

Package ‘BioCor’

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Title Functional similarities

Version 1.31.0

Description Calculates functional similarities based on the pathways described on KEGG and REACTOME or in gene sets. These similarities can be calculated for pathways or gene sets, genes, or clusters and combined with other similarities. They can be used to improve networks, gene selection, testing relationships...

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URL <https://bioconductor.org/packages/BioCor>,
<https://llrs.github.io/BioCor/>

BugReports <https://github.com/llrs/BioCor/issues>

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BioCor-package

BioCor: A package to calculate functional similarities

Description

Calculates a functional similarity measure between gene identifiers based on the pathways described on KEGG and REACTOME.

Important functions

- `pathSim()`: Calculates the similarity between two pathways.
- `geneSim()`: Calculates the similarity (based on `pathSim`) between two genes.
- `clusterSim()`: Calculates the similarity between two clusters of genes by joining pathways of each gene.
- `clusterGeneSim()`: Calculates the similarity between two clusters of genes by comparing the similarity between the genes of a cluster.
- `similarities()`: Allows to combine the value of matrices of similarities.
- `conversions()`: Two functions to convert similarity measures.
- `weighted()`: Functions provided to combine similarities.

Author(s)

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- Pau Sancho-Bru ([ORCID](#)) [thesis advisor]
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See Also

Useful links:

- <https://bioconductor.org/packages/BioCor>
- <https://llrs.github.io/BioCor/>
- Report bugs at <https://github.com/llrs/BioCor/issues>

addSimilarities

Additive integration of similarities

Description

Function that use the previously calculated similarities into a single similarity matrix.

Usage

```
addSimilarities(x, bio_mat, weights = c(0.5, 0.18, 0.1, 0.22))
```

Arguments

| | |
|----------------------|--|
| <code>x</code> | A matrix with the similarity of expression |
| <code>bio_mat</code> | A list of matrices of the same dimension as <code>x</code> . |
| <code>weights</code> | A numeric vector of weight to multiply each similarity |

Details

The total weight can't be higher than 1 to prevent values above 1 but can be below 1. It uses `weighted.sum` with `abs = TRUE` internally.

Value

A square matrix of the same dimensions as the input matrices.

Author(s)

Lluís Revilla

See Also

[similarities\(\)](#), [weighted\(\)](#).

Examples

```
set.seed(100)
a <- seq2mat(LETTERS[1:5], rnorm(10))
b <- seq2mat(LETTERS[1:5], seq(from = 0.1, to = 1, by = 0.1))
sim <- list(b)
addSimilarities(a, sim, c(0.5, 0.5))
```

AintoB

Insert a matrix into another

Description

Insert values from a matrix into another matrix based on the rownames and colnames replacing the values.

Usage

```
AintoB(A, B)
```

Arguments

| | |
|---|--------------------------|
| A | A matrix to be inserted. |
| B | A matrix to insert in. |

Details

If all the genes with pathway information are already calculated but you would like to use more genes when performing analysis. insert the once you have calculated on the matrix of genes.

Value

A matrix with the values of A in the matrix B.

Author(s)

Lluís Revilla

Examples

```

B <- matrix(
  ncol = 10, nrow = 10,
  dimnames = list(letters[1:10], letters[1:10])
)
A <- matrix(c(1:15),
  byrow = TRUE, nrow = 5,
  dimnames = list(letters[1:5], letters[1:3])
)
AintoB(A, B)

# Mixed orders
colnames(A) <- c("c", "h", "e")
rownames(A) <- c("b", "a", "f", "c", "j")
AintoB(A, B)

# Missing columns or rows
colnames(A) <- c("d", "f", "k")
AintoB(A, B)

```

| | |
|----------------|---|
| clusterGeneSim | <i>Similarity score between clusters of genes based on genes similarity</i> |
|----------------|---|

Description

Looks for the similarity between genes of a group and then between each group's genes.

Usage

```

clusterGeneSim(cluster1, cluster2, info, method = c("max", "rcmax.avg"), ...)

## S4 method for signature 'character,character,GeneSetCollection'
clusterGeneSim(cluster1, cluster2, info, method = c("max", "rcmax.avg"), ...)

```

Arguments

| | |
|--------------------|--|
| cluster1, cluster2 | A vector with genes. |
| info | A GeneSetCollection or a list of genes and the pathways they are involved. |
| method | A vector with two or one argument to be passed to combineScores the first one is used to summarize the similarities of genes, the second one for clusters. |
| ... | Other arguments passed to combineScores |

Details

Differs with clusterSim that first each combination between genes is calculated, and with this values then the comparison between the two clusters is done. Thus applying combineScores twice, one at gene level and another one at cluster level.

Value

Returns a similarity score between the genes of the two clusters.

Methods (by class)

- clusterGeneSim(cluster1 = character, cluster2 = character, info = GeneSetCollection): Calculates the gene similarities in a GeneSetCollection and combine them using [combineScoresPar\(\)](#)

Author(s)

Lluís Revilla

See Also

[mclusterGeneSim\(\)](#), [combineScores\(\)](#) and [clusterSim\(\)](#)

Examples

```
if (require("org.Hs.eg.db")) {
  # Extract the paths of all genes of org.Hs.eg.db from KEGG (last update in
  # data of June 31st 2011)
  genes.kegg <- as.list(org.Hs.egPATH)
  clusterGeneSim(c("18", "81", "10"), c("100", "10", "1"), genes.kegg)
  clusterGeneSim(
    c("18", "81", "10"), c("100", "10", "1"), genes.kegg,
    c("avg", "avg")
  )
  clusterGeneSim(
    c("18", "81", "10"), c("100", "10", "1"), genes.kegg,
    c("avg", "rcmax.avg")
  )
  (clus <- clusterGeneSim(
    c("18", "81", "10"), c("100", "10", "1"),
    genes.kegg, "avg"
  ))
  combineScores(clus, "rcmax.avg")
} else {
  warning("You need org.Hs.eg.db package for this example")
}
```

| | |
|------------|--|
| clusterSim | <i>Similarity score between clusters of genes based on pathways similarity</i> |
|------------|--|

Description

Looks for the similarity between genes in groups

Usage

```
clusterSim(cluster1, cluster2, info, method = "max", ...)
```

```
## S4 method for signature 'character,character,GeneSetCollection'
```

```
clusterSim(cluster1, cluster2, info, method = "max", ...)
```

Arguments

cluster1, cluster2

A vector with genes.

info

A GeneSetCollection or a list of genes and the pathways they are involved.

method

one of c("avg", "max", "rcmax", "rcmax.avg", "BMA", "reciprocal"), see Details.

...

Other arguments passed to combineScores

Details

Once the pathways for each cluster are found they are combined using [combineScores\(\)](#).

Value

clusterSim returns a similarity score of the two clusters

Methods (by class)

- `clusterSim(cluster1 = character, cluster2 = character, info = GeneSetCollection)`: Calculates all the similarities of the GeneSetCollection and combine them using [combineScoresPar\(\)](#)

Author(s)

Lluís Revilla

See Also

For a different approach see [clusterGeneSim\(\)](#), [combineScores\(\)](#) and [conversions\(\)](#)

Examples

```
if (require("org.Hs.eg.db")) {
  # Extract the paths of all genes of org.Hs.eg.db from KEGG (last update in
  # data of June 31st 2011)
  genes.kegg <- as.list(org.Hs.egPATH)
  clusterSim(c("9", "15", "10"), c("33", "19", "20"), genes.kegg)
  clusterSim(c("9", "15", "10"), c("33", "19", "20"), genes.kegg, NULL)
  clusterSim(c("9", "15", "10"), c("33", "19", "20"), genes.kegg, "avg")
} else {
  warning("You need org.Hs.eg.db package for this example")
}
```

combinadic

i-th combination of *n* elements taken from *r*

Description

Function similar to `combn` but for larger vectors. To avoid allocating a big vector with all the combinations each one can be computed with this function.

Usage

```
combinadic(n, r, i)
```

Arguments

| | |
|----------------|--|
| <code>n</code> | Elements to extract the combination from |
| <code>r</code> | Number of elements per combination |
| <code>i</code> | ith combination |

Value

The combination `ith` of the elements

Author(s)

Joshua Ulrich

References

[StackOverflow answer 4494469/2886003](#)

See Also

[combn\(\)](#)

Examples

```
# Output of all combinations
combn(LETTERS[1:5], 2)
# Output of the second combination
combinadic(LETTERS[1:5], 2, 2)
```

| | |
|---------------|-------------------------|
| combineScores | <i>Combining values</i> |
|---------------|-------------------------|

Description

Combine several similarities into one using several methods.

Usage

```
combineScores(
  scores,
  method = c("max", "avg", "rcmax", "rcmax.avg", "BMA", "reciprocal"),
  round = FALSE,
  t = 0
)

combineScoresPar(scores, method, subSets = NULL, BPPARAM = NULL, ...)
```

Arguments

| | |
|---------|--|
| scores | Matrix of scores to be combined |
| method | one of c("avg", "max", "rcmax", "rcmax.avg", "BMA", "reciprocal"), see Details. |
| round | Should the resulting value be rounded to the third digit? |
| t | Numeric value to filter scores below this value. Only used in the reciprocal method. |
| subSets | List of combinations as info in other functions. |
| BPPARAM | BiocParallel back-end parameters. By default (NULL) a for loop is used. |
| ... | Other arguments passed to combineScores |

Details

The input matrix can be a base matrix or a matrix from package Matrix. The methods return:

- **avg**: The average or mean value.
- **max**: The max value.
- **rcmax**: The max of the column means or row means.
- **rcmax.avg**: The sum of the max values by rows and columns divided by the number of columns and rows.

- **BMA**: The same as `rcmax.avg`.
- **reciprocal**: The double of the sum of the reciprocal maximal similarities (above a threshold) divided by the number of elements. See equation 3 of the Tao *et al* 2007 article.

Value

A numeric value as described in details.

Note

`combineScores` is a version of the function of the same name in package `GOSemSim` (`GOSemSim::combineScores()`) with optional rounding and some internal differences.

Author(s)

Lluís Revilla based on Guangchuang Yu.

References

Ying Tao, Lee Sam, Jianrong Li, Carol Friedman, Yves A. Lussier; Information theory applied to the sparse gene ontology annotation network to predict novel gene function. *Bioinformatics* 2007; 23 (13): i529-i538. doi: 10.1093/bioinformatics/btm195

See Also

[register](#) in `BiocParallel` about the arguments accepted by `BPPARAM`.

Examples

```
(d <- structure(c(
  0.4, 0.6, 0.222222222222222, 0.4, 0.4, 0, 0.25, 0.5,
  0.285714285714286
),
  .Dim = c(3L, 3L),
  .Dimnames = list(c("a", "b", "c"), c("d", "e", "f"))
))
e <- d
sapply(c("avg", "max", "rcmax", "rcmax.avg", "BMA", "reciprocal"),
  combineScores,
  scores = d
)
d[1, 2] <- NA
sapply(c("avg", "max", "rcmax", "rcmax.avg", "BMA", "reciprocal"),
  combineScores,
  scores = d
)
colnames(e) <- rownames(e)
combineScoresPar(e, list(a = c("a", "b"), b = c("b", "c")),
  method = "max"
)
```

| | |
|----------------|--|
| combineSources | <i>Combine different sources of pathways</i> |
|----------------|--|

Description

Given several sources of pathways with the same for the same id of the genes it merge them.

Usage

```
combineSources(...)
```

Arguments

... Lists of genes and their pathways.

Details

It assumes that the identifier of the genes are the same for both sources but if many aren't equal it issues a warning. Only unique pathways identifiers are returned.

Value

A single list with the pathways of each source on the same gene.

Examples

```
DB1 <- list(g1 = letters[6:8], g2 = letters[1:5], g3 = letters[4:7])
DB2 <- list(
  g1 = c("one", "two"), g2 = c("three", "four"),
  g3 = c("another", "two")
)
combineSources(DB1, DB2)
combineSources(DB1, DB1)
DB3 <- list(
  g1 = c("one", "two"), g2 = c("three", "four"),
  g4 = c("five", "six", "seven"), g5 = c("another", "two")
)
combineSources(DB1, DB3) # A warning is expected
```

| | |
|-------------|---|
| conversions | <i>Convert the similarities formats</i> |
|-------------|---|

Description

Functions to convert the similarity coefficients between Jaccard and Dice. D2J is the opposite of J2D.

Usage

D2J(D)

J2D(J)

Arguments

D Dice coefficient, as returned by `diceSim()`, `geneSim()`, `clusterSim()` and `clusterGeneSim()`

J Jaccard coefficient

Value

A numeric value.

Author(s)

Lluís Revilla

Examples

```
D2J(0.5)
J2D(0.5)
D2J(J2D(0.5))
```

| | |
|---------|-------------------------|
| diceSim | <i>Compare pathways</i> |
|---------|-------------------------|

Description

Function to estimate how much two list of genes overlap by looking how much of the nodes are shared. Calculates the Dice similarity

Usage

```
diceSim(g1, g2)
```

Arguments

g1, g2 A character list with the names of the proteins in each pathway.

Details

It requires a vector of characters otherwise will return an NA.

Value

A score between 0 and 1 calculated as the double of the proteins shared by g1 and g2 divided by the number of genes in both groups.

Author(s)

Lluís Revilla

See Also

Used for [geneSim\(\)](#), see [conversions\(\)](#) help page to transform Dice score to Jaccard score.

Examples

```
genes.id2 <- c("52", "11342", "80895", "57654", "548953", "11586", "45985")
genes.id1 <- c(
  "52", "11342", "80895", "57654", "58493", "1164", "1163",
  "4150", "2130", "159"
)
diceSim(genes.id1, genes.id2)
diceSim(genes.id2, genes.id2)
```

duplicateIndices *Finds the indices of the duplicated events of a vector*

Description

Finds the indices of duplicated elements in the vector given.

Usage

```
duplicateIndices(vec)
```

Arguments

vec Vector of identifiers presumably duplicated

Details

For each duplication it can return a list or if all the duplication events are of the same length it returns a matrix, where each column is duplicated.

Value

The format is determined by the `simplify2array`

Author(s)

Lluís Revilla

See Also

[removeDup\(\)](#)

Examples

```
duplicateIndices(c("52", "52", "53", "55")) # One repeated element
duplicateIndices(c("52", "52", "53", "55", "55")) # Repeated elements
duplicateIndices(c("52", "55", "53", "55", "52")) # Mixed repeated elements
```

geneSim

Similarity score genes based on pathways similarity

Description

Given two genes, calculates the Dice similarity between each pathway which is combined to obtain a similarity between the genes.

Usage

```
geneSim(gene1, gene2, info, method = "max", ...)

## S4 method for signature 'character,character,GeneSetCollection'
geneSim(gene1, gene2, info, method = "max", ...)
```

Arguments

| | |
|--------------|---|
| gene1, gene2 | Ids of the genes to calculate the similarity, to be found in genes. |
| info | A GeneSetCollection or a list of genes and the pathways they are involved. |
| method | one of <code>c("avg", "max", "rcmax", "rcmax.avg", "BMA", "reciprocal")</code> , see Details. |
| ... | Other arguments passed to <code>combineScores</code> |

Details

Given the information about the genes and their pathways, uses the ids of the genes to find the Dice similarity score for each pathway comparison between the genes. Later this similarities are combined using [combineScoresPar\(\)](#).

Value

The highest Dice score of all the combinations of pathways between the two ids compared if a method to combine scores is provided or NA if there isn't information for one gene. If an NA is returned this means that there isn't information available for any pathways for one of the genes. Otherwise a number between 0 and 1 (both included) is returned. Note that there isn't a negative value of similarity.

Methods (by class)

- `geneSim(gene1 = character, gene2 = character, info = GeneSetCollection)`: Calculates all the similarities of the `GeneSetCollection` and combine them using `combineScoresPar()`

Author(s)

Lluís Revilla

See Also

`mgeneSim()`, `conversions()` help page to transform Dice score to Jaccard score. For the method to combine the scores see `combineScoresPar()`.

Examples

```
if (require("org.Hs.eg.db") & require("reactome.db")) {
  # Extract the paths of all genes of org.Hs.eg.db from KEGG
  # (last update in data of June 31st 2011)
  genes.kegg <- as.list(org.Hs.egPATH)
  # Extracts the paths of all genes of org.Hs.eg.db from reactome
  genes.react <- as.list(reactomeEXTID2PATHID)
  geneSim("81", "18", genes.react)
  geneSim("81", "18", genes.kegg)
  geneSim("81", "18", genes.react, NULL)
  geneSim("81", "18", genes.kegg, NULL)
} else {
  warning("You need reactome.db and org.Hs.eg.db package for this example")
}
```

`incidence,list-method` *Creates the incidence matrix*

Description

Given a list of pathways and its genes creates an incidence matrix.

Usage

```
## S4 method for signature 'list'
incidence(x)
```

Arguments

x A list

Value

A matrix with pathways as rows and genes in columns.

Note

Designed to be easier to work with list and GeneSetCollection

Author(s)

Lluís Revilla

inverseList

Invert a list

Description

Calculate the pathways per gene of list

Usage

```
inverseList(x)
```

Arguments

x A list with genes as names and names of pathways as values of the list

Value

The number of pathways each gene has.

Author(s)

Lluís Revilla

| | |
|-----------------|---|
| mclusterGeneSim | <i>Similarity score between clusters of genes based on genes similarity</i> |
|-----------------|---|

Description

Looks for the similarity between genes of a group and then between each group's genes.

Usage

```
mclusterGeneSim(clusters, info, method = c("max", "rcmax.avg"), ...)
```

```
## S4 method for signature 'list, GeneSetCollection'
```

```
mclusterGeneSim(clusters, info, method = c("max", "rcmax.avg"), ...)
```

Arguments

| | |
|----------|--|
| clusters | A list of clusters of genes to be found in id. |
| info | A GeneSetCollection or a list of genes and the pathways they are involved. |
| method | A vector with two or one argument to be passed to combineScores the first one is used to summarize the similarities of genes, the second one for clusters. |
| ... | Other arguments passed to combineScores |

Value

Returns a matrix with the similarity scores for each cluster comparison.

Methods (by class)

- `mclusterGeneSim(clusters = list, info = GeneSetCollection)`: Calculates all the similarities of the GeneSetCollection and combine them using `combineScoresPar()`

Author(s)

Lluís Revilla

See Also

[clusterGeneSim\(\)](#), [clusterSim\(\)](#) and [combineScores\(\)](#)

Examples

```
if (require("org.Hs.eg.db")) {
  genes.kegg <- as.list(org.Hs.egPATH)
  clusters <- list(
    cluster1 = c("18", "81", "10"),
    cluster2 = c("100", "594", "836"),
    cluster3 = c("18", "10", "83")
  )
}
```

```

mclusterGeneSim(clusters, genes.kegg)
mclusterGeneSim(clusters, genes.kegg, c("max", "avg"))
mclusterGeneSim(clusters, genes.kegg, c("max", "BMA"))
} else {
  warning("You need org.Hs.eg.db package for this example")
}

```

| | |
|-------------|--|
| mclusterSim | <i>Similarity score between clusters of genes based on pathways similarity</i> |
|-------------|--|

Description

Looks for the similarity between genes in groups. Once the pathways for each cluster are found they are combined using code [combineScores](#).

Usage

```

mclusterSim(clusters, info, method = "max", ...)

## S4 method for signature 'list, GeneSetCollection'
mclusterSim(clusters, info, method = "max", ...)

```

Arguments

| | |
|----------|--|
| clusters | A list of clusters of genes to be found in id. |
| info | A GeneSetCollection or a list of genes and the pathways they are involved. |
| method | one of c("avg", "max", "rcmax", "rcmax.avg", "BMA", "reciprocal"), see Details . |
| ... | Other arguments passed to combineScores |

Value

mclusterSim returns a matrix with the similarity scores for each cluster comparison.

Methods (by class)

- `mclusterSim(clusters = list, info = GeneSetCollection)`: Calculates all the similarities of the GeneSetCollection and combine them using [combineScoresPar\(\)](#)

Author(s)

Lluís Revilla

See Also

For a different approach see [clusterGeneSim\(\)](#), [combineScores\(\)](#) and [conversions\(\)](#)

Examples

```

if (require("org.Hs.eg.db")) {
  # Extract the paths of all genes of org.Hs.eg.db from KEGG (last update in
  # data of June 31st 2011)
  genes.kegg <- as.list(org.Hs.egPATH)

  clusters <- list(
    cluster1 = c("18", "81", "10"),
    cluster2 = c("100", "10", "1"),
    cluster3 = c("18", "10", "83")
  )
  mclusterSim(clusters, genes.kegg)
  mclusterSim(clusters, genes.kegg, "avg")
} else {
  warning("You need org.Hs.eg.db package for this example")
}

```

mgeneSim

Similarity score genes based on pathways similarity

Description

Given two genes, calculates the Dice similarity between each pathway which is combined to obtain a similarity between the genes.

Usage

```

mgeneSim(genes, info, method = "max", ...)

## S4 method for signature 'character, GeneSetCollection'
mgeneSim(genes, info, method = "max", ...)

## S4 method for signature 'missing, GeneSetCollection'
mgeneSim(genes, info, method = "max", ...)

```

Arguments

| | |
|--------|---|
| genes | A vector of genes. |
| info | A GeneSetCollection or a list of genes and the pathways they are involved. |
| method | one of c("avg", "max", "rcmax", "rcmax.avg", "BMA", "reciprocal"), see Details. |
| ... | Other arguments passed to combineScores |

Details

Given the information about the genes and their pathways, uses the ids of the genes to find the Dice similarity score for each pathway comparison between the genes. Later this similarities are combined using [combineScoresPar\(\)](#).

Value

mgeneSim returns the matrix of similarities between the genes in the vector

Methods (by class)

- mgeneSim(genes = character, info = GeneSetCollection): Calculates all the similarities of the list and combine them using [combineScoresPar\(\)](#)
- mgeneSim(genes = missing, info = GeneSetCollection): Calculates all the similarities of the list and combine them using [combineScoresPar\(\)](#)

Note

genes accept named characters and the output will use the names of the genes.

See Also

[geneSim\(\)](#), [conversions\(\)](#) help page to transform Dice score to Jaccard score. For the method to combine the scores see [combineScoresPar\(\)](#).

Examples

```
if (require("org.Hs.eg.db") & require("reactome.db")) {
  # Extract the paths of all genes of org.Hs.eg.db from KEGG
  # (last update in data of June 31st 2011)
  genes.kegg <- as.list(org.Hs.egPATH)
  # Extracts the paths of all genes of org.Hs.eg.db from reactome
  genes.react <- as.list(reactomeEXTID2PATHID)
  mgeneSim(c("81", "18", "10"), genes.react)
  mgeneSim(c("81", "18", "10"), genes.react, "avg")
  named_genes <- structure(c("81", "18", "10"),
    .Names = c("ACTN4", "ABAT", "NAT2")
  )
  mgeneSim(named_genes, genes.react, "max")
} else {
  warning("You need reactome.db and org.Hs.eg.db package for this example")
}
```

 mpathSim

Calculates the Dice similarity between pathways

Description

Calculates the similarity between several pathways using dice similarity score. If one needs the matrix of similarities between pathways set the argument methods to NULL.

Usage

```

mPathSim(pathways, info, method = NULL, ...)

## S4 method for signature 'character, GeneSetCollection, ANY'
mPathSim(pathways, info, method = NULL, ...)

## S4 method for signature 'missing, GeneSetCollection, ANY'
mPathSim(pathways, info, method = NULL, ...)

## S4 method for signature 'missing, list, ANY'
mPathSim(pathways, info, method = NULL, ...)

## S4 method for signature 'missing, list, missing'
mPathSim(pathways, info, method = NULL, ...)

```

Arguments

| | |
|----------|---|
| pathways | Pathways to calculate the similarity for |
| info | A list of genes and the pathways they are involved or a GeneSetCollection object |
| method | To combine the scores of each pathway, one of c("avg", "max", "rcmax", "rcmax.avg", "BMA"), if NULL returns the matrix of similarities. |
| ... | Other arguments passed to combineScoresPar() |

Value

The similarity between those pathways or all the similarities between each comparison.

Methods (by class)

- `mPathSim(pathways = character, info = GeneSetCollection, method = ANY)`: Calculates the similarity between the provided pathways of the GeneSetCollection using `combineScoresPar`
- `mPathSim(pathways = missing, info = GeneSetCollection, method = ANY)`: Calculates all the similarities of the GeneSetCollection and combine them using `combineScoresPar`
- `mPathSim(pathways = missing, info = list, method = ANY)`: Calculates all the similarities of the list and combine them using `combineScoresPar`
- `mPathSim(pathways = missing, info = list, method = missing)`: Calculates all the similarities of the list

Note

pathways accept named characters, and then the output will have the names

See Also

[pathSim\(\)](#) For single pairwise comparison. [conversions\(\)](#) To convert the Dice similarity to Jaccard similarity

Examples

```

if (require("reactome.db")) {
  genes.react <- as.list(reactomeEXTID2PATHID)
  (pathways <- sample(unique(unlist(genes.react)), 10))
  mpathSim(pathways, genes.react, NULL)
  named_paths <- structure(
    c("R-HSA-112310", "R-HSA-112316", "R-HSA-112315"),
    .Names = c(
      "Neurotransmitter Release Cycle",
      "Neuronal System",
      "Transmission across Chemical Synapses"
    )
  )
  mpathSim(named_paths, genes.react, NULL)
  many_pathways <- sample(unique(unlist(genes.react)), 152)
  mpathSim(many_pathways, genes.react, "avg")
} else {
  warning("You need reactome.db package for this example")
}

```

pathSim

Calculates the Dice similarity between pathways

Description

Calculates the similarity between pathways using dice similarity score. `diceSim` is used to calculate similarities between the two pathways.

Usage

```
pathSim(pathway1, pathway2, info)
```

```
## S4 method for signature 'character,character,GeneSetCollection'
pathSim(pathway1, pathway2, info)
```

Arguments

```
pathway1, pathway2
```

A single pathway to calculate the similarity

```
info
```

A `GeneSetCollection` or a list of genes and the pathways they are involved.

Value

The similarity between those pathways or all the similarities between each comparison.

Methods (by class)

- `pathSim(pathway1 = character, pathway2 = character, info = GeneSetCollection)`: Calculates all the similarities of a `GeneSetCollection` and combine them using `combineScoresPar`

Author(s)

Lluís Revilla

See Also

[conversions\(\)](#) help page to transform Dice score to Jaccard score. [mpathSim\(\)](#) for multiple pairwise comparison of pathways.

Examples

```
if (require("reactome.db")) {  
  # Extracts the paths of all genes of org.Hs.eg.db from reactome  
  genes.react <- as.list(reactomeEXTID2PATHID)  
  (paths <- sample(unique(unlist(genes.react)), 2))  
  pathSim(paths[1], paths[2], genes.react)  
} else {  
  warning("You need reactome.db package for this example")  
}
```

plot_data

The position of the nodes is based on the similarity between them.

Description

The position of the nodes is based on the similarity between them.

Plot how similar are the data

Usage

```
plot_data(x, top)
```

```
plot_similarity(pd)
```

Arguments

| | |
|-----|---|
| x | Matrix with the similarities. |
| top | a number between 0 and 1 to select the edges relating the elements of the matrix. |
| pd | The plot data from plot_data() function. |

Value

A list with two elements:

- nodes: The position and name of the nodes
- edges: The information about the selected edges

A ggplot object

Examples

```

if (require("org.Hs.eg.db") & require("reactome.db")) {
  # Extract the paths of all genes of org.Hs.eg.db from KEGG
  # (last update in data of June 31st 2011)
  genes.kegg <- as.list(org.Hs.egPATH)
  # Extracts the paths of all genes of org.Hs.eg.db from reactome
  genes.react <- as.list(reactomeEXTID2PATHID)

  sim <- mgeneSim(c("81", "18", "10"), genes.react)
  pd <- plot_data(sim, top = 0.25)
  if (requireNamespace("ggplot2", quietly = TRUE)){
    plot_similarity(pd)
  }
}

```

removeDup

Remove duplicated rows and columns

Description

Given the indices of the duplicated entries remove the columns and rows until just one is left, it keeps the duplicated with the highest absolute mean value.

Usage

```
removeDup(cor_mat, dupli)
```

Arguments

| | |
|---------|---|
| cor_mat | List of matrices |
| dupli | List of indices with duplicated entries |

Value

A matrix with only one of the columns and rows duplicated

Author(s)

Lluís Revilla

See Also

[duplicateIndices\(\)](#) to obtain the list of indices with duplicated entries.

Examples

```
a <- seq2mat(c("52", "52", "53", "55"), runif(choose(4, 2)))
b <- seq2mat(c("52", "52", "53", "55"), runif(choose(4, 2)))
mat <- list("kegg" = a, "react" = b)
mat
dupli <- duplicateIndices(rownames(a))
remat <- removeDup(mat, dupli)
remat
```

seq2mat

Transforms a vector to a symmetric matrix

Description

Fills a matrix of `ncol = length(x)` and `nrow = length(x)` with the values in `dat` and setting the diagonal to 1.

Usage

```
seq2mat(x, dat)
```

Arguments

`x` names of columns and rows, used to define the size of the matrix
`dat` Data to fill with the matrix with except the diagonal.

Details

`dat` should be at least `choose(length(x), 2)` of length. It assumes that the data provided comes from using the row and column id to obtain it.

Value

A square matrix with the diagonal set to 1 and `dat` on the upper and lower triangle with the columns ids and row ids from `x`.

Author(s)

Lluís Revilla

See Also

[upper.tri\(\)](#) and [lower.tri\(\)](#)

Examples

```
seq2mat(LETTERS[1:5], 1:10)
seq2mat(LETTERS[1:5], seq(from = 0.1, to = 1, by = 0.1))
```

`similarities`*Apply a function to a list of similarities*

Description

Function to join list of similarities by a function provided by the user.

Usage

```
similarities(sim, func, ...)
```

Arguments

| | |
|-------------------|---|
| <code>sim</code> | list of similarities to be joined. All similarities must have the same dimensions. The genes are assumed to be in the same order for all the matrices. |
| <code>func</code> | function to perform on those similarities: prod, sum... It should accept as many arguments as similarities matrices are provided, and should use numbers. |
| <code>...</code> | Other arguments passed to the function func. Usually <code>na.rm</code> or similar. |

Value

A matrix of the size of the similarities

Note

It doesn't check that the columns and rows of the matrices are in the same order or are the same.

Author(s)

Lluís Revilla

See Also

[weighted\(\)](#) for functions that can be used, and [addSimilarities\(\)](#) for a wrapper to one of them

Examples

```
set.seed(100)
a <- seq2mat(LETTERS[1:5], rnorm(10))
b <- seq2mat(LETTERS[1:5], seq(from = 0.1, to = 1, by = 0.1))
sim <- list(b, a)
similarities(sim, weighted.prod, c(0.5, 0.5))
# Note the differences in the sign of some values
similarities(sim, weighted.sum, c(0.5, 0.5))
```

| | |
|----------|----------------------------|
| weighted | <i>Weighted operations</i> |
|----------|----------------------------|

Description

Calculates the weighted sum or product of x . Each values should have its weight, otherwise it will throw an error.

Usage

```
weighted.sum(x, w, abs = TRUE)
```

```
weighted.prod(x, w)
```

Arguments

| | |
|-------|--|
| x | an object containing the values whose weighted operations is to be computed |
| w | a numerical vector of weights the same length as x giving the weights to use for elements of x . |
| abs | If any x is negative you want the result negative too? |

Details

This functions are thought to be used with *similarities*. As some similarities might be positive and others negative the argument abs is provided for `weighted.sum`, assuming that only one similarity will be negative (usually the one coming from expression correlation).

Value

`weighted.sum` returns the sum of the product of x *weights removing all NA values. See parameter abs if there are any negative values.

`weighted.prod` returns the product of product of x *weights removing all NA values.

Author(s)

Lluís Revilla

See Also

[weighted.mean\(\)](#), [similarities\(\)](#) and [addSimilarities\(\)](#)

Examples

```
expr <- c(-0.2, 0.3, 0.5, 0.8, 0.1)
weighted.sum(expr, c(0.5, 0.2, 0.1, 0.1, 0.1))
weighted.sum(expr, c(0.5, 0.2, 0.1, 0.2, 0.1), FALSE)
weighted.sum(expr, c(0.4, 0.2, 0.1, 0.2, 0.1))
weighted.sum(expr, c(0.4, 0.2, 0.1, 0.2, 0.1), FALSE)
weighted.sum(expr, c(0.4, 0.2, 0, 0.2, 0.1))
weighted.sum(expr, c(0.5, 0.2, 0, 0.2, 0.1))
# Compared to weighted.prod:
weighted.prod(expr, c(0.5, 0.2, 0.1, 0.1, 0.1))
weighted.prod(expr, c(0.4, 0.2, 0.1, 0.2, 0.1))
weighted.prod(expr, c(0.4, 0.2, 0, 0.2, 0.1))
weighted.prod(expr, c(0.5, 0.2, 0, 0.2, 0.1))
```

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