Package 'DTHybrid'

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Title DT-Hybrid Algorithm

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Depends R (>= 3.0), methods, BiocGenerics, stats, gtools

Suggests parallel

LazyLoad yes

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Description An implementation of the DT-Hybrid algorithm which has been described in Alaimo S, Pulvirenti A, Giugno R and Ferro A (2013). Drug-target interaction prediction through domain-tuned network-based inference. Bioinformatics, 29(16), pp. 2004-2008.

biocViews Bioinformatics, Networks, NetworkInference, NetworkAnalysis

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R topics documented:

`computeRecommendation` *Runs the DT-Hybrid algorithm on a bipartite network*

Description

Compute the recommendations on a bipartite network by using the DT-Hybrid algorithm.

Usage

```
computeRecommendation(A, lambda=0.5, alpha=0.5, S=NA, S1=NA, cl=NA)
```

Arguments

A	The adjacency matrix that represents the bipartite network. Given "n" nodes of type "X" and "m" nodes of type "Y", the adjacency matrix is an n by m matrix, where each element A[i,j] contains 1 if the X-node i interacts with the Y-node j, 0 otherwise.
alpha	Tuning parameter (value between 0 and 1) to adjust the performance of the algorithm.
lambda	Tuning parameter (value between 0 and 1) to adjust the performance of the algorithm.
S	A n by n similarity matrix where each element (value between 0 and 1) represents the similarity between two X-nodes.
S1	A m by m similarity matrix where each element (value between 0 and 1) represents the similarity between two Y-nodes.
cl	A cluster, generated with the function `makeCluster` available through packages `snow` or `parallel`, used to speed up the computation when the input matrices are too large.

Details

See cited document for more details.

Value

An n by m matrix where each element represents how much the interaction between an X-node and an Y-node is favorable.

Author(s)

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References

Alaimo S, Pulvirenti A, Giugno R and Ferro A (2013). Drug-target interaction prediction through domain-tuned network-based inference. Bioinformatics, 29(16), pp. 2004-2008.

Examples

```
# Example using a Drug-Target Interaction dataset
data(enzyme)

# Compute recommendation
result <- computeRecommendation(enzyme_r)
## Not run: print(result)

# Compute recommendation using similarity informations
result1 <- computeRecommendation(enzyme_r, S=enzyme_ts, S1=enzyme_ds)
## Not run: print(result1)

# Speeds up the computation process through the use of multiple threads
library(parallel)
cl <- makeCluster(detectCores())
result2 <- computeRecommendation(enzyme_r, S=enzyme_ts, S1=enzyme_ds, cl=cl)
```

```
stopCluster(cl)
## Not run: print(result2)
```

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enzyme *An example Drug-Target interaction network dataset.*

Description

The enzyme dataset consists: i) an n by m matrix enzyme_r, which represents the bipartite network built upon the known drug-target interactions; ii) an n by n matrix enzyme_ts where each element is the sequence similarity between all pairs of genes in the bipartite network, computed using a normalized Smith-Waterman score (Smith and Waterman, J.Mol.Bio, 1981); iii) an m by m matrix enzyme_ds where each element is the 2D chemical similarity between all pairs of drugs in the example network, computed using the SIMCOMP algorithm (Hattori et al, J.Ame.Chem.Soc, 2003).

Usage

```
data(enzyme)
```

References

Yamanishi,Y., Araki,M., Gutteridge,A., Honda,W. and Kanehisa,M. , Prediction of drug-target interaction networks from the integration of chemical and genomic spaces, 2008.
Smith, T. F., Waterman, M. S. (1981), Identification of common molecular subsequences. Journal of molecular biology, 147(1), 195-197.
Hattori, M., Okuno, Y., Goto, S., and Kanehisa, M., Development of a chemical structure comparison method for integrated analysis of chemical and genomic information in the metabolic pathways. J. Am. Chem. Soc. 125, 11853-11865 (2003).

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