# Package 'sims'

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<b>Description</b> This package allows the computation of semantic similarity measures, based on different approaches, between terms of an arbitrary ontology
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ancestors

Ancestors for each term of the ontology

# Description

Given the accesibility matrix, generates a list whose elements are the ancestors for each term of the ontology

# Usage

```
ancestors(m)
```

### **Arguments**

m

matrix of accessibility

### Value

The resulting object is a list whose elements are character vectors with the names of the ancestors associated with each term

### Author(s)

Jose Luis Mosquera

### See Also

getA

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
print(at)</pre>
```

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commonAncestors

Common ancestors for each pair of terms of the ontology

# **Description**

Generates a list whose elements are the common ancestors for each pair of terms of the ontology

# Usage

```
commonAncestors(at)
```

## **Arguments**

at

list of character vectors containing the name of the ancestors of each term of the ontology

### Value

Resulting object is a list whose elements are character vectors with the names of the common ancestors between each pair of terms connected

# Author(s)

Jose Luis Mosquera

### See Also

```
ancestors, getA, inverseIminusG
```

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)

ca <- commonAncestors(at)
print(at)</pre>
```

cosSim 5

cosSim

Cosine similarity measure

### **Description**

This function computes the cosine similarity measure between two columns of a matrix

### Usage

```
cosSim(x, na.rm = FALSE)
```

### **Arguments**

x matrix with two columns

na.rm a logical value indicating whether NA values should be stripped before the computation proceeds. By default is FALSE

#### **Details**

Given the two columns of the matrix, let A and B be the names of such columns, the cosine similarity, is estimated using a dot product and magnitude as

$$sim_{cos}(A, B) = \frac{A \cdot B}{\|A\| \cdot \|B\|} = \frac{\sum_{i=1}^{n} A_i \times B_i}{\sqrt{\sum_{i=1}^{n} (A_i)^2} \times \sqrt{\sum_{i=1}^{n} (B_i)^2}}$$

### Author(s)

Jose Luis Mosquera

```
a <- sample(c(1:100, NA), 20)
idx.na <- sample(1:20, 4)
a[idx.na] <- NA
b <- sample(1:100, 20)
x <- as.matrix(cbind(a,b))

cos.sim <- cosSim(x, na.rm = TRUE)
print(cos.sim)

## Cosine similarity between semantic similarites of Resnik

data(prostateIds)  # Data set from the package goProfiles

pckg <- "org.Hs.eg.db"  # Organism package of humans

eg.we <- welsh01EntrezIDs[1:10]  # Entrez Gene IDs signature Welsh 01
eg.sg <- singh01EntrezIDs[1:10]  # Entrez Gene IDs signature Singh 01</pre>
```

6 depth

```
WEvsSG.nb <- gosimsAvsB(eg1 = eg.we, eg2 = eg.sg, ontology = "MF", pckg = pckg, type = "nb", method = "Res")
idx.Inf <- which(WEvsSG.nb == Inf)
WEvsSG.nb[idx.Inf] <-NA
WEvsSG.cos.sim <- cosSim(WEvsSG.nb , na.rm = TRUE)
print(WEvsSG.cos.sim)</pre>
```

depth

Depth of the ontology

### **Description**

Computes the depth of the ontology. That is, the longest path from the root term to the farthest refinement term end

### Usage

depth(x)

### **Arguments**

Χ

can be an OOC object, a matrix of the refinements between terms, or a list of matrices with the number of paths between each pair of terms that are directly connected for each length

# Value

numeric value indicating the longest path from the root term to the far refinement term end.

### Author(s)

Jose Luis Mosquera

#### See Also

```
getGk, getGr, toOOC
```

```
data(joslyn)
print(mat.g)
d.G <- depth(mat.g)
print(d.G)
## list of matrices with the number of paths</pre>
```

distRada 7

```
## between each pair of terms for each length k

Gk <- getGk(joslyn.00C)
d.Gk <- depth(Gk)

print(d.Gk)

## matrix with all the number of paths of any length
## between each pair of terms

Gr <- getGr(Gk)
d.Gr <- depth(Gr)

print(d.Gr)

distRada

Distances of the shortest paths between each pair of terms in the on-</pre>
```

# Description

This function is a edge-based approach to compute the distance of the shortest between each pair of terms in the ontology.

### Usage

```
distRada(sum.paths, at)
```

# Arguments

sum.paths list of numeric vectors with the lengths (in terms of depth) of the number of

paths between each pair of terms.

at list of ancestors of each term

tology

### **Details**

This function is based on the edge-counting method (i.e. edge-based approach) proposed by Rada *et al.* The measure computes the length of the shortest path (i.e. the number of edges between a pair of terms).

This taxonomical distance was thought to be applied in trees where the shortest path between two terms contains a unique common ancestor, which is known as the Least Common Ancestor (LCA). Note that, in ontologies, this measure is not the most appropriate to be used because DAG structures may show more than one LCA. In any case, the method implemented does not distinguish a unique LCA (see function LCAs)

#### Value

Resulting object is a matrix whose elements show the distance (column) between each pair of different terms (rows)

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#### Author(s)

Jose Luis Mosquera

#### References

Rada, R. et al. Development and application of a metric on semantic nets. Ieee Transactions On Systems Man And Cybernetics, 19(1), pp.17-30, 1989.

#### See Also

```
ancestors, LCAs, simRada, simRes.eb, summaryPaths
```

# Examples

```
data(joslyn)
sum.paths <- summaryPaths(x = joslyn.00C, root = "R", len = TRUE)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
dist.rada <- distRada(sum.paths,at)
print(dist.rada)</pre>
```

getA

Accessibility matrix associated with the DAG structure of the ontology

#### **Description**

Builds the accessibility matrix associated with the DAG structure of the ontology

#### Usage

```
getA(x)
```

### Arguments

Х

matrix of the number of paths of any length between each pair of terms.

#### Value

Resulting object is a matrix whose elements contains a TRUE value, if there exists a path of terms path following the arcs from the term on the rows to the term on the columns.

Depending on the approach applied later on, resulting matrix may be interpreted as the accessibility matrix (i.e. a node-based approach, and an edge-based approach based on distances, or a hybrid-based approach) or the comparability matrix (i.e. an edge-based based on pseudo-distances). In the first case, TRUE values indicate terms that are connected by a path, and FALSE values indicate

getGk

which not. In the second case, TRUE values indicate comparable nodes (i.e. terms), but FALSE values indicate non-comparable nodes.

### Author(s)

Jose Luis Mosquera

### See Also

```
inverseIminusG, getGr
```

### **Examples**

```
data(joslyn)
## (I-Gamma)^{-1}
inv.IminusG <- inverseIminusG(joslyn.00C)
getA(inv.IminusG)

## I + Gamma^1 + Gamma^2 + ... + Gamma^r, where r is the depth of the ontology.
Gr <- getGr(joslyn.00C)

## (I-Gamma)^{-1} = I + Gamma^1 + Gamma^2 + ... + Gamma^r
Gr==inv.IminusG-diag(nrow(inv.IminusG))

## Accessibility matrix
getA(inv.IminusG-diag(nrow(inv.IminusG)))
getA(Gr)</pre>
```

getGk

Builds a list of the matrices with the number of paths between each pair of terms that are directly connected for each length

# **Description**

Builds a list whose elements are the matrices (one per each length) of the number of paths between each pair of terms that are directly connected. That is,  $\Gamma^1, \Gamma^2, \dots, \Gamma^r$ , where r is the depth of the ontology

### Usage

```
getGk(x)
```

## **Arguments**

Χ

an OOC or a matrix of refinements

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### **Details**

Given either an OOC object or a refinement matrix (i.e. G matrix in the OOC object), computes all the number of paths for each length between each pair of terms that are directly connected. Each of these matrices are power matrices of the matrix G. For example, to obtain all the number of paths between each pair of terms connected in the ontology with length 1, the function computes  $D^1$ , to obtain all the number of paths with length 2, calculates  $G^2 = G * G$ , and so on until the length of the largest path, that is, the maximum depth of the ontology

#### Value

The resulting object is a list of matrices. Each matrix is associated with a length of paths between each pair of connected terms. Elements of these matrices are the number of paths for the same length connecting each pair of terms. For example, let r be the depth of the ontology, then the elements of the resulting list are

```
G1 matrix with the number of paths between each pair of terms with length 1 G2 matrix with the number of paths between each pair of terms with length 2 ...
```

# Gr matrix with the number of paths between each pair of terms with length r

### Author(s)

Jose Luis Mosquera

#### See Also

```
getGr, depth, toOOC
```

### **Examples**

```
data(joslyn)

Gk <- getGk(joslyn.00C)  # based on an OOC object
print(Gk)

Gk.2 <- getGk(mat.g)  # based on a matrix
print(Gk.2)</pre>
```

getGr

Number of paths of any length between each pair of terms that are directly connected

### Description

Computes all the number of paths of any length between each pair of terms that are directly connected.

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### Usage

getGr(x)

### **Arguments**

Х

can be an object OOC, a matrix of refinement matrix, or a list of matrices with the number of paths of each length between each pair of terms that are directly connected

#### **Details**

The computation of the number of paths is based on the formula

$$\mathbf{I} + \Gamma^1 + \ldots + \Gamma^r = (\mathbf{I} - \Gamma)^{(-1)}$$

.

There are two ways for performing the computation; first, by calculating the sum of the power matrices of the refinements matrix, and second, by computing the inverse of the matrix  $I - \Gamma$ .

Note that depending on the class of the argument x supplied, the computation requires calculating the power matrices of the refinements matrix. That is,  $\Gamma^1, \Gamma^2, \dots, \Gamma^r$ , where r is the depth of the ontology

### Value

Resulting object is a matrix whose elements are the number of paths of any length between each pair of terms that are directly connected

### Author(s)

Jose Luis Mosquera

#### See Also

```
getGk, toOOC
```

```
data(joslyn)
## Based on the OOC object

Gr <- getGr(joslyn.OOC)
print(Gr)
## Based on the refinement matrix

Gr.2 <- getGr(mat.g)
Gr==Gr.2
## Based on the list of matrices with the number of</pre>
```

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```
## paths of each length between each pair of terms
## that are directly connected

Gk <- getGk(joslyn.00C)
Gr.3 <- getGr(Gk)
Gr==Gr.3</pre>
```

go00C

Builds an Object-Ontology Complex (OOC) whose slots are associated with GO Identifiers

# Description

Given a list of Entrez Gene Identifiers, the name of an R organism package, and a domain of the GO, the function builds an Object-Ontology Complex where the slots are associated with GO ID's and Entrez Gene ID's. But also, if two list of Entrez Gene Identifiers are provided, then the function builds a list with two elements, each one associated with one of the list of Entrez Gene Identifiers and consisting of an object of class OOC

### Usage

```
goOOC(eg1, eg2 = NULL, pckg = "org.Hs.eg.db", ontology = "BP")
```

### **Arguments**

eg1	character vector with the (first list of) Entrez Gene IDs to be interrogated.
eg2	character vector with the second list of Entrez Gene IDs to be interrogated. By default is NULL.
pckg	character with the name of the R organism package. By default is $\operatorname{org.Hs.eg.db}$
ontology	character the ontology from the GO is selected (see <i>Details</i> . By default is BP

### **Details**

This function is similar to the function to00C, but it is particularly adapted to deal with information associated with the Gene Ontology.

If argument eg2 is NULL, then yields an OOC object. Otherwise, the resulting object is a list with two OOC objects. First element is associated with the first list of Entrez Gene Identifiers (provided to the function in argument eg1), and second element is associated with the second list of Entrez Gene Identifiers (provided to the function in argument eg2).

Note that, in case of providing two lists of Entrez Gene Identifiers, both objects 00C from the resulting list have the same refinement matrix (i.e. slot G). This is made in order to compare both lists of Entrez Gene IDs in terms of semantic similarities profiles later on. That is, sometimes the comparison between two list of genes is required. This tasks may be performed by comparing two semantic similarity profiles (i.e. two lists of semantic similarities between each pair of terms and performed with the same measure). Thus, each list of genes yields an induced subgraph from the GO. But, note that both subgraphs might be different. In consequence, no comparison might be

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computed because the number of pairs of GO IDs would be different. This drawback, can be solved by considering a common subgraph induced by both lists of genes.

Argument ontology has three possibilities

```
BP Biological ProcessesCC Cellular Components
```

MF Molecular Functions

### Value

Resulting object

### Author(s)

Jose Luis Mosquera

#### See Also

to00C

```
data(prostateIds)
## Entrez Genes from two different studies
## of prostate cancer
eg.we <- welsh01EntrezIDs[1:10] # Weslh study
eg.sg <- singh01EntrezIDs[1:10] # Singh study</pre>
## OOC associated with Entrez Gene IDs of Welsh
ooc1 \leftarrow goOOC(eg1 = eg.we, eg2 = NULL,
              pckg = "org.Hs.eg.db", ontology = "MF")
class(ooc1)
str(ooc1)
dim(ooc1@G)
dim(ooc1@M)
## OOC associated with Entrez Gene IDs of Singh
ooc2 \leftarrow goOOC(eg1 = eg.sg, eg2 = NULL,
              pckg = "org.Hs.eg.db", ontology = "MF")
class(ooc2)
str(ooc2)
dim(ooc2@G)
dim(ooc2@M)
## List of OOC associated with Entrez Gene IDs of Welsh
## and Singh
ooc \leftarrow goOOC(eg1 = eg.we, eg2 = eg.sg,
```

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```
pckg = "org.Hs.eg.db", ontology = "MF")
class(ooc)
str(ooc)
dim(ooc[[1]]@G)
dim(ooc[[2]]@G)
table(ooc[[1]]@G==ooc[[2]]@G)
dim(ooc[[1]]@M)
dim(ooc[[2]]@M)
```

gosims

Wrapper function that calls different approaches and methods for computing semantic similarities between GO Identifiers given a list of Entrez Gene IDs

### **Description**

Given a list of Entrez Gene Identifiers, the name of an R organism package, and an ontology domain, the function builds an Object-Ontology Complex particularly adapted for dealing with GO Identifiers. But also, if two list of Entrez Gene Identifiers are provided, then the function builds a list with two elements, each one associated with one of the list of Entrez Gene Identifiers and consisting of an object of class OOC

#### **Usage**

```
gosims(eg, ontology = "BP", pckg = "org.Hs.eg.db", type = "nb", method = "Res")
```

### Arguments

eg	character vector with the Entrez Gene IDs to be interrogated.
ontology	character with the ontology domain of the GO (see <i>Details</i> ). By default is BP
pckg	$character\ with\ the\ name\ of\ the\ R\ organism\ package.\ By\ default\ is\ org.\ Hs.\ eg.\ db$
type	character indicating the approach for computing semantic similarities. By default nb
method	character indicating the method used for computing semantic similarities. By default Res

# **Details**

Argument ontology has three possible domains

**BP** Biological Processes

**CC** Cellular Components

MF Molecular Functions

Argument type has three possibilities

nb node-based approach

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eb edge-based approach

eb.pd edge-based approach based on pseudo-distances

Depending on the approach selected in argument type, different methods for computing semantic similarities are available.

• Possible methods of *Node-based approach* (i.e. type = nb) are

Res semantic similarty of Resnik

Lin semantic similarty of Lin

Rel semantic similarty of Schlicker et al.

JC semantic similarty of Jiang and Conrath

Nunivers semantic similarty of Mazandu and Mulder

Psec semantic similarty of Pirro and Seco

Faith semantic similarty of Pirro and Euzenat

all all sementic similarities

• Possible methods of *Edge-based approach* (i.e. type = eb) are

Rada semantic similarty of Rada

Res.eb semantic similarty of Resnik based on the shortest path (see function distRada)

all all semantic similarities of edge-based approaches implemented in the package

• Possible pseudo-distance methods of *Edge-based approach* (i.e. type = eb.pd) are

hm pseudo-distance of the minimum chain length

hx pseudo-distance of the maximum chain length

hax pseudo-distance of the average of extreme chain lengths

hap pseudo-distance of the average of all chain lengths

all all pseudo-distances

### Author(s)

Jose Luis Mosquera

#### See Also

gosimsAvsB, simsBetweenGOIDs, summarySims, goOOC, sims.nb, sims.eb, pseudoDists

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gosimsAvsB

Wrapper function for computing semantic similarities between GO Identifiers for two lists of Entrez Gene IDs

### **Description**

Given two lists of Entrez Gene Identifiers computes semantic similarities between GO Identifiers

# Usage

```
gosimsAvsB(eg1, eg2, ontology = "BP", pckg = "org.Hs.eg.db", type = "nb", method = "Res")
```

### **Arguments**

eg1	character vector with the first list of Entrez Gene IDs to be interrogated.
eg2	character vector with the second list of Entrez Gene IDs to be interrogated.
ontology	character the ontology from the GO is selected (see <i>Details</i> ). By default is BP
pckg	character with the name of the R organism package. By default is org. Hs. eg. db $$
type	character indicating the approach for computing semantic similarities. By default nb
method	character indicating the method used for computing semantic similarities. By default Res

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#### **Details**

Argument ontology has three possible domains

**BP** Biological Processes

CC Cellular Components

MF Molecular Functions

Argument type has three possibilities

nb node-based approach

eb edge-based approach

eb.pd edge-based approach based on pseudo-distances

Depending on the approach selected in argument type, different methods for computing semantic similarities are available.

• Possible methods of *Node-based approach* (i.e. type = nb) are

Res semantic similarty of Resnik

Lin semantic similarty of Lin

Rel semantic similarty of Schlicker et al.

JC semantic similarty of Jiang and Conrath

Nunivers semantic similarty of Mazandu and Mulder

Psec semantic similarty of Pirro and Seco

Faith semantic similarty of Pirro and Euzenat

all all sementic similarities

• Possible methods of *Edge-based approach* (i.e. type = eb) are

Rada semantic similarty of Rada

Res.eb semantic similarty of Resnik based on the shortest path (see function distRada)

all all semantic similarities of edge-based approaches implemented in the package

• Possible pseudo-distance methods of *Edge-based approach* (i.e. type = eb.pd) are

hm pseudo-distance of the minimum chain length

hx pseudo-distance of the maximum chain length

hax pseudo-distance of the average of extreme chain lengths

hap pseudo-distance of the average of all chain lengths

all all pseudo-distances

### Value

Resulting object is a matrix semantic similarity values. On the rows there are the pairs of GO ID's compared and on the columns the method(s) used for the computation of the measures. For each measure there are two columns (one per list of genes)

#### Author(s)

Jose Luis Mosquera

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### See Also

summarySims, gosims, goOOC, sims.nb, sims.eb, pseudoDists

### **Examples**

```
data(prostateIds)
## R organism package
pckg <- "org.Hs.eg.db"</pre>
## Entrez Genes from two different studies
## of prostate cancer
eg.we <- welsh01EntrezIDs[1:10] # Welsh study</pre>
eg.sg <- singh01EntrezIDs[1:10] # Singh study
## Semantic similarity of Resnik (node-based approach)
WEvsSG.nb <- gosimsAvsB(eg1 = eg.we, eg2 = eg.sg,</pre>
                        ontology = "MF", pckg = pckg,
                        type = "nb", method = "Res")
head(WEvsSG.nb, 20)
tail(WEvsSG.nb, 20)
## Semantic similarity of Resnik (edge-based approach)
WEvsSG.eb <- gosimsAvsB(eg1 = eg.we, eg2 = eg.sg,
                        ontology = "MF", pckg = pckg,
                         type = "eb", method = "Res.eb")
head(WEvsSG.eb, 20)
tail(WEvsSG.eb, 20)
## Pseudo-distance of the minimum chains length
## (edge-based approach)
WEvsSG.pd <- gosimsAvsB(eg1 = eg.we, eg2 = eg.sg,</pre>
                        ontology = "MF", pckg = pckg,
                         type = "eb.pd", method = "hm")
head(WEvsSG.pd, 20)
tail(WEvsSG.pd, 20)
```

gosimsProfiles

Plots a vertical bar diagram whose bars are associated with the semantic similarities between each pair of terms, and such that bars on the left side of the plot are the corresponding to the first group of objects and on the bars on the right side are the bars corresponding to the second group of objects

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### **Description**

Given a two-columns matrix (or data.frame), this function yields a vertical bar diagram whose bars are associated with the semantic similarities between each pair of terms, and such that bars on the left side of the plot are the corresponding to the first group of objects and on the bars on the right side are the bars corresponding to the second group of objects

### Usage

### **Arguments**

X	matrix (or data.frame) where for each pair terms (rows) contains the values of the semantic similarity measure estimated for each group of objects (columns)
col	character vector with the two elements containing the colors associated with each group of objects. By default are tomato for the left bars on the left side, and blue for the bars on the right side
cex	numeric value with the expansion for the category labels. By default is 0.4
top.labels	character vector indicating the two categories represented on the left and right sides of the plot and a heading for the labels in the center. By default is NULL
main	character with title for the plot. By default NULL
xlab	character with the label for the units of the plot (i.e. labels on the x-axis).

### Author(s)

Jose Luis Mosquera

### See Also

```
gosimsAvsB, summarySimsAvsB, plotHistSims, plotGODAG
```

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ICA

Information Content (IC) of common ancestors

### **Description**

Builds a list of numeric vectors with the Information Content (IC) associated with each common ancestor of each pair of terms

### Usage

```
ICA(x, ic)
```

### **Arguments**

x list of common ancestors for each pair of terms ic numeric vector with the IC of each term in the ontology

### Value

The resulting object is a list whose elements are numeric vectors with the ICs of the common ancestors for each pair of terms

# Author(s)

Jose Luis Mosquera

### References

Resnik P. "Using information content to evaluate semantic similarity in a taxonomy". Proceedings of the 14th International Joint Conference on Artificial Intelligence, pp. 448-453, 1995.

## See Also

ancestors, commonAncestors, inverseIminusG, resnikSummary

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### **Examples**

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)  # (I - G)^(-1)
A.mat <- getA(inv.IminusG)  # accessibility matrix
at <- ancestors(A.mat)  # ancestors
ca <- commonAncestors(at)  # common ancestors
resnik.sum <- resnikSummary(x = joslyn.00C)  # summary of Resnik measures
ica <- ICA(x = ca, ic = resnik.sum[, "ic"])
print(ica)</pre>
```

inverseIminusG

Computes the number of paths of any length between each pair of terms in the ontology

### **Description**

Builds a matrix with the number of paths of any length between each pair of terms in the ontology

### Usage

```
inverseIminusG(x)
```

### **Arguments**

x can be an object of class OOC or a matrix with the refinements of each term in the ontology

### **Details**

```
In order to compute faster the matrix, applies the formula (I - Gamma)^(-1), instead of using I + Gamma^1 + ... + Gamma^r where r is the depth of the ontology.
```

### Value

The resulting object is a matrix whose elements are the number of paths

## Author(s)

Jose Luis Mosquera

#### See Also

to00C

is.OOC

# Examples

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)
print(inv.IminusG)</pre>
```

is.00C

Tests if its argument is a (strict) OOC object

# Description

Tests if its argument is a (strict) OOC object

# Usage

```
is.00C(x)
```

# Arguments

Х

an R object

### **Details**

is. OOC returns TRUE if argument x is an OOC object, and FALSE otherwise

# Author(s)

Jose Luis Mosquera

# See Also

to00C

```
data(joslyn)
is.00C(mat.m)  # FALSE
is.00C(joslyn.00C) # TRUE
```

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LCAs	Length of the shortest paths containing the Least Common Ancestors
	(LCA) between each pair of terms

### **Description**

Computes the Least Common Ancestors between each pair of nodes

# Usage

```
LCAs(at, sum.paths)
```

### **Arguments**

at list of ancestors of each term

sum.paths list of numeric vectors with the lengths (in terms of depth) of the number of

paths between each pair of terms.

### **Details**

The function looks for all the least common ancestor of each pair of terms and computes the shortest path between such terms containing the corresponding LCA.

### Value

The resulting object is a list whose elements are numeric vectors with the lengths of the shortest paths associated with each LCA.

## Author(s)

```
jose Luis Mosquera
```

#### See Also

```
ancestors, summaryPaths
```

```
data(joslyn)
sum.paths <- summaryPaths(x = joslyn.00C, root = "R", len = TRUE)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)

lcas <- LCAs(at, sum.paths)
print(lcas)</pre>
```

24 mapEG2GO

mapEG2G0

Mapping Entrez Gene IDs to Gene Ontology IDs

### **Description**

This function maps the Entrez Gene IDs on to the GO IDs provided by an R organism package (e.g. org. Hs. eg. db

### Usage

```
mapEG2GO(eg = NULL, pckg = "org.Hs.eg.db")
```

### **Arguments**

eg character vector with the Entrez Gene IDs. By default is NULL, which means

that all the eg from the pckg will be mapped

pckg character with the name of the package of the organism from where the GO

IDs are extracted. By default is org. Hs. eg. db, that is, Homo sapiens specie

### Value

The resulting object is a list with three elements, corresponding to an ontology of the the GO (i.e BP, CC and MF). Each of these elements is a data. frame with two columns. First column consists of the list of Entrez Gene IDs mapping the GO IDs placed in the second column. Note that in both columns, the concepts can be repeated. That is, an Entrez Gene ID can map different GO IDs, and a GO ID can be mapped by different Entrez Gene IDs

### Author(s)

Jose Luis Mosquera

```
data(prostateIds)  # Data set from the package goProfiles

pckg <- "org.Hs.eg.db"  # Names of the organism package
eg <- welsh01EntrezIDs[1:10]  # Entrez Gene IDs

eg2go <- mapEG2GO(eg, pckg)
lapply(eg2go, head)</pre>
```

mappingMatrix 25

mappingMatrix	Mapping matrix from the Entrez Gene IDs to the GO IDs associated
	with the directed subgraph extracted from GO DAG structure

### **Description**

Based on the data.frame of the maps the Entrez Gene IDs on to the GO IDs and the refinement matrix, this function builds the mapping matrix associated with the GO DAG structure

### Usage

```
mappingMatrix(G, df)
```

### **Arguments**

G	binary matrix indicating the refinements of each GO ID
df	data.frame with mapping from the Entrez Gene IDs to the GO ID terms

#### **Details**

Given the data.frame with mapping from the Entrez Gene IDs to the GO IDs, mappingMatrix and the refinement matrix, builds a binary matrix where on rows are the Entrez Gene IDs and on the columns are all the GO IDs associated with the directed subgraph extracted from the GO DAG.

### Value

The resulting object is a binary matrix. Each element of this matrix is either 1 when an Entrez Gene ID on a row is mapping a GO ID on a column, or 0 otherwise.

### Author(s)

Jose Luis Mosquera

### See Also

```
mapEG2GO, refinementMatrix
```

```
data(prostateIds)  # Data set from the package goProfiles

pckg <- "org.Hs.eg.db"  # Names of the organism package
eg <- welsh01EntrezIDs[1:10]  # Entrez Gene IDs

eg2go <- mapEG2GO(eg, pckg)
eg2go.mf <- eg2go$MF  # Get mollecular functions

G <- refinementMatrix(df = eg2go.mf, ontology = "MF")</pre>
```

26 Nt

```
M <- mappingMatrix(G, df = eg2go.mf)
print(M)</pre>
```

Nt

Number of times that each term or any of its specializations references to an ancestor

# Description

Calulates the matrix of the number of times that each term or any of its specializations references to an ancestor

# Usage

Nt(x)

# Arguments

Χ

an object of class OOC

### **Details**

The resulting matrix is based on the Neumann series of a matrix. The function calculates the matrix based on the formula

$$N_t = M(I - \Gamma)^{-1}$$

# Author(s)

Jose Luis Mosquera

### See Also

toOOC,

```
data(joslyn)

N.t <- Nt(joslyn.00C)
print(N.t)</pre>
```

OOC 27

00C

General container for an Object-Ontology Complex (OOC)

### **Description**

Class "00C" is a general container for Object-Ontology Complexes (OOC)

### **Objects from the Class**

Objects can be created by calls of either the form new("OOC", ...) or the function toOOC(T, G, O, M)

#### **Slots**

- T character vector with the names of the terms in the ontology
- G matrix encoding the refinement matrix associated with the DAG of the ontology. Elements of this matrix are 1, when a term on the rows refines a term on the columns, and 0 otherwise
- O character vector with the object identifiers (i.e. features, genes,...) mapping the terms of the ontology
- M matrix encoding the mapping from the set of object identifiers (listed in the slot O to the terms listed in the slot  $\mathsf{T}$

### Methods

No methods defined with class OOC in the signature

### Author(s)

Jose Luis Mosquera

### See Also

to00C

рdНар	Pseudo-distances of the average of all chain lengths between compa-
	rable terms of the ontology.

# Description

This function computes pseudo-distances of the average of all chain lengths proposed by Josly *et al*.

#### Usage

```
pdHap(sum.paths)
```

28 pdHap

### Arguments

sum.paths

list of vectors with the lengths of the chains of each pair of terms

### **Details**

Pseudo-distance concept is an strategy of the edge-based approach for measuring the distances between terms in an ontology. It was proposed by Joslyn *et al*.

pdHap computes the pseudo-distances proposed of the average of all chain lengths. That is, let  $t_i$  and  $t_i$  be two comparable terms, then the average of all chain length is defined as

$$\delta_{ap}(t_i, t_j) = \frac{\sum_{h \in \mathbf{h}(t_i, t_j)} h}{|\mathbf{h}|}$$

In case of non-comparable terms, the resulting value is NA.

### Author(s)

Jose Luis Mosquera

#### References

Cliff A. Joslyn, Susan M. Mniszewski Andy W. Fulmer, and Gary G. Heaton. (2004). "The gene ontology categorizer". Bioinformatics, 20(s1):169-77, 2004.

### See Also

```
pdHm, pdHx, pdHax, pseudoDists
```

### **Examples**

data(joslyn)

```
length.chains <- summaryPaths(x = joslyn.00C, root = "R", len = TRUE) # length of chains
num.chains <- summaryPaths(x = joslyn.00C, root = "R", len = FALSE) # number of chains</pre>
```

##

pdHax 29

pdHax

Pseudo-distances of the average of extreme chain lengths between comparable terms of the ontology.

### **Description**

This function computes pseudo-distances of the average of extreme chain lengths proposed by Josly *et al.* 

### Usage

pdHax(sum.paths)

### **Arguments**

sum.paths

list of vectors with the lengths of the chains of each pair of terms

#### **Details**

Pseudo-distance concept is an strategy of the edge-based approach for measuring the distances between terms in an ontology. It was proposed by Joslyn *et al*.

pdHax computes the pseudo-distances proposed of the average of extreme chain lengths. That is, let  $t_i$  and  $t_j$  be two comparable terms, then the average of extreme chain length is defined as

$$\delta_{ax}(t_i, t_j) = \frac{h_*(t_i, t_j) + h^*(t_i, t_j)}{2}$$

In case of non-comparable terms, the resulting value is NA.

#### Author(s)

Jose Luis Mosquera

#### References

Cliff A. Joslyn, Susan M. Mniszewski Andy W. Fulmer, and Gary G. Heaton. (2004). "The gene ontology categorizer". Bioinformatics, 20(s1):169-77, 2004.

### See Also

pdHm, pdHx, pdHap, pseudoDists

30 pdHm

### **Examples**

```
data(joslyn)
length chains <- summaryPaths;</pre>
```

pdHm

Pseudo-distance of the minimum chain lengths between comparable terms of the ontology.

##

### Description

This function computes pseudo-distances of the minimum chain lengths proposed by Josly et al.

### Usage

pdHm(sum.paths)

### **Arguments**

sum.paths

list of vectors with the lengths of the chains of each pair of terms

### **Details**

Pseudo-distance concept is an strategy of the edge-based approach for measuring the distances between terms in an ontology. It was proposed by Joslyn *et al*.

pdHm computes the pseudo-distances proposed of the minimum chain lengths. That is, let  $t_i$  and  $t_j$  be two comparable terms, then the minimum chain lengths is defined as

$$\delta_m(t_i, t_j) = h_*(t_i, t_j) = \min_{C \in \mathcal{C}(t_i, t_j)} |C|$$

In case of non-comparable terms, the resulting value is NA.

### Author(s)

Jose Luis Mosquera

pdHx 31

### References

Cliff A. Joslyn, Susan M. Mniszewski Andy W. Fulmer, and Gary G. Heaton. (2004). "The gene ontology categorizer". Bioinformatics, 20(s1):169-77, 2004.

#### See Also

```
pdHx, pdHax, pdHap, pseudoDists
```

### **Examples**

pdHx

Pseudo-distance of the maximum chain lengths between comparable terms of the ontology.

##

# Description

This function computes pseudo-distances of the maximum chain lengths proposed by Josly et al.

# Usage

```
pdHx(sum.paths)
```

### **Arguments**

sum.paths

list of vectors with the lengths of the chains of each pair of terms

pdHx

### **Details**

Pseudo-distance concept is an strategy of the edge-based approach for measuring the distances between terms in an ontology. It was proposed by Joslyn *et al*.

pdHx computes the pseudo-distances proposed of the maximum chain lengths. That is, let  $t_i$  and  $t_j$  be two comparable terms, then the maximum chain lengths is defined as

$$\delta_x(t_i, t_j) = h^*(t_i, t_j) = \max_{C \in \mathcal{C}(t_i, t_j)} C|C|$$

In case of non-comparable terms, the resulting value is NA.

### Author(s)

Jose Luis Mosquera

#### References

Cliff A. Joslyn, Susan M. Mniszewski Andy W. Fulmer, and Gary G. Heaton. (2004). "The gene ontology categorizer". Bioinformatics, 20(s1):169-77, 2004.

#### See Also

```
pdHm, pdHax, pdHap, pseudoDists
```

## **Examples**

```
data(joslyn)
```

##

plotGODAG 33

plotGODAG	Plots a subgraph from the GO associated with one or two lists of En-
	trez Gene Identifiers

# **Description**

This function plots a subgraph from the ontology selected from the GO (see *Details*) associated with one or two lists of Entrez Gene IDs

### Usage

```
plotGODAG(eg1, eg2 = NULL, pckg = "org.Hs.eg.db", ontology = "MF", verbose = FALSE)
```

### **Arguments**

eg1	character vector with the (first list of) Entrez Gene IDs
eg2	character vector with the second list of Entrez Gene IDs. By default is NULL
pckg	character with the name of the R organism package. By default is $\operatorname{org.Hs.eg.db}$
ontology	character the ontology from the GO is selected (see <i>Details</i> . By default is BP
verbose	logical. By default FALSE

### **Details**

There are three possibilities, of course, in argument ontology

- BPBiological Processes
- CCCellular Components
- MFMolecular Functions

The subgraph shows two types of shapes for each node. Circles are nodes not mapped directly and rectangles are nodes mapped directly.

The color of nodes indicate the type of relation with the Entrez Gene IDs. That is, when argument eg2 is NULL, there are two possibilities: nodes mapped directly are shown in red color and their ancestors are shown in yellow color. But, if argument eg2 is not NULL, then there are six different colors. Nodes mapped directly from the first list of Entrez Gene IDs are shown in red color and their ancestors are shown in yellow color. Nodes mapped directly from the second list of Entrez Gene IDs are shown in lightblue color and their ancestors are shown in blue color. Nodes mapped directly from both lists of Entrez Gene IDs are shown in magenta color and their ancestors are shown in violet color.

### Author(s)

Jose Luis Mosquera

#### See Also

gosimsAvsB, summarySimsAvsB, gosimsProfiles

34 plotHistSims

### **Examples**

```
data(prostateIds)  # Data set from the package goProfiles

pckg = "org.Hs.eg.db"  # Organism package of humans

eg.we <- welsh01EntrezIDs[1:10]  # Entrez Gene IDs signature Welsh 01

eg.sg <- singh01EntrezIDs[1:10]  # Entrez Gene IDs signature Singh 01

plotGODAG(eg1 = eg.we, eg2 = NULL, pckg = pckg, ontology = "MF")

plotGODAG(eg1 = eg.sg, eg2 = NULL, pckg = pckg, ontology = "MF")

plotGODAG(eg1 = eg.we, eg2 = eg.sg, pckg = pckg, ontology = "MF")</pre>
```

plotHistSims

Histogram of two semantic similarity profiles

### **Description**

This function plots an histogram of two semantic similarity profiles in the same plot

#### Usage

```
plotHistSims(x, freq = TRUE, main = "Histogram of Semantic Similarities", xlab = "Semantic Similarity")
```

### Arguments

Х	$\label{eq:matrix} \mbox{matrix with measures of semantic similarity measures provided by the function} \\ \mbox{gosimsAvsB}$
freq	logical value. If TRUE, histogram graphic is a representation of frequencies, the "counts" component of the result. If FALSE, probability densities, component "density", are plotted (so that the histogram has a total area of one). By default is TRUE
main	character to title the graphic
xlab	character to label x-axis

#### **Details**

The plot shows two "curves" in the same figure overlapped. Area colored in red is associated with the first column of the matrix provided in argument x, and area colored in blue is associated with the second column of the matrix. Intersected area is colored in *violet*.

### Value

Resulting object is of class histogram

### Author(s)

Jose Luis Mosquera

pseudoDists 35

### See Also

```
gosimsAvsB, summarySimsAvsB, gosimsProfiles
```

### **Examples**

pseudoDists

Wrapper function that calls different methods for computing pseudodistances

### **Description**

It is a wrapper function that calls different methods for computing pseudo-distances

### Usage

```
pseudoDists(x, root = NULL, method = "hm")
```

#### Arguments

X

00C object

root method character with the name of the root term of the ontology in the OOC object character indicating the method for computing the pseudo-distance. The op-

tions implemented in sims package are

- hmpseudo-distance of the minimum chain length
- hxpseudo-distance of the maximum chain length
- haxpseudo-distance of the average of extreme chain lengths
- happseudo-distance of the average of all chain lengths
- allall pseudo-distances

By default computes the pseudo-distance of the minimum chain length, i.e. hm

36 refinementMatrix

### **Details**

In case of non-comparable terms, the resulting value is NA

### Value

The resulting object is a data.frame where for each pair of different terms (rows) are shown the pseudo-distances proposed by Joslyn *et al.* (columns).

### Author(s)

Jose Luis Mosquera

#### References

Cliff A. Joslyn, Susan M. Mniszewski Andy W. Fulmer, and Gary G. Heaton. (2004). "The gene ontology categorizer". Bioinformatics, 20(s1):169-77, 2004.

#### See Also

```
toOOC, pdHm, pdHx, pdHax, pdHap
```

# Examples

refinementMatrix Builds the refinement matrix associated with the DAG structure of Gene Ontology

### **Description**

Based on the data. frame of the maps the Entrez Gene IDs on to the GO IDs, this function builds the refinement matrix (i.e. in terms of the graph theory the accessibility matrix) associated with the GO DAG structure

### Usage

```
refinementMatrix(df, ontology = "BP")
```

refinementMatrix 37

# Arguments

df	data.frame with mapping from the Entrez Gene IDs to the GO ID terms
ontology	character indicating which ontologies is selected (see Details). By default is
	BP (i.e. Biological Processes

## **Details**

Given the data. frame with mapping from the Entrez Gene IDs to the GO IDs, refinementMatrix looks for all the ancestors and builds the matrix with the refinements associated with the directed subgraph extracted from the GO DAG.

ontology argument requires to indicate which of the ontologies in GO is selected for building the refinement matrix. Obviously, there are three possibilities

- BPBiological Processes
- CCCellular Components
- BPMolecular Functions

#### Value

The resulting object is a binary matrix whose rows and columns are all the GO IDs that make up the subgraph of the GO DAG. Each element of this matrix is either 1 when there exists a refinement from the GO ID on the row to the GO ID on the column, or 0 otherwise.

## Author(s)

Jose Luis Mosquera

# See Also

```
mapEG2GO, mappingMatrix
```

```
data(prostateIds)  # Data set from the package goProfiles

pckg <- "org.Hs.eg.db"  # Names of the organism package

eg <- welsh01EntrezIDs[1:10]  # Entrez Gene IDs

eg2go <- mapEG2GO(eg, pckg)
eg2go.mf <- eg2go$MF

G <- refinementMatrix(df = eg2go.mf, ontology = "MF")
print(G)</pre>
```

38 resnikSummary

resnikSummary	Summary table providing with the number of times that each term or any of its refinements appears in the OOC, the probability of finding the term, and the Information Content of the term
	· · · · · · · · · · · · · · · · · · ·

## **Description**

Builds a data. frame providing the number of times that each term or any of its refinements appears in the OOC (i.e.  $n(t_{i})$ ), the probability of finding the term (i.e.  $p(t_{i})$ ), and the Information Content of the term (i.e.  $IC(t_{i})$ )

## Usage

```
resnikSummary(x, root = NULL)
```

## **Arguments**

X	an object of class OOC
X	all object of class ooc

root a character with the name of the root term in the ontology. If NULL, it takes the

first element of vocabulary, that is, the first element of the slot T from the object

00C x)

#### Value

The resulting object is a data.frame where on rows are all the terms of the ontology, and on columns are the following measures

nt the number of times that each term or any of its refinements appears in the OOC

pt the probability of finding the term ic the Information Content of the term

## Author(s)

Jose Luis Mosquera

## References

Resnik, P. "Using information content to evaluate semantic similarity in a taxonomy". Proceeding of the 14th International Joint Conference on Artificial Intelligence. pp. 448-453, 1995.

# See Also

Nt, toOOC

simFaith 39

## **Examples**

```
data(joslyn)
sum.resnik <- resnikSummary(joslyn.00C)
print(sum.resnik)</pre>
```

simFaith

Semantic similarity of Pirro and Euzenat for each pair of terms

## **Description**

Computes the semantic similarity proposed by Pirro and Euzenat for each pair of terms

## Usage

```
simFaith(sum.mica)
```

## **Arguments**

sum.mica

data. frame generated with function summaryMICA

## **Details**

Pirro and Euzenat introduced a semantic similarity based on the Most Informative Common Ancestor (MICA). It is a node-based approach, such that

$$sim_{Faith}(t_i, t_j) = \frac{IC(MICA)}{/}IC(t_i + IC(t_j - IC(MICA)))$$

## Author(s)

Jose Luis Mosquera

# References

Pirro, G. and Euzenat, J. "A Feature and Information Theoretic Framework for Semantic Similarity and Relatedness". In Proceedings of the 9th International Semantic Web Conference ISWC. Springer, pp.615-630, 2010.

# See Also

ancestors, resnikSummary, simJC, simLin, simNunivers, simPsec, simRel, simRes, sims.nb, summaryMICA

40 simJC

## **Examples**

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
resnik.sum <- resnikSummary(x = joslyn.00C)
ic <- resnik.sum[, "ic"]
sum.mica <- summaryMICA(at, ic)

sim.Faith <- simFaith(sum.mica)
print(sim.Faith)</pre>
```

simJC

Semantic similarity of Jiang and Conrath for each pair of terms

## **Description**

Computes the semantic similarity proposed by Jiang and Conrath for each pair of terms

## Usage

```
simJC(sum.mica)
```

## **Arguments**

sum.mica

data. frame generated with function summaryMICA

## **Details**

Jiang and Conrath introduced a semantic similarity based on the Most Informative Common Ancestor (MICA). It is a node-based approach, such that

$$sim_{JC}(t_i, t_j) = \frac{1}{1 + dist_{JC}(t_i, t_j)} = \frac{1}{1 + (IC(t_i) + IC(t_j) - (2MICA))}$$

## Author(s)

Jose Luis Mosquera

#### References

Jiang, J.J. and Conrath, D.W. "Semantic similarity based on corpus statistics and lexical taxonomy". In Proceedings of International Conference Research on Computational Linguistics (ROCLING X), pp.19-33, 1997.

simLin 41

## See Also

ancestors, resnik Summary, sim Faith, sim Lin, sim Nunivers, sim Psec, sim Rel, sim Res, sim s. nb, summary MICA

## **Examples**

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
resnik.sum <- resnikSummary(x = joslyn.00C)
ic <- resnik.sum[, "ic"]
sum.mica <- summaryMICA(at, ic)
sim.JC <- simJC(sum.mica)
print(sim.JC)</pre>
```

simLin

Semantic similarity of Lin for each pair of terms

# **Description**

Computes the semantic similarity proposed by Lin for each pair of terms

## Usage

```
simLin(sum.mica)
```

## **Arguments**

sum.mica

data. frame generated with function summaryMICA

# **Details**

Lin introduced a semantic similarity based on the Most Informative Common Ancestor (MICA). It is a node-based approach, such that

$$sim_{Lin}(t_i, t_j) = 2IC(MICA)/(IC(t_i) + IC(t_j))$$

## Author(s)

Jose Luis Mosquera

## References

Lin, D. "An information-theoretic definition of similarity". In Proceedings of the Fifteenth International Conference on Machine Learning, Morgan Kaufmann Publishers, pp. 296<e2><80><93>304, 1998.

42 simNunivers

## See Also

ancestors, resnikSummary, simJC, simFaith, simNunivers, simPsec, simRel, simRes, sims.nb, summaryMICA

## **Examples**

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
resnik.sum <- resnikSummary(x = joslyn.00C)
ic <- resnik.sum[, "ic"]
sum.mica <- summaryMICA(at, ic)
sim.Lin <- simLin(sum.mica)
print(sim.Lin)</pre>
```

simNunivers

Semantic similarity of Mazandu and Mulder for each pair of terms

## **Description**

Computes the semantic similarity proposed by Mazandu and Mulder for each pair of terms

## Usage

```
simNunivers(sum.mica)
```

# Arguments

sum.mica

data.frame generated with function summaryMICA

## **Details**

Mazandu and Mulder introduced a semantic similarity based on the Most Informative Common Ancestor (MICA). It is a node-based approach, such that

$$sim_{Nunivers}(t_i,t_j) = \frac{IC(MICA)}{\max\{IC(t_i),IC(t_j\}}$$

## Author(s)

Jose Luis Mosquera

#### References

Mazandu, G.K. and Mulder, N.J. "Information content-based Gene Ontology semantic similarity approaches: Toward a unified framework theory". BioMed Research International, 2013.

simPsec 43

## See Also

ancestors, resnikSummary, simJC, simLin, simFaith, simPsec, simRel, simRes, sims.nb, summaryMICA

## **Examples**

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
resnik.sum <- resnikSummary(x = joslyn.00C)
ic <- resnik.sum[, "ic"]
sum.mica <- summaryMICA(at, ic)
sim.Nunivers <- simNunivers(sum.mica)
print(sim.Nunivers)</pre>
```

simPsec

Semantic similarity of Pirro and Seco for each pair of terms

# Description

Computes the semantic similarity proposed by Pirro and Seco for each pair of terms

## Usage

```
simPsec(sum.mica)
```

# **Arguments**

sum.mica

data. frame generated with function summaryMICA

## **Details**

Pirro and Seco introduced a semantic similarity based on the Most Informative Common Ancestor (MICA). It is a node-based approach, such that

$$sim_{Psec}(t_i, t_j) = (3IC(MICA)) - IC(t_i - IC(t_j))$$

# Author(s)

Jose Luis Mosquera

44 simRada

## References

Pirro, G. and Seco, N. "Design, Implementation and Evaluation of a New Semantic Similarity Metric Combining Features and Intrinsic Information Content". Meersman, R. and Tari, Z. eds. Lecture Notes in Computer Science, 5332:1271-1288, 2008.

Pirro, G. "A semantic similarity metric combining features and intrinsic information content". Data and Knowledge Engineering, 68(11):1289-1308, 2009.

## See Also

ancestors, resnik Summary, sim JC, sim Lin, sim Nunivers, sim Faith, sim Rel, sim Res, sim s. nb, summary MICA

## **Examples**

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
resnik.sum <- resnikSummary(x = joslyn.00C)
ic <- resnik.sum[, "ic"]
sum.mica <- summaryMICA(at, ic)
sim.Psec <- simPsec(sum.mica)
print(sim.Psec)</pre>
```

simRada

Semantic similarity measure of Rada et al. for each pair of terms

# Description

Computes the semantic similarity, based on the shortest path, proposed by Rada *et al.* between each pair of terms

## Usage

```
simRada(sum.paths, at)
```

# Arguments

sum.paths list of numeric vectors with the lengths (in terms of depth) of the number of

paths between each pair of terms.

at list of ancestors of each term

simRel 45

## **Details**

The measure involved in this function is an edge-based approach. It was proposed by Rada et al.. The measure is a transformation from the distance of Rada et al. (see function distRada) to semantic similarity through the formula  $sim = \frac{1}{1+dist}$ . That is, the semantic similarity proposed by Rada et al. is defined as

$$sim_{Rada}(t_i, t_j) = \frac{1}{1 + d_{Rada}(t_i, t_j)}$$

## Value

The resulting object is a matrix where for each pair of different terms (rows) is shown the numeric value of the semantic similarity computed (column).

## Author(s)

Jose Luis Mosquera

#### References

Rada, R. et al. Development and application of a metric on semantic nets. Ieee Transactions On Systems Man And Cybernetics, 19(1), pp.17-30, 1989.

#### See Also

```
ancestors, simRes.eb, distRada, LCAs, summaryPaths
```

## **Examples**

```
data(joslyn)
sum.paths <- summaryPaths(x = joslyn.00C, root = "R", len = TRUE)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
sim.Rada <- simRada(sum.paths, at)
print(sim.Rada)</pre>
```

simRel

Semantic similarity of Schlicker et al. for each pair of terms

## **Description**

Computes the semantic similarity proposed by Schlicker et al. for each pair of terms

46 simRel

## Usage

```
simRel(sum.mica, ic)
```

#### **Arguments**

sum.mica data.frame generated with function summaryMICA ic numeric vector with the IC of each term in the ontology

#### **Details**

Schlicker  $et\ al.$  noted that by taking into account specificities of compared terms can lead to high similarities when comparing general terms. For instance, when comparing general terms the semantic similarity of Lin (see function 'simLin'), the maximal similarity will be obtained comparing a (general) term to itself. Actually, the identity of the indiscernible is generally ensured, with the exception of the root which has an IC=0. However, some treatments require this property not to be respected. Therefore, Schlicker  $et\ al.$  introduced a semantic similarity based on a modification of the semantic similarity of Lin, such that

$$sim_{Rel}(t_i, t_i) = sim_{Lin}(t_i, t_i)(1 - P(MICA))$$

#### Value

The resulting object is a matrix where for each pair of different terms (rows) is shown the numeric value of the semantic similarity computed (column)

## Author(s)

Jose Luis Mosquera

## References

Schlicker, A. *et al.* "A new measure for functional similarity of gene products based on Gene Ontology". BMC Bioinformatics, 7(1):302, 2006.

#### See Also

ancestors, resnik Summary, simJC, simLin, simNunivers, simPsec, simFaith, simRes, sims.nb, summary MICA

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
resnik.sum <- resnikSummary(x = joslyn.00C)
ic <- resnik.sum[, "ic"]
sum.mica <- summaryMICA(at, ic)</pre>
```

simRes 47

```
sim.Rel <- simRel(sum.mica, ic)
print(sim.Rel)</pre>
```

simRes

Semantic similarity of Resnik for each pair of terms

# Description

Computes the semantic similarity proposed by Resnik for each pair of terms

#### Usage

```
simRes(at, ic, subs = FALSE)
```

## Arguments

at list whose elements are the ancestors of each term

ic numeric vector with the IC of each term in the ontology

subs logical value. If TRUE, then the resulting data.frame will show an etra column with the name of the subsumer term associated with MICA value

#### **Details**

Given two terms of an ontology the Most Informative Common Ancestor (MICA) is the common ancestor with the highest Information Content (IC). This measure is a semantic similarity, from the node-based approaches, introduced by Resnik and defined as

$$sim_{Res}(t_i, t_j) = IC(MICA) = \max_{t \in S(t_i, t_j)} (IC(t)$$

where  $S(t_i, t_j)$  is the set of terms that subsumes both terms  $t_i$  and  $t_j$ , and IC(t) is the information content measure of t.

MICA does not take into account the disjoint common ancestors, that is, those common ancestors that do not subsume any other common ancestor.

#### Value

The resulting object is a matrix where for each pair of different terms (rows) is shown the numeric value of the semantic similarity computed (column)

## Author(s)

Jose Luis Mosquera

#### References

Resnik P. "Using information content to evaluate semantic similarity in a taxonomy". Proceedings of the 14th International Joint Conference on Artificial Intelligence. 448-453, 1995

48 simRes.eb

## See Also

ancestors, commonAncestors, resnikSummary, simJC, simLin, simNunivers, simPsec, simRel, simFaith, sims.nb, summaryMICA

## **Examples**

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
ca <- commonAncestors(at)
resnik.sum <- resnikSummary(x = joslyn.00C)
sim.Res <- simRes(at, ic = resnik.sum[, "ic"])
print(sim.Res)</pre>
```

simRes.eb

Semantic similarity measure of Resnik et al. for each pair of terms, considering the maximal depth of the ontology

## **Description**

Computes the semantic similarity measure of Resnik between each pair of node, considering the maximal depth of the ontology.

# Usage

```
simRes.eb(sum.paths, at, x)
```

## **Arguments**

sum.paths list of numeric vectors with the lengths (in terms of depth) of the number of

paths between each pair of terms.

at list of ancestors of each term

x 00C object

#### **Details**

This function computes a measure proposed by Resnik in order to normalize the measure of semantic evidences from the graph of the ontology and computed with the shortest path containing the LCAs of the terms involved int (see function distRada). It is an edge-based approach, and given two terms  $t_i$  and  $t_j$ , it is defined as

sims 49

#### Value

The resulting object is a matrix where for each pair of different terms (rows) is shown the numeric value of the semantic similarity computed (column).

#### Author(s)

Jose Luis Mosquera

#### References

Resnik P. "Using information content to evaluate semantic similarity in a taxonomy". Proceedings of the 14th International Joint Conference on Artificial Intelligence. 448-453, 1995

Rada, R. et al. Development and application of a metric on semantic nets. Ieee Transactions On Systems Man And Cybernetics, 19(1), pp.17-30, 1989.

#### See Also

```
distRada, simRada
```

## **Examples**

```
data(joslyn)
sum.paths <- summaryPaths(x = joslyn.00C, root = "R", len = TRUE)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
sim.Res.eb <- simRes.eb(sum.paths, at, x = joslyn.00C)
print(sim.Res.eb)</pre>
```

sims

Computation of semantic similarity measures between terms of an ontology

#### **Description**

sims package is devoted to compute semantic similarity measures between terms of an ontology, and some functions are particularly addressed to manage the Gene Ontology terms.

## **Details**

This package is designed to compute semantic similarities between terms of any ontology. Fourteen measures from different approaches are implemented. Specifically, from node-based approach there are implemented seven semantic similarity measures proposed by Resnik, Lin, Schlicker et al., Jiang and Conrath, Mazandu and Mulder, Pirro and Seco, and Pirro and Euzenat. With regard to edge-based approaches there are implemented: two semantic similarity measures proposed by Resnik,

50 sims.eb

and Rada et al, one distance measure proposed by Rada and four pseudo-distances proposed by Joslyn et al. The package can manage any ontology, but it is particularly focused on the Gene Ontology. In this regard, there are some functions that allow building the refinements matrix (i.e. the accessibility matrix in terms of graph theory), the mapping matrix (i.e the matrix that maps from Entrez Gene IDs to GO IDs) and plot the DAG structure in order to compare two different list of GO terms. sims package can manage Entrez Gene IDs and GO IDs from any organism R package.

Package: sims
Type: Package
Version: 1.0

Date: 31-08-2014 License: GPL-2

Depends: AnnotationDbi, expm, goProfiles, GOstats, igraph, methods, plotrix, Rgraphviz, vegan

Imports: Matrix, plyr, knitr Suggests: org.Hs.eg.db

The most important functions are sims.nb, sims.eb, pseudoDists, gosims and gosimsAvsB

#### Author(s)

Jose Luis Mosquera and Alex Sanchez

Maintainer: Jose Luis Mosquera <jlmosquera@gmail.com>

#### See Also

```
sims.nb, sims.eb, pseudoDists, gosims, gosimsAvsB
```

similarities based on edge-based approaches

Wrapper function that calls different methods for computing semantic

## **Description**

sims.eb

It is wrapper function that calls different methods for computing semantic similarities based on edge-based approaches

#### Usage

```
sims.eb(x, root = NULL, at, method = "Rada")
```

#### **Arguments**

x 00C object

root charcter with the name of the root term of the ontology. By default, it takes

the first element of vocabulary (i.e. the first element of the slot T from the OOC

object passed in the argument x

sims.eb 51

at list of character vectors with the ancestors of each term

method character indicating the method for computing the semantic similarity. The

options implemented in sims package are

Rada semantic similarty of Rada

Res.eb semantic similarty of Resnik based on the shortest path (see function distRada)

all all semantic similarities of edge-based approaches implemented in the package

By default computes the semantic similarity of Rada, that is, Rada

#### **Details**

This function computes either all the semantic similarities implemented in the package or the one indicated.

## Value

The resulting object is an data.frame where for each pair of different terms (rows) are shown the numeric values of the semantic similarities computed (columns)

## Author(s)

Jose Luis Mosquera

## See Also

```
ancestors, simRada, simRes.eb, sims.nb, pseudoDists
```

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)

sims.eb(x = joslyn.00C, root = "R", at, method = "Rada")
sims.eb(x = joslyn.00C, root = "R", at, method = "Res.eb")
sims.eb(x = joslyn.00C, root = "R", at, method = "all")</pre>
```

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sims.nb	Wrapper function that calls different methods for computing semantic similarities based on node-based approaches
	**

## **Description**

It is a wrapper function that calls different methods for computing semantic similarities based on node-based approaches

# Usage

```
sims.nb(at, ic, method = "Res")
```

# **Arguments**

at list of character vectors with the ancestors of each term ic numeric vector with the IC of each term in the ontology

method character indicating the method for computing the semantic similarity. The op-

tions implemented in sims package are

Res semantic similarty of Resnik Lin semantic similarty of Lin

Rel semantic similarty of Schlicker *et al.*JC semantic similarty of Jiang and Conrath

Nunivers semantic similarty of Mazandu and Mulder

Psec semantic similarty of Pirro and Seco Faith semantic similarty of Pirro and Euzenat

all all sementic similarities

By default computes the semantic similarity of Resnik, that is, Res

## **Details**

This function computes either all the semantic similarities implemented in the packages or the one indicated.

# Value

The resulting object is an data. frame where for each pair of different terms (rows) are shown the numeric values of the semantic similarities computed (columns)

# Author(s)

Jose Luis Mosquera

simsBetweenGOIDs 53

#### See Also

ancestors, simRes, simLin, simRel, simJC, simNunivers, simPsec, simFaith, summaryMICA, sims.eb, pseudoDists,resnikSummary

## **Examples**

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)</pre>
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)</pre>
resnik.sum <- resnikSummary(x = joslyn.00C)</pre>
ic <- resnik.sum[, "ic"]</pre>
sims.nb(at, ic, method = "Res")
                                     # Renik
sims.nb(at, ic, method = "Lin")
                                    # Lin
sims.nb(at, ic, method = "Rel")
                                    # Schlicker et al.
sims.nb(at, ic, method = "JC")
                                   # Jiang and Conrath
sims.nb(at, ic, method = "Nuviers") # Mazandu and Mulder
sims.nb(at, ic, method = "Psec") # Pirro & Seco
sims.nb(at, ic, method = "Faith") # Pirro & Euzenat
                                     # All semantic similarities
sims.nb(at, ic, method = "all")
```

simsBetweenGOIDs

Wrapper function that calls different approaches and methods for computing semantic similarities between GO ID ancestors of a list of GO ID's

## **Description**

Given a list of GO ID's, a GO ontology domain, a type of approach for computing semantic similarities and a specific method, the function calculates the semantic similarities between all the pairs of GO ID ancestors of the induced graph.

# Usage

```
simsBetweenGOIDs(goids, ontology = "BP", type = "nb", method = "Res")
```

# Arguments

goids	character vector with the GO IDs.
ontology	character with the ontology domain (see Details). By default is BP
type	character indicating the approach for computing semantic similarities. By default nb
method	character indicating the method used for computing semantic similarities. By

default Res

54 simsBetweenGOIDs

#### **Details**

There are three possibilities, of course, in argument ontology

**BP** Biological Processes

**CC** Cellular Components

MF Molecular Functions

There are three possibilities in argument type

nb node-based approach

eb edge-based approach

eb.pd edge-based approach based on psedudo-distances

According to the approach selected in argument type, there are different methods for computing semantic similarities.

• Node-based approach (i.e. type = nb)

Res semantic similarty of Resnik

Lin semantic similarty of Lin

Rel semantic similarty of Schlicker et al.

JC semantic similarty of Jiang and Conrath

Nunivers semantic similarty of Mazandu and Mulder

Psec semantic similarty of Pirro and Seco

Faith semantic similarty of Pirro and Euzenat

all all sementic similarities

• Edge-based approach (i.e. type = eb)

Rada semantic similarty of Rada

Res.eb semantic similarty of Resnik based on the shortest path (see function distRada

all all semantic similarities of edge-based approaches implemented in the package

• Edge-based approach pseudo-distance (i.e. type = eb.pd)

hm pseudo-distance of the minimum chain length

hx pseudo-distance of the maximum chain length

hax pseudo-distance of the average of extreme chain lengths

hap pseudo-distance of the average of all chain lengths

all all pseudo-distances

#### Author(s)

Jose Luis Mosquera

# See Also

```
gosims, gosimsAvsB
```

```
goids <- c("GO:0004022","GO:0005515")
a <- simsBetweenGOIDs(goids, ontology = "MF", type = "nb", method = "Res")</pre>
```

simsMat 55

simsMat

Coerces a 1-column data.frame resulting from semantic similarity functions to be an object of class dist.

## **Description**

Given a data.frame with one column resulting from one of the functions for computing semantic similarities, builds a matrix of class dist

# Usage

```
simsMat(x)
```

#### **Arguments**

Х

data.frame with one column resulting from one of the functions for computing semantic similarities

## Value

The resulting object is of class dist

## Author(s)

Jose Luis Mosquera

# See Also

```
toMat, sims.nb, sims.eb, pseudoDists, gosims
```

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
resnik.sum <- resnikSummary(x = joslyn.00C)
ic <- resnik.sum[, "ic"]
sims.Res <- sims.nb(at, ic, method = "Res")
simsMat(sims.Res)</pre>
```

56 summaryMICA

summaryMICA	Computes for each pair of terms the Information Content (IC) of each
	term the Most Informative Common Ancestor (MICA), and the sub- sumer associated with the MICA

# Description

Builds a data.frame that for each pair of terms gives the Information Content (IC) of each term the Most Informative Common Ancestor (MICA), and the subsumer associated with the MICA

# Usage

```
summaryMICA(at, ic)
```

# Arguments

at list whose elements are the ancestors of each term

ic numeric vector with the IC of each term in the ontology

# Author(s)

Jose Luis Mosquera

#### See Also

ancestors, commonAncestors, inverseIminusG, getA, resnikSummary

```
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.00C)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
ca <- commonAncestors(at)
resnik.sum <- resnikSummary(x = joslyn.00C)
ic <- resnik.sum[, "ic"]
sum.mica <- summaryMICA(at, ic)
print(sum.mica)</pre>
```

summaryPaths 57

summaryPaths	Lengths of the chains (in terms of depth) or number of paths between each pair of terms.

## **Description**

Builds a list of numeric vectors with either the lengths of the chains (in terms of depth) or the number of paths between each pair of terms.

## Usage

```
summaryPaths(x, root = NULL, len = TRUE)
```

## **Arguments**

x 00C object

root character indicating the name of the root term of the ontology in the OOC

object

len logical value. If TRUE, computes the length (depth) of the chain. If FALSE,

computes the number of chains. By default is TRUE

## Author(s)

Jose Luis Mosquera

#### See Also

00C

## **Examples**

data(joslyn)

summary Sims

Summary of semantic similarity estimates between each pair of terms and measure

## **Description**

For estimates of each measure (columns) provided on matrix, this function builds a data.frame with the number of pairs, the number of NA's, the minimum value and the number of minimum values, the maximum value and the number of minimum values, the mean, the standard deviation and the median

58 summarySims

## Usage

```
summarySims(x)
```

## **Arguments**

Х

matrix with the semantic similarity estimates

#### **Details**

If any value of the semantic similarities is Inf, then it is converted to an NA value, and it is removed from the computation of the statistics

## Value

The resulting object is a data. frame that for each measure (rows) shows the estimates of statistics provided (columns)

#### Author(s)

Jose Luis Mosquera

#### See Also

ancestors, inverse Iminus G, get A, resnik Summary, sims, eb, pseudo Dists, gosims, gosims Avs B, summary Sims Avs B

```
## An arbitrary OOC
data(joslyn)
inv.IminusG <- inverseIminusG(joslyn.OOC)
A.mat <- getA(inv.IminusG)
at <- ancestors(A.mat)
resnik.sum <- resnikSummary(x = joslyn.OOC)
ic <- resnik.sum[, "ic"]
sims.all <- sims.nb(at, ic, method = "all")
summarySims(sims.all)
## An OOC associated with the GO
data(prostateIds)  # Data set from the package goProfiles
eg.we <- welsh01EntrezIDs[1:10]  # Entrez Gene IS signature Welsh 01
all.nb <- gosims(eg = eg.we, ontology = "MF", pckg = "org.Hs.eg.db", type = "nb", method = "all")
summarySims(as.matrix(all.nb))</pre>
```

59 summarySimsAvsB

ates
u

## **Description**

This function provides a summary of estimates calculated with the same semantic similarity measure for two lists of objects (i.e. genes). The summary consists of a list with three elements: first, a data. frame with basic statistics for each column, second, the Pearson's Correlation and the correlation test associated with, and three, the Cosine Similarity Measure

## Usage

```
summarySimsAvsB(x)
```

# **Arguments** х

a matrix with two columns where for each pair of terms (rows) contains the estimates of the semantic similarity measure for each list of objects (columns)

#### **Details**

If any value of the semantic similarities is Inf, then it is converted to an NA value, and it is removed from the computation of the statistics.

This function can be used with an arbitrary OOC object, but is particularly thought for using Entrex Gene Identifiers (objects) and GO Identifiers (terms).

## Author(s)

Jose Luis Mosquera

#### See Also

summarySims, sims, sims.eb, pseudoDists, gosims, gosimsAvsB, summarySims, cosSim

```
data(prostateIds)
                                 # Data set from the package goProfiles
eg.we <- welsh01EntrezIDs[1:10] # Entrez Gene IS signature Welsh 01
eg.sg <- singh01EntrezIDs[1:10]  # Entrez Gene IS signature Singh 01
WEvsSG.nb <- gosimsAvsB(eg1 = eg.we, eg2 = eg.sg, ontology = "MF", pckg = "org.Hs.eg.db", type = "nb", method = "Res
summarySimsAvsB(WEvsSG.nb)
```

60 toMat

termPairs

Builds the pairs of different terms or characters

## **Description**

Builds a character vector whose elements are the pairs of different terms or characters

# Usage

```
termPairs(x)
```

## **Arguments**

Х

it can be an object of class OOC or character vector with the names of each term

## **Details**

Given a character vector, builds all the pairs of different elements in the vector

## Author(s)

Jose Luis Mosquera

## See Also

00C

## **Examples**

```
termPairs(letters[1:5])
data(joslyn)
termPairs(joslyn.00C)
```

toMat

Builds a matrix of zero and one elements such that zero indicates there is no a relation between row and column, and one there is a relation.

# **Description**

Given two character vectors and a 2-columns data.frame, that relates an element of the first character vector with an element of the second character vector, builds a matrix whose rownames are the elements of the first character vector, colnames are the elements of the second character vector, and elements are 0 and 1. The values indicate that there is no a relation between a row and a column, when the value is zero, and there is a relation between a row and a column, when the value is one

toOOC 61

## Usage

```
toMat(df, rnames, cnames)
```

## **Arguments**

df data.frame with mapping from the Entrez Gene IDs to the GO ID terms

rnames character indicating which ontologies is selected (see *Details*) cnames character indicating which ontologies is selected (see *Details*)

#### Value

The resulting object is a matrix

#### Author(s)

Jose Luis Mosquera

## See Also

toPairs, mappingMatrix, refinementMatrix

# **Examples**

to00C

Builds an Object-Ontology Complex (OOC)

## **Description**

Builds a object of class OOC that is used as a container of an Object-Ontology Object (OOC)

## Usage

```
to00C(T, G, 0, M)
```

62 toOOC

# **Arguments**

Т	character vector with the names of the terms in the ontology
G	matrix encoding the refinement matrix associated with the DAG of the ontology. Elements of this matrix are 1, when a term on the rows refines a term on the columns, and $0$ otherwise
0	character vector with the object identifiers (i.e. features, genes,) mapping the terms of the ontology ${\bf r}$
М	matrix encoding the mapping from the set of object identifiers (listed in the argument 0 to the terms listed in the argument $T$

# Value

The resulting object is an OOC

## Author(s)

Jose Luis Mosquera

## See Also

00C

```
## Terms in the ontology
terms <- c("R", "B", "C", "K", "F", "G", "I", "E", "J", "H", "A", "D")
## Object identifiers
object.ids <- letters[1:10]</pre>
## Matrix of refinements
1,0,0,0,0,0,0,0,0,0,0,0,0,
             1,0,0,0,0,0,0,0,0,0,0,0,0,
             1,0,0,0,0,0,0,0,0,0,0,0,0,
             0,1,0,0,0,0,0,0,0,0,0,0,0,
             0,1,0,0,0,0,0,0,0,0,0,0,0,
             0,1,1,0,0,0,0,0,0,0,0,0,0,
             0,0,1,1,0,0,1,0,0,0,0,0,
             0,0,1,1,0,0,0,0,0,0,0,0,0,
             0,0,0,0,0,0,1,0,0,0,0,0,
             0,0,0,0,1,1,0,0,0,1,0,0,
             0,0,0,0,0,0,0,1,1,0,0,0),
            nrow = 12, ncol = 12, byrow = TRUE)
colnames(G) <-rownames(G) <- terms</pre>
## Mapping matrix
```

toPairs 63

toPairs

Builds a 2-columns data.frame relating elements of a matrix with value one.

## **Description**

Given a matrix of zero's and one's, builds a 2-columns data. frame where on the first columns are the names of the rows and on the second column the names of columns for those elements of the matrix with value one.

## Usage

```
toPairs(mat)
```

## **Arguments**

mat

matrix with 0's and 1's

# Value

The resulting object is a 2-columns data. frame

## Author(s)

Jose Luis Mosquera

## See Also

```
toMat, mappingMatrix, refinementMatrix
```

toPairs

```
a <- sample(0:1, 20, replace = TRUE)
A <- matrix(a, nrow = 5)
colnames(A) <- LETTERS[1:4]
rownames(A) <- letters[1:5]

toPairs(A)</pre>
```

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