# Package 'dcGOR'

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Type Package

Title Analysis of Ontologies and Protein Domain Annotations

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**Depends** R (>= 3.1.0), Matrix, igraph, dnet

Imports methods

Suggests foreach, doMC, ape

Description The package is used to analyse domain-centric ontologies and annotations, particularly those in the dcGO database. The dcGO (http://supfam.org/SUPERFAMILY/dcGO) is a comprehensive domain-centric database for annotating protein domains using a panel of ontologies including Gene Ontology. With the package, users are expected to analyse and visualise domain-centric ontologies and annotations. Supported analyses include but are not limited to: easy access to a wide range of ontologies and their domain-centric annotations; able to build customised ontologies and annotations; domain-based enrichment analysis and visualisation; construction of a domain (semantic similarity) network according to ontology annotations; significance analysis for estimating a contact (statistical significance) network via Random Walk with Restart; and high-performance parallel computing. The under-development functionalities are: 1) to create domain-centric ontologies; 2) to predict ontology terms for input protein sequences (precisely domain content in the form of architectures) plus to assess the predictions; 3) to reconstruct ancestral discrete characters using maximum likelihood/parsimony.

URL http://supfam.org/dcGOR, http://dcgor.r-forge.r-project.org, http:
//cran.r-project.org/package=dcGOR, https://github.com/hfang-bristol/dcGOR

Collate 'ClassMethod-dcGOR.r' 'dcDAGannotate.r' 'dcRDataLoader.r' 'dcEnrichment.r' 'visEnrichment.r' 'dcDAGdomainSim.r' 'dcRWRpipeline.r' 'dcConverter.r' 'dcBuildInfoDataFrame.r' 'dcBuildAnno.r' 'dcBuildOnto.r' 'dcAlgoPropagate.r' 'dcAlgoPredict.r' 'dcAlgoPredictMain.r' 'dcAlgoPredictGenome.r' 'dcAncestralML.r' 'dcAncestralMP.r' 'dcSubtreeClade.r' 'dcSubtreeTips.r' 'dcTreeConnectivity.r' 'dcDuplicated.r' 'dcSplitArch.r' 'dcAlgo.r' 'dcFunArgs.r' 'dcSparseMatrix.r' 'dcList2Matrix.r' 'dcAlgoPredictPR.r' 'dcSupraBetter.r'

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AdjData-class

Definition for VIRTUAL S4 class AdjData

# **Description**

AdjData is union of other classes: either matrix or dgCMatrix (a sparse matrix in the package Matrix). It is used as a virtual class

#### Value

Class AdjData

#### See Also

Onto-class

Ancestral\_domainome

Ancestral superfamily domain repertoires in Eukaryotes

# **Description**

An object of class "Anno" that contains information about domain repertoires (a complete set of domains: domain-ome) in Eukaryotes (including extant and ancestral genomes). This data is prepared based on 1) SUPERFAMILY database which provides domain and architecture assignments to all completely sequenced genomes including eukaryotic genomes; 2) ancestral domain architecture repertoires inferred by applying Dollo parsimony to eukaryotic part of species tree of life (sTOL), from which ancestral superfamily domain and architecture repertoires at all branching points in eukaryotic evolution are inferred. This allows us to list ancestral domain and architecture repertoires that were present at these points. Based on the observed/inferred domain and architecture repertoires, we also define genome-specific plasticity potential for an individual domain as how many different architectures (or architecture diversity) it can be formed in an extant/ancestral genome. As a result, for each genome, domain repertoires (domainome) are represented as a profile of states on domains, where non-zero entry indicates a domain for which how many different architectures have occurred in the genome.

# Usage

data(Ancestral\_domainome)

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#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

• annoData: a sparse matrix of 2019 domains X 875 terms/genomes (including 438 extant genomes and 437 ancestral genomes), with each entry telling how many different architectures a domain has in a genome. Note: zero entry also means that this domain is absent in the genome

- termData: variables describing terms/genomes (i.e. columns in annoData), including extant/ancestral genome information: "left\_id" (unique and used as internal id), "right\_id" (used in combination with "left\_id" to define the post-ordered binary tree structure), "taxon\_id" (NCBI taxonomy id, if matched), "genome" (2-letter genome identifiers used in SUPER-FAMILY, if being extant), "name" (NCBI taxonomy name, if matched), "rank" (NCBI taxonomy rank, if matched), "branchlength" (branch length in relevance to the parent), and "common name" (NCBI taxonomy common name, if matched and existed)
- domainData: variables describing domains (i.e. rows in annoData), including information about domains: "sunid" for SCOP id, "level" for SCOP level, "classification" for SCOP classification, "description" for SCOP description

#### References

Fang et al. (2013) A daily-updated tree of (sequenced) life as a reference for genome research. *Scientific reports*, 3:2015.

Morais et al. (2011) SUPERFAMILY 1.75 including a domain-centric gene ontology method. *Nucleic Acids Res*, 39(Database issue):D427-34.

Andreeva et al. (2008) Data growth and its impact on the SCOP database: new developments. *Nucleic Acids Res*, 36(Database issue):D419-425

# **Examples**

```
data(Ancestral_domainome)
Ancestral_domainome
# retrieve info on terms/genomes
termData(Ancestral_domainome)
# retrieve info on SCOP domains
domainData(Ancestral_domainome)
# retrieve the first 5 rows and columns of data
x <- annoData(Ancestral_domainome)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

Anno-class

Definition for S4 class Anno

# **Description**

Anno has 3 slots: annoData, termData and domainData

# Value

Class Anno

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#### **Slots**

annoData An object of S4 class AnnoData, containing data matrix with the column number equal to nrow(termData) and the row number equal to nrow(domainData).

termData An object of S4 class InfoDataFrame, describing information on columns in annoData. domainData An object of S4 class InfoDataFrame, describing information on rows in annoData.

### Creation

An object of this class can be created via: new("Anno", annoData, termData, domainData)

#### Methods

Class-specific methods:

- dim(): retrieve the dimension in the object
- annoData(): retrieve the slot 'annoData' in the object
- termData(): retrieve the slot 'termData' (as class InfoDataFrame) in the object
- domainData(): retrieve the slot 'domainData' (as class InfoDataFrame) in the object
- tData(): retrieve termData (as data.frame) in the object
- dData(): retrieve domainData (as data.frame) in the object
- termNames(): retrieve term names (ie, row names of termData) in the object
- domanNames(): retrieve domain names (ie, row names of domainData) in the object

### Standard generic methods:

- str(): compact display of the content in the object
- show(): abbreviated display of the object
- as(matrix, "Anno"): convert a matrix to an object of class Anno
- as(dgCMatrix, "Anno"): convert a dgCMatrix (a sparse matrix) to an object of class Anno
- [i,j]: get the subset of the same class

### Access

Ways to access information on this class:

- showClass("Anno"): show the class definition
- showMethods(classes="Anno"): show the method definition upon this class
- getSlots("Anno"): get the name and class of each slot in this class
- slotNames("Anno"): get the name of each slot in this class
- selectMethod(f, signature="Anno"): retrieve the definition code for the method 'f' defined in this class

# See Also

Anno-method

Anno-method 7

#### **Examples**

```
# create an object of class Anno, only given a matrix
annoData <- matrix(runif(50),nrow=10,ncol=5)</pre>
as(annoData, "Anno")
# create an object of class Anno, given a matrix plus information on its columns/rows
# 1) create termData: an object of class InfoDataFrame
data <- data.frame(x=1:5, y=I(LETTERS[1:5]), row.names=paste("Term",</pre>
1:5, sep="_"))
termData <- new("InfoDataFrame", data=data)</pre>
termData
# 2) create domainData: an object of class InfoDataFrame
data <- data.frame(x=1:10, y=I(LETTERS[1:10]),</pre>
row.names=paste("Domain", 1:10, sep="_"))
domainData <- new("InfoDataFrame", data=data)</pre>
domainData
# 3) create an object of class Anno
# VERY IMPORTANT: make sure having consistent names between annoData and domainData (and termData)
annoData <- matrix(runif(50),nrow=10,ncol=5)</pre>
rownames(annoData) <- rowNames(domainData)</pre>
colnames(annoData) <- rowNames(termData)</pre>
x \leftarrow new("Anno", annoData=annoData, domainData=domainData,
termData=termData)
# 4) look at various methods defined on class Anno
dim(x)
annoData(x)
termData(x)
tData(x)
domainData(x)
dData(x)
termNames(x)
domainNames(x)
# 5) get the subset
x[1:3,1:2]
```

Anno-method

Methods defined for S4 class Anno

# Description

Methods defined for class Anno.

# Usage

```
## S4 method for signature Anno
dim(x)
## S4 method for signature Anno
annoData(x)
## S4 method for signature Anno
termData(x)
```

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```
## S4 method for signature Anno
domainData(x)

## S4 method for signature Anno
tData(object)

## S4 method for signature Anno
dData(object)

## S4 method for signature Anno
termNames(object)

## S4 method for signature Anno
domainNames(object)

## S4 method for signature Anno
show(object)

## S4 method for signature Anno
show(object)

## S4 method for signature Anno,ANY,ANY,ANY
x[i, j, ..., drop = FALSE]
```

# **Arguments**

Χ	an object of class Anno
object	an object of class Anno

i an index j an index

... additional parameters

drop a logic for matrices and arrays. If TRUE the result is coerced to the lowest possi-

ble dimension. This only works for extracting elements, not for the replacement

# See Also

Anno-class

AnnoData-class

Definition for VIRTUAL S4 class AnnoData

# **Description**

AnnoData is union of other classes: either matrix or dgCMatrix (a sparse matrix in the package Matrix). It is used as a virtual class

### Value

Class AnnoData

# See Also

Anno-class

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Cnetwork-class

Definition for S4 class Cnetwork

### **Description**

Cnetwork is an S4 class to store a contact network, such as the one from RWR-based contact between samples/terms by dcRWRpipeline. It has 2 slots: nodeInfo and adjMatrix

### Value

Class Cnetwork

#### **Slots**

nodeInfo An object of S4 class InfoDataFrame, describing information on nodes/domains.
adjMatrix An object of S4 class AdjData, containing symmetric adjacency data matrix for an indirect domain network

#### Creation

An object of this class can be created via: new("Cnetwork", nodeInfo, adjMatrix)

#### Methods

Class-specific methods:

- dim(): retrieve the dimension in the object
- adjMatrix(): retrieve the slot 'adjMatrix' in the object
- nodeInfo(): retrieve the slot 'nodeInfo' (as class InfoDataFrame) in the object
- nInfo(): retrieve nodeInfo (as data.frame) in the object
- nodeNames(): retrieve node/term names (ie, row names of nodeInfo) in the object

# Standard generic methods:

- str(): compact display of the content in the object
- show(): abbreviated display of the object
- as(matrix, "Cnetwork"): convert a matrix to an object of class Cnetwork
- as(dgCMatrix, "Cnetwork"): convert a dgCMatrix (a sparse matrix) to an object of class Cnetwork
- [i]: get the subset of the same class

# Access

Ways to access information on this class:

- showClass("Cnetwork"): show the class definition
- showMethods(classes="Cnetwork"): show the method definition upon this class
- getSlots("Cnetwork"): get the name and class of each slot in this class
- slotNames("Cnetwork"): get the name of each slot in this class
- selectMethod(f, signature="Cnetwork"): retrieve the definition code for the method 'f' defined in this class

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#### See Also

Cnetwork-method

### **Examples**

```
# create an object of class Cnetwork, only given a matrix
adjM <- matrix(runif(25),nrow=5,ncol=5)</pre>
as(adjM, "Cnetwork")
# create an object of class Cnetwork, given a matrix plus information on nodes
# 1) create nodeI: an object of class InfoDataFrame
data <- data.frame(id=paste("Domain", 1:5, sep="_"),</pre>
level=rep("SCOP",5), description=I(LETTERS[1:5]),
row.names=paste("Domain", 1:5, sep="_"))
nodeI <- new("InfoDataFrame", data=data)</pre>
nodeI
# 2) create an object of class Cnetwork
# VERY IMPORTANT: make sure having consistent names between nodeInfo and adjMatrix
adjM <- matrix(runif(25),nrow=5,ncol=5)</pre>
colnames(adjM) <- rownames(adjM) <- rowNames(nodeI)</pre>
x <- new("Cnetwork", adjMatrix=adjM, nodeInfo=nodeI)</pre>
# 3) look at various methods defined on class Cnetwork
dim(x)
adjMatrix(x)
nodeInfo(x)
nInfo(x)
nodeNames(x)
# 4) get the subset
x[1:2]
```

Cnetwork-method

Methods defined for S4 class Cnetwork

# **Description**

Methods defined for class Cnetwork.

# Usage

```
## $4 method for signature Cnetwork
dim(x)

## $4 method for signature Cnetwork
adjMatrix(x)

## $4 method for signature Cnetwork
nodeInfo(x)

## $4 method for signature Cnetwork
nInfo(object)

## $4 method for signature Cnetwork
```

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```
nodeNames(object)
## $4 method for signature Cnetwork
show(object)
## $4 method for signature Cnetwork, ANY, ANY, ANY
x[i, j, ..., drop = FALSE]
```

# **Arguments**

x an object of class Cnetwork
object an object of class Cnetwork
i an index
j an index
... additional parameters
drop a logic for matrices and arrays. If TRUE the result is coerced to the lowest poss

a logic for matrices and arrays. If TRUE the result is coerced to the lowest possible dimension. This only works for extracting elements, not for the replacement

### See Also

Cnetwork-class

Coutput-class Definition for S4 class Coutput

# **Description**

Coutput is an S4 class to store output by dcRWRpipeline.

### Value

Class Coutput

# Slots

```
ratio A symmetrix matrix, containing ratio
zscore A symmetrix matrix, containing z-scores
pvalue A symmetrix matrix, containing p-values
adjp A symmetrix matrix, containing adjusted p-values
cnetwork An object of S4 class Cnetwork, storing contact network.
```

# Creation

An object of this class can be created via: new("Coutput", ratio,zscore, pvalue, adjp, cnetwork)

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#### Methods

Class-specific methods:

- ratio(): retrieve the slot 'ratio' in the object
- zscore(): retrieve the slot 'zscore' in the object
- pvalue(): retrieve the slot 'pvalue' in the object
- adjp(): retrieve the slot 'adjp' in the object
- cnetwork(): retrieve the slot 'cnetwork' in the object
- write(): write the object into a local file

# Standard generic methods:

- str(): compact display of the content in the object
- show(): abbreviated display of the object

#### Access

Ways to access information on this class:

- showClass("Coutput"): show the class definition
- showMethods(classes="Coutput"): show the method definition upon this class
- getSlots("Coutput"): get the name and class of each slot in this class
- slotNames("Coutput"): get the name of each slot in this class
- selectMethod(f, signature="Coutput"): retrieve the definition code for the method 'f' defined in this class

# See Also

Coutput-method

# **Examples**

```
# 1) load onto.GOMF (as Onto object)
g <- dcRDataLoader(onto.GOMF)</pre>
# 2) load SCOP superfamilies annotated by GOMF (as Anno object)
Anno <- dcRDataLoader(SCOP.sf2GOMF)</pre>
# 3) prepare for ontology appended with annotation information
dag <- dcDAGannotate(g, annotations=Anno, path.mode="shortest_paths",</pre>
verbose=TRUE)
# 4) calculate pair-wise semantic similarity between 10 randomly chosen domains
alldomains <- unique(unlist(nInfo(dag)$annotations))</pre>
domains <- sample(alldomains,10)</pre>
dnetwork <- dcDAGdomainSim(g=dag, domains=domains,</pre>
method.domain="BM.average", method.term="Resnik", parallel=FALSE,
verbose=TRUE)
dnetwork
# 5) estimate RWR dating based sample/term relationships
# define sets of seeds as data
# each seed with equal weight (i.e. all non-zero entries are 1)
```

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```
data <- data.frame(aSeeds=c(1,0,1,0,1), bSeeds=c(0,0,1,0,1))
rownames(data) <- id(dnetwork)[1:5]
# calcualte their two contact graph
coutput <- dcRWRpipeline(data=data, g=dnetwork, parallel=FALSE)
coutput
# 6) write into the file Coutput.txt in your local directory
write(coutput, file=Coutput.txt, saveBy="adjp")
# 7) retrieve several slots directly
ratio(coutput)
zscore(coutput)
pvalue(coutput)
adjp(coutput)
cnetwork(coutput)</pre>
```

Coutput-method

Methods defined for S4 class Coutput

# **Description**

Methods defined for S4 class Coutput.

# Usage

```
## S4 method for signature Coutput
show(object)

## S4 method for signature Coutput
ratio(x)

## S4 method for signature Coutput
zscore(x)

## S4 method for signature Coutput
pvalue(x)

## S4 method for signature Coutput
adjp(x)

## S4 method for signature Coutput
cnetwork(x)

## S4 method for signature Coutput
write(x, file = "Coutput.txt", saveBy = c("adjp",
"pvalue", "zscore", "ratio"), verbose = T)
```

# **Arguments**

object an object of S4 class Coutput. Usually this is an output from dcRWRpipeline

x an object of S4 class Coutput. Usually this is part of the output from dcRWRpipeline

file a character specifying a file name written into. By default, it is 'Coutput.txt'

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saveBy which statistics will be saved. It can be "pvalue" for p value, "adjp" for adjusted

p value, "zscore" for z-score, "ratio" for ratio

verbose logical to indicate whether the messages will be displayed in the screen. By

default, it sets to true for display

#### Value

write(x) also returns a symmetrix matrix storing the specific statistics

#### See Also

Coutput-class

dcAlgo

Function to apply dcGO algorithm to infer domain-centric ontology

# **Description**

dcAlgo is supposed to apply dcGO algorithm to infer domain-centric ontology from input files. It requires two input files: 1) an annotation file containing annotations between proteins/genes and ontology terms; 2) an architecture file containing domain architectures for proteins/genes.

# Usage

```
dcAlgo(anno.file, architecture.file, output.file = NULL, ontology =
c(NA,
   "GOBP", "GOMF", "GOCC", "DO", "HPPA", "HPMI", "HPON", "MP", "EC", "KW",
   "UP"),
feature.mode = c("supra", "individual", "comb"), min.overlap = 3,
fdr.cutoff = 0.001, hscore.type = c("zscore", "fdr"), parallel = TRUE,
multicores = NULL, verbose = T, RData.ontology.customised = NULL,
RData.location = "http://dcgor.r-forge.r-project.org/data")
```

# Arguments

anno.file

an annotation file containing annotations between proteins/genes and ontology terms. For example, a file containing annotations between human genes and HP terms can be found in http://dcgor.r-forge.r-project.org/data/Algo/HP\_anno.txt. As seen in this example, the input file must contain the header (in the first row) and two columns: 1st column for 'SeqID' (actually these IDs can be anything), 2nd column for 'termID' (HP terms). Note: the file should use the tab delimiter as the field separator between columns

architecture.file

an architecture file containing domain architectures (including individual domains) for proteins/genes. For example, a file containing human genes and domain architectures can be found in <a href="http://dcgor.r-forge.r-project.org/data/Algo/SCOP\_architecture.txt">http://dcgor.r-forge.r-project.org/data/Algo/SCOP\_architecture.txt</a>. As seen in this example, the input file must contain the header (in the first row) and two columns: 1st column for 'SeqID' (actually these IDs can be anything), 2nd column for 'Architecture' (SCOP domain architectures, each represented as comma-separated domains). Note: the file should use the tab delimiter as the field separator between columns

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output.file

an output file containing results. If not NULL, a tab-delimited text file will be also written out, with 1st column 'Feature id' for features/domains, 2nd column 'Term\_id' for ontology terms, 3rd column 'Score' for hypergeometric scores (indicative of strength for feature-term associations). Otherwise, there is no output file (by default)

ontology

the ontology identity. It can be "GOBP" for Gene Ontology Biological Process, "GOMF" for Gene Ontology Molecular Function, "GOCC" for Gene Ontology Cellular Component, "DO" for Disease Ontology, "HPPA" for Human Phenotype Phenotypic Abnormality, "HPMI" for Human Phenotype Mode of Inheritance, "HPON" for Human Phenotype ONset and clinical course, "MP" for Mammalian Phenotype, "EC" for Enzyme Commission, "KW" for UniProtKB KeyWords, "UP" for UniProtKB UniPathway. For details on the eligibility for pairs of input domain and ontology, please refer to the online Documentations at http://supfam.org/dcGOR/docs.html. If NA, then the user has to input a customised RData-formatted file (see RData.ontology.customised below)

feature.mode

the mode of how to define the features thereof. It can be: "supra" for combinations of one or two successive domains (including individual domains; considering the order), "individual" for individual domains only, and "comb" for all possible combinations (including individual domains; ignoring the order)

min.overlap

the minimum number of overlaps with each term in consideration. By default, it sets to a minimum of 3

fdr.cutoff

the fdr cutoff to call the significant associations between features and terms. By default, it sets to 1e-3

hscore.type

the type of defining the hypergeometric score. It can be: "zscore" for z-score (by default), "fdr" for fdr (after being transformed via  $-1 * log_2(fdr)$ )

parallel

logical to indicate whether parallel computation with multicores is used. By default, it sets to true, but not necessarily does so. Partly because parallel backends available will be system-specific (now only Linux or Mac OS). Also, it will depend on whether these two packages "foreach" and "doMC" have been installed. It can be installed via: source("http://bioconductor.org/biocLite.R"); biocLite(c("foreach", "doMC")). If not yet installed, this option will be disabled

multicores

an integer to specify how many cores will be registered as the multicore parallel backend to the 'foreach' package. If NULL, it will use a half of cores available in a user's computer. This option only works when parallel computation is enabled

verbose

logical to indicate whether the messages will be displayed in the screen. By default, it sets to TRUE for display

RData.ontology.customised

a file name for RData-formatted file containing an object of S4 class 'Onto' (i.g. ontology). By default, it is NULL. It is only needed when the user wants to perform customised analysis using their own ontology. See dcBuildOnto for how to creat this object

RData.location the characters to tell the location of built-in RData files. By default, it remotely locates at "http://supfam.org/dcGOR/data" or "http://dcgor.r-forge.r-project.org/data". For the user equipped with fast internet connection, this option can be just left as default. But it is always advisable to download these files locally. Especially when the user needs to run this function many times, there is no need to ask the function to remotely download every time (also it will unnecessarily increase the runtime). For examples, these files (as a whole or part of them) can be first downloaded into your current working directory, and then set this option as:

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RData.location = ".". If RData to load is already part of package itself, this parameter can be ignored (since this function will try to load it via function data first)

### Value

a data frame containing three columns: 1st column 'Feature\_id' for features, 2nd 'Term\_id' for terms, and 3rd 'Score' for the hypergeometric score indicative of strength of associations beteen features and terms

### Note

When 'output.file' is specified, a tab-delimited text file is output, with the column names: 1st column 'Feature\_id' for features, 2nd 'Term\_id' for terms, and 3rd 'Score' for the hypergeometric score indicative of strength of associations beteen features and terms

#### See Also

dcRDataLoader, dcSplitArch, dcConverter, dcDuplicated, dcAlgoPropagate

### **Examples**

```
# 1) Prepare input file: anno.file and architecture.file
anno.file <- "http://dcgor.r-forge.r-project.org/data/Algo/HP_anno.txt"</pre>
architecture.file <-
"http://dcgor.r-forge.r-project.org/data/Algo/SCOP_architecture.txt"
# 2) Do inference using built-in data
res <- dcAlgo(anno.file, architecture.file, ontology="HPPA",
feature.mode="supra", parallel=FALSE)
res[1:5,]
# 3) Advanced usage: using customised data
base::load(base::url("http://dcgor.r-forge.r-project.org/data/onto.HPPA.RData"))
RData.ontology.customised <- onto.HPPA.RData
base::save(list=x, file=RData.ontology.customised)
#list.files(pattern=*.RData)
## you will see an RData file onto.HPPA.RData in local directory
res <- dcAlgo(anno.file, architecture.file, feature.mode="supra",</pre>
parallel=FALSE, RData.ontology.customised=RData.ontology.customised)
res[1:5,]
```

dcAlgoPredict

Function to predict ontology terms given domain architectures (including individual domains)

# Description

dcAlgoPredict is supposed to predict ontology terms given domain architectures (including individual domains). It involves 3 steps: 1) splitting an architecture into individual domains and all possible consecutive domain combinations (viewed as component features); 2) merging hscores among component features; 3) scaling merged hscores into predictive scores across terms.

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#### Usage

```
dcAlgoPredict(data, RData.HIS = c(NA, "Feature2GOBP.sf",
   "Feature2GOMF.sf",
   "Feature2GOCC.sf", "Feature2HPPA.sf", "Feature2GOBP.pfam",
   "Feature2GOMF.pfam", "Feature2GOCC.pfam", "Feature2HPPA.pfam",
   "Feature2GOBP.interpro", "Feature2GOMF.interpro",
   "Feature2GOCC.interpro",
   "Feature2HPPA.interpro"), merge.method = c("sum", "max", "sequential"),
   scale.method = c("log", "linear", "none"), feature.mode = c("supra",
   "individual", "comb"), slim.level = NULL, max.num = NULL,
   parallel = TRUE, multicores = NULL, verbose = T,
   RData.HIS.customised = NULL,
   RData.location = "http://dcgor.r-forge.r-project.org/data")
```

# Arguments

data

an input data vector containing domain architectures. An architecture is represented in the form of comma-separated domains

RData.HIS

RData to load. This RData conveys two bits of information: 1) feature (domain) type; 2) ontology. It stores the hypergeometric scores (hscore) between features (individual domains or consecutive domain combinations) and ontology terms. The RData name tells which domain type and which ontology to use. It can be: SCOP sf domains/combinations (including "Feature2GOBP.sf", "Feature2GOMF.sf", "Feature2GOCC.sf", "Feature2HPPA.sf"), Pfam domains/combinations (including "Feature2GOBP.pfam", "Feature2GOMF.pfam", "Feature2GOCC.pfam", "Feature2HPPA.pfam"), InterPro domains (including "Feature2GOBP.interpro", "Feature2GOMF.interpro", "Feature2HPPA.interpro"). If NA, then the user has to input a customised RData-formatted file (see RData.HIS.customised below)

merge.method

the method used to merge predictions for each component feature (individual domains and their combinations derived from domain architecture). It can be one of "sum" for summing up, "max" for the maximum, and "sequential" for the sequential weighting. The sequential weighting is done via:  $\sum_{i=1}^{R_i} \frac{R_i}{i}$ , where  $R_i$  is the  $i^{th}$  ranked highest hscore

scale.method

the method used to scale the predictive scores. It can be: "none" for no scaling, "linear" for being linearily scaled into the range between 0 and 1, "log" for the same as "linear" but being first log-transformed before being scaled. The scaling between 0 and 1 is done via:  $\frac{S-S_{min}}{S_{max}-S_{min}}$ , where  $S_{min}$  and  $S_{max}$  are the minimum and maximum values for S

feature.mode

the mode of how to define the features thereof. It can be: "supra" for combinations of one or two successive domains (including individual domains; considering the order), "individual" for individual domains only, and "comb" for all possible combinations (including individual domains; ignoring the order)

slim.level

whether only slim terms are returned. By defaut, it is NULL and all predicted terms will be reported. If it is specified as a vector containing any values from 1 to 4, then only slim terms at these levels will be reported. Here is the meaning of these values: '1' for very general terms, '2' for general terms, '3' for specific terms, and '4' for very specific terms

max.num

whether only top terms per sequence are returned. By defaut, it is NULL and no constraint is imposed. If an integer is specified, then all predicted terms (with

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> scores in a decreasing order) beyond this number will be discarded. Notably, this parameter works after the preceding parameter slim.level

parallel

logical to indicate whether parallel computation with multicores is used. By default, it sets to true, but not necessarily does so. Partly because parallel backends available will be system-specific (now only Linux or Mac OS). Also, it will depend on whether these two packages "foreach" and "doMC" have been installed. It can be installed via: source("http://bioconductor.org/biocLite.R"); biocLite(c("foreach", "doMC")). If not yet installed, this option will be disabled

multicores

an integer to specify how many cores will be registered as the multicore parallel backend to the 'foreach' package. If NULL, it will use a half of cores available in a user's computer. This option only works when parallel computation is enabled

verbose

logical to indicate whether the messages will be displayed in the screen. By

default, it sets to TRUE for display

RData.HIS.customised

a file name for RData-formatted file containing an object of S3 class 'HIS'. By default, it is NULL. It is only needed when the user wants to perform customised analysis. See dcAlgoPropagate on how this object is created

RData.location the characters to tell the location of built-in RData files. By default, it remotely locates at "http://supfam.org/dcGOR/data" or "http://dcgor.r-forge.r-project.org/data". For the user equipped with fast internet connection, this option can be just left as default. But it is always advisable to download these files locally. Especially when the user needs to run this function many times, there is no need to ask the function to remotely download every time (also it will unnecessarily increase the runtime). For examples, these files (as a whole or part of them) can be first downloaded into your current working directory, and then set this option as: RData.location = ".". If RData to load is already part of package itself, this parameter can be ignored (since this function will try to load it via function data first)

# Value

a named list of architectures, each containing predictive scores

#### Note

none

### See Also

dcRDataLoader, dcSplitArch, dcConverter, dcAlgoPropagate, dcAlgoPredictMain, dcAlgoPredictGenome

# **Examples**

```
# 1) randomly generate 5 domains and/or domain architectures
x <- dcRDataLoader(RData="Feature2GOMF.sf")</pre>
data <- sample(names(x$hscore), 5)</pre>
# 2) get predictive scores of all predicted terms for this domain architecture
## using sequential method (by default)
pscore <- dcAlgoPredict(data=data, RData.HIS="Feature2GOMF.sf",</pre>
parallel=FALSE)
## using max method
```

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```
pscore_max <- dcAlgoPredict(data=data, RData.HIS="Feature2GOMF.sf",</pre>
merge.method="max", parallel=FALSE)
## using sum method
pscore_sum <- dcAlgoPredict(data=data, RData.HIS="Feature2GOMF.sf",</pre>
merge.method="sum", parallel=FALSE)
# 3) advanced usage
## a) focus on those terms at the 2nd level (general)
pscore <- dcAlgoPredict(data=data, RData.HIS="Feature2GOMF.sf",</pre>
slim.level=2, parallel=FALSE)
## b) visualise predictive scores in the ontology hierarchy
### load the ontology
g <- dcRDataLoader("onto.GOMF", verbose=FALSE)</pre>
ig <- dcConverter(g, from=Onto, to=igraph, verbose=FALSE)</pre>
### do visualisation for the 1st architecture
data <- pscore[[1]]</pre>
subg <- dnet::dDAGinduce(ig, nodes_query=names(data),</pre>
path.mode="shortest_paths")
dnet::visDAG(g=subg, data=data, node.info="term_id")
```

dcAlgoPredictGenome

Function to predict ontology terms for genomes with domain architectures (including individual domains)

# **Description**

dcAlgoPredictGenome is supposed to predict ontology terms for genomes with domain architectures (including individual domains).

## Usage

```
dcAlgoPredictGenome(input.file, RData.HIS = c(NULL, "Feature2GOBP.sf",
   "Feature2GOMF.sf", "Feature2GOCC.sf", "Feature2HPPA.sf",
   "Feature2GOBP.pfam",
   "Feature2GOMF.pfam", "Feature2GOCC.pfam", "Feature2HPPA.pfam",
   "Feature2GOBP.interpro", "Feature2GOMF.interpro",
   "Feature2GOCC.interpro",
   "Feature2HPPA.interpro"), weight.method = c("none", "copynum", "ic",
   "both"), merge.method = c("sum", "max", "sequential"),
   scale.method = c("log", "linear", "none"), feature.mode = c("supra",
   "individual", "comb"), slim.level = NULL, max.num = NULL,
   parallel = TRUE, multicores = NULL, verbose = T,
   RData.HIS.customised = NULL,
   RData.location = "http://dcgor.r-forge.r-project.org/data")
```

# **Arguments**

input.file

an input file containing genomes and their domain architectures (including individual domains). For example, a file containing Hominidae genomes and their domain architectures can be found in <a href="http://dcgor.r-forge.r-project.org/data/Feature/Hominidae.txt">http://dcgor.r-forge.r-project.org/data/Feature/Hominidae.txt</a>. As seen in this example, the input file must contain the header (in the first row) and two columns: 1st column for 'Genome'

(a genome like a container), 2nd column for 'Architecture' (SCOP domain architectures, each represented as comma-separated domains). Alternatively, the input file can be a matrix or data frame, assuming that input file has been read. Note: the file should use the tab delimiter as the field separator between columns

RData.HIS

RData to load. This RData conveys two bits of information: 1) feature (domain) type; 2) ontology. It stores the hypergeometric scores (hscore) between features (individual domains or consecutive domain combinations) and ontology terms. The RData name tells which domain type and which ontology to use. It can be: SCOP sf domains/combinations (including "Feature2GOBP.sf", "Feature2GOMF.sf", "Feature2GOCC.sf", "Feature2HPPA.sf"), Pfam domains/combinations (including "Feature2GOBP.pfam", "Feature2GOMF.pfam", "Feature2GOCC.pfam", "Feature2HPPA.pfam"), InterPro domains (including "Feature2GOBP.interpro", "Feature2GOMF.interpro", "Feature2HPPA.interpro"). If NA, then the user has to input a customised RData-formatted file (see RData.HIS.customised below)

weight.method

the method used how to weight predictions. It can be one of "none" (no weighting; by default), "copynum" for weighting copynumber of architectures, and "ic" for weighting information content (ic) of the term, "both" for weighting both copynumber and ic

merge.method

the method used to merge predictions for each component feature (individual domains and their combinations derived from domain architecture). It can be one of "sum" for summing up, "max" for the maximum, and "sequential" for the sequential merging. The sequential merging is done via:  $\sum_{i=1}^{R_i} \frac{R_i}{i}$ , where  $R_i$  is the  $i^{th}$  ranked highest hscore

scale.method

the method used to scale the predictive scores. It can be: "none" for no scaling, "linear" for being linearily scaled into the range between 0 and 1, "log" for the same as "linear" but being first log-transformed before being scaled. The scaling between 0 and 1 is done via:  $\frac{S-S_{min}}{S_{max}-S_{min}}$ , where  $S_{min}$  and  $S_{max}$  are the minimum and maximum values for S

feature.mode

the mode of how to define the features thereof. It can be: "supra" for combinations of one or two successive domains (including individual domains; considering the order), "individual" for individual domains only, and "comb" for all possible combinations (including individual domains; ignoring the order)

slim.level

whether only slim terms are returned. By defaut, it is NULL and all predicted terms will be reported. If it is specified as a vector containing any values from 1 to 4, then only slim terms at these levels will be reported. Here is the meaning of these values: '1' for very general terms, '2' for general terms, '3' for specific terms, and '4' for very specific terms

max.num

whether only top terms per sequence are returned. By defaut, it is NULL and no constraint is imposed. If an integer is specified, then all predicted terms (with scores in a decreasing order) beyond this number will be discarded. Notably, this parameter works after the preceding parameter slim.level

parallel

logical to indicate whether parallel computation with multicores is used. By default, it sets to true, but not necessarily does so. Partly because parallel backends available will be system-specific (now only Linux or Mac OS). Also, it will depend on whether these two packages "foreach" and "doMC" have been installed. It can be installed via: source("http://bioconductor.org/biocLite.R"); biocLite(c("foreach", "doMC")). If not yet installed, this option will be disabled

multicores

an integer to specify how many cores will be registered as the multicore parallel backend to the 'foreach' package. If NULL, it will use a half of cores available in a user's computer. This option only works when parallel computation is enabled

verbose

logical to indicate whether the messages will be displayed in the screen. By default, it sets to TRUE for display

RData.HIS.customised

a file name for RData-formatted file containing an object of S3 class 'HIS'. By default, it is NULL. It is only needed when the user wants to perform customised analysis. See dcAlgoPropagate on how this object is created

RData.location the characters to tell the location of built-in RData files. By default, it remotely locates at "http://supfam.org/dcGOR/data" or "http://dcgor.r-forge.r-project.org/data". For the user equipped with fast internet connection, this option can be just left as default. But it is always advisable to download these files locally. Especially when the user needs to run this function many times, there is no need to ask the function to remotely download every time (also it will unnecessarily increase the runtime). For examples, these files (as a whole or part of them) can be first downloaded into your current working directory, and then set this option as: RData.location = ".". If RData to load is already part of package itself, this parameter can be ignored (since this function will try to load it via function data first)

### Value

a matrix of terms X genomes, containing the predicted scores (per genome) as a whole

# Note

none

#### See Also

dcRDataLoader, dcAlgoPropagate, dcAlgoPredict

#### **Examples**

```
# 1) Prepare an input file containing domain architectures
input file <-
"http://dcgor.r-forge.r-project.org/data/Feature/Hominidae.txt"
# 2) Do prediction using built-in data
output <- dcAlgoPredictGenome(input.file, RData.HIS="Feature2GOMF.sf",</pre>
parallel=FALSE)
dim(output)
output[1:10,]
# 3) Advanced usage: using customised data
base::load(base::url("http://dcgor.r-forge.r-project.org/data/Feature2GOMF.sf.RData"))
RData.HIS.customised <- Feature2GOMF.sf.RData
base::save(list=x, file=RData.HIS.customised)
#list.files(pattern=*.RData)
## you will see an RData file Feature2GOMF.sf.RData in local directory
output <- dcAlgoPredictGenome(input.file, parallel=FALSE,</pre>
RData.HIS.customised=RData.HIS.customised)
```

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```
dim(output)
output[1:10,]
```

dcAlgoPredictMain

Function to predict ontology terms given an input file containing domain architectures (including individual domains)

# **Description**

dcAlgoPredictMain is supposed to predict ontology terms given an input file containing domain architectures (including individual domains).

# Usage

```
dcAlgoPredictMain(input.file, output.file = NULL, RData.HIS = c(NA,
    "Feature2GOBP.sf",    "Feature2GOMF.sf",    "Feature2GOCC.sf",
    "Feature2HPPA.sf",
    "Feature2GOBP.pfam",    "Feature2GOMF.pfam",    "Feature2GOCC.pfam",
    "Feature2HPPA.pfam",    "Feature2GOBP.interpro",    "Feature2GOMF.interpro",
    "Feature2GOCC.interpro",    "Feature2HPPA.interpro"),    merge.method = c("sum",
    "max",    "sequential"),    scale.method = c("log",    "linear",    "none"),
    feature.mode = c("supra",    "individual",    "comb"),    slim.level = NULL,
    max.num = NULL,    parallel = TRUE,    multicores = NULL,    verbose = T,
    RData.HIS.customised = NULL,
    RData.location = "http://dcgor.r-forge.r-project.org/data")
```

# Arguments

input.file

an input file containing domain architectures (including individual domains). For example, a file containing UniProt ID and domain architectures for human proteins can be found in <a href="http://dcgor.r-forge.r-project.org/data/Feature/hs.txt">http://dcgor.r-forge.r-project.org/data/Feature/hs.txt</a>. As seen in this example, the input file must contain the header (in the first row) and two columns: 1st column for 'SeqID' (actually these IDs can be anything), 2nd column for 'Architecture' (SCOP domain architectures, each represented as comma-separated domains). Alternatively, the input.file can be a matrix or data frame, assuming that input file has been read. Note: the file should use the tab delimiter as the field separator between columns

output.file

an output file containing predicted results. If not NULL, a tab-delimited text file will be also written out; otherwise, there is no output file (by default)

RData.HIS

RData to load. This RData conveys two bits of information: 1) feature (domain) type; 2) ontology. It stores the hypergeometric scores (hscore) between features (individual domains or consecutive domain combinations) and ontology terms. The RData name tells which domain type and which ontology to use. It can be: SCOP sf domains/combinations (including "Feature2GOBP.sf", "Feature2GOMF.sf", "Feature2GOCC.sf", "Feature2HPPA.sf"), Pfam domains/combinations (including "Feature2GOBP.pfam", "Feature2GOMF.pfam", "Feature2GOCC.pfam", "Feature2HPPA.pfam"), InterPro domains (including "Feature2GOBP.interpro", "Feature2GOMF.interpro", "Feature2HPPA.interpro"). If NA, then the user has to input a customised RData-formatted file (see RData.HIS.customised below)

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merge.method

the method used to merge predictions for each component feature (individual domains and their combinations derived from domain architecture). It can be one of "sum" for summing up, "max" for the maximum, and "sequential" for the sequential merging. The sequential merging is done via:  $\sum_{i=1}^{\infty} \frac{R_i}{i}$ , where  $R_i$  is the  $i^{th}$  ranked highest hscore

scale.method

the method used to scale the predictive scores. It can be: "none" for no scaling, "linear" for being linearily scaled into the range between 0 and 1, "log" for the same as "linear" but being first log-transformed before being scaled. The scaling between 0 and 1 is done via:  $\frac{S-S_{min}}{S_{max}-S_{min}}$ , where  $S_{min}$  and  $S_{max}$  are the minimum and maximum values for S

feature.mode

the mode of how to define the features thereof. It can be: "supra" for combinations of one or two successive domains (including individual domains; considering the order), "individual" for individual domains only, and "comb" for all possible combinations (including individual domains; ignoring the order)

slim.level

whether only slim terms are returned. By defaut, it is NULL and all predicted terms will be reported. If it is specified as a vector containing any values from 1 to 4, then only slim terms at these levels will be reported. Here is the meaning of these values: '1' for very general terms, '2' for general terms, '3' for specific terms, and '4' for very specific terms

max.num

whether only top terms per sequence are returned. By defaut, it is NULL and no constraint is imposed. If an integer is specified, then all predicted terms (with scores in a decreasing order) beyond this number will be discarded. Notably, this parameter works after the preceding parameter slim.level

parallel

logical to indicate whether parallel computation with multicores is used. By default, it sets to true, but not necessarily does so. Partly because parallel backends available will be system-specific (now only Linux or Mac OS). Also, it will depend on whether these two packages "foreach" and "doMC" have been installed. It can be installed via: source("http://bioconductor.org/biocLite.R"); biocLite(c("foreach", "doMC")). If not yet installed, this option will be dis-

multicores

an integer to specify how many cores will be registered as the multicore parallel backend to the 'foreach' package. If NULL, it will use a half of cores available in a user's computer. This option only works when parallel computation is enabled

verbose

logical to indicate whether the messages will be displayed in the screen. By default, it sets to TRUE for display

RData.HIS.customised

a file name for RData-formatted file containing an object of S3 class 'HIS'. By default, it is NULL. It is only needed when the user wants to perform customised analysis. See dcAlgoPropagate on how this object is created

RData.location the characters to tell the location of built-in RData files. By default, it remotely locates at "http://supfam.org/dcGOR/data" or "http://dcgor.r-forge.r-project.org/data". For the user equipped with fast internet connection, this option can be just left as default. But it is always advisable to download these files locally. Especially when the user needs to run this function many times, there is no need to ask the function to remotely download every time (also it will unnecessarily increase the runtime). For examples, these files (as a whole or part of them) can be first downloaded into your current working directory, and then set this option as: RData.location = ".". If RData to load is already part of package itself, this parameter can be ignored (since this function will try to load it via function data first)

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#### Value

a data frame containing three columns: 1st column the same as the input file (e.g. 'SeqID'), 2nd for 'Term' (predicted ontology terms), 3rd for 'Score' (along with predicted scores)

#### Note

When 'output.file' is specified, a tab-delimited text file is written out, with the column names: 1st column the same as the input file (e.g. 'SeqID'), 2nd for 'Term' (predicted ontology terms), 3rd for 'Score' (along with predicted scores)

#### See Also

dcRDataLoader, dcAlgoPropagate, dcAlgoPredict

### **Examples**

```
# 1) Prepare an input file containing domain architectures
input.file <- "http://dcgor.r-forge.r-project.org/data/Feature/hs.txt"

# 2) Do prediction using built-in data
output <- dcAlgoPredictMain(input.file, RData.HIS="Feature2GOMF.sf",
parallel=FALSE)
output[1:5,]

# 3) Advanced usage: using customised data
x <-
base::load(base::url("http://dcgor.r-forge.r-project.org/data/Feature2GOMF.sf.RData"))
RData.HIS.customised <- Feature2GOMF.sf.RData
base::save(list=x, file=RData.HIS.customised)
#list.files(pattern=*.RData)
## you will see an RData file Feature2GOMF.sf.RData in local directory
output <- dcAlgoPredictMain(input.file, parallel=FALSE,
RData.HIS.customised=RData.HIS.customised)
output[1:5,]</pre>
```

dcAlgoPredictPR

Function to assess the prediction performance via Precision-Recall (PR) analysis

# Description

dcAlgoPredictPR is supposed to assess the prediction performance via Precision-Recall (PR) analysis. It requires two input files: 1) a Glod Standard Positive (GSP) file containing known annotations between proteins/genes and ontology terms; 2) a prediction file containing predicted terms for proteins/genes. Note: the known annotations will be recursively propagated towards the root of the ontology.

# Usage

```
dcAlgoPredictPR(GSP.file, prediction.file, ontology = c(NA, "GOBP",
"GOMF",
"GOCC", "DO", "HPPA", "HPMI", "HPON", "MP", "EC", "KW", "UP"),
num.threshold = 10, verbose = T, RData.ontology.customised = NULL,
RData.location = "http://dcgor.r-forge.r-project.org/data")
```

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### **Arguments**

GSP.file

a Glod Standard Positive (GSP) file containing known annotations between proteins/genes and ontology terms. For example, a file containing annotations between human genes and HP terms can be found in http://dcgor.r-forge. r-project.org/data/Algo/HP\_anno.txt. As seen in this example, the input file must contain the header (in the first row) and two columns: 1st column for 'SeqID' (actually these IDs can be anything), 2nd column for 'termID' (HP terms). Note: the file should use the tab delimiter as the field separator between columns

prediction.file

a prediction file containing proteins/genes, their predicted terms along with predictive scores. As seen in an example below, this file is usually created via dcAlgoPredictMain, containing three columns: 1st column for 'SeqID' (actually these IDs can be anything), 2nd column for 'Term' (ontology terms), 3rd column for 'Score' (predictive score). Note: the file should use the tab delimiter as the field separator between columns

ontology

the ontology identity. It can be "GOBP" for Gene Ontology Biological Process, "GOMF" for Gene Ontology Molecular Function, "GOCC" for Gene Ontology Cellular Component, "DO" for Disease Ontology, "HPPA" for Human Phenotype Phenotypic Abnormality, "HPMI" for Human Phenotype Mode of Inheritance, "HPON" for Human Phenotype ONset and clinical course, "MP" for Mammalian Phenotype, "EC" for Enzyme Commission, "KW" for UniProtKB KeyWords, "UP" for UniProtKB UniPathway. For details on the eligibility for pairs of input domain and ontology, please refer to the online Documentations at http://supfam.org/dcGOR/docs.html. If NA, then the user has to input a customised RData-formatted file (see RData.ontology.customised below)

num.threshold

an integer to specify how many PR points (as a function of the score threshold) will be calculated

verbose

logical to indicate whether the messages will be displayed in the screen. By default, it sets to TRUE for display

RData.ontology.customised

a file name for RData-formatted file containing an object of S4 class 'Onto' (i.g. ontology). By default, it is NULL. It is only needed when the user wants to perform customised analysis using their own ontology. See dcBuildOnto for how to creat this object

RData.location the characters to tell the location of built-in RData files. By default, it remotely locates at "http://supfam.org/dcGOR/data" or "http://dcgor.r-forge.r-project.org/data". For the user equipped with fast internet connection, this option can be just left as default. But it is always advisable to download these files locally. Especially when the user needs to run this function many times, there is no need to ask the function to remotely download every time (also it will unnecessarily increase the runtime). For examples, these files (as a whole or part of them) can be first downloaded into your current working directory, and then set this option as: RData.location = ".". If RData to load is already part of package itself, this parameter can be ignored (since this function will try to load it via function data first)

# Value

a data frame containing two columns: 1st column 'Precision' for precision, 2nd 'Recall' for recall. The row has the names corresponding to the score threshold.

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#### Note

Prediction coverage: the ratio between predicted targets in number and GSP targets in number F-measure: the maximum of a harmonic mean between precision and recall along PR curve

#### See Also

dcRDataLoader, dcConverter, dcDuplicated, dcAlgoPredictMain

# **Examples**

```
# 1) Generate prediction file with HPPA predicitions for human genes
architecture.file <-
"http://dcgor.r-forge.r-project.org/data/Algo/SCOP_architecture.txt"
prediction.file <- "SCOP_architecture.txt.HPPA_predicted"
res <- dcAlgoPredictMain(input.file=architecture.file,
output.file=prediction.file, RData.HIS="Feature2HPPA.sf",
parallel=FALSE)

# 2) Calculate Precision and Recall
GSP.file <- "http://dcgor.r-forge.r-project.org/data/Algo/HP_anno.txt"
res_PR <- dcAlgoPredictPR(GSP.file=GSP.file,
prediction.file=prediction.file, ontology="HPPA")
res_PR

# 3) Plot PR-curve
plot(res_PR[,2], res_PR[,1], type="b", xlab="Recall", ylab="Precision")</pre>
```

 ${\tt dcAlgoPropagate}$ 

Function to propagate ontology annotations according to an input file

### **Description**

dcAlgoPropagate is supposed to propagate ontology annotations, given an input file. This input file contains original annotations between domains/features and ontology terms, along with the hypergeometric scores (hscore) in support for their annotations. The annotations are propagated to the ontology root (retaining the maximum hscore). After the propogation, the ontology terms of increasing levels are determined based on the concept of Information Content (IC) to product a slim version of ontology. It returns an object of S3 class "HIS" with three components: "hscore", "ic" and "slim".

# Usage

```
dcAlgoPropagate(input.file, ontology = c("GOBP", "GOMF", "GOCC", "DO",
"HPPA",
"HPMI", "HPON", "MP", "EC", "KW", "UP"), output.file = "HIS.RData",
verbose = T, RData.location =
"http://dcgor.r-forge.r-project.org/data")
```

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### **Arguments**

input.file

an input file used to build the object. This input file contains original annotations between domains/features and ontology terms, along with the hypergeometric scores (hscore) in support for their annotations. For example, a file containing original annotations between SCOP domain architectures and GO terms can be found in <a href="http://dcgor.r-forge.r-project.org/data/Feature/Feature2GO.sf.txt">http://dcgor.r-forge.r-project.org/data/Feature/Feature2GO.sf.txt</a>. As seen in this example, the input file must contain the header (in the first row) and three columns: 1st column for 'Feature\_id' (here SCOP domain architectures), 2nd column for 'Term\_id' (GO terms), and 3rd column for 'Score' (hscore)

ontology

the ontology identity. It can be "GOBP" for Gene Ontology Biological Process, "GOMF" for Gene Ontology Molecular Function, "GOCC" for Gene Ontology Cellular Component, "DO" for Disease Ontology, "HPPA" for Human Phenotype Phenotypic Abnormality, "HPMI" for Human Phenotype Mode of Inheritance, "HPON" for Human Phenotype ONset and clinical course, "MP" for Mammalian Phenotype, "EC" for Enzyme Commission, "KW" for UniProtKB KeyWords, "UP" for UniProtKB UniPathway. For details on the eligibility for pairs of input domain and ontology, please refer to the online Documentations at http://supfam.org/dcGOR/docs.html

output.file

an output file used to save the HIS object as an RData-formatted file (see 'Value' for details). If NULL, this file will be saved into "HIS.RData" in the current working local directory

verbose

logical to indicate whether the messages will be displayed in the screen. By default, it sets to TRUE for display

RData.location

the characters to tell the location of built-in RData files. By default, it remotely locates at "http://supfam.org/dcGOR/data" or "http://dcgor.r-forge.r-project.org/data". For the user equipped with fast internet connection, this option can be just left as default. But it is always advisable to download these files locally. Especially when the user needs to run this function many times, there is no need to ask the function to remotely download every time (also it will unnecessarily increase the runtime). For examples, these files (as a whole or part of them) can be first downloaded into your current working directory, and then set this option as: RData.location = "." If RData to load is already part of package itself, this parameter can be ignored (since this function will try to load it via function data first)

# Value

an object of S3 class HIS, with following components:

- hscore: a list of features, each with a term-named vector containing hscore
- ic: a term-named vector containing information content (IC). Terms are ordered first by IC and then by longest-path level, making sure that for terms with the same IC, parental terms always come first
- slim: a list of four slims, each with a term-named vector containing information content (IC). Slim '1' for very general terms, '2' for general terms, '3' for specific terms, '4' for very specific terms

# Note

None

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#### See Also

dcRDataLoader, dcConverter, dcAlgo

# **Examples**

```
# build an "HIS" object for GO Molecular Function
Feature2GOMF.sf <-
dcAlgoPropagate(input.file="http://dcgor.r-forge.r-project.org/data/Feature/Feature2GO.sf.txt",
ontology="GOMF", output.file="Feature2GOMF.sf.RData")
names(Feature2GOMF.sf)
Feature2GOMF.sf$hscore[1]
Feature2GOMF.sf$ic[1:10]
Feature2GOMF.sf$slim[1]
# extract hscore as a matrix with 3 columns (Feature_id, Term_id, Score)
hscore <- Feature2GOMF.sf$hscore
output_list <- lapply(1:length(hscore), function(i){</pre>
x <- hscore[[i]]
y <- rep(names(hscore)[i],length(x))</pre>
cbind(Feature_id=y, Term_id=names(x), Score=as.numeric(x))
hscore_mat <- base::do.call(base::rbind, output_list)</pre>
dim(hscore_mat)
hscore_mat[1:10,]
```

dcAncestralML

Function to reconstruct ancestral discrete states using fast maximum likelihood algorithm

# Description

dcAncestralML is supposed to reconstruct ancestral discrete states using fast maximum likelihood algorithm. It takes inputs both the phylo-formatted tree and discrete states in the tips. The algorithm assumes that state changes can be described by a probablistic reversible model. It first determines transition matrix between states (also considering branch lengths), then uses dynamic programming (from tips to the root) to estimate conditional maximum likelihood, and finally reconstructs the ancestral states (from the root to tips). If the ties occur at the root, the state at the root is set to the last state in ties (for example, usually being 'present' for 'present'-'absent' two states).

#### **Usage**

```
dcAncestralML(data, phy, transition.model = c("different", "symmetric",
    "same", "customised"), customised.model = NULL, edge.length.power = 1,
    initial.estimate = 0.1, output.detail = F, parallel = T,
    multicores = NULL, verbose = T)
```

# **Arguments**

data

an input data matrix storing discrete states for tips (in rows) X characters (in columns). The rows in the matrix are for tips. If the row names do not exist, then addumedly they have the same order as in the tree tips. More wisely, users provide row names which can be matched to the tip labels of the tree. The row

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names can be more than found in the tree labels, and they should contain all those in the tree labels

phy

an object of class 'phylo'

transition.model

a character specifying the transition model. It can be: "different" for all-transition-different model (such as matrix(c(0,1,2,0),2)), "symmetric" for the symmetric model (such as matrix(c(0,1,1,0),2) or matrix(c(0,1,2,1,0,3,2,3,0),3)), "same" for all-transition-same model (such as matrix(c(0,1,1,0),2)), "customised" for the user-customised model (see the next parameter)

customised.model

a matrix customised for the transition model. It can be: matrix(c(0,1,1,0),2), matrix(c(0,1,2,0),2), or matrix(c(0,1,2,1,0,3,2,3,0),3)

edge.length.power

a non-negative value giving the exponent transformation of the branch lengths. It is useful when determining transition matrix between states

initial.estimate

the initial value used for the maximum likelihood estimation

output.detail

logical to indicate whether the output is returned as a detailed list. If TRUE, a nested list is returned: a list of characters (corresponding to columns of input data matrix), in which each element is a list consisting of three components ("states", "transition" and "relative"). If FALSE, a matrix is returned: the columns respond to the input data columns, and rows responding to all node index in the phylo-formatted tree

parallel

logical to indicate whether parallel computation with multicores is used. By default, it sets to true, but not necessarily does so. Partly because parallel backends available will be system-specific (now only Linux or Mac OS). Also, it will depend on whether these two packages "foreach" and "doMC" have been installed. It can be installed via: source("http://bioconductor.org/biocLite.R"); biocLite(c("foreach", "doMC")). If not yet installed, this option will be disabled

multicores

an integer to specify how many cores will be registered as the multicore parallel backend to the 'foreach' package. If NULL, it will use a half of cores available in a user's computer. This option only works when parallel computation is enabled

verbose

logical to indicate whether the messages will be displayed in the screen. By default, it sets to TRUE for display

# Value

It depends on the 'output.detail'. If FALSE (by default), a matrix is returned, with the columns responding to the input data columns, and rows responding to node index in the phylo-formatted tree. If TRUE, a nested list is returned. Outer-most list is for characters (corresponding to columns of input data matrix), in which each elemenl is a list (inner-most) consisting of three components ("states", "transition" and "relative"):

- states: a named vector storing states (extant and ancestral states)
- transition: an estimated transition matrix between states
- relative: a matrix of nodes X states, storing conditional maximum likelihood being relative to each state

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#### Note

This fast dynamic programming for ancestral discrete state reconstruction is partially inspired by a joint estimation procedure as described in http://mbe.oxfordjournals.org/content/17/6/890.full

#### See Also

dcAncestralMP, dcDuplicated

# **Examples**

```
# 1) a newick tree that is imported as a phylo-formatted tree
tree <- "(((t1:5,t2:5):2,(t3:4,t4:4):3):2,(t5:4,t6:4):6);"
phy <- ape::read.tree(text=tree)</pre>
# 2) an input data matrix storing discrete states for tips (in rows) X four characters (in columns)
data1 <- matrix(c(0, rep(1,3), rep(0,2)), ncol=1)
data2 \leftarrow matrix(c(rep(0,4),rep(1,2)), ncol=1)
data <- cbind(data1, data1, data1, data2)</pre>
colnames(data) <- c("C1", "C2", "C3", "C4")</pre>
## reconstruct ancestral states, without detailed output
res <- dcAncestralML(data, phy, parallel=FALSE)</pre>
res
# 3) an input data matrix storing discrete states for tips (in rows) X only one character
data <- matrix(c(0,rep(1,3),rep(0,2)), ncol=1)</pre>
## reconstruct ancestral states, with detailed output
res <- dcAncestralML(data, phy, parallel=FALSE, output.detail=TRUE)</pre>
res
## get the inner-most list
res <- res[[1]]
## visualise the tree with ancestral states and their conditional probability
Ntip <- ape::Ntip(phy)</pre>
Nnode <- ape::Nnode(phy)</pre>
color <- c("white", "gray")</pre>
## visualise main tree
ape::plot.phylo(phy, type="p", use.edge.length=TRUE, label.offset=1,
show.tip.label=TRUE, show.node.label=FALSE)
## visualise tips (state 1 in gray, state 0 in white)
x <- data[,1]</pre>
ape::tiplabels(pch=22, bg=color[as.numeric(x)+1], cex=2, adj=1)
## visualise internal nodes
### thermo bar to illustrate relative probability (state 1 in gray, state 0 in white)
ape::nodelabels(thermo=res$relative[Ntip+1:Nnode,2:1],
piecol=color[2:1], cex=0.75)
### labeling reconstructed ancestral states
ape::nodelabels(text=res$states[Ntip+1:Nnode], node=Ntip+1:Nnode,
frame="none", col="red", bg="transparent", cex=0.75)
```

dcAncestralMP

Function to reconstruct ancestral discrete states using maximum parsimony algorithm dcAncestralMP 31

#### **Description**

dcAncestralMP is supposed to reconstruct ancestral discrete states using a maximum parsimony-modified Fitch algorithm. In a from-tip-to-root manner, ancestral state for an internal node is determined if a state is shared in a majority by all its children. If two or more states in a majority are equally shared, this internal node is temporarily marked as an unknown tie, which is further resolved in a from-root-to-tip manner: always being the same state as its direct parent holds. If the ties also occur at the root, the state at the root is set to the last state in ties (for example, usually being 'present' for 'present'-'absent' two states).

### Usage

```
dcAncestralMP(data, phy, output.detail = F, parallel = T,
multicores = NULL, verbose = T)
```

# **Arguments**

data an input data matrix/frame storing discrete states for tips (in rows) X characters

(in columns). The rows in the matrix are for tips. If the row names do not exist, then addumedly they have the same order as in the tree tips. More wisely, users provide row names which can be matched to the tip labels of the tree. The row names can be more than found in the tree labels, and they should contain all

those in the tree labels

phy an object of class 'phylo'

output.detail logical to indicate whether the output is returned as a detailed list. If TRUE,

a nested list is returned: a list of characters (corresponding to columns of input data matrix), in which each element is a list consisting of three components ("states", "transition" and "relative"). If FALSE, a matrix is returned: the columns respond to the input data columns, and rows responding to all node

index in the phylo-formatted tree

parallel logical to indicate whether parallel computation with multicores is used. By de-

fault, it sets to true, but not necessarily does so. Partly because parallel backends available will be system-specific (now only Linux or Mac OS). Also, it will depend on whether these two packages "foreach" and "doMC" have been installed. It can be installed via: source("http://bioconductor.org/biocLite.R"); biocLite(c("foreach", "doMC")). If not yet installed, this option will be dis-

abled

multicores an integer to specify how many cores will be registered as the multicore parallel

backend to the 'foreach' package. If NULL, it will use a half of cores available in a user's computer. This option only works when parallel computation is enabled

verbose logical to indicate whether the messages will be displayed in the screen. By

default, it sets to TRUE for display

### Value

It depends on the 'output.detail'. If FALSE (by default), a matrix is returned, with the columns responding to the input data columns, and rows responding to node index in the phylo-formatted tree. If TRUE, a nested list is returned. Outer-most list is for characters (corresponding to columns of input data matrix), in which each element is a list (inner-most) consisting of three components ("states", "transition" and "relative"):

• states: a named vector storing states (extant and ancestral states)

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- transition: a posterior transition matrix between states
- relative: a matrix of nodes X states, storing relative probability

#### Note

This maximum parsimony algorithm for ancestral discrete state reconstruction is attributable to the basic idea as described in http://sysbio.oxfordjournals.org/content/20/4/406.short

# See Also

dcAncestralML, dcTreeConnectivity, dcDuplicated

# **Examples**

```
# 1) a newick tree that is imported as a phylo-formatted tree
tree <- "(((t1:5,t2:5):2,(t3:4,t4:4):3):2,(t5:4,t6:4):6);"
phy <- ape::read.tree(text=tree)</pre>
# 2) an input data matrix storing discrete states for tips (in rows) X four characters (in columns)
data1 <- matrix(c(0,rep(1,3),rep(0,2)), ncol=1)
data2 <- matrix(c(rep(0,4),rep(1,2)), ncol=1)</pre>
data <- cbind(data1, data1, data1, data2)</pre>
colnames(data) <- c("C1", "C2", "C3", "C4")</pre>
## reconstruct ancestral states, without detailed output
res <- dcAncestralMP(data, phy, parallel=FALSE)</pre>
res
# 3) an input data matrix storing discrete states for tips (in rows) X only one character
data <- matrix(c(0,rep(1,3),rep(0,2)), ncol=1)</pre>
## reconstruct ancestral states, with detailed output
res <- dcAncestralMP(data, phy, parallel=FALSE, output.detail=TRUE)</pre>
res
## get the inner-most list
res <- res[[1]]
## visualise the tree with ancestral states and their conditional probability
Ntip <- ape::Ntip(phy)</pre>
Nnode <- ape::Nnode(phy)</pre>
color <- c("white", "gray")</pre>
## visualise main tree
ape::plot.phylo(phy, type="p", use.edge.length=TRUE, label.offset=1,
show.tip.label=TRUE, show.node.label=FALSE)
## visualise tips (state 1 in gray, state 0 in white)
x <- data[,1]
ape::tiplabels(pch=22, bg=color[as.numeric(x)+1], cex=2, adj=1)
## visualise internal nodes
### thermo bar to illustrate relative probability (state 1 in gray, state 0 in white)
ape::nodelabels(thermo=res$relative[Ntip+1:Nnode,2:1],
piecol=color[2:1], cex=0.75)
### labeling reconstructed ancestral states
ape::nodelabels(text=res$states[Ntip+1:Nnode], node=Ntip+1:Nnode,
frame="none", col="red", bg="transparent", cex=0.75)
```

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dcBuildAnno

Function to build an object of the S4 class Anno from input files

# **Description**

dcBuildAnno is supposed to build an object of of the S4 class Anno, given input files. These input files include 1) a file containing domain information, 2) a file containing term information, and 3) a file containing associations between domains and terms.

#### Usage

```
dcBuildAnno(domain_info.file, term_info.file, association.file,
output.file = "Anno.RData")
```

# **Arguments**

domain\_info.file

an input file containing domain information. For example, a file containing InterPro domains (InterPro) can be found in http://dcgor.r-forge.r-project. org/data/InterPro/InterPro.txt. As seen in this example, the input file must contain the header (in the first row), and entries in the first column intend to be domain ID (and must be unique). Note: the file should use the tab delimiter as the field separator between columns

term\_info.file an input file containing term information. For example, a file containing Gene Ontology (GO) terms can be found in http://dcgor.r-forge.r-project. org/data/InterPro/GO. txt. As seen in this example, the input file must contain the header (in the first row) and four columns: 1st column for term ID (must be unique), 2nd column for term name, 3rd column for term namespace, and 4th column for term distance. These four columns must be provided, but the content for the last column can be arbitrary (if it is hard to prepare). Note: the file should use the tab delimiter as the field separator between columns

association.file

an input file containing associations between domains and terms. For example, a file containing associations between InterPro domains and GO Molecular Function (GOMF) terms can be found in http://dcgor.r-forge.r-project. org/data/InterPro/Domain2GOMF.txt. As seen in this example, the input file must contain the header (in the first row) and two columns: 1st column for domain ID (corresponding to the first column in 'domain\_info.file'), 2nd column for term ID (corresponding to the first column in 'term info.file'). If there are additional columns, these columns will be ignored. Note: the file should use the tab delimiter as the field separator between columns

output.file

an output file used to save the built object as an RData-formatted file. If NULL, this file will be saved into "Anno.RData" in the current working local directory

#### Value

Any use-specified variable that is given on the right side of the assignment sign '<-', which contains the built Anno object. Also, an RData file specified in "output.file" is saved in the local directory.

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#### Note

If there are no use-specified variable that is given on the right side of the assignment sign '<-', then no object will be loaded onto the working environment.

#### See Also

Anno

### **Examples**

```
# build an "Anno" object that contains SCOP domain superfamilies (sf) annotated by GOBP terms
InterPro2GOMF <-
dcBuildAnno(domain_info.file="http://dcgor.r-forge.r-project.org/data/InterPro/InterPro.txt",
term_info.file="http://dcgor.r-forge.r-project.org/data/InterPro/GO.txt",
association.file="http://dcgor.r-forge.r-project.org/data/InterPro/Domain2GOMF.txt",
output.file="InterPro2GOMF.RData")
InterPro2GOMF</pre>
```

 ${\tt dcBuildInfoDataFrame}$ 

Function to build an object of the S4 class InfoDataframe from an input file

### **Description**

dcBuildInfoDataFrame is supposed to build an object of of the S4 class InfoDataFrame, given an input file. This input file can, for example, contain the domain information.

# Usage

```
dcBuildInfoDataFrame(input.file, output.file = "InfoDataFrame.RData")
```

# **Arguments**

input.file an input file used to build the object. For example, a file containing InterPro

domains (InterPro) can be found in <a href="http://dcgor.r-forge.r-project.org/data/InterPro/InterPro.txt">http://dcgor.r-forge.r-project.org/data/InterPro/InterPro.txt</a>. As seen in this example, the input file must contain the header (in the first row), and entries in the first column intend to be domain identities (and must be unique). Note: the file should use the tab

delimiter as the field separator between columns

output.file an output file used to save the built object as an RData-formatted file. If NULL,

this file will be saved into "InfoDataFrame.RData" in the current working local

directory

# Value

Any use-specified variable that is given on the right side of the assignment sign '<-', which contains the built dcBuildInfoDataFrame object. Also, an RData file specified in "output.file" is saved in the local directory.

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#### Note

If there are no use-specified variable that is given on the right side of the assignment sign '<-', then no object will be loaded onto the working environment.

#### See Also

InfoDataFrame

#### **Examples**

```
# build an "InfoDataFrame" object that contains information on InterPro domains (InterPro)
InterPro <-
dcBuildInfoDataFrame(input.file="http://dcgor.r-forge.r-project.org/data/InterPro/InterPro.txt",
output.file="InterPro.RData")
InterPro</pre>
```

dcBuildOnto

Function to build an object of the S4 class Onto from input files

### **Description**

dcBuildOnto is supposed to build an object of of the S4 class Onto, given input files. These input files include 1) a file containing term relations, and 2) a file containing term/node information.

# Usage

```
dcBuildOnto(relations.file, nodes.file, output.file = "Onto.RData")
```

# **Arguments**

relations.file an input file containing term relations (i.e. edges from parent terms to child terms). For example, a file containing relations between GO Molecular Function (GOMF) terms can be found in <a href="http://dcgor.r-forge.r-project.org/data/onto/igraph\_GOMF\_edges.txt">http://dcgor.r-forge.r-project.org/data/onto/igraph\_GOMF\_edges.txt</a>. As seen in this example, the input file must contain the header (in the first row) and two columns: 1st column for parent term ID, and 2nd column for child term ID. Note: the file should use the tab delimiter as the field separator between columns

nodes.file

an input file containing term/node information. For example, a file containing GO Molecular Function (GOMF) terms can be found in <a href="http://dcgor.r-forge.r-project.org/data/onto/igraph\_GOMF\_nodes.txt">http://dcgor.r-forge.r-project.org/data/onto/igraph\_GOMF\_nodes.txt</a>. As seen in this example, the input file must contain the header (in the first row) and five columns: 1st column 'name' for node names (actually term ID; must be unique), 2nd column 'term\_id' for term ID, 3rd 'term\_name' for term name, 4th column 'term\_namespace' for term namespace, and 5th column 'term\_distance' for term distance. These five columns must be provided, the content in the first two columns are identical, and the content for the last column can be arbitrary (if it is hard to prepare). Note: the file should use the tab delimiter as the field separator between columns

output.file

an output file used to save the built object as an RData-formatted file. If NULL, this file will be saved into "Onto.RData" in the current working local directory

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#### Value

Any use-specified variable that is given on the right side of the assignment sign '<-', which contains the built Onto object. Also, an RData file specified in "output.file" is saved in the local directory.

### Note

If there are no use-specified variable that is given on the right side of the assignment sign '<-', then no object will be loaded onto the working environment.

### See Also

Onto

# Examples

```
# build an "Onto" object for GO Molecular Function
onto.GOMF <-
dcBuildOnto(relations.file="http://dcgor.r-forge.r-project.org/data/onto/igraph_GOMF_edges.txt",
nodes.file="http://dcgor.r-forge.r-project.org/data/onto/igraph_GOMF_nodes.txt",
output.file="onto.GOMF.RData")
onto.GOMF</pre>
```

dcConverter

Function to convert an object between graph classes

# Description

dcConverter is supposed to convert an object between classes 'Onto' and 'igraph', or between 'Dnetwork' and 'igraph', or between 'Cnetwork' and 'igraph'.

# Usage

```
dcConverter(obj, from = c("Onto", "igraph", "Dnetwork", "Cnetwork"),
to = c("igraph", "Onto", "Dnetwork", "Cnetwork"), verbose = TRUE)
```

# **Arguments**

obj	an object of class "Onto", "igraph", "Dnetwork" or "Cnetwork"
from	a character specifying the class converted from. It can be one of "Onto", "igraph", "Dnetwork" and "Dnetwork"
to	a character specifying the class converted to. It can be one of "Onto", "igraph", "Dnetwork" and "Dnetwork"
verbose	logical to indicate whether the messages will be displayed in the screen. By default, it sets to true for display

### Value

```
an object of class "Onto", "igraph", "Dnetwork" or "Cnetwork"
```

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#### Note

Conversion is also supported between classes 'Onto' and 'igraph', or between 'Dnetwork' and 'igraph', or between 'Cnetwork' and 'igraph'

### See Also

dcRDataLoader, Onto-class, Dnetwork-class, Cnetwork-class

#### **Examples**

```
# 1) conversion between Onto and igraph
# 1a) load onto.GOMF (as Onto object)
on <- dcRDataLoader(onto.GOMF)</pre>
# 1b) convert the object from Onto to igraph class
ig <- dcConverter(on, from=Onto, to=igraph)</pre>
# 1c) convert the object from igraph to Onto class
dcConverter(ig, from=igraph, to=Onto)
# 2) conversion between Dnetwork and igraph
# 2a) computer a domain semantic network (as Dnetwork object)
g <- dcRDataLoader(onto.GOMF)</pre>
Anno <- dcRDataLoader(SCOP.sf2GOMF)</pre>
dag <- dcDAGannotate(g, annotations=Anno, path.mode="shortest_paths",</pre>
verbose=FALSE)
alldomains <- unique(unlist(nInfo(dag)$annotations))</pre>
domains <- sample(alldomains,5) # randomly sample 5 domains</pre>
dnetwork <- dcDAGdomainSim(g=dag, domains=domains,</pre>
method.domain="BM.average", method.term="Resnik", parallel=FALSE,
verbose=FALSE)
dnetwork
# 2b) convert the object from Dnetwork to igraph class
ig <- dcConverter(dnetwork, from=Dnetwork, to=igraph)</pre>
ig
# 2c) convert the object from igraph to Dnetwork class
dcConverter(ig, from=igraph, to=Dnetwork)
```

dcDAGannotate

Function to generate a subgraph of a direct acyclic graph (DAG) induced by the input annotation data

## Description

dcDAGannotate is supposed to produce a subgraph induced by the input annotation data, given a direct acyclic graph (DAG; an ontology). The input is a graph of "igraph" or "Onto" object, a list of the vertices containing annotation data, and the mode defining the paths to the root of DAG. The induced subgraph contains vertices (with annotation data) and their ancestors along with the defined paths to the root of DAG. The annotations at these vertices (including their ancestors) are also updated according to the true-path rule: a domain annotated to a term should also be annotated by its all ancestor terms.

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#### Usage

```
dcDAGannotate(g, annotations, path.mode = c("all_paths",
  "shortest_paths",
  "all_shortest_paths"), verbose = TRUE)
```

### **Arguments**

g an object of class "igraph" or Onto

annotations an object of class Anno, that is, the vertices/nodes for which annotation data are

provided

path. mode the mode of paths induced by vertices/nodes with input annotation data. It can be

"all\_paths" for all possible paths to the root, "shortest\_paths" for only one path to the root (for each node in query), "all\_shortest\_paths" for all shortest paths to

the root (i.e. for each node, find all shortest paths with the equal lengths)

verbose logical to indicate whether the messages will be displayed in the screen. By

default, it sets to true for display

#### Value

• subg: an induced subgraph, an object of class "igraph" or "Onto" (the same as input). In addition to the original attributes to nodes and edges, the return subgraph is also appended by new node attributes: "annotations", which contains a list of domains either as original annotations or inherited annotations; "IC", which stands for information content defined as negative 10-based log-transformed frequency of domains annotated to that term.

#### Note

For the mode "shortest\_paths", the induced subgraph is the most concise, and thus informative for visualisation when there are many nodes in query, while the mode "all\_paths" results in the complete subgraph.

#### See Also

dcRDataLoader, dcEnrichment, dcDAGdomainSim, dcConverter

```
# 1) load onto.GOMF (as Onto object)
g <- dcRDataLoader(onto.GOMF)

# 2) load SCOP superfamilies annotated by GOMF (as Anno object)
Anno <- dcRDataLoader(SCOP.sf2GOMF)

# 3) prepare for annotation data
# randomly select 5 terms vertices (and their annotation data)
annotations <- Anno[,sample(1:dim(Anno)[2], 5)]

# 4) obtain the induced subgraph according to the input annotation data
# 4a) based on all possible paths (i.e. the complete subgraph induced)
dcDAGannotate(g, annotations, path.mode="all_paths", verbose=TRUE)
# 4b) based on shortest paths (i.e. the most concise subgraph induced)
dag <- dcDAGannotate(g, annotations, path.mode="shortest_paths",
verbose=TRUE)</pre>
```

```
# 5) color-code nodes/terms according to the number of annotations
if(class(dag)==Onto) dag <- dcConverter(dag, from=Onto,
to=igraph)
data <- sapply(V(dag)$annotations, length)
names(data) <- V(dag)$name
dnet::visDAG(g=dag, data=data, node.info="both")</pre>
```

dcDAGdomainSim

Function to calculate pair-wise semantic similarity between domains based on a direct acyclic graph (DAG) with annotated data

### **Description**

dcDAGdomainSim is supposed to calculate pair-wise semantic similarity between domains based on a direct acyclic graph (DAG) with annotated data. It first calculates semantic similarity between terms and then derives semantic similarity between domains from terms-term semantic similarity. Parallel computing is also supported for Linux or Mac operating systems.

### Usage

```
dcDAGdomainSim(g, domains = NULL, method.domain = c("BM.average",
"BM.max",
"BM.complete", "average", "max"), method.term = c("Resnik", "Lin",
"Schlicker", "Jiang", "Pesquita"), force = TRUE, fast = TRUE,
parallel = TRUE, multicores = NULL, verbose = TRUE)
```

#### **Arguments**

g

an object of class "igraph" or Onto. It must contain a node attribute called 'annotations' for storing annotation data (see example for howto)

domains

the domains between which pair-wise semantic similarity is calculated. If NULL, all domains annotatable in the input dag will be used for calculation, which is very prohibitively expensive!

method.domain

the method used for how to derive semantic similarity between domains from semantic similarity between terms. It can be "average" for average similarity between any two terms (one from domain 1, the other from domain 2), "max" for the maximum similarity between any two terms, "BM.average" for bestmatching (BM) based average similarity (i.e. for each term of either domain, first calculate maximum similarity to any term in the other domain, then take average of maximum similarity; the final BM-based average similiary is the pre-calculated average between two domains in pair), "BM.max" for BM based maximum similarity (i.e. the same as "BM.average", but the final BM-based maximum similiary is the maximum of the pre-calculated average between two domains in pair), "BM.complete" for BM-based complete-linkage similarity (inspired by complete-linkage concept: the least of any maximum similarity between a term of one domain and a term of the other domain). When comparing BM-based similarity between domains, "BM.average" and "BM.max" are sensitive to the number of terms invovled; instead, "BM.complete" is much robust in this aspect. By default, it uses "BM.average".

method.term

the method used to measure semantic similarity between terms. It can be "Resnik" for information content (IC) of most informative common ancestor (MICA) (see http://arxiv.org/pdf/cmp-lg/9511007.pdf), "Lin" for 2\*IC at MICA divided by the sum of IC at pairs of terms (see http://webdocs.cs.ualberta.ca/~lindek/papers/sim.pdf), "Schlicker" for weighted version of 'Lin' by the 1-prob(MICA) (see http://www.ncbi.nlm.nih.gov/pubmed/16776819), "Jiang" for 1 - difference between the sum of IC at pairs of terms and 2\*IC at MICA (see http://arxiv.org/pdf/cmp-lg/9709008.pdf), "Pesquita" for graph information content similarity related to Tanimoto-Jacard index (ie. summed information content of common ancestors divided by summed information content of all ancestors of term1 and term2 (see http://www.ncbi.nlm.nih.gov/pubmed/18460186))

force

logical to indicate whether the only most specific terms (for each domain) will be used. By default, it sets to true. It is always advisable to use this since it is computationally fast but without compromising accuracy (considering the fact that true-path-rule has been applied when running dcDAGannotate)

fast

logical to indicate whether a vectorised fast computation is used. By default, it sets to true. It is always advisable to use this vectorised fast computation; since the conventional computation is just used for understanding scripts

parallel

logical to indicate whether parallel computation with multicores is used. By default, it sets to true, but not necessarily does so. Partly because parallel backends available will be system-specific (now only Linux or Mac OS). Also, it will depend on whether these two packages "foreach" and "doMC" have been installed. It can be installed via: source("http://bioconductor.org/biocLite.R"); biocLite(c("foreach", "doMC")). If not yet installed, this option will be disabled

multicores

an integer to specify how many cores will be registered as the multicore parallel backend to the 'foreach' package. If NULL, it will use a half of cores available in a user's computer. This option only works when parallel computation is enabled

verbose

logical to indicate whether the messages will be displayed in the screen. By default, it sets to true for display

#### Value

an object of S4 class Dnetwork. It is a weighted and undirect graph, with following slots:

- nodeInfo: an object of S4 class, describing information on nodes/domains
- adjMatrix: an object of S4 class AdjData, containing symmetric adjacency data matrix for pair-wise semantic similarity between domains

### Note

For the mode "shortest\_paths", the induced subgraph is the most concise, and thus informative for visualisation when there are many nodes in query, while the mode "all\_paths" results in the complete subgraph.

#### See Also

 ${\tt dcRDataLoader, dcDAGannotate, dcConverter, Dnetwork-class}$ 

```
# 1) Semantic similarity between SCOP domain superfamilies (sf)
## 1a) load onto.GOMF (as Onto object)
g <- dcRDataLoader(onto.GOMF)</pre>
## 1b) load SCOP superfamilies annotated by GOMF (as Anno object)
Anno <- dcRDataLoader(SCOP.sf2GOMF)</pre>
## 1c) prepare for ontology appended with annotation information
dag <- dcDAGannotate(g, annotations=Anno, path.mode="shortest_paths",</pre>
verbose=FALSE)
## 1d) calculate pair-wise semantic similarity between 8 randomly chosen domains
alldomains <- unique(unlist(nInfo(dag)$annotations))</pre>
domains <- sample(alldomains,8)</pre>
dnetwork <- dcDAGdomainSim(g=dag, domains=domains,</pre>
method.domain="BM.average", method.term="Resnik", parallel=FALSE,
verbose=TRUE)
dnetwork
## 1e) convert it to an object of class igraph
ig <- dcConverter(dnetwork, from=Dnetwork, to=igraph)</pre>
ig
## 1f) visualise the domain network
### extract edge weight (with 2-digit precision)
x <- signif(E(ig)$weight, digits=2)</pre>
### rescale into an interval [1,4] as edge width
edge.width <-1 + (x-min(x))/(max(x)-min(x))*3
### do visualisation
dnet::visNet(g=ig, vertex.shape="sphere", edge.width=edge.width,
edge.label=x, edge.label.cex=0.7)
# 2) Semantic similarity between Pfam domains (Pfam)
## 2a) load onto.GOMF (as Onto object)
g <- dcRDataLoader(onto.GOMF)</pre>
## 2b) load Pfam domains annotated by GOMF (as Anno object)
Anno <- dcRDataLoader(Pfam2GOMF)</pre>
## 2c) prepare for ontology appended with annotation information
dag <- dcDAGannotate(g, annotations=Anno, path.mode="shortest_paths",</pre>
verbose=FALSE)
## 2d) calculate pair-wise semantic similarity between 8 randomly chosen domains
alldomains <- unique(unlist(nInfo(dag)$annotations))</pre>
domains <- sample(alldomains,8)</pre>
dnetwork <- dcDAGdomainSim(g=dag, domains=domains,</pre>
method.domain="BM.average", method.term="Resnik", parallel=FALSE,
verbose=TRUE)
dnetwork
## 2e) convert it to an object of class igraph
ig <- dcConverter(dnetwork, from=Dnetwork, to=igraph)</pre>
## 2f) visualise the domain network
### extract edge weight (with 2-digit precision)
x <- signif(E(ig)$weight, digits=2)</pre>
### rescale into an interval [1,4] as edge width
edge.width <-1 + (x-min(x))/(max(x)-min(x))*3
### do visualisation
dnet::visNet(g=ig, vertex.shape="sphere", edge.width=edge.width,
edge.label=x, edge.label.cex=0.7)
```

```
# 3) Semantic similarity between InterPro domains (InterPro)
## 3a) load onto.GOMF (as Onto object)
g <- dcRDataLoader(onto.GOMF)</pre>
## 3b) load InterPro domains annotated by GOMF (as Anno object)
Anno <- dcRDataLoader(InterPro2GOMF)</pre>
## 3c) prepare for ontology appended with annotation information
dag <- dcDAGannotate(g, annotations=Anno, path.mode="shortest_paths",</pre>
verbose=FALSE)
## 3d) calculate pair-wise semantic similarity between 8 randomly chosen domains
alldomains <- unique(unlist(nInfo(dag)$annotations))</pre>
domains <- sample(alldomains,8)</pre>
dnetwork <- dcDAGdomainSim(g=dag, domains=domains,</pre>
method.domain="BM.average", method.term="Resnik", parallel=FALSE,
verbose=TRUE)
dnetwork
## 3e) convert it to an object of class igraph
ig <- dcConverter(dnetwork, from=Dnetwork, to=igraph)</pre>
## 3f) visualise the domain network
### extract edge weight (with 2-digit precision)
x <- signif(E(ig)$weight, digits=2)</pre>
### rescale into an interval [1,4] as edge width
edge.width \leftarrow 1 + (x-min(x))/(max(x)-min(x))*3
### do visualisation
dnet::visNet(g=ig, vertex.shape="sphere", edge.width=edge.width,
edge.label=x, edge.label.cex=0.7)
# 4) Semantic similarity between Rfam RNA families (Rfam)
## 4a) load onto.GOBP (as Onto object)
g <- dcRDataLoader(onto.GOBP)</pre>
## 4b) load Rfam families annotated by GOBP (as Anno object)
Anno <- dcRDataLoader(Rfam2GOBP)</pre>
## 4c) prepare for ontology appended with annotation information
dag <- dcDAGannotate(g, annotations=Anno, path.mode="shortest_paths",</pre>
verbose=FALSE)
## 4d) calculate pair-wise semantic similarity between 8 randomly chosen RNAs
alldomains <- unique(unlist(nInfo(dag)$annotations))</pre>
domains <- sample(alldomains,8)</pre>
dnetwork <- dcDAGdomainSim(g=dag, domains=domains,</pre>
method.domain="BM.average", method.term="Resnik", parallel=FALSE,
verbose=TRUE)
## 4e) convert it to an object of class igraph
ig <- dcConverter(dnetwork, from=Dnetwork, to=igraph)</pre>
ig
## 4f) visualise the domain network
### extract edge weight (with 2-digit precision)
x <- signif(E(ig)$weight, digits=2)</pre>
### rescale into an interval [1,4] as edge width
edge.width <-1 + (x-min(x))/(max(x)-min(x))*3
### do visualisation
dnet::visNet(g=ig, vertex.shape="sphere", edge.width=edge.width,
edge.label=x, edge.label.cex=0.7)
```

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```
# 5) Advanced usage: customised data for ontology and annotations
# 5a) customise ontology
g <-
nodes.file="http://dcgor.r-forge.r-project.org/data/onto/igraph_GOMF_nodes.txt",
output.file="ontology.RData")
# 5b) customise Anno
Anno <-
dcBuildAnno(domain_info.file="http://dcgor.r-forge.r-project.org/data/InterPro/InterPro.txt",
term_info.file="http://dcgor.r-forge.r-project.org/data/InterPro/GO.txt",
association.file="http://dcgor.r-forge.r-project.org/data/InterPro/Domain2GOMF.txt",
output.file="annotations.RData")
## 5c) prepare for ontology appended with annotation information
dag <- dcDAGannotate(g, annotations=Anno, path.mode="shortest_paths",</pre>
verbose=FALSE)
## 5d) calculate pair-wise semantic similarity between 8 randomly chosen domains
alldomains <- unique(unlist(nInfo(dag)$annotations))</pre>
domains <- sample(alldomains,8)</pre>
dnetwork <- dcDAGdomainSim(g=dag, domains=domains,</pre>
method.domain="BM.average", method.term="Resnik", parallel=FALSE,
verbose=TRUE)
dnetwork
## 5e) convert it to an object of class igraph
ig <- dcConverter(dnetwork, from=Dnetwork, to=igraph)</pre>
## 5f) visualise the domain network
### extract edge weight (with 2-digit precision)
x <- signif(E(ig)$weight, digits=2)</pre>
### rescale into an interval [1,4] as edge width
edge.width <- 1 + (x-min(x))/(max(x)-min(x))*3
### do visualisation
dnet::visNet(g=ig, vertex.shape="sphere", edge.width=edge.width,
edge.label=x, edge.label.cex=0.7)
```

dcDuplicated

Function to determine the duplicated patterns from input data matrix

## Description

dcDuplicated is supposed to determine the duplicated vectorised patterns from a matrix or data frame. The patterns can come from column-wise vectors or row-wise vectors. It returns an integer vector, in which the value indicates from which it duplicats.

## Usage

```
dcDuplicated(data, pattern.wise = c("column", "row"), verbose = T)
```

### **Arguments**

data an input data matrix/frame

pattern.wise a character specifying in which wise to define patterns from input data. It can

be 'column' for column-wise vectors, and 'row' for row-wise vectors

verbose logical to indicate whether the messages will be displayed in the screen. By

default, it sets to TRUE for display

#### Value

an interger vector, in which an entry indicates from which it duplicats. When viewing column-wise patterns (or row-wise patterns), the returned integer vector has the same length as the column number (or the row number) of input data.

#### Note

none

#### See Also

dcAncestralMP, dcAncestralMP, dcAlgo

### **Examples**

```
# an input data matrix storing discrete states for tips (in rows) X four characters (in columns)
data1 <- matrix(c(0,rep(1,3),rep(0,2)), ncol=1)
data2 <- matrix(c(rep(0,4),rep(1,2)), ncol=1)
data3 <- matrix(c(1,rep(0,3),rep(1,2)), ncol=1)
data <- cbind(data1, data2, data1, data3)
colnames(data) <- c("C1", "C2", "C3", "C4")
data

# determine the duplicated patterns from inut data matrix
res <- dcDuplicated(data, pattern.wise="column")
## return an integer vector
res
## get index for unique patterns
ind <- sort(unique(res))
## As seen above, the returned integer vector tells there are 3 unique patterns:
## they are in columns (1, 2, 4). The column 3 is duplicated from column 1.</pre>
```

dcEnrichment

Function to conduct ontology enrichment analysis given a group of domains

### **Description**

dcEnrichment is supposed to conduct enrichment analysis for an input group of domains using a specified ontology. It returns an object of S4 class "Eoutput". Enrichment analysis is based on either Fisher's exact test or Hypergeometric test. The test can respect the hierarchy of the ontology. The user can customise the background domains; otherwise, the function will use all annotatable domains as the test background

### Usage

```
dcEnrichment(data, background = NULL, domain = c(NA, "SCOP.sf",
  "SCOP.fa",
  "Pfam", "InterPro", "Rfam"), ontology = c(NA, "GOBP", "GOMF", "GOCC",
  "DO",
  "HPPA", "HPMI", "HPON", "MP", "EC", "KW", "UP"), sizeRange = c(10,
1000),
```

```
min.overlap = 3, which_distance = NULL, test = c("HypergeoTest",
   "FisherTest", "BinomialTest"), p.adjust.method = c("BH", "BY",
   "bonferroni",
   "holm", "hochberg", "hommel"), ontology.algorithm = c("none", "pc",
   "elim",
   "lea"), elim.pvalue = 0.01, lea.depth = 2, verbose = T,
   domain.RData = NULL, ontology.RData = NULL, annotations.RData = NULL,
   RData.location = "http://dcgor.r-forge.r-project.org/data")
```

#### **Arguments**

data an input vector. It contains id for a list of domains, for example, sunids for

**SCOP** domains

background a background vector. It contains id for a list of background domains, for exam-

ple, sunids for SCOP domains. If NULL, by default all annotatable domains are

used as background

domain the domain identity. It can be one of 'SCOP.sf' for SCOP superfamilies, 'SCOP.fa'

for SCOP families, 'Pfam' for Pfam domains, 'InterPro' for InterPro domains,

'Rfam' for Rfam RNA families

ontology the ontology identity. It can be "GOBP" for Gene Ontology Biological Process,

"GOMF" for Gene Ontology Molecular Function, "GOCC" for Gene Ontology Cellular Component, "DO" for Disease Ontology, "HPPA" for Human Phenotype Phenotypic Abnormality, "HPMI" for Human Phenotype Mode of Inheritance, "HPON" for Human Phenotype ONset and clinical course, "MP" for Mammalian Phenotype, "EC" for Enzyme Commission, "KW" for UniProtKB KeyWords, "UP" for UniProtKB UniPathway. For details on the eligibility for pairs of input domain and ontology, please refer to the online Documentations

at http://supfam.org/dcGOR/docs.html

sizeRange the minimum and maximum size of members of each term in consideration. By

default, it sets to a minimum of 10 but no more than 1000

min.overlap the minimum number of overlaps. Only those terms that overlap with input data

at least min.overlap (3 domains by default) will be processed

which\_distance which distance of terms in the ontology is used to restrict terms in consideration.

By default, it sets to 'NULL' to consider all distances

the statistic test used. It can be "FisherTest" for using fisher's exact test, "Hyper-

geoTest" for using hypergeometric test, or "BinomialTest" for using binomial test. Fisher's exact test is to test the independence between domain group (domains belonging to a group or not) and domain annotation (domains annotated by a term or not), and thus compare sampling to the left part of background (after sampling without replacement). Hypergeometric test is to sample at random (without replacement) from the background containing annotated and non-annotated domains, and thus compare sampling to background. Unlike hypergeometric test, binomial test is to sample at random (with replacement) from the background with the constant probability. In terms of the ease of finding the significance, they are in order: hypergeometric test > binomial test > fisher's exact test. In other words, in terms of the calculated p-value, hypergeometric test <

binomial test < fisher's exact test

p.adjust.method

the method used to adjust p-values. It can be one of "BH", "BY", "bonferroni", "holm", "hochberg" and "hommel". The first two methods "BH" (widely used) and "BY" control the false discovery rate (FDR: the expected proportion of false

discoveries amongst the rejected hypotheses); the last four methods "bonferroni", "holm", "hochberg" and "hommel" are designed to give strong control of the family-wise error rate (FWER). Notes: FDR is a less stringent condition than FWER

ontology.algorithm

the algorithm used to account for the hierarchy of the ontology. It can be one of "none", "pc", "elim" and "lea". For details, please see 'Note'

elim.pvalue the parameter only used when "ontology.algorithm" is "elim". It is used to con-

trol how to declare a signficantly enriched term (and subsequently all domains

in this term are eliminated from all its ancestors)

lea.depth the parameter only used when "ontology.algorithm" is "lea". It is used to con-

trol how many maximum depth is uded to consider the children of a term (and subsequently all domains in these children term are eliminated from the use for

the recalculation of the signifiance at this term)

verbose logical to indicate whether the messages will be displayed in the screen. By

default, it sets to TRUE for display

domain.RData a file name for RData-formatted file containing an object of S4 class 'Info-DataFrame' (i.g. domain). By default, it is NULL. It is only needed when

the user wants to customise enrichment analysis using their own data. See

dcBuildInfoDataFrame for how to creat this object

ontology.RData a file name for RData-formatted file containing an object of S4 class 'Onto' (i.g.

ontology). By default, it is NULL. It is only needed when the user wants to customise enrichment analysis using their own data. See dcBuildOnto for how

to creat this object

annotations.RData

a file name for RData-formatted file containing an object of S4 class 'Anno' (i.g. annotations). By default, it is NULL. It is only needed when the user wants to customise enrichment analysis using their own data. See dcBuildAnno for how

to creat this object

RData.location the characters to tell the location of built-in RData files. By default, it remotely locates at "http://supfam.org/dcGOR/data" or "http://dcgor.r-forge.r-project.org/data".

For the user equipped with fast internet connection, this option can be just left as default. But it is always advisable to download these files locally. Especially when the user needs to run this function many times, there is no need to ask the function to remotely download every time (also it will unnecessarily increase the runtime). For examples, these files (as a whole or part of them) can be first downloaded into your current working directory, and then set this option as: RData.location = ".". If RData to load is already part of package itself, this parameter can be ignored (since this function will try to load it via function data

first)

## Value

an object of S4 class Eoutput, with following slots:

- domain: a character specifying the domain identity
- ontology: a character specifying the ontology used
- term\_info: a matrix of nTerm X 5 containing term information, where nTerm is the number of terms in consideration, and the 5 columns are "term\_id" (i.e. "Term ID"), "term\_name" (i.e. "Term Name"), "namespace" (i.e. "Term Namespace"), "distance" (i.e. "Term Distance") and "IC" (i.e. "Information Content for the term based on annotation frequency by it")

 anno: a list of terms, each storing annotated domain members (also within the background domains). Always, terms are identified by "term\_id" and domain members identified by their ids (e.g. sunids for SCOP domains)

- data: a vector containing input data in consideration. It is not always the same as the input data as only those mappable and annotatable are retained
- background: a vector containing background in consideration. It is not always the same as the input background as only those mappable/annotatable are retained
- overlap: a list of terms, each storing domains overlapped between domains annotated by a term and domains in the input data (i.e. the domains of interest). Always, terms are identified by "term\_id" and domain members identified by their IDs (e.g. sunids for SCOP domains)
- zscore: a vector containing z-scores
- pvalue: a vector containing p-values
- adjp: a vector containing adjusted p-values. It is the p value but after being adjusted for multiple comparisons

#### Note

The interpretation of the algorithms used to account for the hierarchy of the ontology is:

- "none": does not consider the ontology hierarchy at all.
- "lea": computers the significance of a term in terms of the significance of its children at the maximum depth (e.g. 2). Precisely, once domains are already annotated to any children terms with a more significance than itself, then all these domains are eliminated from the use for the recalculation of the significance at that term. The final p-values takes the maximum of the original p-value and the recalculated p-value.
- "elim": computers the significance of a term in terms of the significance of its all children. Precisely, once domains are already annotated to a significantly enriched term under the cutoff of e.g. pvalue<1e-2, all these domains are eliminated from the ancestors of that term).
- "pc": requires the significance of a term not only using the whole domains as background but also using domains annotated to all its direct parents/ancestors as background. The final p-value takes the maximum of both p-values in these two calculations.
- "Notes": the order of the number of significant terms is: "none" > "lea" > "elim" > "pc".

## See Also

dcRDataLoader, dcDAGannotate, Eoutput-class, visEnrichment, dcConverter

```
# 1) Enrichment analysis for SCOP domain superfamilies (sf)
## 1a) load SCOP.sf (as InfoDataFrame object)
SCOP.sf <- dcRDataLoader(SCOP.sf)
### randomly select 50 domains as a list of domains of interest
data <- sample(rowNames(SCOP.sf), 50)
## 1b) perform enrichment analysis, producing an object of S4 class Eoutput
eoutput <- dcEnrichment(data, domain="SCOP.sf", ontology="GOMF")
eoutput
## 1c) view the top 10 significance terms
view(eoutput, top_num=10, sortBy="pvalue", details=TRUE)
## 1d) visualise the top 10 significant terms in the ontology hierarchy
### color-coded according to 10-based negative logarithm of adjusted p-values (adjp)</pre>
```

```
visEnrichment(eoutput)
## 1e) the same as above but using a customised background
### randomly select 500 domains as background
background <- sample(rowNames(SCOP.sf), 500)</pre>
### perform enrichment analysis, producing an object of S4 class Eoutput
eoutput <- dcEnrichment(data, background=background, domain="SCOP.sf",</pre>
ontology="GOMF")
eoutput
### view the top 10 significance terms
view(eoutput, top_num=10, sortBy="pvalue", details=TRUE)
### visualise the top 10 significant terms in the ontology hierarchy
### color-coded according to 10-based negative logarithm of adjusted p-values (adjp)
visEnrichment(eoutput)
# 2) Enrichment analysis for Pfam domains (Pfam)
## 2a) load Pfam (as InfoDataFrame object)
Pfam <- dcRDataLoader(Pfam)</pre>
### randomly select 100 domains as a list of domains of interest
data <- sample(rowNames(Pfam), 100)</pre>
## 2b) perform enrichment analysis, producing an object of S4 class Eoutput
eoutput <- dcEnrichment(data, domain="Pfam", ontology="GOMF")</pre>
eoutput
## 2c) view the top 10 significance terms
view(eoutput, top_num=10, sortBy="pvalue", details=TRUE)
## 2d) visualise the top 10 significant terms in the ontology hierarchy
### color-coded according to 10-based negative logarithm of adjusted p-values (adjp)
visEnrichment(eoutput)
## 2e) the same as above but using a customised background
### randomly select 1000 domains as background
background <- sample(rowNames(Pfam), 1000)</pre>
### perform enrichment analysis, producing an object of S4 class Eoutput
eoutput <- dcEnrichment(data, background=background, domain="Pfam",</pre>
ontology="GOMF")
eoutput
### view the top 10 significance terms
view(eoutput, top_num=10, sortBy="pvalue", details=TRUE)
\#\#\# visualise the top 10 significant terms in the ontology hierarchy
### color-coded according to 10-based negative logarithm of adjusted p-values (adjp)
visEnrichment(eoutput)
# 3) Enrichment analysis for InterPro domains (InterPro)
## 3a) load InterPro (as InfoDataFrame object)
InterPro <- dcRDataLoader(InterPro)</pre>
\#\#\# randomly select 100 domains as a list of domains of interest
data <- sample(rowNames(InterPro), 100)</pre>
## 3b) perform enrichment analysis, producing an object of S4 class Eoutput
eoutput <- dcEnrichment(data, domain="InterPro", ontology="GOMF")</pre>
## 3c) view the top 10 significance terms
view(eoutput, top_num=10, sortBy="pvalue", details=TRUE)
## 3d) visualise the top 10 significant terms in the ontology hierarchy
### color-coded according to 10-based negative logarithm of adjusted p-values (adjp)
visEnrichment(eoutput)
## 3e) the same as above but using a customised background
### randomly select 1000 domains as background
```

```
background <- sample(rowNames(InterPro), 1000)</pre>
### perform enrichment analysis, producing an object of S4 class Eoutput
eoutput <- dcEnrichment(data, background=background, domain="InterPro",</pre>
ontology="GOMF")
eoutput
### view the top 10 significance terms
view(eoutput, top_num=10, sortBy="pvalue", details=TRUE)
### visualise the top 10 significant terms in the ontology hierarchy
### color-coded according to 10-based negative logarithm of adjusted p-values (adjp)
visEnrichment(eoutput)
# 4) Enrichment analysis for Rfam RNA families (Rfam)
## 4a) load Rfam (as InfoDataFrame object)
Rfam <- dcRDataLoader(Rfam)</pre>
### randomly select 100 RNAs as a list of RNAs of interest
data <- sample(rowNames(Rfam), 100)</pre>
## 4b) perform enrichment analysis, producing an object of S4 class Eoutput
eoutput <- dcEnrichment(data, domain="Rfam", ontology="GOBP")</pre>
eoutput
## 4c) view the top 10 significance terms
view(eoutput, top_num=10, sortBy="pvalue", details=FALSE)
## 4d) visualise the top 10 significant terms in the ontology hierarchy
### color-coded according to 10-based negative logarithm of adjusted p-values (adjp)
visEnrichment(eoutput)
## 4e) the same as above but using a customised background
### randomly select 1000 RNAs as background
background <- sample(rowNames(Rfam), 1000)</pre>
### perform enrichment analysis, producing an object of S4 class Eoutput
eoutput <- dcEnrichment(data, background=background, domain="Rfam",</pre>
ontology="GOBP")
eoutput
### view the top 10 significance terms
view(eoutput, top_num=10, sortBy="pvalue", details=FALSE)
### visualise the top 10 significant terms in the ontology hierarchy
### color-coded according to 10-based negative logarithm of adjusted p-values (adjp)
visEnrichment(eoutput)
# 5) Advanced usage: customised data for domain, ontology and annotations
# 5a) create domain, ontology and annotations
## for domain
domain <-
dcBuildInfoDataFrame(input.file="http://dcgor.r-forge.r-project.org/data/InterPro/InterPro.txt",
output.file="domain.RData")
## for ontology
dcBuildOnto(relations.file="http://dcgor.r-forge.r-project.org/data/onto/igraph_GOMF_edges.txt",
nodes.file="http://dcgor.r-forge.r-project.org/data/onto/igraph_GOMF_nodes.txt",
output.file="ontology.RData")
## for annotations
dcBuildAnno(domain_info.file="http://dcgor.r-forge.r-project.org/data/InterPro/InterPro.txt",
term_info.file="http://dcgor.r-forge.r-project.org/data/InterPro/GO.txt",
association.file="http://dcgor.r-forge.r-project.org/data/InterPro/Domain2GOMF.txt",
output.file="annotations.RData")
## 5b) prepare data and background
### randomly select 100 domains as a list of domains of interest
data <- sample(rowNames(domain), 100)</pre>
```

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```
### randomly select 1000 domains as background
background <- sample(rowNames(domain), 1000)
## 5c) perform enrichment analysis, producing an object of S4 class Eoutput
eoutput <- dcEnrichment(data, background=background,
domain.RData=domain.RData, ontology.RData=ontology.RData,
annotations.RData=annotations.RData)
eoutput
## 5d) view the top 10 significance terms
view(eoutput, top_num=10, sortBy="pvalue", details=TRUE)
### visualise the top 10 significant terms in the ontology hierarchy
### color-coded according to 10-based negative logarithm of adjusted p-values (adjp)
visEnrichment(eoutput)</pre>
```

dcFunArgs

Function to assign (and evaluate) arguments with default values for

an input function

## **Description**

dcFunArgs is supposed to assign (and evaluate) arguments with default values for an input function.

### Usage

```
dcFunArgs(fun, action = F, verbose = T)
```

## **Arguments**

fun an input function name (character string)

action logical to indicate whether the function will act as it should be (with assigned

values in the current environment). By default, it sets to FALSE

verbose logical to indicate whether the messages will be displayed in the screen. By

default, it sets to TRUE for display

### Value

a list containing arguments and their default values

### Note

This function is potentially useful when debugging. Because the developer does not have to specify default values for all arguments except those arguments are of interest

#### See Also

dcAlgoPredictMain

```
fun <- "dcAlgoPredictMain"
dcFunArgs(fun)</pre>
```

dcList2Matrix 51

dcList2Matrix

Function to convert a list into a matrix containing three columns

## Description

dcList2Matrix is supposed to convert a list into a matrix containing three columns

## Usage

```
dcList2Matrix(x, verbose = T)
```

# Arguments

x a list, its each component must be a named vector

verbose logical to indicate whether the messages will be displayed in the screen. By

default, it sets to TRUE for display

### Value

a matrix containing three columns: 1st for the input list names (if exist, otherises an increasing integer), 2nd for the vector names of each list component, and 3rd for the vector values of each list component

## Note

none

### See Also

dcAlgoPropagate

```
# load an object HIS
Feature2GOMF.sf <- dcRDataLoader(RData=Feature2GOMF.sf)
# get a list
x <- Feature2GOMF.sf$hscore
# convert the list into a matrix
res <- dcList2Matrix(x)
dim(res)
res[1:10,]</pre>
```

52 dcRDataLoader

dcRDataLoader

Function to load dcGOR built-in RData

## **Description**

dcRDataLoader is supposed to load RData that are used by package dcGOR.

### Usage

```
dcRDataLoader(RData = c(NA, "SCOP.sf", "SCOP.fa", "Pfam", "InterPro",
"onto.GOBP", "onto.GOMF", "onto.GOCC", "onto.DO", "onto.HPPA",
"onto.HPMI"
"onto.HPON", "onto.MP", "onto.EC", "onto.KW", "onto.UP",
"SCOP.sf2GOBP"
"SCOP.sf2GOMF", "SCOP.sf2GOCC", "SCOP.sf2DO", "SCOP.sf2HPPA",
"SCOP.sf2HPMI",
"SCOP.sf2HPON", "SCOP.sf2MP", "SCOP.sf2EC", "SCOP.sf2KW", "SCOP.sf2UP",
"SCOP.fa2GOBP", "SCOP.fa2GOMF", "SCOP.fa2GOCC", "SCOP.fa2DO",
"SCOP.fa2HPPA"
"SCOP.fa2HPMI", "SCOP.fa2HPON", "SCOP.fa2MP", "SCOP.fa2EC",
"SCOP.fa2KW"
"SCOP.fa2UP", "Pfam2GOBP", "Pfam2GOMF", "Pfam2GOCC", "InterPro2GOBP",
"InterPro2GOMF", "InterPro2GOCC", "Rfam2GOBP", "Rfam2GOMF",
"Rfam2GOCC",
"Ancestral_domainome", "eTOL", "Feature2GOBP.sf", "Feature2GOMF.sf",
"Feature2GOCC.sf", "Feature2HPPA.sf", "Feature2GOBP.pfam",
"Feature2GOMF.pfam", "Feature2GOCC.pfam", "Feature2HPPA.pfam",
"Feature2GOBP.interpro", "Feature2GOMF.interpro",
"Feature2GOCC.interpro",
"Feature2HPPA.interpro"), domain = c(NA, "SCOP.sf", "SCOP.fa", "Pfam",
"InterPro", "Rfam"), ontology = c(NA, "GOBP", "GOMF", "GOCC", "DO",
"HPPA",
"HPMI", "HPON", "MP", "EC", "KW", "UP"), verbose = T,
RData.location = "http://dcgor.r-forge.r-project.org/data")
```

### **Arguments**

RData

which built-in RData to load. If NOT NA, this RData will be always loaded. It can be: domains/RNAs (including 'SCOP.sf', 'SCOP.fa', 'Pfam', 'InterPro', 'Rfam'), ontologies (including 'onto.GOBP', 'onto.GOMF', 'onto.GOCC', 'onto.DO', 'onto.HPPA', 'onto.HPMI', 'onto.HPON', 'onto.MP', 'onto.EC', 'onto.KW', 'onto.UP'), annotations (including 'SCOP.sf2GOBP', 'SCOP.sf2GOMF', 'SCOP.sf2GOCC', 'SCOP.sf2HPPA', 'SCOP.sf2HPMI', 'SCOP.sf2HPON', 'SCOP.sf2MP', 'SCOP.sf2EC', 'SCOP.sf2KW', 'SCOP.sf2UP', 'SCOP.fa2GOBP', 'SCOP.fa2GOMF', 'SCOP.fa2GOCC', 'SCOP.fa2DO', 'SCOP.fa2HPPA', 'SCOP.fa2HPMI', 'SCOP.fa2HPON', 'SCOP.fa2MP', 'SCOP.fa2EC', 'SCOP.fa2KW', 'SCOP.fa2UP', 'Pfam2GOBP', 'InterPro2GOMF', 'InterPro2GOMF', 'InterPro2GOCC', 'Rfam2GOBP', 'Rfam2GOMF', 'Rfam2GOCC'), domainome in eukaryotic genomes (including 'Ancestral\_domainome', 'eTOL'), and databases used for predicting ontology terms from input protein domain contents. On the meanings, please refer to the Documentations

dcRDataLoader 53

domain part of annotation RData to load. When RData is NA and this plus

next are NOT NA, then this plus next one are used to specify which annotation RData to load. In addition to NA, it can also be: 'SCOP.sf', 'SCOP.fa', 'Pfam'

and 'InterPro'

ontology ontology part of annotation RData to load. This only works together with the

previous 'domain' parameter. In addition to NA, it can also be: 'GOBP', 'GOMF',

'GOCC', 'DO', 'HPPA', 'HPMI', 'HPON', 'MP', 'EC', 'KW', 'UP'

verbose logical to indicate whether the messages will be displayed in the screen. By

default, it sets to TRUE for display

RData.location the characters to tell the location of built-in RData files. By default, it remotely

locates at "http://supfam.org/dcGOR/data" or "http://dcgor.r-forge.r-project.org/data". For the user equipped with fast internet connection, this option can be just left as default. But it is always advisable to download these files locally. Especially when the user needs to run this function many times, there is no need to ask the function to remotely download every time (also it will unnecessarily increase the runtime). For examples, these files (as a whole or part of them) can be first downloaded into your current working directory, and then set this option as: RData.location = ".". If RData to load is already part of package itself, this parameter can be ignored (since this function will try to load it via function data

first)

#### Value

any use-specified variable that is given on the right side of the assignment sign '<-', which contains the loaded RData.

#### Note

If there are no use-specified variable that is given on the right side of the assignment sign '<-', then no RData will be loaded onto the working environment.

#### See Also

dcEnrichment

```
# Always, load from specified RData directly
SCOP.sf <- dcRDataLoader(RData=SCOP.sf)
Pfam <- dcRDataLoader(RData=Pfam)
InterPro <- dcRDataLoader(RData=InterPro)
Rfam <- dcRDataLoader(RData=Rfam)
onto.GOMF <- dcRDataLoader(RData=onto.GOMF)
# But for annotaion data, there are two ways to do so:
# 1) in a direct way
SCOP.sf2GOMF <- dcRDataLoader(RData=SCOP.sf2GOMF)
# 2) in an indirect way: specify both domain and ontology
SCOP.sf2GOMF <- dcRDataLoader(domain=SCOP.sf, ontology=GOMF)</pre>
```

54 dcRWRpipeline

dcRWRpipeline	Function to setup a pipeine to estimate RWR-based contact strength
	between samples from an input domain-sample data matrix and an input graph

#### **Description**

dcRWRpipeline is supposed to estimate sample relationships (ie. contact strength between samples) from an input domain-sample matrix and an input graph (such as a domain-domain semantic network). The pipeline includes: 1) random walk restart (RWR) of the input graph using the input matrix as seeds; 2) calculation of contact strength (inner products of RWR-smoothed columns of input matrix); 3) estimation of the contact signficance by a randomalisation procedure. It supports two methods how to use RWR: 'direct' for directly applying RWR in the given seeds; 'indirectly' for first pre-computing affinity matrix of the input graph, and then deriving the affinity score. Parallel computing is also supported for Linux or Mac operating systems.

## Usage

```
dcRWRpipeline(data, g, method = c("indirect", "direct"),
normalise = c("laplacian", "row", "column", "none"), restart = 0.75,
normalise.affinity.matrix = c("none", "quantile"),
permutation = c("random", "degree"), num.permutation = 100,
p.adjust.method = c("BH", "BY", "bonferroni", "holm", "hochberg",
    "hommel"),
adjp.cutoff = 0.05, parallel = TRUE, multicores = NULL, verbose = T)
```

#### **Arguments**

data	an input domain-sample	data matrix used for seeds.	Each value in input domain-

sample matrix does not necessarily have to be binary (non-zeros will be used as

a weight, but should be non-negative for easy interpretation).

g an object of class "igraph" or Dnetwork

method the method used to calculate RWR. It can be 'direct' for directly applying RWR,

'indirect' for indirectly applying RWR (first pre-compute affinity matrix and

then derive the affinity score)

normalise the way to normalise the adjacency matrix of the input graph. It can be 'lapla-

cian' for laplacian normalisation, 'row' for row-wise normalisation, 'column'

for column-wise normalisation, or 'none'

restart the restart probability used for RWR. The restart probability takes the value from

0 to 1, controlling the range from the starting nodes/seeds that the walker will explore. The higher the value, the more likely the walker is to visit the nodes centered on the starting nodes. At the extreme when the restart probability is zero, the walker moves freely to the neighbors at each step without restarting

from seeds, i.e., following a random walk (RW)

normalise.affinity.matrix

the way to normalise the output affinity matrix. It can be 'none' for no normalisation, 'quantile' for quantile normalisation to ensure that columns (if multiple)

of the output affinity matrix have the same quantiles

permutation how to do permutation. It can be 'degree' for degree-preserving permutation,

'random' for permutation in random

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num.permutation

the number of permutations used to for generating the distribution of contact strength under randomalisation

p.adjust.method

the method used to adjust p-values. It can be one of "BH", "BY", "bonferroni", "holm", "hochberg" and "hommel". The first two methods "BH" (widely used) and "BY" control the false discovery rate (FDR: the expected proportion of false discoveries amongst the rejected hypotheses); the last four methods "bonferroni", "holm", "hochberg" and "hommel" are designed to give strong control of the family-wise error rate (FWER). Notes: FDR is a less stringent condition than FWER

adjp.cutoff

the cutoff of adjusted pvalue to construct the contact graph

parallel

logical to indicate whether parallel computation with multicores is used. By default, it sets to true, but not necessarily does so. Partly because parallel backends available will be system-specific (now only Linux or Mac OS). Also, it will depend on whether these two packages "foreach" and "doMC" have been installed. It can be installed via: source("http://bioconductor.org/biocLite.R"); biocLite(c("foreach", "doMC")). If not yet installed, this option will be disabled

multicores

an integer to specify how many cores will be registered as the multicore parallel backend to the 'foreach' package. If NULL, it will use a half of cores available in a user's computer. This option only works when parallel computation is enabled

verbose

logical to indicate whether the messages will be displayed in the screen. By

default, it sets to true for display

### Value

an object of class "iContact", a list with following components:

- ratio: a symmetric matrix storing ratio (the observed against the expected) between pairwise samples
- zscore: a symmetric matrix storing zscore between pairwise samples
- pval: a symmetric matrix storing pvalue between pairwise samples
- adjpval: a symmetric matrix storing adjusted pvalue between pairwise samples
- icontact: the constructed contact graph (as an 'igraph' object) under the cutoff of adjusted value
- Amatrix: a pre-computated affinity matrix when using 'inderect' method; NULL otherwise
- call: the call that produced this result

### Note

The choice of which method to use RWR depends on the number of seed sets and the number of permutations for statistical test. If the total product of both numbers are huge, it is better to use 'indrect' method (for a single run).

### See Also

 $\tt dcRDataLoader, dcDAGannotate, dcDAGdomainSim, dcConverter$ 

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#### **Examples**

```
# 1) load onto.GOMF (as Onto object)
g <- dcRDataLoader(onto.GOMF)</pre>
# 2) load SCOP superfamilies annotated by GOMF (as Anno object)
Anno <- dcRDataLoader(SCOP.sf2GOMF)</pre>
# 3) prepare for ontology appended with annotation information
dag <- dcDAGannotate(g, annotations=Anno, path.mode="shortest_paths",</pre>
verbose=TRUE)
# 4) calculate pair-wise semantic similarity between 10 randomly chosen domains
alldomains <- unique(unlist(nInfo(dag)$annotations))</pre>
domains <- sample(alldomains,10)</pre>
dnetwork <- dcDAGdomainSim(g=dag, domains=domains,</pre>
method.domain="BM.average", method.term="Resnik", parallel=FALSE,
verbose=TRUE)
dnetwork
# 5) estimate RWR dating based sample/term relationships
# define sets of seeds as data
# each seed with equal weight (i.e. all non-zero entries are 1)
data <- data.frame(aSeeds=c(1,0,1,0,1), bSeeds=c(0,0,1,0,1))</pre>
rownames(data) <- id(dnetwork)[1:5]</pre>
# calcualte their two contact graph
coutput <- dcRWRpipeline(data=data, g=dnetwork, parallel=FALSE)</pre>
coutput
```

dcSparseMatrix

Function to create a sparse matrix for an input file with three columns

## **Description**

dcSparseMatrix is supposed to create a sparse matrix for an input file with three columns.

# Usage

```
dcSparseMatrix(input.file, verbose = T)
```

#### **Arguments**

input.file an input file containing three columns: 1st column for rows, 2nd for columns,

and 3rd for numeric values. Alternatively, the input file can be a matrix or data frame, assuming that input file has been read. Note: the file should use the tab

delimiter as the field separator between columns

verbose logical to indicate whether the messages will be displayed in the screen. By

default, it sets to TRUE for display

### Value

a list containing arguments and their default values

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#### Note

This function is potentially useful when debugging. Because the developer does not have to specify default values for all arguments except those arguments are of interest

#### See Also

```
dcAlgoPredictMain
```

## **Examples**

```
# create a sparse matrix of 4 X 2
input.file <- rbind(c(R1,C1,1), c(R2,C1,1), c(R2,C2,1),
c(R3,C2,1), c(R4,C1,1))
res <- dcSparseMatrix(input.file)
res
# get a full matrix
as.matrix(res)</pre>
```

dcSplitArch

Function to obtain a list of features via splitting an input architecture

## **Description**

dcSplitArch is supposed to obtain a list of features via splitting an input architecture.

## Usage

```
dcSplitArch(da, feature.mode = c("supra", "individual", "comb"), sep =
",",
ignore = "_gap_", verbose = T)
```

### **Arguments**

da an input architecture. For example, a comma-separated string

feature.mode the mode of how to define the features thereof. It can be: "supra" for combi-

nations of one or two successive domains (including individual domains; considering the order), "individual" for individual domains only, and "comb" for all possible combinations (including individual domains; ignoring the order)

sep a character string to separate. By default, it is comma','

ignore a character string to ignore. By default, it is '\_gap\_'. Ihis ignored character will

affect the features defined as being 'supra' (see examples below)

verbose logical to indicate whether the messages will be displayed in the screen. By

default, it sets to TRUE for display

## Value

a vector containing splitted features.

### Note

none

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#### See Also

```
dcAlgo, dcAlgoPredict
```

### **Examples**

```
da <- "_gap_,100895,57610,_gap_,57610,47473"
# get features defined as being "supra"
dcSplitArch(da, feature.mode="supra")
# get features defined as being "individual"
dcSplitArch(da, feature.mode="individual")
# get features defined as being "comb"
dcSplitArch(da, feature.mode="comb")</pre>
```

dcSubtreeClade

Function to extract a subtree under a given clade from a phyloformatted phylogenetic tree

## **Description**

dcSubtreeClade is supposed to extract a subtree under a given clade from a phylo-formatted phylogenetic tree. In addition to the tree in subject, another input is a built-in integer specifying an internal node/clade of interest. Alternatively, the internal node of interest can be given by its label (if there are internal node labels). As a result, a subtree under a given clade is also represented as an object of class 'phylo'.

### Usage

```
dcSubtreeClade(phy, choose.node = NULL, choose.node.label = NULL,
verbose = T)
```

## **Arguments**

phy an object of class 'phylo'

choose.node an integer specifying which internal node is chosen. For an object of class

'phylo', the tree has built-in ID for internal nodes, ranging from Ntip+1 to Ntip+Nnode, where Ntip and Nnode are the number of tips and internal nodes. Internal nodes are indexed in a pre-ordered manner. The subtree under

the given interna node will be extracted

choose.node.label

a character specifying which internal node is chosen. For the tree with internal

node labels, the extraction of subtree can be done in this way

verbose logical to indicate whether the messages will be displayed in the screen. By

default, it sets to TRUE for display

### Value

```
an object of class 'phylo'
```

#### Note

If a valid 'choose.node' is given, then 'choose.node.label' will be ignored.

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#### See Also

dcTreeConnectivity

#### **Examples**

```
# 1) a newick tree without internal node labels
tree <- "(((t1:5,t2:5):2,(t3:4,t4:4):3):2,(t5:4,t6:4):6);"
phy <- ape::read.tree(text=tree)</pre>
phy
Ntip <- ape::Ntip(phy)</pre>
Nnode <- ape::Nnode(phy)</pre>
ape::plot.phylo(phy, type="p", use.edge.length=TRUE)
ape::nodelabels(node=Ntip+1:Nnode, col="red", bg="white")
# a subtree specified via a built-in internal node ID
subphy <- dcSubtreeClade(phy, choose.node=Ntip+2)</pre>
subphy
ape::plot.phylo(subphy, type="p", use.edge.length=TRUE)
# 2) a newick tree with internal node labels
tree <- "(((t1:5,t2:5)i3:2,(t3:4,t4:4)i4:3)i2:2,(t5:4,t6:4)i5:6)i1;"
phy <- ape::read.tree(text=tree)</pre>
phy
ape::plot.phylo(phy, type="p", use.edge.length=TRUE,
show.node.label=TRUE)
# a subtree specified via an internal node label
subphy <- dcSubtreeClade(phy, choose.node.label=i2)</pre>
subphy
ape::plot.phylo(subphy, type="p", use.edge.length=TRUE,
show.node.label=TRUE)
```

dcSubtreeTips

Function to extract a tip-induced subtree from a phylo-formatted phylogenetic tree

## **Description**

dcSubtreeTips is supposed to extract a tip-induced subtree from a phylo-formatted phylogenetic tree. In addition to the tree in subject, another input is a vector containing tip labels of interest. From valid tip labels, there are two types of subtree to extract. One is first induce clade (an internal node) from tip labels, and then the subtree is extracted under the induced clade. Another type is to extract a subtree only containing given tip labels; in this situation, some internal nodes perhaps need to further trimmed. The resulting subtree is also represented as an object of class 'phylo'.

## Usage

```
dcSubtreeTips(phy, choose.tip.labels = NULL, subtree.type = c("clade",
"tips_only"), verbose = T)
```

### Arguments

```
phy an object of class 'phylo' choose.tip.labels a character specifying which tips are chosen
```

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subtree.type a character specifying how to extract subtree from given tips. It can be 'clade'

or 'tips\_only'. The former is first induce clade (an internal node) from tip labels, and then to extract the subtree under the induced clade. The latter is to directly extract the subtree only containing given tip labels, (if necessary), after trimming

out unnecessary internal nodes

verbose logical to indicate whether the messages will be displayed in the screen. By

default, it sets to TRUE for display

#### Value

an object of class 'phylo'

#### Note

nonde

#### See Also

dcTreeConnectivity, dcSubtreeClade

## **Examples**

```
# 1) with internal node labels
tree <- "(((t1:5,t2:5)i3:2,(t3:4,t4:4)i4:3)i2:2,(t5:4,t6:4)i5:6)i1;"
phy <- ape::read.tree(text=tree)</pre>
ape::plot.phylo(phy, type="p", use.edge.length=TRUE,
show.node.label=TRUE)
# 2) tip labels of interest
choose.tip.labels <- c(t1,t2,t3)
# 2a) extract subtree via an induced clade
subphy <- dcSubtreeTips(phy, choose.tip.labels, subtree.type="clade")</pre>
ape::plot.phylo(subphy, type="p", use.edge.length=TRUE,
show.node.label=TRUE)
# 2b) extract subtree containing only tips
subphy <- dcSubtreeTips(phy, choose.tip.labels,</pre>
subtree.type="tips_only")
ape::plot.phylo(subphy, type="p", use.edge.length=TRUE,
show.node.label=TRUE)
```

dcSupraBetter

Function to find supra-domains with better scores than their individual domains

## **Description**

dcSupraBetter is supposed to find supra-domains with better scores than their individual domains.

## Usage

```
dcSupraBetter(input.file, output.file = NULL, verbose = T)
```

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### **Arguments**

input.file

an input file used to build the object. This input file contains original annotations between domains/features and ontology terms, along with the hypergeometric scores (hscore) in support for their annotations. For example, a file containing original annotations between SCOP domain architectures and GO terms can be found in <a href="http://dcgor.r-forge.r-project.org/data/Feature/Feature2GO.sf.txt">http://dcgor.r-forge.r-project.org/data/Feature/Feature2GO.sf.txt</a>. As seen in this example, the input file must contain the header (in the first row) and three columns: 1st column for 'Feature\_id' (here SCOP domain architectures), 2nd column for 'Term\_id' (GO terms), and 3rd column for 'Score' (hscore)

output.file

an output file containing results. If not NULL, a tab-delimited text file will be also written out, with 1st column 'Feature\_id' for features/domains, 2nd column 'Term\_id' for ontology terms, 3rd column 'Score' for hypergeometric scores (indicative of strength for feature-term associations). Otherwise, there is no output file (by default)

verbose

logical to indicate whether the messages will be displayed in the screen. By default, it sets to TRUE for display

#### Value

a data frame containing three columns: 1st column 'Feature\_id' for features, 2nd 'Term\_id' for terms, and 3rd 'Score' for the hypergeometric score indicative of strength of associations beteen features and terms

#### Note

When 'output.file' is specified, a tab-delimited text file is output, with the column names: 1st column 'Feature\_id' for features, 2nd 'Term\_id' for terms, and 3rd 'Score' for the hypergeometric score indicative of strength of associations beteen features and terms

# See Also

dcList2Matrix

## **Examples**

```
input.file <-
"http://dcgor.r-forge.r-project.org/data/Feature/Feature2GO.sf.txt"
res <- dcSupraBetter(input.file)
res[1:10,]</pre>
```

dcTreeConnectivity

Function to calculate the sparse connectivity matrix between parents and children from a phylo-formatted phylogenetic tree

## Description

dcTreeConnectivity is supposed to calculate the sparse connectivity matrix between parents and children from a phylo-formatted phylogenetic tree. The matrix has internal nodes (in rows) and tips plus internal nodes (in columns). For a row (an internal node; as a parent), the non-zeros indicate all its descendants/children.

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### Usage

```
dcTreeConnectivity(phy, verbose = T)
```

## **Arguments**

phy an object of class 'phylo'

verbose logical to indicate whether the messages will be displayed in the screen. By

default, it sets to TRUE for display

### Value

a sparse matrix of  $Nnode \times Ntip + Nnode$ , where Ntip and Nnode are the number of tips and internal nodes. A non-zero entry indicates a pair of a parent and its child.

### Note

None

### See Also

dcTreeConnectivity

## **Examples**

```
# a newick tree
tree <- "(((t1:5,t2:5):2,(t3:4,t4:4):3):2,(t5:4,t6:4):6);"
phy <- ape::read.tree(text=tree)

# connectivity matrix
res <- dcTreeConnectivity(phy)
dim(res)
# convert to a full Matrix
as.matrix(res)</pre>
```

Dnetwork-class

Definition for S4 class Dnetwork

# Description

Dnetwork is an S4 class to store a domain network, such as the one from semantic similarity between pairs of domains by dcDAGdomainSim. It has 2 slots: nodeInfo and adjMatrix

# Value

Class Dnetwork

indirect domain network

#### **Slots**

nodeInfo An object of S4 class InfoDataFrame, describing information on nodes/domains. adjMatrix An object of S4 class AdjData, containing symmetric adjacency data matrix for an

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#### Creation

An object of this class can be created via: new("Dnetwork", nodeInfo, adjMatrix)

#### Methods

Class-specific methods:

- dim(): retrieve the dimension in the object
- adjMatrix(): retrieve the slot 'adjMatrix' in the object
- nodeInfo(): retrieve the slot 'nodeInfo' (as class InfoDataFrame) in the object
- nInfo(): retrieve nodeInfo (as data.frame) in the object
- nodeNames(): retrieve node/term names (ie, row names of nodeInfo) in the object
- id(): retrieve domain id (ie, column 'id' of nodeInfo) in the object, if any
- level(): retrieve domain level (ie, column 'level' of nodeInfo) in the object, if any
- description(): retrieve domain description (ie, column 'description' of nodeInfo) in the object, if any

## Standard generic methods:

- str(): compact display of the content in the object
- show(): abbreviated display of the object
- as(matrix, "Dnetwork"): convert a matrix to an object of class Dnetwork
- as(dgCMatrix, "Dnetwork"): convert a dgCMatrix (a sparse matrix) to an object of class Dnetwork
- [i]: get the subset of the same class

### Access

Ways to access information on this class:

- showClass("Dnetwork"): show the class definition
- showMethods(classes="Dnetwork"): show the method definition upon this class
- getSlots("Dnetwork"): get the name and class of each slot in this class
- slotNames("Dnetwork"): get the name of each slot in this class
- selectMethod(f, signature="Dnetwork"): retrieve the definition code for the method 'f' defined in this class

## See Also

Dnetwork-method

```
# create an object of class Dnetwork, only given a matrix
adjM <- matrix(runif(25),nrow=5,ncol=5)
as(adjM, "Dnetwork")

# create an object of class Dnetwork, given a matrix plus information on nodes
# 1) create nodeI: an object of class InfoDataFrame
data <- data.frame(id=paste("Domain", 1:5, sep="_"),</pre>
```

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```
level=rep("SCOP",5), description=I(LETTERS[1:5]),
row.names=paste("Domain", 1:5, sep="_"))
nodeI <- new("InfoDataFrame", data=data)</pre>
nodeI
# 2) create an object of class Dnetwork
# VERY IMPORTANT: make sure having consistent names between nodeInfo and adjMatrix
adjM <- matrix(runif(25),nrow=5,ncol=5)</pre>
colnames(adjM) <- rownames(adjM) <- rowNames(nodeI)</pre>
x <- new("Dnetwork", adjMatrix=adjM, nodeInfo=nodeI)</pre>
# 3) look at various methods defined on class Dnetwork
dim(x)
adjMatrix(x)
nodeInfo(x)
nInfo(x)
nodeNames(x)
id(x)
level(x)
description(x)
# 4) get the subset
x[1:2]
```

Dnetwork-method

Methods defined for S4 class Dnetwork

## **Description**

Methods defined for class Dnetwork.

## Usage

```
## S4 method for signature Dnetwork
dim(x)

## S4 method for signature Dnetwork
adjMatrix(x)

## S4 method for signature Dnetwork
nodeInfo(x)

## S4 method for signature Dnetwork
nInfo(object)

## S4 method for signature Dnetwork
nodeNames(object)

## S4 method for signature Dnetwork
id(object)

## S4 method for signature Dnetwork
level(object)

## S4 method for signature Dnetwork
```

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```
description(object)
## S4 method for signature Dnetwork
show(object)
## S4 method for signature Dnetwork, ANY, ANY, ANY
x[i, j, ..., drop = FALSE]
```

### **Arguments**

X	an object of class Dnetwork
object	an object of class Dnetwork

i an indexj an index

... additional parameters

drop a logic for matrices and arrays. If TRUE the result is coerced to the lowest possi-

ble dimension. This only works for extracting elements, not for the replacement

#### See Also

Dnetwork-class

Eoutput-class

Definition for S4 class Eoutput

## Description

Eoutput is an S4 class to store output from enrichment analysis by dcEnrichment.

### Value

Class Eoutput

### **Slots**

domain A character specifying the domain identity

ontology A character specifying the ontology identity

term\_info A data.frame of nTerm X 5 containing term information, where nTerm is the number of terms in consideration, and the 5 columns are "term\_id" (i.e. "Term ID"), "term\_name" (i.e. "Term Name"), "namespace" (i.e. "Term Namespace"), "distance" (i.e. "Term Distance") and "IC" (i.e. "Information Content for the term based on annotation frequency by it")

anno A list of terms, each storing annotated domains (also within the background domains). Always, terms are identified by "term\_id" and domain members identified by their ids (e.g. sunids for SCOP domains)

data A vector containing input data in dcEnrichment. It is not always the same as the input data as only those mappable are retained

background A vector containing background in dcEnrichment. It is not always the same as the input background (if provided by the user) as only those mappable are retained

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overlap A list of terms, each storing domains overlapped between domains annotated by a term and domains in the input data (i.e. the domains of interest). Always, terms are identified by "term\_id" and domain members identified by their ids (e.g. sunids for SCOP domains)

zscore A vector of terms, containing z-scores

pvalue A vector of terms, containing p-values

adjp A vector of terms, containing adjusted p-values. It is the p value but after being adjusted for multiple comparisons

#### Creation

An object of this class can be created via: new("Eoutput", domain, ontology, term\_info, anno, data, overlap,

#### Methods

Class-specific methods:

- zscore(): retrieve the slot 'zscore' in the object
- pvalue(): retrieve the slot 'pvalue' in the object
- adjp(): retrieve the slot 'adjp' in the object
- view(): retrieve an integrated data.frame used for viewing the object
- write(): write the object into a local file

Standard generic methods:

- str(): compact display of the content in the object
- show(): abbreviated display of the object

#### Access

Ways to access information on this class:

- showClass("Eoutput"): show the class definition
- showMethods(classes="Eoutput"): show the method definition upon this class
- getSlots("Eoutput"): get the name and class of each slot in this class
- slotNames("Eoutput"): get the name of each slot in this class
- selectMethod(f, signature="Eoutput"): retrieve the definition code for the method 'f' defined in this class

#### See Also

Eoutput-method

```
# 1) load SCOP.sf (as InfoDataFrame object)
SCOP.sf <- dcRDataLoader(SCOP.sf)
# randomly select 20 domains
data <- sample(rowNames(SCOP.sf), 20)
# 2) perform enrichment analysis, producing an object of S4 class Eoutput
eoutput <- dcEnrichment(data, domain="SCOP.sf", ontology="GOMF")
eoutput</pre>
```

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```
# 3) write into the file Eoutput.txt in your local directory
write(eoutput, file=Eoutput.txt)

# 4) view the top 5 significant terms
view(eoutput, top_num=5, sortBy="pvalue", details=TRUE)

# 4) retrieve several slots directly
zscore(eoutput)[1:5]
pvalue(eoutput)[1:5]
adjp(eoutput)[1:5]
```

Eoutput-method

Methods defined for S4 class Eoutput

## **Description**

Methods defined for S4 class Eoutput.

### Usage

```
## S4 method for signature Eoutput
show(object)

## S4 method for signature Eoutput
zscore(x)

## S4 method for signature Eoutput
pvalue(x)

## S4 method for signature Eoutput
adjp(x)

## S4 method for signature Eoutput
view(x, top_num = 5, sortBy = c("pvalue", "adjp",
"zscore", "nAnno", "nOverlap", "none"), decreasing = NULL, details = T)

## S4 method for signature Eoutput
write(x, file = "Eoutput.txt", verbose = T)
```

# Arguments

object	an object of S4 class Eoutput. Usually this is an output from dcEnrichment
x	an object of S4 class Eoutput. Usually this is an output from dcEnrichment
top_num	the maximum number (5, by default) of terms will be viewed. If NULL or NA, all terms will be viewed (this can be used for the subsequent saving)
sortBy	which statistics will be used for sorting and viewing terms. It can be "pvalue" for p value, "adjp" for adjusted p value, "zscore" for enrichment z-score, "nAnno" for the number in domains annotated by a term, "nOverlap" for the number in overlaps, and "none" for ordering simply according to ID of terms

eTOL

decreasing	logical to indicate whether to sort in a decreasing order. If it is null, by default it will be true for "zscore", "nAnno" or "nOverlap"; otherwise false
details	logical to indicate whether the detailed information of terms is also viewed. By default, it sets to TRUE for the inclusion
file	a character specifying a file name written into. By default, it is 'Eoutput.txt'
verbose	logical to indicate whether the messages will be displayed in the screen. By default, it sets to true for display

#### Value

view(x) returns a data frame with following components:

• term\_id: term ID

• nAnno: number in domains annotated by a term

• nGroup: number in domains from the input group

• nOverlap: number in overlaps

• zscore: enrichment z-score

• pvalue: p value

• adjp: adjusted p value

• term\_name: term name

• term\_namespace: term namespace; optional, it is only appended when "details" is true

• term\_distance: term distance; optional, it is only appended when "details" is true

• members: members (represented as domain IDs) in overlaps; optional, it is only appended when "details" is true

write(x) also returns the same data frame as view(x), in addition to a specified local file.

### See Also

Eoutput-class

eT0L

eukaryotic Tree Of Life (eTOL)

## **Description**

A 'phylo' object that contains information about eukaryotic part of species tree of life (eTOL). It is a rooted binary tree. Tips represent extant genomes. Since its reconstruction is guided under the NCBI taxonomy, each internal node is either mapped onto a unique taxonomic identifier or left empty (assumedly a hypothetical unknown ancestral genome).

## Usage

data(eTOL)

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#### Value

an object of class "phylo" with the following components:

- Nnode: the number of (internal) nodes
- tip.label: a vector giving the names of the tips (i.e., "left\_id" to define the post-ordered binary tree structure)
- node.label: a vector giving the names of the internal nodes (i.e., "left\_id" to define the postordered binary tree structure)
- genome\_info: a matrix of all nodes (including tips and internal nodes) X 8, giving extant/ancestral genome information: "left\_id" (unique and used as internal id), "right\_id" (used in combination with "left\_id" to define the post-ordered binary tree structure), "taxon\_id" (NCBI taxonomy id, if matched), "genome" (2-letter genome identifiers used in SUPER-FAMILY, if being extant), "name" (NCBI taxonomy name, if matched), "rank" (NCBI taxonomy rank, if matched), "branchlength" (branch length in relevance to the parent), and "common\_name" (NCBI taxonomy common name, if matched and existed)
- edge: a two-column matrix of mode numeric where each row represents an edge of the tree; the nodes and the tips are symbolized with numbers; the tips are numbered 1, 2, ..., and the internal nodes are numbered after the tips. For each row, the first column gives the ancestor
- edge.length: a numeric vector giving the lengths of the branches given by 'edge'
- root.length: a numeric value giving the length of the branch at the root
- connectivity: a matrix of internal nodes X all nodes (including tips and internal nodes), with 1 for the presence of a ancestor-descenant path, and 0 otherwise

### References

Fang et al. (2013) A daily-updated tree of (sequenced) life as a reference for genome research. *Scientific reports*, 3:2015.

```
data(eTOL)
eTOL
# list all components
names(eTOL)
# extract information about the first 5 genomes
eTOL$genome_info[1:5,]
# look at the dimension of connectivity
dim(eTOL$connectivity)
## Not run:
# visualise the connectivity matrix
Ntip <- length(eTOL$tip.label) # number of tips
Nnode <- eTOL$Nnode # number of internal nodes
data <- eTOL$connectivity
visHeatmapAdv(data, Rowv=FALSE,Colv=FALSE, zlim=c(0,1), colormap="gray-black", add.expr=abline(v=c(1,Ntip+""))
## End(Not run)</pre>
```

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Feature2GOBP.interpro Annotations and scores between InterPro domains and Gene Ontology Biological Process (GOBP).

### **Description**

An object of class "HIS" that contains annotations and scores between Gene Ontology Biological Process terms and InterPro domains. This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

### Usage

Feature2GOBP.interpro <- dcRDataLoader(RData=Feature2GOBP.interpro)</pre>

### Value

an object of class HIS. It has three components for "hscore", "ic" and "slim":

- hscore: a list of domain-related features, each with a term-named vector containing hypergeometric score (hscore)
- ic: a term-named vector containing information content (IC). Terms are ordered first by IC and then by longest-path level, making sure that for terms with the same IC, parental terms always come first
- slim: a list of four slims, each with a term-named vector containing information content (IC). Slim '1' for very general terms, '2' for general terms, '3' for specific terms, '4' for very specific terms

#### References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

Fang H and Gough J. (2013) A domain-centric solution to functional genomics via dcGO Predictor. *BMC Bioinformatics*, 14(Suppl 3):S9.

## **Examples**

# load data
Feature2GOBP.interpro <- dcRDataLoader(RData=Feature2GOBP.interpro)
names(Feature2GOBP.interpro)</pre>

Feature2GOBP.pfam

Annotations and scores between Pfam domains/combinations and Gene Ontology Biological Process (GOBP).

### **Description**

An object of class "HIS" that contains annotations and scores between Gene Ontology Biological Process terms and Pfam domains/combinations. This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

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#### Usage

Feature2GOBP.pfam <- dcRDataLoader(RData=Feature2GOBP.pfam)</pre>

#### Value

an object of class HIS. It has three components for "hscore", "ic" and "slim":

- hscore: a list of domain-related features, each with a term-named vector containing hypergeometric score (hscore)
- ic: a term-named vector containing information content (IC). Terms are ordered first by IC and then by longest-path level, making sure that for terms with the same IC, parental terms always come first
- slim: a list of four slims, each with a term-named vector containing information content (IC). Slim '1' for very general terms, '2' for general terms, '3' for specific terms, '4' for very specific terms

#### References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

Fang H and Gough J. (2013) A domain-centric solution to functional genomics via dcGO Predictor. *BMC Bioinformatics*, 14(Suppl 3):S9.

## **Examples**

```
# load data
Feature2GOBP.pfam <- dcRDataLoader(RData=Feature2GOBP.pfam)
names(Feature2GOBP.pfam)</pre>
```

Feature2GOBP.sf

Annotations and scores between SCOP domains/combinations (at the superfamily level; sf) and Gene Ontology Biological Process (GOBP).

## **Description**

An object of class "HIS" that contains annotations and scores between Gene Ontology Biological Process terms and SCOP domains/combinations (at the superfamily level; sf). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

# Usage

```
Feature2GOBP.sf <- dcRDataLoader(RData=Feature2GOBP.sf)</pre>
```

### Value

an object of class HIS. It has three components for "hscore", "ic" and "slim":

- hscore: a list of domain-related features, each with a term-named vector containing hypergeometric score (hscore)
- ic: a term-named vector containing information content (IC). Terms are ordered first by IC and then by longest-path level, making sure that for terms with the same IC, parental terms always come first

• slim: a list of four slims, each with a term-named vector containing information content (IC). Slim '1' for very general terms, '2' for general terms, '3' for specific terms, '4' for very specific terms

#### References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

Fang H and Gough J. (2013) A domain-centric solution to functional genomics via dcGO Predictor. *BMC Bioinformatics*, 14(Suppl 3):S9.

## **Examples**

```
# load data
Feature2GOBP.sf <- dcRDataLoader(RData=Feature2GOBP.sf)
names(Feature2GOBP.sf)</pre>
```

Feature2GOCC.interpro Annotations and scores between InterPro domains and Gene Ontology Cellular Component (GOCC).

## Description

An object of class "HIS" that contains annotations and scores between Gene Ontology Cellular Component terms and InterPro domains. This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

### Usage

```
Feature2GOCC.interpro <- dcRDataLoader(RData=Feature2GOCC.interpro)</pre>
```

#### Value

an object of class HIS. It has three components for "hscore", "ic" and "slim":

- hscore: a list of domain-related features, each with a term-named vector containing hypergeometric score (hscore)
- ic: a term-named vector containing information content (IC). Terms are ordered first by IC and then by longest-path level, making sure that for terms with the same IC, parental terms always come first
- slim: a list of four slims, each with a term-named vector containing information content (IC). Slim '1' for very general terms, '2' for general terms, '3' for specific terms, '4' for very specific terms

#### References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

Fang H and Gough J. (2013) A domain-centric solution to functional genomics via dcGO Predictor. *BMC Bioinformatics*, 14(Suppl 3):S9.

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### **Examples**

```
# load data
Feature2GOCC.interpro <- dcRDataLoader(RData=Feature2GOCC.interpro)
names(Feature2GOCC.interpro)</pre>
```

Feature2GOCC.pfam Annotations and scores between Pfam domains/combinations and Gene Ontology Cellular Component (GOCC).

### **Description**

An object of class "HIS" that contains annotations and scores between Gene Ontology Cellular Component terms and Pfam domains/combinations. This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

## Usage

Feature2GOCC.pfam <- dcRDataLoader(RData=Feature2GOCC.pfam)</pre>

### Value

an object of class HIS. It has three components for "hscore", "ic" and "slim":

- hscore: a list of domain-related features, each with a term-named vector containing hypergeometric score (hscore)
- ic: a term-named vector containing information content (IC). Terms are ordered first by IC and then by longest-path level, making sure that for terms with the same IC, parental terms always come first
- slim: a list of four slims, each with a term-named vector containing information content (IC). Slim '1' for very general terms, '2' for general terms, '3' for specific terms, '4' for very specific terms

#### References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

Fang H and Gough J. (2013) A domain-centric solution to functional genomics via dcGO Predictor. *BMC Bioinformatics*, 14(Suppl 3):S9.

```
# load data
Feature2GOCC.pfam <- dcRDataLoader(RData=Feature2GOCC.pfam)
names(Feature2GOCC.pfam)</pre>
```

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Feature2GOCC.sf	Annotations and scores between SCOP domains/combinations (at
	the superfamily level; sf) and Gene Ontology Cellular Component (GOCC).

## **Description**

An object of class "HIS" that contains annotations and scores between Gene Ontology Cellular Component terms and SCOP domains/combinations (at the superfamily level; sf). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

# Usage

```
Feature2GOCC.sf <- dcRDataLoader(RData=Feature2GOCC.sf)</pre>
```

### Value

an object of class HIS. It has three components for "hscore", "ic" and "slim":

- hscore: a list of domain-related features, each with a term-named vector containing hypergeometric score (hscore)
- ic: a term-named vector containing information content (IC). Terms are ordered first by IC and then by longest-path level, making sure that for terms with the same IC, parental terms always come first
- slim: a list of four slims, each with a term-named vector containing information content (IC). Slim '1' for very general terms, '2' for general terms, '3' for specific terms, '4' for very specific terms

### References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

Fang H and Gough J. (2013) A domain-centric solution to functional genomics via dcGO Predictor. *BMC Bioinformatics*, 14(Suppl 3):S9.

```
# load data
Feature2GOCC.sf <- dcRDataLoader(RData=Feature2GOCC.sf)
names(Feature2GOCC.sf)</pre>
```

Feature2GOMF.interpro Annotations and scores between InterPro domains and Gene Ontology Molecular Function (GOMF).

### **Description**

An object of class "HIS" that contains annotations and scores between Gene Ontology Molecular Function terms and InterPro domains. This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

### Usage

Feature2GOMF.interpro <- dcRDataLoader(RData=Feature2GOMF.interpro)</pre>

### Value

an object of class HIS. It has three components for "hscore", "ic" and "slim":

- hscore: a list of domain-related features, each with a term-named vector containing hypergeometric score (hscore)
- ic: a term-named vector containing information content (IC). Terms are ordered first by IC and then by longest-path level, making sure that for terms with the same IC, parental terms always come first
- slim: a list of four slims, each with a term-named vector containing information content (IC). Slim '1' for very general terms, '2' for general terms, '3' for specific terms, '4' for very specific terms

#### References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

Fang H and Gough J. (2013) A domain-centric solution to functional genomics via dcGO Predictor. *BMC Bioinformatics*, 14(Suppl 3):S9.

## **Examples**

```
# load data
Feature2GOMF.interpro <- dcRDataLoader(RData=Feature2GOMF.interpro)
names(Feature2GOMF.interpro)</pre>
```

Feature2GOMF.pfam

Annotations and scores between Pfam domains/combinations and Gene Ontology Molecular Function (GOMF).

### **Description**

An object of class "HIS" that contains annotations and scores between Gene Ontology Molecular Function terms and Pfam domains/combinations. This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

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### **Usage**

Feature2GOMF.pfam <- dcRDataLoader(RData=Feature2GOMF.pfam)</pre>

#### Value

an object of class HIS. It has three components for "hscore", "ic" and "slim":

- hscore: a list of domain-related features, each with a term-named vector containing hypergeometric score (hscore)
- ic: a term-named vector containing information content (IC). Terms are ordered first by IC and then by longest-path level, making sure that for terms with the same IC, parental terms always come first
- slim: a list of four slims, each with a term-named vector containing information content (IC). Slim '1' for very general terms, '2' for general terms, '3' for specific terms, '4' for very specific terms

#### References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

Fang H and Gough J. (2013) A domain-centric solution to functional genomics via dcGO Predictor. *BMC Bioinformatics*, 14(Suppl 3):S9.

## **Examples**

```
# load data
Feature2GOMF.pfam <- dcRDataLoader(RData=Feature2GOMF.pfam)
names(Feature2GOMF.pfam)</pre>
```

Feature2GOMF.sf

Annotations and scores between SCOP domains/combinations (at the superfamily level; sf) and Gene Ontology Molecular Function (GOMF).

## **Description**

An object of class "HIS" that contains annotations and scores between Gene Ontology Molecular Function terms and SCOP domains/combinations (at the superfamily level; sf). This data is prepared based on the dcGO database (see <a href="http://supfam.org/SUPERFAMILY/dcGO/">http://supfam.org/SUPERFAMILY/dcGO/</a>).

# Usage

```
Feature2GOMF.sf <- dcRDataLoader(RData=Feature2GOMF.sf)</pre>
```

## Value

an object of class HIS. It has three components for "hscore", "ic" and "slim":

 hscore: a list of domain-related features, each with a term-named vector containing hypergeometric score (hscore)

- ic: a term-named vector containing information content (IC). Terms are ordered first by IC and then by longest-path level, making sure that for terms with the same IC, parental terms always come first
- slim: a list of four slims, each with a term-named vector containing information content (IC). Slim '1' for very general terms, '2' for general terms, '3' for specific terms, '4' for very specific terms

#### References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

Fang H and Gough J. (2013) A domain-centric solution to functional genomics via dcGO Predictor. *BMC Bioinformatics*, 14(Suppl 3):S9.

### **Examples**

```
# load data
Feature2GOMF.sf <- dcRDataLoader(RData=Feature2GOMF.sf)
names(Feature2GOMF.sf)</pre>
```

Feature2HPPA.interpro Annotations and scores between InterPro domains and Human Phenotype Phenotypic Abnormality (HPPA).

### **Description**

An object of class "HIS" that contains annotations and scores between Human Phenotype Phenotypic Abnormality terms and InterPro domains. This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

# Usage

Feature2HPPA.interpro <- dcRDataLoader(RData=Feature2HPPA.interpro)</pre>

### Value

an object of class HIS. It has three components for "hscore", "ic" and "slim":

- hscore: a list of domain-related features, each with a term-named vector containing hypergeometric score (hscore)
- ic: a term-named vector containing information content (IC). Terms are ordered first by IC and then by longest-path level, making sure that for terms with the same IC, parental terms always come first
- slim: a list of four slims, each with a term-named vector containing information content (IC). Slim '1' for very general terms, '2' for general terms, '3' for specific terms, '4' for very specific terms

### References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

Fang H and Gough J. (2013) A domain-centric solution to functional genomics via dcGO Predictor. *BMC Bioinformatics*, 14(Suppl 3):S9.

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### **Examples**

```
# load data
Feature2HPPA.interpro <- dcRDataLoader(RData=Feature2HPPA.interpro)
names(Feature2HPPA.interpro)</pre>
```

Feature2HPPA.pfam

Annotations and scores between Pfam domains/combinations and Human Phenotype Phenotypic Abnormality (HPPA).

### **Description**

An object of class "HIS" that contains annotations and scores between Human Phenotype Phenotypic Abnormality terms and Pfam domains/combinations. This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

## Usage

Feature2HPPA.pfam <- dcRDataLoader(RData=Feature2HPPA.pfam)

### Value

an object of class HIS. It has three components for "hscore", "ic" and "slim":

- hscore: a list of domain-related features, each with a term-named vector containing hypergeometric score (hscore)
- ic: a term-named vector containing information content (IC). Terms are ordered first by IC and then by longest-path level, making sure that for terms with the same IC, parental terms always come first
- slim: a list of four slims, each with a term-named vector containing information content (IC). Slim '1' for very general terms, '2' for general terms, '3' for specific terms, '4' for very specific terms

#### References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

Fang H and Gough J. (2013) A domain-centric solution to functional genomics via dcGO Predictor. *BMC Bioinformatics*, 14(Suppl 3):S9.

```
# load data
Feature2HPPA.pfam <- dcRDataLoader(RData=Feature2HPPA.pfam)
names(Feature2HPPA.pfam)</pre>
```

Feature2HPPA.sf 79

Feature2HPPA.sf	Ametations and accuse between SCOD demains (a white ations (at the
reatureznera.Sr	Annotations and scores between SCOP domains/combinations (at the
	superfamily level; sf) and Human Phenotype Phenotypic Abnormality
	(HPPA).

## **Description**

An object of class "HIS" that contains annotations and scores between Human Phenotype Phenotypic Abnormality terms and SCOP domains/combinations (at the superfamily level; sf). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

## Usage

```
Feature2HPPA.sf <- dcRDataLoader(RData=Feature2HPPA.sf)</pre>
```

### Value

an object of class HIS. It has three components for "hscore", "ic" and "slim":

- hscore: a list of domain-related features, each with a term-named vector containing hypergeometric score (hscore)
- ic: a term-named vector containing information content (IC). Terms are ordered first by IC and then by longest-path level, making sure that for terms with the same IC, parental terms always come first
- slim: a list of four slims, each with a term-named vector containing information content (IC). Slim '1' for very general terms, '2' for general terms, '3' for specific terms, '4' for very specific terms

### References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

Fang H and Gough J. (2013) A domain-centric solution to functional genomics via dcGO Predictor. *BMC Bioinformatics*, 14(Suppl 3):S9.

```
# load data
Feature2HPPA.sf <- dcRDataLoader(RData=Feature2HPPA.sf)
names(Feature2HPPA.sf)</pre>
```

80 InfoDataFrame-class

InfoDataFrame-class Definition for S4 class InfoDataFrame

# Description

InfoDataFrame has two slots: data and dimLabels.

### Value

Class InfoDataFrame

#### Slots

data A data.frame containing terms (rows) and measured variables (columns). dimLabels A character descripting labels for rows and columns.

#### Creation

An object of this class can be created via: new("InfoDataFrame", data, dimLabels)

#### Methods

Class-specific methods:

- dim(): retrieve the dimension in the object
- nrow(): retrieve number of rows in the object
- ncol(): retrieve number of columns in the object
- rowNames(): retrieve names of rows in the object
- colNames(): retrieve names of columns in the object
- dimLabels(): retrieve the slot 'dimLabels', containing labels used for display of rows and columns in the object
- Data(): retrieve the slot 'data' in the object

## Standard generic methods:

- str(): compact display of the content in the object
- show(): abbreviated display of the object
- as(data.frame, "InfoDataFrame"): convert a data.frame to an object of class InfoDataFrame
- [i,j]: get the subset of the same class

#### Access

Ways to access information on this class:

- showClass("InfoDataFrame"): show the class definition
- showMethods(classes="InfoDataFrame"): show the method definition upon this class
- getSlots("InfoDataFrame"): get the name and class of each slot in this class
- slotNames("InfoDataFrame"): get the name of each slot in this class
- selectMethod(f, signature="InfoDataFrame"): retrieve the definition code for the method 'f' defined in this class

InfoDataFrame-method 81

### See Also

InfoDataFrame-method

### **Examples**

```
# generate data on domain information on
data <- data.frame(x=1:10, y=I(LETTERS[1:10]),</pre>
row.names=paste("Domain", 1:10, sep="_"))
dimLabels <- c("rowLabels", "colLabels")</pre>
# create an object of class InfoDataFrame
x <- new("InfoDataFrame", data=data, dimLabels=dimLabels)</pre>
# alternatively, using coerce methods
x <- as(data, "InfoDataFrame")</pre>
# look at various methods defined on class Anno
dimLabels(x)
dim(x)
nrow(x)
ncol(x)
rowNames(x)
colNames(x)
Data(x)
x[1:3,]
```

InfoDataFrame-method Methods defined for S4 class InfoDataFrame

### **Description**

Methods defined for class InfoDataFrame.

## Usage

```
dimLabels(x)
## S4 method for signature InfoDataFrame
dimLabels(x)
## S4 method for signature InfoDataFrame
dim(x)
## S4 method for signature InfoDataFrame
nrow(x)
## S4 method for signature InfoDataFrame
ncol(x)
## S4 method for signature InfoDataFrame
rowNames(x)
## S4 method for signature InfoDataFrame
```

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```
colNames(x)
## S4 method for signature InfoDataFrame
Data(x)
## S4 method for signature InfoDataFrame
show(object)
## S4 method for signature InfoDataFrame,ANY,ANY,ANY
x[i, j, ..., drop = FALSE]
```

### **Arguments**

x an object of class InfoDataFrame
object an object of class InfoDataFrame
i an index

j an index

... additional parameters

drop a logic for matrices and arrays. If TRUE the result is coerced to the lowest possi-

ble dimension. This only works for extracting elements, not for the replacement

#### See Also

InfoDataFrame-class

InterPro

InterPro domains (InterPro).

## **Description**

An object of class "InfoDataFrame" that contains information on InterPro domains (InterPro). This data is prepared based on ftp://anonymous@ftp.ebi.ac.uk/pub/databases/interpro/Current/entry.list.

# Usage

```
data(InterPro)
```

#### Value

an object of class InfoDataFrame. It has slots for data and dimLabels:

- data: a data.frame containing information about 11638 annotatable domains (in rows), with 3 columns ("id" for InterPro ID, and "level" always equals "InterPro", "description" for InterPro description)
- dimLabels: a character describing labels for rows and columns in data

# References

Hunter et al. (2012) InterPro in 2011: new developments in the family and domain prediction database. *Nucleic Acids Res*, 40(Database issue):D306-12.

InterPro2GOBP 83

#### See Also

InfoDataFrame-class

### **Examples**

```
# load data
data(InterPro)
InterPro
# retrieve the dimension
dim(InterPro)
# retrieve names of columns
colNames(InterPro)
# retrieve the first 5 rows of data
Data(InterPro)[1:5,]
```

InterPro2GOBP

Annotations of InterPro domains by Gene Ontology Biological Process (GOBP).

## **Description**

An object of class "Anno" that contains associations between Gene Ontology Biological Process terms and InterPro domains. This data is prepared based on the InterPro database (see <a href="http://www.ebi.ac.uk/interpro/">http://www.ebi.ac.uk/interpro/</a>) and <a href="http://anonymous@ftp.ebi.ac.uk/pub/databases/interpro/Current/interpro2go">http://anonymous@ftp.ebi.ac.uk/pub/databases/interpro/Current/interpro2go</a>.

### Usage

data(InterPro2GOBP)

## Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- $\bullet\,$  annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for Inter-Pro ID, and "level" always equals "InterPro", "description" for InterPro description

#### References

Hunter et al. (2012) Manual GO annotation of predictive protein signatures: the InterPro approach to GO curation. *Database (Oxford)*, 2012:bar068.

## See Also

84 InterPro2GOCC

## **Examples**

```
# load data
data(InterPro2GOBP)
InterPro2GOBP
# retrieve info on ontology terms
termData(InterPro2GOBP)
# retrieve info on InterPro domains
domainData(InterPro2GOBP)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(InterPro2GOBP)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

InterPro2GOCC

Annotations of InterPro domains by Gene Ontology Cellular Component (GOCC).

## **Description**

An object of class "Anno" that contains associations between Gene Ontology Cellular Component terms and InterPro domains. This data is prepared based on the InterPro database (see <a href="http://www.ebi.ac.uk/interpro/">http://www.ebi.ac.uk/interpro/</a>) and <a href="http://anonymous@ftp.ebi.ac.uk/pub/databases/interpro/Current/interpro2go">http://anonymous@ftp.ebi.ac.uk/pub/databases/interpro/Current/interpro2go</a>.

# Usage

data(InterPro2GOCC)

## Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID"
   (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for Inter-Pro ID, and "level" always equals "InterPro", "description" for InterPro description

### References

Hunter et al. (2012) Manual GO annotation of predictive protein signatures: the InterPro approach to GO curation. *Database (Oxford)*, 2012:bar068.

## See Also

InterPro2GOMF 85

### **Examples**

```
# load data
data(InterPro2GOCC)
InterPro2GOCC
# retrieve info on ontology terms
termData(InterPro2GOCC)
# retrieve info on InterPro domains
domainData(InterPro2GOCC)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(InterPro2GOCC)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

InterPro2GOMF

Annotations of InterPro domains by Gene Ontology Molecular Function (GOMF).

## **Description**

An object of class "Anno" that contains associations between Gene Ontology Molecular Function terms and InterPro domains. This data is prepared based on the InterPro database (see <a href="http://www.ebi.ac.uk/interpro/">http://www.ebi.ac.uk/interpro/</a>) and <a href="http://anonymous@ftp.ebi.ac.uk/pub/databases/interpro/Current/interpro2go">http://anonymous@ftp.ebi.ac.uk/pub/databases/interpro/Current/interpro2go</a>.

# Usage

data(InterPro2GOMF)

## Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID"
   (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for Inter-Pro ID, and "level" always equals "InterPro", "description" for InterPro description

### References

Hunter et al. (2012) Manual GO annotation of predictive protein signatures: the InterPro approach to GO curation. *Database (Oxford)*, 2012:bar068.

## See Also

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### **Examples**

```
# load data
data(InterPro2GOMF)
InterPro2GOMF
# retrieve info on ontology terms
termData(InterPro2GOMF)
# retrieve info on InterPro domains
domainData(InterPro2GOMF)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(InterPro2GOMF)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

Onto-class

Definition for S4 class Onto

### **Description**

Onto has 2 slots: nodeInfo and adjMatrix

#### Value

Class Onto

## **Slots**

nodeInfo An object of S4 class InfoDataFrame, describing information on nodes/terms.

adjMatrix An object of S4 class AdjData, containing adjacency data matrix (for a direct graph), with rows for parent (arrow-outbound) and columns for children (arrow-inbound)

### Creation

An object of this class can be created via: new("Onto", nodeInfo,adjMatrix)

# Methods

Class-specific methods:

- dim(): retrieve the dimension in the object
- adjMatrix(): retrieve the slot 'adjMatrix' in the object
- nodeInfo(): retrieve the slot 'nodeInfo' (as class InfoDataFrame) in the object
- nInfo(): retrieve nodeInfo (as data.frame) in the object
- nodeNames(): retrieve node/term names (ie, row names of nodeInfo) in the object
- term\_id(): retrieve term id (ie, column 'term\_id' of nodeInfo) in the object, if any
- term\_name(): retrieve term id (ie, column 'term\_name' of nodeInfo) in the object, if any
- term\_namespace(): retrieve term id (ie, column 'term\_namespace' of nodeInfo) in the object, if any
- term\_distance(): retrieve term id (ie, column 'term\_distance' of nodeInfo) in the object, if any

Onto-class 87

### Standard generic methods:

- str(): compact display of the content in the object
- show(): abbreviated display of the object
- as(matrix, "Onto"): convert a matrix to an object of class Onto
- as (dgCMatrix, "Onto"): convert a dgCMatrix (a sparse matrix) to an object of class Onto
- [i]: get the subset of the same class

#### Access

Ways to access information on this class:

- showClass("Onto"): show the class definition
- showMethods(classes="Onto"): show the method definition upon this class
- getSlots("Onto"): get the name and class of each slot in this class
- slotNames("Onto"): get the name of each slot in this class
- selectMethod(f, signature="Onto"): retrieve the definition code for the method 'f' defined in this class

#### See Also

Onto-method

```
# create an object of class Onto, only given a matrix
adjM <- matrix(runif(25),nrow=5,ncol=5)</pre>
as(adjM, "Onto")
# create an object of class Onto, given a matrix plus information on nodes
# 1) create nodeI: an object of class InfoDataFrame
data <- data.frame(term_id=paste("Term", 1:5, sep="_"),</pre>
term_name=I(LETTERS[1:5]), term_namespace=rep("Namespace",5),
term_distance=1:5, row.names=paste("Term", 1:5, sep="_"))
nodeI <- new("InfoDataFrame", data=data)</pre>
nodeI
# 2) create an object of class Onto
# VERY IMPORTANT: make sure having consistent names between nodeInfo and adjMatrix
adjM <- matrix(runif(25),nrow=5,ncol=5)</pre>
colnames(adjM) <- rownames(adjM) <- rowNames(nodeI)</pre>
x <- new("Onto", adjMatrix=adjM, nodeInfo=nodeI)</pre>
# 3) look at various methods defined on class Onto
dim(x)
adjMatrix(x)
nodeInfo(x)
nInfo(x)
nodeNames(x)
term_id(x)
term_namespace(x)
term_distance(x)
# 4) get the subset
x[1:2]
```

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Onto-method

Methods defined for S4 class Onto

# Description

Methods defined for class Onto.

# Usage

```
## S4 method for signature Onto
dim(x)
## S4 method for signature Onto
adjMatrix(x)
## S4 method for signature Onto
nodeInfo(x)
## S4 method for signature Onto
nInfo(object)
## S4 method for signature Onto
nodeNames(object)
## S4 method for signature Onto
term_id(object)
## S4 method for signature Onto
term_name(object)
## S4 method for signature Onto
term_namespace(object)
## S4 method for signature Onto
term_distance(object)
## S4 method for signature Onto
show(object)
## S4 method for signature Onto, ANY, ANY, ANY
x[i, j, ..., drop = FALSE]
```

# Arguments

x	an object of class Onto
object	an object of class Onto
i	an index
j	an index
	additional parameters
drop	a logic for matrices and arrays. If TRUE the result is coerced to the lowest possible dimension. This only works for extracting elements, not for the replacement

onto.DO 89

#### See Also

Onto-class

onto.D0

Disease Ontology (DO).

### **Description**

An R object that contains information on Gene Ontology Biological Process terms. These terms are organised as a direct acyclic graph (DAG), which is further stored as an object of the class 'igraph' (see http://igraph.org/r/doc/aaa-igraph-package.html). This data is prepared based on http://sourceforge.net/p/diseaseontology/code/HEAD/tree/trunk/HumanDO.obo.

### Usage

data(onto.DO)

## Value

an object of S4 class Onto. It has slots for "nodeInfo" and "adjMatrix"

- nodeInfo: an object of S4 class InfoDataFrame, describing information on nodes/terms including: "term\_id" (i.e. Term ID), "term\_name" (i.e. Term Name), "term\_namespace" (i.e. Term Namespace), and "term\_distance" (i.e. Term Distance: the distance to the root; always 0 for the root itself)
- adjMatrix: an object of S4 class AdjData, containing adjacency data matrix, with rows for parent (arrow-outbound) and columns for children (arrow-inbound)

### References

Schriml et al. (2012) Disease Ontology: a backbone for disease semantic integration. *Nucleic Acids Res*, 40:D940-946.

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

## **Examples**

data(onto.DO)
onto.DO

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onto.EC

Enzyme Commission (EC).

### **Description**

An R object that contains information on Enzyme Commission terms. These terms are organised as a direct acyclic graph (DAG), which is further stored as an object of the class 'igraph' (see http://igraph.org/r/doc/aaa-igraph-package.html). Enzyme Commission (EC) is a resource focused on enzyme nomenclature, which is a system of naming enzymes (protein catalysts) with Cross-references to UniProt sequences. It uses four-digit EC numbers to define the reaction catalysed. The first three digits are to define the reaction catalysed and the fourth for a unique identifier (serial number).

# Usage

```
onto.EC <- dcRDataLoader(RData=onto.EC)</pre>
```

#### Value

an object of S4 class Onto. It has slots for "nodeInfo" and "adjMatrix"

- nodeInfo: an object of S4 class InfoDataFrame, describing information on nodes/terms including: "term\_id" (i.e. Term ID), "term\_name" (i.e. Term Name), "term\_namespace" (i.e. Term Namespace), and "term\_distance" (i.e. Term Distance: the distance to the root; always 0 for the root itself)
- adjMatrix: an object of S4 class AdjData, containing adjacency data matrix, with rows for parent (arrow-outbound) and columns for children (arrow-inbound)

### References

Fleischmann et al. (2004) IntEnz, the integrated relational enzyme database. *Nucleic Acids Res*, 32:D434-7.

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

### **Examples**

```
onto.EC <- dcRDataLoader(RData=onto.EC)
onto.EC</pre>
```

onto.GOBP

Gene Ontology Biological Process (GOBP).

## **Description**

An R object that contains information on Gene Ontology Biological Process terms. These terms are organised as a direct acyclic graph (DAG), which is further stored as an object of the class 'igraph' (see http://igraph.org/r/doc/aaa-igraph-package.html). This data is prepared based on http://www.geneontology.org/ontology/obo\_format\_1\_2/gene\_ontology.1\_2.obo. Only the edges with the relation (either 'is\_a' or 'part\_of') are retained.

onto.GOCC 91

## Usage

```
data(onto.GOBP)
```

#### Value

an object of S4 class Onto. It has slots for "nodeInfo" and "adjMatrix"

- nodeInfo: an object of S4 class InfoDataFrame, describing information on nodes/terms including: "term\_id" (i.e. Term ID), "term\_name" (i.e. Term Name), "term\_namespace" (i.e. Term Namespace), and "term\_distance" (i.e. Term Distance: the distance to the root; always 0 for the root itself)
- adjMatrix: an object of S4 class AdjData, containing adjacency data matrix, with rows for parent (arrow-outbound) and columns for children (arrow-inbound)

#### References

Ashburner et al. (2000) Gene ontology: tool for the unification of biology. *Nat Genet*, 25:25-29. Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

### **Examples**

data(onto.GOBP)
onto.GOBP

onto.GOCC

Gene Ontology Cellular Component (GOCC).

# Description

An R object that contains information on Gene Ontology Cellular Component terms. These terms are organised as a direct acyclic graph (DAG), which is further stored as an object of the class 'igraph' (see http://igraph.org/r/doc/aaa-igraph-package.html). This data is prepared based on http://www.geneontology.org/ontology/obo\_format\_1\_2/gene\_ontology.1\_2.obo. Only the edges with the relation (either 'is\_a' or 'part\_of') are retained.

### Usage

```
data(onto.GOCC)
```

#### Value

an object of S4 class Onto. It has slots for "nodeInfo" and "adjMatrix"

- nodeInfo: an object of S4 class InfoDataFrame, describing information on nodes/terms including: "term\_id" (i.e. Term ID), "term\_name" (i.e. Term Name), "term\_namespace" (i.e. Term Namespace), and "term\_distance" (i.e. Term Distance: the distance to the root; always 0 for the root itself)
- adjMatrix: an object of S4 class AdjData, containing adjacency data matrix, with rows for parent (arrow-outbound) and columns for children (arrow-inbound)

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### References

Ashburner et al. (2000) Gene ontology: tool for the unification of biology. *Nat Genet*, 25:25-29. Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

## **Examples**

data(onto.GOCC)
onto.GOCC

onto.GOMF

Gene Ontology Molecular Function (GOMF).

### **Description**

An R object that contains information on Gene Ontology Molecular Function terms. These terms are organised as a direct acyclic graph (DAG), which is further stored as an object of the class 'igraph' (see http://igraph.org/r/doc/aaa-igraph-package.html). This data is prepared based on http://www.geneontology.org/ontology/obo\_format\_1\_2/gene\_ontology.1\_2.obo. Only the edges with the relation (either 'is\_a' or 'part\_of') are retained.

## Usage

```
data(onto.GOMF)
```

## Value

an object of S4 class Onto. It has slots for "nodeInfo" and "adjMatrix"

- nodeInfo: an object of S4 class InfoDataFrame, describing information on nodes/terms including: "term\_id" (i.e. Term ID), "term\_name" (i.e. Term Name), "term\_namespace" (i.e. Term Namespace), and "term\_distance" (i.e. Term Distance: the distance to the root; always 0 for the root itself)
- adjMatrix: an object of S4 class AdjData, containing adjacency data matrix, with rows for parent (arrow-outbound) and columns for children (arrow-inbound)

## References

Ashburner et al. (2000) Gene ontology: tool for the unification of biology. *Nat Genet*, 25:25-29. Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

```
data(onto.GOMF)
onto.GOMF
```

onto.HPMI 93

onto.HPMI

Human Phenotype Mode of Inheritance (HPMI).

### **Description**

An R object that contains information on Human Phenotype Mode of Inheritance terms. These terms are organised as a direct acyclic graph (DAG), which is further stored as an object of the class 'igraph' (see http://igraph.org/r/doc/aaa-igraph-package.html). This data is prepared based on http://compbio.charite.de/svn/hpo/trunk/src/ontology/human-phenotype-ontology.obo.

### Usage

data(onto.HPMI)

#### Value

an object of S4 class Onto. It has slots for "nodeInfo" and "adjMatrix"

- nodeInfo: an object of S4 class InfoDataFrame, describing information on nodes/terms including: "term\_id" (i.e. Term ID), "term\_name" (i.e. Term Name), "term\_namespace" (i.e. Term Namespace), and "term\_distance" (i.e. Term Distance: the distance to the root; always 0 for the root itself)
- adjMatrix: an object of S4 class AdjData, containing adjacency data matrix, with rows for parent (arrow-outbound) and columns for children (arrow-inbound)

#### References

Robinson et al. (2012) The Human Phenotype Ontology: a tool for annotating and analyzing human hereditary disease. *Am J Hum Genet*, 83:610-615.

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

## **Examples**

data(onto.HPMI)
onto.HPMI

onto.HPON

Human Phenotype ONset and clinical course (HPON).

## **Description**

An R object that contains information on Human Phenotype ONset and clinical course terms. These terms are organised as a direct acyclic graph (DAG), which is further stored as an object of the class 'igraph' (see http://igraph.org/r/doc/aaa-igraph-package.html). This data is prepared based on http://compbio.charite.de/svn/hpo/trunk/src/ontology/human-phenotype-ontology.obo.

94 onto.HPPA

## Usage

```
data(onto.HPON)
```

#### Value

an object of S4 class Onto. It has slots for "nodeInfo" and "adjMatrix"

- nodeInfo: an object of S4 class InfoDataFrame, describing information on nodes/terms including: "term\_id" (i.e. Term ID), "term\_name" (i.e. Term Name), "term\_namespace" (i.e. Term Namespace), and "term\_distance" (i.e. Term Distance: the distance to the root; always 0 for the root itself)
- adjMatrix: an object of S4 class AdjData, containing adjacency data matrix, with rows for parent (arrow-outbound) and columns for children (arrow-inbound)

#### References

Robinson et al. (2012) The Human Phenotype Ontology: a tool for annotating and analyzing human hereditary disease. *Am J Hum Genet*, 83:610-615.

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

## **Examples**

```
data(onto.HPON)
onto.HPON
```

onto.HPPA

Human Phenotype Phenotypic Abnormality (HPPA).

# **Description**

An R object that contains information on Human Phenotype Phenotypic Abnormality terms. These terms are organised as a direct acyclic graph (DAG), which is further stored as an object of the class 'igraph' (see http://igraph.org/r/doc/aaa-igraph-package.html). This data is prepared based on http://compbio.charite.de/svn/hpo/trunk/src/ontology/human-phenotype-ontology.obo.

## Usage

```
data(onto.HPPA)
```

### Value

an object of S4 class Onto. It has slots for "nodeInfo" and "adjMatrix"

- nodeInfo: an object of S4 class InfoDataFrame, describing information on nodes/terms including: "term\_id" (i.e. Term ID), "term\_name" (i.e. Term Name), "term\_namespace" (i.e. Term Namespace), and "term\_distance" (i.e. Term Distance: the distance to the root; always 0 for the root itself)
- adjMatrix: an object of S4 class AdjData, containing adjacency data matrix, with rows for parent (arrow-outbound) and columns for children (arrow-inbound)

onto.KW 95

#### References

Robinson et al. (2012) The Human Phenotype Ontology: a tool for annotating and analyzing human hereditary disease. *Am J Hum Genet*, 83:610-615.

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

## **Examples**

```
data(onto.HPPA)
onto.HPPA
```

onto.KW

UniProtKB KeyWords (KW).

# Description

An R object that contains information on UniProtKB KeyWords terms. These terms are organised as a direct acyclic graph (DAG), which is further stored as an object of the class 'igraph' (see <a href="http://igraph.org/r/doc/aaa-igraph-package.html">http://igraph.org/r/doc/aaa-igraph-package.html</a>). UniProtKB KeyWords (KW) controlled vocabulary provides a summary of the entry content and is used to index UniProtKB/Swiss-Prot entries based on 10 categories (the category "Technical term" being excluded here).

## Usage

```
onto.KW <- dcRDataLoader(RData=onto.KW)</pre>
```

## Value

an object of S4 class Onto. It has slots for "nodeInfo" and "adjMatrix"

- nodeInfo: an object of S4 class InfoDataFrame, describing information on nodes/terms including: "term\_id" (i.e. Term ID), "term\_name" (i.e. Term Name), "term\_namespace" (i.e. Term Namespace), and "term\_distance" (i.e. Term Distance: the distance to the root; always 0 for the root itself)
- adjMatrix: an object of S4 class AdjData, containing adjacency data matrix, with rows for parent (arrow-outbound) and columns for children (arrow-inbound)

#### References

Bairoch et al. (2005) The Universal Protein Resource (UniProt). *Nucleic Acids Res*, 33:D154-9. Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

```
onto.KW <- dcRDataLoader(RData=onto.KW)
onto.KW</pre>
```

96 onto.UP

onto.MP

Mammalian Phenotype (MP).

## **Description**

An R object that contains information on Mammalian Phenotype terms. These terms are organised as a direct acyclic graph (DAG), which is further stored as an object of the class 'igraph' (see http://igraph.org/r/doc/aaa-igraph-package.html). This data is prepared based on http://sourceforge.net/p/diseaseontology/code/HEAD/tree/trunk/HumanMP.obo.

### Usage

```
data(onto.MP)
```

#### Value

an object of S4 class Onto. It has slots for "nodeInfo" and "adjMatrix"

- nodeInfo: an object of S4 class InfoDataFrame, describing information on nodes/terms including: "term\_id" (i.e. Term ID), "term\_name" (i.e. Term Name), "term\_namespace" (i.e. Term Namespace), and "term\_distance" (i.e. Term Distance: the distance to the root; always 0 for the root itself)
- adjMatrix: an object of S4 class AdjData, containing adjacency data matrix, with rows for parent (arrow-outbound) and columns for children (arrow-inbound)

### References

Smith et al. (2009) The Mammalian Phenotype Ontology: enabling robust annotation and comparative analysis. *Wiley Interdiscip Rev Syst Biol Med*, 1:390-399.

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

## **Examples**

```
data(onto.MP)
onto.MP
```

onto.UP

UniProtKB UniPathway (UP).

### **Description**

An R object that contains information on UniProtKB UniPathway terms. These terms are organised as a direct acyclic graph (DAG), which is further stored as an object of the class 'igraph' (see http://igraph.org/r/doc/aaa-igraph-package.html). UniProtKB UniPathway (UP) is a fully manually curated resource for the representation and annotation of metabolic pathways, being used as a controlled vocabulary for pathway annotation in UniProtKB.

## Usage

```
onto.UP <- dcRDataLoader(RData=onto.UP)</pre>
```

Pfam 97

#### Value

an object of S4 class Onto. It has slots for "nodeInfo" and "adjMatrix"

• nodeInfo: an object of S4 class InfoDataFrame, describing information on nodes/terms including: "term\_id" (i.e. Term ID), "term\_name" (i.e. Term Name), "term\_namespace" (i.e. Term Namespace), and "term\_distance" (i.e. Term Distance: the distance to the root; always 0 for the root itself)

• adjMatrix: an object of S4 class AdjData, containing adjacency data matrix, with rows for parent (arrow-outbound) and columns for children (arrow-inbound)

#### References

Morgat et al. (2006) UniPathway: a resource for the exploration and annotation of metabolic pathways. *Nucleic Acids Res*, 40:D761-9.

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

## **Examples**

```
onto.UP <- dcRDataLoader(RData=onto.UP)
onto.UP</pre>
```

Pfam

Pfam domains (Pfam).

# Description

An object of class "InfoDataFrame" that contains information on Pfam domains (Pfam). This data is prepared based on ftp://ftp.sanger.ac.uk/pub/databases/Pfam/current\_release/database\_files/pfamA.txt.gz.

## Usage

data(Pfam)

## Value

an object of class InfoDataFrame. It has slots for data and dimLabels:

- data: a data.frame containing information about 14831 domains (in rows), with 3 columns ("id" for Pfam accession ID, and "level" always equals "Pfam", "description" for Pfam description)
- dimLabels: a character describing labels for rows and columns in data

# References

Finn et al. (2014) The Pfam protein families database. *Nucleic Acids Res*, 42(Database issue):D222-D230.

### See Also

InfoDataFrame-class

98 Pfam2GOBP

## **Examples**

```
# load data
data(Pfam)
Pfam
# retrieve the dimension
dim(Pfam)
# retrieve names of columns
colNames(Pfam)
# retrieve the first 5 rows of data
Data(Pfam)[1:5,]
```

Pfam2GOBP

Annotations of Pfam domains by Gene Ontology Biological Process (GOBP).

## **Description**

An object of class "Anno" that contains associations between Gene Ontology Biological Process terms and Pfam domains. This data is prepared based on the Pfam database (see http://pfam.xfam.org) and ftp://ftp.geneontology.org/pub/go/external2go/pfam2go.

## Usage

```
data(Pfam2GOBP)
```

## Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for Pfam accession ID, and "level" always equals "Pfam", "description" for Pfam description

## References

Finn et al. (2014) The Pfam protein families database. *Nucleic Acids Res*, 42(Database issue):D222-D230.

### See Also

Pfam2GOCC 99

### **Examples**

```
# load data
data(Pfam2GOBP)
Pfam2GOBP
# retrieve info on ontology terms
termData(Pfam2GOBP)
# retrieve info on Pfam domains
domainData(Pfam2GOBP)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(Pfam2GOBP)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

Pfam2GOCC

Annotations of Pfam domains by Gene Ontology Cellular Component (GOCC).

## **Description**

An object of class "Anno" that contains associations between Gene Ontology Cellular Component terms and Pfam domains. This data is prepared based on the Pfam database (see http://pfam.xfam.org) and ftp://ftp.geneontology.org/pub/go/external2go/pfam2go.

## Usage

```
data(Pfam2GOCC)
```

# Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for Pfam accession ID, and "level" always equals "Pfam", "description" for Pfam description

### References

Finn et al. (2014) The Pfam protein families database. *Nucleic Acids Res*, 42(Database issue):D222-D230.

### See Also

100 Pfam2GOMF

## **Examples**

```
# load data
data(Pfam2GOCC)
Pfam2GOCC
# retrieve info on ontology terms
termData(Pfam2GOCC)
# retrieve info on Pfam domains
domainData(Pfam2GOCC)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(Pfam2GOCC)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

Pfam2GOMF

Annotations of Pfam domains by Gene Ontology Molecular Function (GOMF).

## **Description**

An object of class "Anno" that contains associations between Gene Ontology Molecular Function terms and Pfam domains. This data is prepared based on the Pfam database (see http://pfam.xfam.org) and ftp://ftp.geneontology.org/pub/go/external2go/pfam2go.

## Usage

```
data(Pfam2GOMF)
```

# Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for Pfam accession ID, and "level" always equals "Pfam", "description" for Pfam description

### References

Finn et al. (2014) The Pfam protein families database. *Nucleic Acids Res*, 42(Database issue):D222-D230.

### See Also

Rfam 101

## **Examples**

```
# load data
data(Pfam2GOMF)
Pfam2GOMF
# retrieve info on ontology terms
termData(Pfam2GOMF)
# retrieve info on Pfam domains
domainData(Pfam2GOMF)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(Pfam2GOMF)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

Rfam

RNA families (Rfam).

## **Description**

An object of class "InfoDataFrame" that contains information on RNA families (Rfam). This data is prepared based on ftp://anonymous@ftp.sanger.ac.uk/pub/databases/Rfam/11.0/database\_files/rfam.txt.gz.

### Usage

data(Rfam)

# Value

an object of class InfoDataFrame. It has slots for data and dimLabels:

- data: a data.frame containing information about 2208 RNA families (in rows), with 3 columns ("id" for Rfam accession ID, and "level" always equals "Rfam", "description" for Rfam description)
- dimLabels: a character describing labels for rows and columns in data

# References

Gardner et al. (2011) Rfam: Wikipedia, clans and the "decimal" release. *Nucleic Acids Res*, 39(Database issue):D141-D145.

# See Also

InfoDataFrame-class

```
# load data
data(Rfam)
Rfam
# retrieve the dimension
dim(Rfam)
# retrieve names of columns
```

102 Rfam2GOBP

```
colNames(Rfam)
# retrieve the first 5 rows of data
Data(Rfam)[1:5,]
```

Rfam2GOBP

Annotations of Rfam RNA families by Gene Ontology Biological Process (GOBP).

## **Description**

An object of class "Anno" that contains associations between Gene Ontology Biological Process terms and Rfam RNA families. This data is prepared based on the Rfam database (see <a href="http://rfam.xfam.org">http://geneontology.org/external2go/rfam2go</a>.

### **Usage**

```
data(Rfam2GOBP)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of RNAs X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing RNAs (i.e. rows in annoData), including: "id" for Rfam accession ID, and "level" always equals "Rfam", "description" for Rfam description

### References

Gardner et al. (2011) Rfam: Wikipedia, clans and the "decimal" release. *Nucleic Acids Res*, 39(Database issue):D141-D145.

### See Also

Anno-class

```
# load data
data(Rfam2GOBP)
Rfam2GOBP
# retrieve info on ontology terms
termData(Rfam2GOBP)
# retrieve info on Rfam RNAs
domainData(Rfam2GOBP)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(Rfam2GOBP)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

Rfam2GOCC 103

Rfam2GOCC

Annotations of Rfam RNA families by Gene Ontology Cellular Component (GOCC).

## **Description**

An object of class "Anno" that contains associations between Gene Ontology Cellular Component terms and Rfam RNA families. This data is prepared based on the Rfam database (see <a href="http://rfam.xfam.org">http://geneontology.org/external2go/rfam2go</a>.

### Usage

```
data(Rfam2GOCC)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of RNAs X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing RNAs (i.e. rows in annoData), including: "id" for Rfam accession ID, and "level" always equals "Rfam", "description" for Rfam description

## References

Gardner et al. (2011) Rfam: Wikipedia, clans and the "decimal" release. *Nucleic Acids Res*, 39(Database issue):D141-D145.

### See Also

Anno-class

```
# load data
data(Rfam2GOCC)
Rfam2GOCC
# retrieve info on ontology terms
termData(Rfam2GOCC)
# retrieve info on Rfam RNAs
domainData(Rfam2GOCC)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(Rfam2GOCC)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

104 Rfam2GOMF

Rfam2GOMF

Annotations of Rfam RNA families by Gene Ontology Molecular Function (GOMF).

# Description

An object of class "Anno" that contains associations between Gene Ontology Molecular Function terms and Rfam RNA families. This data is prepared based on the Rfam database (see <a href="http://rfam.xfam.org">http://geneontology.org/external2go/rfam2go</a>.

#### **Usage**

```
data(Rfam2GOMF)
```

### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of RNAs X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing RNAs (i.e. rows in annoData), including: "id" for Rfam accession ID, and "level" always equals "Rfam", "description" for Rfam description

## References

Gardner et al. (2011) Rfam: Wikipedia, clans and the "decimal" release. *Nucleic Acids Res*, 39(Database issue):D141-D145.

### See Also

Anno-class

```
# load data
data(Rfam2GOMF)
Rfam2GOMF
# retrieve info on ontology terms
termData(Rfam2GOMF)
# retrieve info on Rfam RNAs
domainData(Rfam2GOMF)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(Rfam2GOMF)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

SCOP.fa 105

SCOP.fa

SCOP domain families (fa).

## **Description**

An object of class "InfoDataFrame" that contains information on SCOP domain families (fa).

# Usage

```
data(SCOP.fa)
```

### Value

an object of class InfoDataFrame. It has slots for data and dimLabels:

- data: a data.frame containing information about 2223 domains (in rows), with 3 columns ("id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description)
- dimLabels: a character describing labels for rows and columns in data

## References

Morais et al. (2011) SUPERFAMILY 1.75 including a domain-centric gene ontology method. *Nucleic Acids Res*, 39(Database issue):D427-34.

Andreeva et al. (2008) Data growth and its impact on the SCOP database: new developments. *Nucleic Acids Res*, 36(Database issue):D419-425

## See Also

InfoDataFrame-class

```
# load data
data(SCOP.fa)
SCOP.fa
# retrieve the dimension
dim(SCOP.fa)
# retrieve names of columns
colNames(SCOP.fa)
# retrieve the first 5 rows of data
Data(SCOP.fa)[1:5,]
```

106 SCOP.fa2DO

SCOP.fa2D0

Annotations of SCOP domain families (fa) by Disease Ontology (DO).

## **Description**

An object of class "Anno" that contains associations between Disease Ontology terms and SCOP domain families (fa). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

### Usage

```
data(SCOP.fa2D0)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

```
Anno-class
```

```
# load data
data(SCOP.fa2DO)
SCOP.fa2DO
# retrieve info on ontology terms
termData(SCOP.fa2DO)
# retrieve info on SCOP domains
domainData(SCOP.fa2DO)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.fa2DO)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

SCOP.fa2EC 107

SCOP.fa2EC

Annotations of SCOP domain families (fa) by Enzyme Commission (EC).

# Description

An object of class "Anno" that contains associations between Enzyme Commission terms and SCOP domain families (fa). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

#### Usage

```
SCOP.fa2EC <- dcRDataLoader(RData=SCOP.fa2EC)</pre>
```

### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

## See Also

Anno-class

```
# load data
SCOP.fa2EC <- dcRDataLoader(RData=SCOP.fa2EC)
SCOP.fa2EC
# retrieve info on ontology terms
termData(SCOP.fa2EC)
# retrieve info on SCOP domains
domainData(SCOP.fa2EC)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.fa2EC)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

108 SCOP.fa2GOBP

SCOP.fa2GOBP

Annotations of SCOP domain families (fa) by Gene Ontology Biological Process (GOBP).

# Description

An object of class "Anno" that contains associations between Gene Ontology Biological Process terms and SCOP domain families (fa). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

#### **Usage**

```
data(SCOP.fa2GOBP)
```

### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

### See Also

Anno-class

```
# load data
data(SCOP.fa2GOBP)
SCOP.fa2GOBP
# retrieve info on ontology terms
termData(SCOP.fa2GOBP)
# retrieve info on SCOP domains
domainData(SCOP.fa2GOBP)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.fa2GOBP)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

SCOP.fa2GOCC 109

SCOP.fa2GOCC	Annotations of SCOP domain families (fa) by Gene Ontology Cellular
	Component (GOCC).

# **Description**

An object of class "Anno" that contains associations between Gene Ontology Cellular Component terms and SCOP domain families (fa). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

#### Usage

```
data(SCOP.fa2GOCC)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.fa2GOCC)
SCOP.fa2GOCC
# retrieve info on ontology terms
termData(SCOP.fa2GOCC)
# retrieve info on SCOP domains
domainData(SCOP.fa2GOCC)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.fa2GOCC)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

110 SCOP.fa2GOMF

SCOP.fa2GOMF

Annotations of SCOP domain families (fa) by Gene Ontology Molecular Function (GOMF).

# Description

An object of class "Anno" that contains associations between Gene Ontology Molecular Function terms and SCOP domain families (fa). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

#### **Usage**

```
data(SCOP.fa2GOMF)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.fa2GOMF)
SCOP.fa2GOMF
# retrieve info on ontology terms
termData(SCOP.fa2GOMF)
# retrieve info on SCOP domains
domainData(SCOP.fa2GOMF)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.fa2GOMF)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

SCOP.fa2HPMI 111

SCOP.fa2HPMI

Annotations of SCOP domain families (fa) by Human Phenotype Mode of Inheritance (HPMI).

# **Description**

An object of class "Anno" that contains associations between HPMI terms and SCOP domain families (fa). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

#### Usage

```
data(SCOP.fa2HPMI)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.fa2HPMI)
SCOP.fa2HPMI
# retrieve info on ontology terms
termData(SCOP.fa2HPMI)
# retrieve info on SCOP domains
domainData(SCOP.fa2HPMI)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.fa2HPMI)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

112 SCOP.fa2HPON

SCOP.fa2HPON

Annotations of SCOP domain families (fa) by Human Phenotype ONset and clinical course (HPON).

# Description

An object of class "Anno" that contains associations between HPON terms and SCOP domain families (fa). This data is prepared based on the dcGO database (see <a href="http://supfam.org/SUPERFAMILY/dcGO/">http://supfam.org/SUPERFAMILY/dcGO/</a>).

#### **Usage**

```
data(SCOP.fa2HPON)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.fa2HPON)
SCOP.fa2HPON
# retrieve info on ontology terms
termData(SCOP.fa2HPON)
# retrieve info on SCOP domains
domainData(SCOP.fa2HPON)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.fa2HPON)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

SCOP.fa2HPPA 113

SCOP.fa2HPPA	Annotations of SCOP domain families (fa) by Human Phenotype Phe-
	notypic Abnormality (HPPA).

# **Description**

An object of class "Anno" that contains associations between HPPA terms and SCOP domain families (fa). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

#### Usage

```
data(SCOP.fa2HPPA)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.fa2HPPA)
SCOP.fa2HPPA
# retrieve info on ontology terms
termData(SCOP.fa2HPPA)
# retrieve info on SCOP domains
domainData(SCOP.fa2HPPA)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.fa2HPPA)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

114 SCOP.fa2KW

SCOP.fa2KW

Annotations of SCOP domain families (fa) by UniProtKB KeyWords (KW).

# Description

An object of class "Anno" that contains associations between UniProtKB KeyWords terms and SCOP domain families (fa). This data is prepared based on the dcGO database (see <a href="http://supfam.org/SUPERFAMILY/dcGO/">http://supfam.org/SUPERFAMILY/dcGO/</a>).

#### **Usage**

```
SCOP.fa2KW <- dcRDataLoader(RData=SCOP.fa2KW)</pre>
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
SCOP.fa2KW <- dcRDataLoader(RData=SCOP.fa2KW)
SCOP.fa2KW
# retrieve info on ontology terms
termData(SCOP.fa2KW)
# retrieve info on SCOP domains
domainData(SCOP.fa2KW)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.fa2KW)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

SCOP.fa2MP

SCOP.fa2MP

Annotations of SCOP domain families (fa) by Mammalian Phenotype (MP).

# Description

An object of class "Anno" that contains associations between Mammalian Phenotype terms and SCOP domain families (fa). This data is prepared based on the dcGO database (see <a href="http://supfam.org/SUPERFAMILY/dcGO/">http://supfam.org/SUPERFAMILY/dcGO/</a>).

#### **Usage**

```
data(SCOP.fa2MP)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.fa2MP)
SCOP.fa2MP
# retrieve info on ontology terms
termData(SCOP.fa2MP)
# retrieve info on SCOP domains
domainData(SCOP.fa2MP)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.fa2MP)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

116 SCOP.fa2UP

SCOP.fa2UP

Annotations of SCOP domain families (fa) by UniProtKB UniPathway (UP).

# Description

An object of class "Anno" that contains associations between UniProtKB UniPathway terms and SCOP domain families (fa). This data is prepared based on the dcGO database (see <a href="http://supfam.org/SUPERFAMILY/dcGO/">http://supfam.org/SUPERFAMILY/dcGO/</a>).

#### **Usage**

```
SCOP.fa2UP <- dcRDataLoader(RData=SCOP.fa2UP)</pre>
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
SCOP.fa2UP <- dcRDataLoader(RData=SCOP.fa2UP)
SCOP.fa2UP
# retrieve info on ontology terms
termData(SCOP.fa2UP)
# retrieve info on SCOP domains
domainData(SCOP.fa2UP)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.fa2UP)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

SCOPsf 117

SCOP.sf

SCOP domain superfamilies (sf).

# **Description**

An object of class "InfoDataFrame" that contains information on SCOP domain superfamilies (sf).

# Usage

```
data(SCOP.sf)
```

#### Value

an object of class InfoDataFrame. It has slots for data and dimLabels:

- data: a data.frame containing information about 2223 domains (in rows), with 3 columns ("id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description)
- dimLabels: a character describing labels for rows and columns in data

# References

Morais et al. (2011) SUPERFAMILY 1.75 including a domain-centric gene ontology method. *Nucleic Acids Res*, 39(Database issue):D427-34.

Andreeva et al. (2008) Data growth and its impact on the SCOP database: new developments. *Nucleic Acids Res*, 36(Database issue):D419-425

# See Also

InfoDataFrame-class

```
# load data
data(SCOP.sf)
SCOP.sf
# retrieve the dimension
dim(SCOP.sf)
# retrieve names of columns
colNames(SCOP.sf)
# retrieve the first 5 rows of data
Data(SCOP.sf)[1:5,]
```

118 SCOP.sf2DO

SCOP.sf2D0

Annotations of SCOP domain superfamilies (sf) by Disease Ontology (DO).

# Description

An object of class "Anno" that contains associations between Disease Ontology terms and SCOP domain superfamilies (sf). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

#### Usage

```
data(SCOP.sf2D0)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.sf2DO)
SCOP.sf2DO
# retrieve info on ontology terms
termData(SCOP.sf2DO)
# retrieve info on SCOP domains
domainData(SCOP.sf2DO)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.sf2DO)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

SCOP.sf2EC 119

SCOP.sf2EC

Annotations of SCOP domain superfamilies (sf) by Enzyme Commission (EC).

# Description

An object of class "Anno" that contains associations between Enzyme Commission terms and SCOP domain superfamilies (sf). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

#### Usage

```
SCOP.sf2EC <- dcRDataLoader(RData=SCOP.sf2EC)</pre>
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
SCOP.sf2EC <- dcRDataLoader(RData=SCOP.sf2EC)
SCOP.sf2EC
# retrieve info on ontology terms
termData(SCOP.sf2EC)
# retrieve info on SCOP domains
domainData(SCOP.sf2EC)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.sf2EC)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

120 SCOP.sf2GOBP

SCOP.sf2GOBP Annotations of SCOP domain superfamilies (sf) by Gene Ontology Biological Process (GOBP).

# **Description**

An object of class "Anno" that contains associations between Gene Ontology Biological Process terms and SCOP domain superfamilies (sf). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

#### Usage

```
data(SCOP.sf2GOBP)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.sf2GOBP)
SCOP.sf2GOBP
# retrieve info on ontology terms
termData(SCOP.sf2GOBP)
# retrieve info on SCOP domains
domainData(SCOP.sf2GOBP)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.sf2GOBP)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

SCOP.sf2GOCC 121

SCOP.sf2GOCC	Annotations of SCOP domain superfamilies (sf) by Gene Ontology
	Cellular Component (GOCC).

# **Description**

An object of class "Anno" that contains associations between Gene Ontology Cellular Component terms and SCOP domain superfamilies (sf). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

#### Usage

```
data(SCOP.sf2GOCC)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.sf2GOCC)
SCOP.sf2GOCC
# retrieve info on ontology terms
termData(SCOP.sf2GOCC)
# retrieve info on SCOP domains
domainData(SCOP.sf2GOCC)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.sf2GOCC)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

122 SCOP.sf2GOMF

SCOP.sf2GOMF	Annotations of SCOP domain superfamilies (sf) by Gene Ontology
	Molecular Function (GOMF).

# Description

An object of class "Anno" that contains associations between Gene Ontology Molecular Function terms and SCOP domain superfamilies (sf). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

#### **Usage**

```
data(SCOP.sf2GOMF)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.sf2GOMF)
SCOP.sf2GOMF
# retrieve info on ontology terms
termData(SCOP.sf2GOMF)
# retrieve info on SCOP domains
domainData(SCOP.sf2GOMF)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.sf2GOMF)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

SCOP.sf2HPMI 123

SCOP.sf2HPMI	Annotations of SCOP domain superfamilies (sf) by Human Phenotype
	Mode of Inheritance (HPMI).

# **Description**

An object of class "Anno" that contains associations between HPMI terms and SCOP domain superfamilies (sf). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

# Usage

```
data(SCOP.sf2HPMI)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.sf2HPMI)
SCOP.sf2HPMI
# retrieve info on ontology terms
termData(SCOP.sf2HPMI)
# retrieve info on SCOP domains
domainData(SCOP.sf2HPMI)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.sf2HPMI)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

124 SCOP.sf2HPON

SCOP.sf2HPON

Annotations of SCOP domain superfamilies (sf) by Human Phenotype ONset and clinical course (HPON).

# Description

An object of class "Anno" that contains associations between HPON terms and SCOP domain superfamilies (sf). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

#### Usage

```
data(SCOP.sf2HPON)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.sf2HPON)
SCOP.sf2HPON
# retrieve info on ontology terms
termData(SCOP.sf2HPON)
# retrieve info on SCOP domains
domainData(SCOP.sf2HPON)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.sf2HPON)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

SCOP.sf2HPPA 125

SCOP.sf2HPPA	Annotations of SCOP domain superfamilies (sf) by Human Phenotype
	Phenotypic Abnormality (HPPA).

# **Description**

An object of class "Anno" that contains associations between HPPA terms and SCOP domain superfamilies (sf). This data is prepared based on the dcGO database (see http://supfam.org/SUPERFAMILY/dcGO/).

# Usage

```
data(SCOP.sf2HPPA)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.sf2HPPA)
SCOP.sf2HPPA
# retrieve info on ontology terms
termData(SCOP.sf2HPPA)
# retrieve info on SCOP domains
domainData(SCOP.sf2HPPA)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.sf2HPPA)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

126 SCOP.sf2KW

SCOP.sf2KW

Annotations of SCOP domain superfamilies (sf) by UniProtKB Key-Words (KW).

# Description

An object of class "Anno" that contains associations between UniProtKB KeyWords terms and SCOP domain superfamilies (sf). This data is prepared based on the dcGO database (see <a href="http://supfam.org/SUPERFAMILY/dcGO/">http://supfam.org/SUPERFAMILY/dcGO/</a>).

#### Usage

```
SCOP.sf2KW <- dcRDataLoader(RData=SCOP.sf2KW)</pre>
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
SCOP.sf2KW <- dcRDataLoader(RData=SCOP.sf2KW)
SCOP.sf2KW
# retrieve info on ontology terms
termData(SCOP.sf2KW)
# retrieve info on SCOP domains
domainData(SCOP.sf2KW)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.sf2KW)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

SCOP.sf2MP

SCOP.sf2MP

Annotations of SCOP domain superfamilies (sf) by Mammalian Phenotype (MP).

# **Description**

An object of class "Anno" that contains associations between Mammalian Phenotype terms and SCOP domain superfamilies (sf). This data is prepared based on the dcGO database (see <a href="http://supfam.org/SUPERFAMILY/dcGO/">http://supfam.org/SUPERFAMILY/dcGO/</a>).

#### Usage

```
data(SCOP.sf2MP)
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
data(SCOP.sf2MP)
SCOP.sf2MP
# retrieve info on ontology terms
termData(SCOP.sf2MP)
# retrieve info on SCOP domains
domainData(SCOP.sf2MP)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.sf2MP)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

128 SCOP.sf2UP

SCOP.sf2UP

Annotations of SCOP domain superfamilies (sf) by UniProtKB Uni-Pathway (UP).

# **Description**

An object of class "Anno" that contains associations between UniProtKB UniPathway terms and SCOP domain superfamilies (sf). This data is prepared based on the dcGO database (see <a href="http://supfam.org/SUPERFAMILY/dcGO/">http://supfam.org/SUPERFAMILY/dcGO/</a>).

#### Usage

```
SCOP.sf2UP <- dcRDataLoader(RData=SCOP.sf2UP)</pre>
```

#### Value

an object of class Anno. It has slots for "annoData", "termData" and "domainData":

- annoData: a sparse matrix of domains X terms
- termData: variables describing ontology terms (i.e. columns in annoData), including: "ID" (i.e. term ID), "Name" (i.e. term Names), "Namespace" (i.e. term Namespace), and "Distance" (i.e. term Distance to the ontology root)
- domainData: variables describing domains (i.e. rows in annoData), including: "id" for SCOP sunid, and "level" for SCOP level, "description" for SCOP description

## References

Fang H and Gough J. (2013) dcGO: database of domain-centric ontologies on functions, phenotypes, diseases and more. *Nucleic Acids Res*, 41(Database issue):D536-44.

#### See Also

Anno-class

```
# load data
SCOP.sf2UP <- dcRDataLoader(RData=SCOP.sf2UP)
SCOP.sf2UP
# retrieve info on ontology terms
termData(SCOP.sf2UP)
# retrieve info on SCOP domains
domainData(SCOP.sf2UP)
# retrieve the first 5 rows and columns of annotation data
x <- annoData(SCOP.sf2UP)[1:5,1:5]
x
# convert the above retrieval to the full matrix
as.matrix(x)</pre>
```

visEnrichment	Function to visualise enrichment analysis outputs in the context of the
	ontology hierarchy

#### **Description**

visEnrichment is supposed to visualise enrichment analysis outputs (represented as an 'Eoutput' object) in the context of the ontology hierarchy (direct acyclic graph; DAG). Only part of DAG induced by those nodes/terms specified in query nodes (and the mode defining the paths to the root of DAG) will be visualised. Nodes in query are framed in black (by default), and all nodes (in query plus induced) will be color-coded according to a given data.type ('zscore'; otherwise taking the form of 10-based negative logarithm for 'adjp' or 'pvalue'). If no nodes in query, the top 5 significant terms (in terms of adjusted p-value) will be used for visualisation

# Usage

```
visEnrichment(e, nodes_query = NULL, num_top_nodes = 5,
path.mode = c("all_shortest_paths", "shortest_paths", "all_paths"),
data.type = c("adjp", "pvalue", "zscore"), height = 7, width = 7,
margin = rep(0.1, 4), colormap = c("yr", "bwr", "jet", "gbr", "wyr",
"br",
"rainbow", "wb", "lightyellow-orange"), ncolors = 40, zlim = NULL,
colorbar = T, colorbar.fraction = 0.1, newpage = T,
layout.orientation = c("left_right", "top_bottom", "bottom_top",
"right_left"), node.info = c("both", "none", "term_id", "term_name",
"full_term_name"), graph.node.attrs = NULL, graph.edge.attrs = NULL,
node.attrs = NULL)
```

# Arguments

e	an object of S4 class Eoutput
nodes_query	a verctor containing a list of nodes/terms in query. These nodes are used to produce a subgraph of the ontology DAG induced by them. If NULL, the top significant terms (in terms of p-value) will be determined by the next 'num_top_nodes'
num_top_nodes	a numeric value specifying the number of the top significant terms (in terms of p-value) will be used. This parameter does not work if the previous 'nodes_query' has been specified
path.mode	the mode of paths induced by nodes in query. It can be "all_paths" for all possible paths to the root, "shortest_paths" for only one path to the root (for each node in query), "all_shortest_paths" for all shortest paths to the root (i.e. for each node, find all shortest paths with the equal lengths)
data.type	a character telling which data type for nodes in query is used to color-code nodes. It can be one of 'adjp' for adjusted p-values (by default), 'pvalue' for p-values and 'zscore' for z-scores. When 'adjp' or 'pvalue' is used, 10-based negative logarithm is taken. For the style of how to color-code, please see the next arguments: colormap, ncolors, zlim and colorbar
height	a numeric value specifying the height of device
width	a numeric value specifying the width of device
margin	margins as units of length 4 or 1

colormap

short name for the colormap. It can be one of "yr" (yellow-red colormap; by default), "jet" (jet colormap), "bwr" (blue-white-red colormap), "gbr" (green-black-red colormap), "wyr" (white-yellow-red colormap), "br" (black-red colormap), "wb" (white-black colormap), and "rainbow" (rainbow colormap, that is, red-yellow-green-cyan-blue-magenta). Alternatively, any hyphen-separated HTML color names, e.g. "lightyellow-orange" (by default), "blue-black-yellow", "royalblue-white-sandybrown", "darkgreen-white-darkviolet". A list of standard color names can be found in http://html-color-codes.info/color-names

ncolors

the number of colors specified over the colormap

zlim

the minimum and maximum z/data values for which colors should be plotted, defaulting to the range of the finite values of z. Each of the given colors will be used to color an equispaced interval of this range. The midpoints of the intervals cover the range, so that values just outside the range will be plotted

colorbar

logical to indicate whether to append a colorbar. If data is null, it always sets to

false

colorbar.fraction

the relative fraction of colorbar block against the device size

newpage

logical to indicate whether to open a new page. By default, it sets to true for opening a new page

layout.orientation

the orientation of the DAG layout. It can be one of "left\_right" for the left-right layout (viewed from the DAG root point; by default), "top\_bottom" for the top-bottom layout, "bottom\_top" for the bottom-top layout, and "right\_left" for the right-left layout

node.info

tells the ontology term information used to label nodes. It can be one of "both" for using both of Term ID and Name (the first 15 characters; by default), "none" for no node labeling, "term\_id" for using Term ID, "term\_name" for using Term Name (the first 15 characters), and "full\_term\_name" for using the full Term Name

graph.node.attrs

a list of global node attributes. These node attributes will be changed globally. See 'Note' below for details on the attributes

graph.edge.attrs

a list of global edge attributes. These edge attributes will be changed globally. See 'Note' below for details on the attributes

node.attrs

a list of local edge attributes. These node attributes will be changed locally; as such, for each attribute, the input value must be a named vector (i.e. using Term ID as names). See 'Note' below for details on the attributes

#### Value

An object of class 'Ragraph'

# Note

A list of global node attributes used in "graph.node.attrs":

- "shape": the shape of the node: "circle", "rectangle", "rect", "box" and "ellipse"
- "fixedsize": the logical to use only width and height attributes. By default, it sets to true for not expanding for the width of the label
- "fillcolor": the background color of the node

- "color": the color for the node, corresponding to the outside edge of the node
- "fontcolor": the color for the node text/labelings
- "fontsize": the font size for the node text/labelings
- "height": the height (in inches) of the node: 0.5 by default
- "width": the width (in inches) of the node: 0.75 by default
- "style": the line style for the node: "solid", "dashed", "dotted", "invis" and "bold"

A list of global edge attributes used in "graph.edge.attrs":

- "color": the color of the edge: gray by default
- "weight": the weight of the edge: 1 by default
- "style": the line style for the edge: "solid", "dashed", "dotted", "invis" and "bold"

A list of local node attributes used in "node.attrs" (only those named Term IDs will be changed locally!):

- "label": a named vector specifying the node text/labelings
- "shape": a named vector specifying the shape of the node: "circle", "rectangle", "rect", "box" and "ellipse"
- "fixedsize": a named vector specifying whether it sets to true for not expanding for the width of the label
- "fillcolor": a named vector specifying the background color of the node
- "color": a named vector specifying the color for the node, corresponding to the outside edge of the node
- "fontcolor": a named vector specifying the color for the node text/labelings
- "fontsize": a named vector specifying the font size for the node text/labelings
- "height": a named vector specifying the height (in inches) of the node: 0.5 by default
- "width": a named vector specifying the width (in inches) of the node: 0.75 by default
- "style": a named vector specifying the line style for the node: "solid", "dashed", "dotted", "invis" and "bold"

#### See Also

```
dcEnrichment, dcRDataLoader, dcConverter
```

```
# 1) load SCOP.sf (as InfoDataFrame object)
SCOP.sf <- dcRDataLoader(SCOP.sf)
# randomly select 20 domains
data <- sample(rowNames(SCOP.sf), 20)

# 2) perform enrichment analysis, producing an object of S4 class Eoutput eoutput <- dcEnrichment(data, domain="SCOP.sf", ontology="GOMF") eoutput

# 3) visualise the top 10 significant terms
# color-coded according to 10-based negative logarithm of p-values visEnrichment(eoutput)
# color-coded according to zscore
visEnrichment(eoutput, data.type=zscore)</pre>
```

```
# 4) visualise the top 5 significant terms in the ontology hierarchy
nodes_query <- names(sort(adjp(eoutput))[1:5])
visEnrichment(eoutput, nodes_query=nodes_query)
# change the frame color: highlight (framed in blue) nodes/terms in query
nodes.highlight <- rep("blue", length(nodes_query))
names(nodes.highlight) <- nodes_query
visEnrichment(eoutput, nodes_query=nodes_query,
node.attrs=list(color=nodes.highlight))</pre>
```

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