canberra'= $\sum \text{abs}(x-y) / \sum (\text{abs}(x)-\text{abs}(y))$, Terms with zero numerator and denominator are omitted from the sum and treated as if the values were missing. This is intended for non-negative values (e.g., counts): taking the absolute value of the denominator is a 1998 R modification to avoid negative distances.

'braycur'= $\sum \text{abs}(x - y) / \text{abs}(x+y)$

'pearsonM' metric, see [Legendre, 1986] or [Bock,1974, pp.77-79] $\sqrt{((1 - r)+1)/2}$ with r beeing the Pearson's correlation coefficient.

'spearmanM' metric, see [Legendre, 1986] or [Bock,1974, pp.77-79] $\sqrt{((1 - r)+1)/2}$ with r beeing Spearman's correlation coefficient.

'kendallM' metric, see [Legendre, 1986] or [Bock,1974, pp.77-79] $\sqrt{((1 - r)+1)/2}$ with tau beeing Kendalls's correlation coefficient.

'pearsonD' dissimilarity $1 - r$ with r beeing the Pearson's correlation coefficient.

'spearmanD' dissimilarity $1 - r$ with r beeing Spearman's correlation coefficient.

'kendallD' dissimilarity $1 - r$ with tau beeing Kendalls's correlation coefficient.

'cosine' s. wiki for similarity conversion: $\max(S) - S(i,j)$

Value

Dmatrix [1:n,1:n] Distance Marix: Pairwise distance between pairs of objects

Author(s)

Michael Thrun

References

Sneath, P. H. A. (1957) Some thoughts on bacterial classification. *Journal of General Microbiology* 17, pages 184-200.

Leydesdorff, L. (2005) Similarity Measures, Author Cocitation Analysis, and Information Theory. In: *JASIST* 56(7), pp.769-772.

Becker, R. A., Chambers, J. M. and Wilks, A. R. (1988) *The New S Language*. Wadsworth & Brooks/Cole.

Mardia, K. V., Kent, J. T. and Bibby, J. M. (1979) *Multivariate Analysis*. Academic Press.

Borg, I. and Groenen, P. (1997) *Modern Multidimensional Scaling. Theory and Applications*. Springer.

Mahalanobis, P. C. (1936) On the generalized distance in statistics. *Proceedings of The National Institute of Sciences of India*, 12:49-55.

Examples

```
data(Hepta)
Dmatrix = DistanceMatrix(Hepta$Data,method='euclidean')
```

fastPdist	<i>fastPdist</i>
-----------	------------------

Description

calculates pairwise euclidean distances

Usage

```
fastPdist(X)
```

Arguments

X [1:n,1:m] data to calculate distances to

Value

dist[1:n,1:n] distances

Author(s)

Michael Thrun

Examples

```
fastPdist(as.matrix(iris[,1:4]))
```

fastPdistC

fastPdist

Description

calculates pairwise euclidean distances

Usage

```
fastPdistC(Ar, Br)
```

Arguments

Ar [1:n,1:m] data to calculate distances to
Br [1:n,1:m] data to calculate distances to

Value

dist[1:n,1:n] distances

Author(s)

Felix Riede

References

<https://blog.felixriedel.com/2013/05/pairwise-distances-in-r/>

FractionalDistance*Calculates fractional distances*

Description

Calculates distance matrix, through $(\sum_{i=1}^n |x_i - y_i|^p)^{1/p}$

Usage

```
FractionalDistance(Data, p)
```

Arguments

Data [1:n,1:d] Matrix, with n cases, d variables
p Scalar, value for p

Details

Values of $p < 1$ can be used, which can be useful for high-dimensional data, see references.

Value

DistanceMatrix [1:n,1:n] symmetric Matrix, containing the distances between the cases (rows) of the input matrix

Author(s)

Michael Thrun

References

Aggrawal, C. C., Hinneburg, A., Keim, D. (2001), On the Suprising Behavior of Distance Metrics in High Dimensional Space.

Examples

```
data(Hepta)
distMatrix = FractionalDistance(Hepta$Data, p = 1/2)
```

GiniDist

GiniDist

Description

Calculates pairwise gini distances

Usage

```
GiniDist(Data)
```

Arguments

Data [1:n,1:d] data to calculate distances to

Value

dist[1:n,1:n] distances

Author(s)

Michael Thrun

Examples

```
GiniDist(as.matrix(iris[,1:4]))
```

Hearingloss_N109 *Hearingloss data*

Description

Hearingloss data, with Gene2GoTerm matrix.

Usage

```
data('Hearingloss_N109')
```

Details

FeatureMatrix_Gene2Term contains the dataset, NCBI are the row names for the genes and GoTerm_Header contains the column names for the GoTerms. Size of data matrix is 109 with dimension 829.

Source

[NCBI OtoGenome Test for Hearing Loss](#), accessed 24 June 2022.

References

GeneTestingRegistry (2018). OtoGenome Test for Hearing Loss Retrieved 2017

Examples

```
data(Hearingloss_N109)
str(Hearingloss_N109)
```

Hepta *Hepta introduced in [Ultsch, 2003]*

Description

Clearly defined clusters, different variances. Detailed description of dataset and its clustering challenge is provided in [Thrun/Ultsch, 2020].

Usage

```
data('Hepta')
```

Details

Size 212, Dimensions 3, stored in Hepta\$Data

Classes 7, stored in Hepta\$C1s

References

[Ultsch, 2003] Ultsch, A.: Maps for the visualization of high-dimensional data spaces, Proc. Workshop on Self organizing Maps (WSOM), pp. 225-230, Kyushu, Japan, 2003.

[Thrun/Ultsch, 2020] Thrun, M. C., & Ultsch, A.: Clustering Benchmark Datasets Exploiting the Fundamental Clustering Problems, Data in Brief, Vol. 30(C), pp. 105501, doi:10.1016/j.dib.2020.105501, 2020.

Examples

```
data(Hepta)
str(Hepta)
```

jaccard	<i>Computes dissimilarity indices Jaccard</i>
---------	---

Description

The function computes dissimilarity indices Jaccard, which index is computed as $2B/(1+B)$, where B is Bray-Curtis dissimilarity

Usage

```
jaccard(X)
```

Arguments

X	Distance Matrix
---	-----------------

Value

Kosinusdistanz der beiden Vektoren x,y

Author(s)

MT

Examples

```
jaccard(as.matrix(iris[,1:4]))
```

Mahalanobis

Pairwise Squared Generalized Mahalanobis Distances

Description

Function to calculate the squared generalized Mahalanobis distance between all pairs of rows in a data frame with respect to a covariance matrix. The element of the i -th row and j -th column of the distance matrix is defined as

$$D_{ij}^2 = (\mathbf{x}_i - \mathbf{x}_j)' \boldsymbol{\Sigma}^{-1} (\mathbf{x}_i - \mathbf{x}_j)$$

Usage

```
Mahalanobis(X, cov, inverted = FALSE)
```

Arguments

`X` a matrix of data ($n \times d$) n cases, d variables
`cov` a variance-covariance matrix ($p \times p$).
`inverted` logical. If FALSE (default), `cov` is supposed to be a variance-covariance matrix.

Value

Distances[1:n,1:n]

Note

copy of function in biotools package, because this packages doesnt work under mac os

Author(s)

Anderson Rodrigo da Silva <anderson.agro@hotmail.com>

References

Mahalanobis, P. C. (1936) On the generalized distance in statistics. *Proceedings of The National Institute of Sciences of India*, 12:49-55.

See Also

[dist](#)

Examples

```

# Manly (2004, p.65-66)
x1 <- c(131.37, 132.37, 134.47, 135.50, 136.17)
x2 <- c(133.60, 132.70, 133.80, 132.30, 130.33)
x3 <- c(99.17, 99.07, 96.03, 94.53, 93.50)
x4 <- c(50.53, 50.23, 50.57, 51.97, 51.37)
x <- cbind(x1, x2, x3, x4)
Cov <- matrix(c(21.112,0.038,0.078,2.01, 0.038,23.486,5.2,2.844,
0.078,5.2,24.18,1.134, 2.01,2.844,1.134,10.154), 4, 4)
Mahalanobis(x, Cov)

# End (not run)

```

msmd

msmd

Description

msmd

Usage

msmd(Values1, Values2, ParameterC)

Arguments

Values1	[1:N1] Numeric vector with values of the first time series.
Values2	[1:N1] Numeric vector with values of the second time series.
ParameterC	Numeric vector with time stamps of the first time series.

Value

List with elements

Value Distance measure

Author(s)

Quirin Stier

Examples

msmd(1:10, 1:10)

nearest	<i>Nearest</i>
---------	----------------

Description

returns the index of the nearest neighbour of a given data point.

Usage

```
nearest(Data, i, defined)
```

Arguments

Data	A matrix holding n data points as row vectors.
i	the index of the data point, who's nearest neighbour is sought.
defined	A row vector with 1 for all columns of data that are used for the computation. If missing, all columns are used.

Value

nNInd	The index of the nearest neighbour of data[i,]
-------	---

Author(s)

Michael Thrun, Raphael Paebst

Examples

```
nearest(Data = as.matrix(iris[,1:4]), i = 1)
```

SharedNeighborDistance	<i>Shared Neighbor Distance</i>
------------------------	---------------------------------

Description

Calculates the Shared Neighbor Distance

Usage

```
SharedNeighborDistance(Data, k = 5, NThreads = NULL, ComputationInR = FALSE)
```

Arguments

Data	[1:n,1:d] matrix with n cases, d variables
k	Integer defining the number of nearest neighbors
NThreads	Number of threads in parallel computation.
ComputationInR	Boolean (Default ComputationInR = FALSE). If FALSE, do computation in Rcpp, else in R (very slow).

Value

Distance	[1:n,1:n] symmetric matrix, containing the distances of the cases (rows) for the given data
----------	---

Author(s)

Quirin Stier

References

<https://github.com/albert-espin/snn-clustering/blob/master/SNN/snn.py>

Examples

```
data(Hepta)
distMatrix = SharedNeighborDistance(Hepta$Data, NThreads = 1, ComputationInR=TRUE)
```

Tfidf_dist

Term frequency-inverse document frequency distance

Description

Computes the term frequency inverse document frequency (tfidf) distance for a FeatureMatrix_Gene2GoTerm. In case of genes with annotated GOterms from gene ontology genes can be interpreted as documents and GOterms as terms.

Usage

```
Tfidf_dist(FeatureMatrix_Gene2GoTerm, tf_fun = mean)
```

Arguments

FeatureMatrix_Gene2GoTerm	[1:n,1:d] Matrix, with n genes and d GO-Terms.
tf_fun	Function, defining the numerator value in the normalized Term-frequency. The default is the mean of the not 0 values.

Details

For the FeatureMatrix_Gene2GoTerm it is:

FeatureMatrix_Gene2GoTerm[i,j] > 0 iff GOterm j is relevant for gene i. The FeatureMatrix_Gene2GoTerm[i,j] > 1 if the specific gene is annotated by in a specific GO-Term with more than one evidence code
 FeatureMatrix_Gene2GoTerm[i,j] is the frequency of term js occurrence in document i.

Value

List with

dist	Numeric vector containing the tfidf distances between the documents = absolute difference of TfidfWeights
TfidfWeights	[1:n] Numeric vector containing the term frequency inverse document frequency weights used for the distance, given as the Term frequency*Inverse document frequency

Author(s)

Michael Thrun

References

Stier, Q. and Thrun, M., C.: Deriving homogeneous subsets from gene sets by exploiting the Gene Ontology, Informatica, in review, 2023

Examples

```
data(Hearingloss_N109)
V = Tfidf_dist(Hearingloss_N109$FeatureMatrix_Gene2Term)
dist = V$dist
TfidfWeights = V$TfidfWeights
```

ToroidDist2All

Calculate toroid Euclidean Distances

Description

Calculate toroid Euclidean Distances

Arguments

positionxy	One datapoint
AllPositions(1:AnzData:2)	All Other dataPoints
Lines, Columns	Size of planar grid

Value

Dist2All(1:AnzData,1:AnzData); distance(s) between XY and AllPositions

Author(s)

MT

Examples

```
positionxy = c(1,1)
AllPositions = rbind(c(2,3), c(5,2))
Lines = 40
Columns = 80
ToroidDist2All(positionxy, AllPositions, Lines, Columns)
```

TransformSimilarity2MetricDistance

TransformSimilarity2MetricDistance

Description

TransformSimilarity2MetricDistance

Usage

TransformSimilarity2MetricDistance(Similarity)

Arguments

Similarity Similarity

Value

Similarity

Author(s)

Michael Thrun

Examples

```
Data_S = fastPdist(as.matrix(iris[,1:4]))
Data_S = Data_S-min(Data_S)
Data_S = Data_S/max(Data_S)
diag(Data_S) = 1
TransformSimilarity2MetricDistance(Data_S)
```

twed	<i>twed</i>
------	-------------

Description

twed

Usage

```
twed(Values1, Values2, Time1, Time2, Nu = 1, Lambda = 1, Degree = 2)
```

Arguments

Values1	[1:N1] Numeric vector with values of the first time series.
Values2	[1:N1] Numeric vector with values of the second time series.
Time1	[1:N1] Numeric vector with time stamps of the first time series.
Time2	[1:N1] Numeric vector with time stamps of the second time series.
Nu	Optional, Numeric: Elasticity parameter - nu >=0 needed for distance measure.
Lambda	Optional, Numeric: Penalty for deletion operation.
Degree	Optional, Integer: Degree of the p norm for local cost.

Value

List with elements

TWED	TWED distance between time series Values1 (Time1) and Values2 (Time2)
DPMatrix	[1:n, 1:m] Numeric matrix

Author(s)

Quirin Stier

Examples

```
twed(1:10, 1:10, 1:10, 1:10)
```

VariablePrecision	<i>VariablePrecision</i>
-------------------	--------------------------

Description

Computes the variable precision

Usage

```
VariablePrecision(Variable)
```

Arguments

Variable	Numeric vector [1:n] or matrix [1:n, 1:d]
----------	---

Value

MinAbsDiff, MinAbsNZDiff, MinExpo

Author(s)

Michael Thrun

Examples

```
data(Hepta)
distMat = VariablePrecision(as.matrix(iris[, 1]))

distMat = VariablePrecision(as.matrix(iris[, 1:4]))
```

WassersteinDist	<i>Wasserstein Distance</i>
-----------------	-----------------------------

Description

Computes the Wasserstein distance for a data matrix

Usage

```
WassersteinDist(Data, p = 1, InverseWeighting = FALSE)
```

Arguments

Data	data matrix of n cases and d features
p	scalar higher than one, the power to which the Euclidean distance between points is taken in order to compute transportation costs.
InverseWeighting	weighting per row can be either 1 (FALSE) or 1/n (TRUE)

Details

Wasserstein distance, also known as Earth Mover's Distance (EMD) is the distance between two probability distributions over a region D . The Wasserstein distance of order p is defined as the p -th root of the total cost incurred when transporting measure a to measure b in an optimal way, where the cost of transporting a unit of mass from x to y is given as the p -th power of the Euclidean distance.

It is claimed to be useful for distributions that do not align well with traditional measures like Euclidean distance.

Value

matrix of distances, symmetric

Author(s)

Michae Thrun

References

...

See Also

[wasserstein1d](#)

Examples

```
data(Hepta)
distMat=WassersteinDist(Hepta$Data)
```

Index

- * **Bioinformatic Distance**
 - CosinusDistance, 2
 - Dist2All, 3
 - FractionalDistance, 8
 - SharedNeighborDistance, 14
 - Tfidf_dist, 15
- * **Cosine Distance**
 - CosinusDistance, 2
- * **Cosine**
 - CosinusDistance, 2
- * **Distance**
 - CosinusDistance, 2
 - Dist2All, 3
 - FractionalDistance, 8
 - SharedNeighborDistance, 14
 - Tfidf_dist, 15
- * **FCPS**
 - Hepta, 10
- * **Fractional Distance**
 - FractionalDistance, 8
- * **Genes**
 - Hearingloss_N109, 10
- * **GoTerm**
 - Hearingloss_N109, 10
- * **Hepta**
 - Hepta, 10
- * **Inverse frequency**
 - Tfidf_dist, 15
- * **Metric**
 - FractionalDistance, 8
- * **Nearest Neighbors**
 - Dist2All, 3
- * **Shared Neighbor Distance**
 - SharedNeighborDistance, 14
- * **Term frequency**
 - Tfidf_dist, 15
- * **TermFrequency**
 - Tfidf_dist, 15
- * **datasets**
 - Hearingloss_N109, 10
 - Hepta, 10
- * **fastPdist**
 - fastPdist, 7
 - fastPdistC, 8
- * **wasserstein distance**
 - WassersteinDist, 19
- * **wasserstein**
 - WassersteinDist, 19
- CosinusDistance, 2
- dist, 12
- Dist2All, 3
- DistanceDistributions, 4
- DistanceMatrix, 5
- fastPdist, 7
- fastPdistC, 8
- FractionalDistance, 8
- GiniDist, 9
- Hearingloss_N109, 10
- Hepta, 10
- jaccard, 11
- Mahalanobis, 12
- msmd, 13
- nearest, 14
- pdist (DistanceMatrix), 5
- SharedNeighborDistance, 14
- Tfidf_dist, 15
- ToroidDist2All, 16
- TransformSimilarity2MetricDistance, 17
- twed, 18

VariablePrecision, [19](#)

wasserstein1d, [20](#)

WassersteinDist, [19](#)