Package 'dcGOR'

October 13, 2022

Type Package

Title Analysis of Ontologies and Protein Domain Annotations

Version 1.0.6

Date 2015-7-26

Author Hai Fang and Julian Gough

Maintainer Hai Fang <hfang@well.ox.ac.uk>

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

Imports methods

Suggests foreach, doMC, ape

- **Description** There lacks a package for analysing 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 new 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://cran.r-project.org/package=dcGOR,

http://dcgor.r-forge.r-project.org,

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' 'dcRWRpredict.r' 'dcNaivePredict.r'

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biocViews Bioinformatics

NeedsCompilation no

Repository CRAN

Date/Publication 2015-07-27 10:52:03

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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, 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)

Anno-class

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)
- 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)
```

Anno-class

Definition for S4 class Anno

Description

Anno has 3 slots: annoData, termData and domainData

Class Anno

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

Anno-method

See Also

Anno-method

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 <- new("Anno", annoData=annoData, domainData=domainData,</pre>
termData=termData)
х
# 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)
## 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,ANY,ANY,ANY'
x[i, j, ..., drop = FALSE]

Arguments

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

See Also

Anno-class

AnnoData-class

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

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

See Also

Cnetwork-method

Examples

```
# create an object of class Cnetwork, only given a matrix
adjM <- matrix(runif(25),nrow=5,ncol=5)
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="_"),
level=rep("SCOP",5), description=I(LETTERS[1:5]),
row.names=paste("Domain", 1:5, sep="_"))
nodeI <- new("InfoDataFrame", data=data)
nodeI
# 2) create an object of class Cnetwork
```

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Cnetwork-method

```
# VERY IMPORTANT: make sure having consistent names between nodeInfo and adjMatrix
adjM <- matrix(runif(25),nrow=5,ncol=5)
colnames(adjM) <- rowNames(nodeI)
x <- new("Cnetwork", adjMatrix=adjM, nodeInfo=nodeI)
x
# 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

```
## S4 method for signature 'Cnetwork'
dim(x)
## S4 method for signature 'Cnetwork'
adjMatrix(x)
```

S4 method for signature 'Cnetwork'
nodeInfo(x)

S4 method for signature 'Cnetwork'
nInfo(object)

S4 method for signature 'Cnetwork'
nodeNames(object)

S4 method for signature 'Cnetwork'
show(object)

S4 method for signature 'Cnetwork,ANY,ANY,ANY'
x[i, j, ..., drop = FALSE]

Arguments

Х	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 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)

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

Coutput-class

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

```
## Not run:
# 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
# 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)
```

End(Not run)

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 ${\tt dcRWRpipeline}$
file	a character specifying a file name written into. By default, it is 'Coutput.txt'
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

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dcAlgo

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 =
    "https://github.com/hfang-bristol/RDataCentre/blob/master/dcGOR")
```

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 http://dcgor.r-forge.r-project.org/ data/Algo/SCOP_architecture.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 'Architecture' (SCOP domain architectures, each represented as comma-separated domains). Note: the file should use the tab delimiter as the field separator between columns

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. See dcRDataLoader for details

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

```
## Not run:
# 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 ontology
res <- dcAlgo(anno.file, architecture.file, ontology="HPPA",</pre>
feature.mode="supra", parallel=FALSE)
res[1:5,]
# 3) Advanced usage: using customised ontology
x <-
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,]
## End(Not run)
```

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.

Usage

```
dcAlgoPredict(data, RData.HIS = c(NA, "Feature2GOBP.sf",
  "Feature2GOMF.sf",
  "Feature2GOMF.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 =
  "https://github.com/hfang-bristol/RDataCentre/blob/master/dcGOR")
```

Arguments

data	an input data vector containing domain architectures. An architecture is repre- sented 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 fea- tures (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", "Fea- ture2GOMF.sf", "Feature2GOCC.sf", "Feature2HPPA.sf"), Pfam domains/combinations (including "Feature2GOBP.pfam", "Feature2GOMF.pfam", "Feature2GODC.pfam", "Feature2HPPA.pfam"), InterPro domains (including "Feature2GOBP.interpro", "Feature2GOMF.interpro", "Feature2GOCC.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: $\sum_{i=1}^{n} \frac{R_i}{i}$, 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 linearly 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
- 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. See dcRDataLoader for details

Value

a named list of architectures, each containing predictive scores

Note

none

See Also

dcRDataLoader, dcSplitArch, dcConverter, dcAlgoPropagate, dcAlgoPredictMain, dcAlgoPredictGenome and dcAlgoPredictGenome and

Examples

```
## Not run:
# 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
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")
## End(Not run)
```

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",
```

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```
"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 =
"https://github.com/hfang-bristol/RDataCentre/blob/master/dcGOR")
```

Arguments

input.file	an input file containing genomes and their domain architectures (including indi- vidual domains). For example, a file containing Hominidae genomes and their domain architectures can be found in http://dcgor.r-forge.r-project.org/ data/Feature/Hominidae.txt. 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 ar- chitectures, 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", "Feature2GOBP.pfam", "Feature2GOMF.pfam", "Feature2GOMF.nterpro", "Feature2GOMF.interpro", "Feature2GOMF.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 weight- ing; 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>i</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 combi- nations of one or two successive domains (including individual domains; con-

	sidering 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 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 de- pend 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
RData.HIS.custo	mised
	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. See dcRDataLoader for details

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

Note

none

See Also

dcRDataLoader, dcAlgoPropagate, dcAlgoPredict

Examples

```
## Not run:
# 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
x <-
base::load(base::url("http://dcgor.r-forge.r-project.org/data/Feature2GOMF.sf.RData"))
RData.HIS.customised <- 'Feature2GOMF.sf.RData'</pre>
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)
dim(output)
output[1:10,]
## End(Not run)
```

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 =
 "https://github.com/hfang-bristol/RDataCentre/blob/master/dcGOR")
```

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 http://dcgor.r-forge.r-project.org/data/ Feature/hs.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 '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 an output file containing predicted results. If not NULL, a tab-delimited text file output.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", "Feature2GOCC.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 merging. The sequential merging is done via: $\sum_{i=1}^{k} \frac{R_i}{i}$, 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 Sfeature.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 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 de- pend 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	
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. See dcRDataLoader for details	

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

```
## Not run:
# 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'</pre>
```

```
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,]
## End(Not run)</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, bin = c("uniform", "quantile"), verbose = T,
RData.ontology.customised = NULL,
RData.location =
"https://github.com/hfang-bristol/RDataCentre/blob/master/dcGOR")
```

Arguments

```
GSP.file a Glod Standard Positive (GSP) file containing known annotations between pro-
teins/genes and ontology terms. For example, a file containing annotations be-
tween 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 in-
put 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). Alternatively, the GSP.file can be a matrix or data frame, assuming that
GSP file has been read. 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

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column for 'Score' (predictive score). Alternatively, the prediction file can be a matrix or data frame, assuming that prediction file has been read. 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
- bin how to bin the scores. It can be "uniform" for binning scores with equal interval (ie with uniform distribution), and 'quantile' for binning scores with eual frequency (ie with equal number)
- 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. See dcRDataLoader for details

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.

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

```
## Not run:
# 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.HPPA_predicted.txt"
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], xlim=c(0,1), ylim=c(0,1), type="b",
xlab="Recall", ylab="Precision")
## End(Not run)</pre>
```

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 (either retaining the maximum hscore or additively accumulating the 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(NA, "GOBP", "GOMF", "GOCC",
  "DO",
  "HPPA", "HPMI", "HPON", "MP", "EC", "KW", "UP"), propagation = c("max",
  "sum"), output.file = "HIS.RData", verbose = T,
  RData.ontology.customised = NULL,
  RData.location =
  "https://github.com/hfang-bristol/RDataCentre/blob/master/dcGOR")
```

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 http://dcgor.r-forge.r-project.org/data/
Feature/Feature2G0.sf.txt. 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). 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
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 Pheno- type Phenotypic Abnormality, "HPMI" for Human Phenotype Mode of Inher- itance, "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)
propagation	how to propagate the score. It can be "max" for retaining the maximum hscore (by default), "sum" for additively accumulating the hscore
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. If NA, there will be no output file
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. See dcRDataLoader for details

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

See Also

dcRDataLoader, dcConverter, dcAlgo, dcList2Matrix

Examples

```
## Not run:
# build an "HIS" object for GO Molecular Function
input.file <-</pre>
"http://dcgor.r-forge.r-project.org/data/Feature/Feature2G0.sf.txt"
Feature2GOMF.sf <- dcAlgoPropagate(input.file=input.file,</pre>
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</pre>
hscore_mat <- dcList2Matrix(hscore)</pre>
colnames(hscore_mat) <- c("Feature_id", "Term_id", "Score")</pre>
dim(hscore_mat)
hscore_mat[1:10,]
## End(Not run)
```

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.mod	el	
	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 symmet- ric 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 $matrix(c(0, 1, 1, 0), 2)$), "cus- tomised" for the user-customised model (see the next parameter)	
customised.mod	el	
	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.po	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.estima	te	
	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 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 de- pend 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	

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)
- transition: an estimated transition matrix between states
- relative: a matrix of nodes X states, storing conditional maximum likelihood being relative to each state

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);"</pre>
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)</pre>
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 <- dcAncestralML(data, phy, parallel=FALSE)
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)
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)
```

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dcAncestralMP

Function to reconstruct ancestral discrete states using maximum parsimony algorithm

Description

dcAncestralMP is supposed to reconstruct ancestral discrete states using a maximum parsimonymodified 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 de- pend 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

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)
- 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);"</pre>
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)</pre>
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)
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)
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]
```

dcBuildAnno

```
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)
```

```
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

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.

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

```
## Not run:
# 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
```

End(Not run)

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")
```

dcBuildOnto

Arguments

input.file	an input file used to build the object. 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 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.

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

```
## Not run:
# 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
```

End(Not run)

dcBuildOnto

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

Description

dcBuildOnto is supposed to build an object 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 http://dcgor.r-forge.r-project.org/ data/onto/igraph_GOMF_edges.txt. 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 http://dcgor. r-forge.r-project.org/data/onto/igraph_GOMF_nodes.txt. 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

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

```
## Not run:
# 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
```

End(Not run)

dcConverter

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"

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

```
## Not run:
# 1) conversion between 'Onto' and 'igraph'
# 1a) load onto.GOMF (as 'Onto' object)
on <- dcRDataLoader('onto.GOMF')
on
# 1b) convert the object from 'Onto' to 'igraph' class
ig <- dcConverter(on, from='Onto', to='igraph')
ig
# 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')
## End(Not run)
```

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.

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

```
## Not run:
# 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 annotation data
# randomly select 5 terms vertices (and their annotation data)
annotations <- Anno[,sample(1:dim(Anno)[2], 5)]</pre>
# 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",</pre>
verbose=TRUE)
# 5) color-code nodes/terms according to the number of annotations
if(class(dag)=='Onto') dag <- dcConverter(dag, from='Onto',</pre>
to='igraph')
data <- sapply(V(dag)$annotations, length)</pre>
names(data) <- V(dag)$name</pre>
dnet::visDAG(g=dag, data=data, node.info="both")
```

End(Not run)

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 'an- notations' 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 best- matching (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 similarity is the maximum of the pre-calculated average between two domains in pair), "BM.complete" for BM-based complete-linkage similarity (in- spired by complete-linkage concept: the least of any maximum similarity be- tween 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 sen- sitive 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 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 de- pend 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

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

dcRDataLoader, dcDAGannotate, dcConverter, Dnetwork-class

Examples

```
## Not run:
# 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)$annotations))
domains <- sample(alldomains,8)</pre>
dnetwork <- dcDAGdomainSim(g=dag, domains=domains,</pre>
method.domain="BM.average", method.term="Resnik", parallel=FALSE,
verbose=TRUE)
dnetwork
## 1e) convert it to an object of class 'igraph'
ig <- dcConverter(dnetwork, from='Dnetwork', to='igraph')</pre>
ig
## 1f) visualise the domain network
### extract edge weight (with 2-digit precision)
x <- signif(E(ig)$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)$annotations))
domains <- sample(alldomains,8)</pre>
dnetwork <- dcDAGdomainSim(g=dag, domains=domains,</pre>
method.domain="BM.average", method.term="Resnik", parallel=FALSE,
verbose=TRUE)
dnetwork
## 2e) convert it to an object of class 'igraph'
ig <- dcConverter(dnetwork, from='Dnetwork', to='igraph')</pre>
ig
## 2f) visualise the domain network
### extract edge weight (with 2-digit precision)
x <- signif(E(ig)$weight, digits=2)</pre>
### rescale into an interval [1,4] as edge width
```

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dcDAGdomainSim

```
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)$annotations))</pre>
domains <- sample(alldomains,8)</pre>
dnetwork <- dcDAGdomainSim(g=dag, domains=domains,</pre>
method.domain="BM.average", method.term="Resnik", parallel=FALSE,
verbose=TRUE)
dnetwork
## 3e) convert it to an object of class 'igraph'
ig <- dcConverter(dnetwork, from='Dnetwork', to='igraph')</pre>
ig
## 3f) visualise the domain network
### extract edge weight (with 2-digit precision)
x <- signif(E(ig)$weight, digits=2)</pre>
### rescale into an interval [1,4] as edge width
edge.width <- 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)
dnetwork
## 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)$weight, digits=2)</pre>
### rescale into an interval [1,4] as edge width
edge.width <- 1 + (x-min(x))/(max(x)-min(x))*3
### do visualisation
dnet::visNet(g=ig, vertex.shape="sphere", edge.width=edge.width,
edge.label=x, edge.label.cex=0.7)
*****
# 5) Advanced usage: customised data for ontology and annotations
# 5a) customise ontology
g <-
dcBuildOnto(relations.file="http://dcgor.r-forge.r-project.org/data/onto/igraph_GOMF_edges.txt",
nodes.file="http://dcgor.r-forge.r-project.org/data/onto/igraph_GOMF_nodes.txt",
output.file="ontology.RData")
# 5b) customise Anno
Anno <-
dcBuildAnno(domain_info.file="http://dcgor.r-forge.r-project.org/data/InterPro/InterPro.txt",
term_info.file="http://dcgor.r-forge.r-project.org/data/InterPro/GO.txt",
association.file="http://dcgor.r-forge.r-project.org/data/InterPro/Domain2GOMF.txt",
output.file="annotations.RData")
## 5c) prepare for ontology appended with annotation information
dag <- dcDAGannotate(g, annotations=Anno, path.mode="shortest_paths",</pre>
verbose=FALSE)
## 5d) calculate pair-wise semantic similarity between 8 randomly chosen domains
alldomains <- unique(unlist(nInfo(dag)$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>
ig
## 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)
## End(Not run)
```

```
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

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dcDuplicated

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 columnwise 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

```
# 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

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 Pheno- type Phenotypic Abnormality, "HPMI" for Human Phenotype Mode of Inher- itance, "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
test	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 (do- mains 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 ran- dom (without replacement) from the background containing annotated and non- annotated domains, and thus compare sampling to background. Unlike hyper- geometric 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 sig- nificance, 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.algori	thm
	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 significantly 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 signifance 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.RDa	ita
	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. See dcRDataLoader for details

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 signifance 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

```
## Not run:
# 1) Enrichment analysis for SCOP domain superfamilies (sf)
## 1a) load SCOP.sf (as 'InfoDataFrame' object)
SCOP.sf <- dcRDataLoader('SCOP.sf')</pre>
### randomly select 50 domains as a list of domains of interest
data <- sample(rowNames(SCOP.sf), 50)</pre>
## 1b) perform enrichment analysis, producing an object of S4 class 'Eoutput'
eoutput <- dcEnrichment(data, domain="SCOP.sf", ontology="GOMF")</pre>
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)
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> eoutput ## 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

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dcEnrichment

```
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>
### randomly select 1000 domains as background
background <- sample(rowNames(domain), 1000)</pre>
## 5c) perform enrichment analysis, producing an object of S4 class 'Eoutput'
eoutput <- dcEnrichment(data, background=background,</pre>
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)
```

End(Not run)

dcFunArgs

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

Description

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

Usage

dcList2Matrix(x, verbose = T)

Arguments

х	a list, its each component must be a named vector	
verbose	logical to indicate whether the messages will be displayed in the screen. E default, it sets to TRUE for display	3y

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

Examples

```
## Not run:
# 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,]
```

End(Not run)

```
dcNaivePredict
```

Description

dcNaivePredict is supposed to perform naive prediction from input known annotations. For each gene/protein, a term to be predicted are simply the frequency of that term appearing in the known annotations.

Usage

```
dcNaivePredict(data, GSP.file, output.file = NULL, ontology = c(NA,
 "GOBP",
 "GOMF", "GOCC", "DO", "HPPA", "HPMI", "HPON", "MP", "EC", "KW", "UP"),
 max.num = 1000, verbose = T, RData.ontology.customised = NULL,
 RData.location =
 "https://github.com/hfang-bristol/RDataCentre/blob/master/dcGOR")
```

Arguments

data	an input vector containing genes/proteins to be predicted
GSP.file	a Glod Standard Positive (GSP) file containing known annotations between pro- teins/genes and ontology terms. For example, a file containing annotations be- tween 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 in- put 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). Alternatively, the GSP.file can be a matrix or data frame, assuming that GSP 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)
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 Pheno- type Phenotypic Abnormality, "HPMI" for Human Phenotype Mode of Inher- itance, "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)
max.num	an integer to specify how many terms will be predicted for each gene/protein
verbose	logical to indicate whether the messages will be displayed in the screen. By default, it sets to TRUE for display

dcNaivePredict

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. See dcRDataLoader for details	

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

Examples

```
## Not run:
# 1) prepare genes to be predicted
input.file <-
"http://dcgor.r-forge.r-project.org/data/Algo/HP_anno.txt"
#input.file <- "http://dcgor.r-forge.r-project.org/data/Algo/SCOP_architecture.txt"
input <- utils::read.delim(input.file, header=TRUE, sep="\t",
colClasses="character")
data <- unique(input[,1])
# 2) do naive prediction
GSP.file <- "http://dcgor.r-forge.r-project.org/data/Algo/HP_anno.txt"
res <- dcNaivePredict(data=data, GSP.file=GSP.file, ontology="HPPA")
res[1:10,]
# 3) calculate Precision and Recall
res_PR <- dcAlgoPredictPR(GSP.file=GSP.file, prediction.file=res,</pre>
```

```
ontology="HPPA")
res_PR
```

```
# 4) plot PR-curve
plot(res_PR[,2], res_PR[,1], xlim=c(0,1), ylim=c(0,1), type="b",
xlab="Recall", ylab="Precision")
```

End(Not run)

dcRDataLoader

Description

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

Usage

```
dcRDataLoader(RData = c(NA, "SCOP.sf", "SCOP.fa", "Pfam", "InterPro",
"Rfam",
"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 =
"https://github.com/hfang-bristol/RDataCentre/blob/master/dcGOR")
```

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.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', 'Inter-Pro2GOCC', '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

- domain 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 https://github.com/hfang-bristol/RDataCentre/blob/master/ dcGOR and 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). Here is the UNIX command for downloading all RData files (preserving the directory structure): wget - r - l2 - A" * .RData" - np - nH - -cut - dirs = 0" http ://dcgor.r - forge.r - project.org/data"

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

Examples

Always, load from specified RData directly
SCOP.sf <- dcRDataLoader(RData='SCOP.sf')</pre>

```
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>
```

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 significance 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'

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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

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

dcRDataLoader, dcDAGannotate, dcDAGdomainSim, dcConverter

Examples

```
## Not run:
# 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
```

End(Not run)

dcRWRpredict

Function to perform RWR-based ontology term predictions from input known annotations and an input graph

Description

dcRWRpredict is supposed to perform ontology term predictions based on Random Walk with Restart (RWR) from input known annotations and an input graph.

Usage

```
dcRWRpredict(data, g, output.file = NULL, ontology = c(NA, "GOBP",
 "GOMF",
 "GOCC", "DO", "HPPA", "HPMI", "HPON", "MP", "EC", "KW", "UP"),
 method = c("indirect", "direct"), normalise = c("laplacian", "row",
 "column", "none"), restart = 0.75, normalise.affinity.matrix =
 c("none",
 "quantile"), leave.one.out = T, propagation = c("max", "sum"),
 scale.method = c("log", "linear", "none"), parallel = TRUE,
 multicores = NULL, verbose = T, RData.ontology.customised = NULL,
 RData.location =
 "https://github.com/hfang-bristol/RDataCentre/blob/master/dcGOR")
```

Arguments

data	an input gene-term data matrix containing known annotations used for seeds. Each value in input matrix does not necessarily have to be binary (non-zeros will be used as a weight, but should be non-negative for easy interpretation). Also, data can be a list, each containing the known annotated genes
g	an object of class "igraph" or Dnetwork
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)
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 Pheno- type Phenotypic Abnormality, "HPMI" for Human Phenotype Mode of Inher- itance, "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)
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.affin	
	the way to normalise the output affinity matrix. It can be 'none' for no normali- sation, 'quantile' for quantile normalisation to ensure that columns (if multiple) of the output affinity matrix have the same quantiles
leave.one.out	logical to indicate whether the leave-one-out test is used for predictions. By default, it sets to true for doing leave-one-out test (that is, known seeds are removed)
propagation	how to propagate the score. It can be "max" for retaining the maximum score (by default), "sum" for additively accumulating the score
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
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 de- pend 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
RData.ontology.	
	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. See dcRDataLoader for details

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)

dcRWRpredict

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). The choice of which method to use RWR depends on the number of seed sets and whether using leave-one-out test. If the total product of both numbers are huge, it is better to use 'indrect' method (for a single run). Also, when using leave-one-out test, it has to be use 'indrect' method.

See Also

dcRDataLoader, dcAlgoPropagate, dcList2Matrix

```
## Not run:
# 1) define an input network
## 1a) an igraph object that contains a functional protein association network in human.
### The network is extracted from the STRING database (version 9.1).
### Only those associations with medium confidence (score>=400) are retained
org.Hs.string <- dnet::dRDataLoader(RData='org.Hs.string')</pre>
## 1b) restrict to those edges with confidence score>=999
### keep the largest connected component
network <- igraph::subgraph.edges(org.Hs.string,</pre>
eids=E(org.Hs.string)[combined_score>=999])
g <- dnet::dNetInduce(g=network, nodes_query=V(network)$name,</pre>
largest.comp=TRUE)
## Notably, in reality, 1b) can be replaced by:
#g <- igraph::subgraph.edges(org.Hs.string, eids=E(org.Hs.string)[combined_score>=400])
## 1c) make sure there is a 'weight' edge attribute
E(g)$weight <- E(g)$combined_score</pre>
### use EntrezGene ID as default 'name' node attribute
V(g)$name <- V(g)$geneid
g
# 2) define the known annotations as seeds
anno.file <- "http://dcgor.r-forge.r-project.org/data/Algo/HP_anno.txt"
data <- dcSparseMatrix(anno.file)</pre>
# 3) perform RWR-based ontology term predictions
res <- dcRWRpredict(data=data, g=g, ontology="HPPA", parallel=FALSE)</pre>
res[1:10,]
# 4) calculate Precision and Recall
GSP.file <- anno.file
prediction.file <- res</pre>
res_PR <- dcAlgoPredictPR(GSP.file=GSP.file,</pre>
prediction.file=prediction.file, ontology="HPPA")
res_PR
# 5) Plot PR-curve
plot(res_PR[,2], res_PR[,1], xlim=c(0,1), ylim=c(0,1), type="b",
xlab="Recall", ylab="Precision")
```

End(Not run)

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

Note

None

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>
```

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dcSplitArch

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; con- sidering 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

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.

See Also

dcTreeConnectivity

dcSubtreeTips

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);"</pre>
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

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;"</pre>
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')</pre>
# 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.

dcSupraBetter

Usage

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

Arguments

input.file	an input file used to build the object. This input file contains original an- notations between domains/features and ontology terms, along with the hy- pergeometric 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 http://dcgor.r-forge.r-project.org/data/ Feature/Feature2GO.sf.txt. As seen in this example, the input file must con- tain 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

```
## Not run:
input.file <-
"http://dcgor.r-forge.r-project.org/data/Feature/Feature2G0.sf.txt"
res <- dcSupraBetter(input.file)
res[1:10,]
```

End(Not run)

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.

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. B default, it sets to TRUE for display	By

Value

a sparse matrix of $Nnode \ge Ntip + Nnode$, 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

```
# 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)</pre>
```

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

Dnetwork-class

Description

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

Value

Class Dnetwork

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("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)</pre>
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>
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>
Х
# 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

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

Arguments

Х	an object of class Dnetwork
object	an object of class Dnetwork
i	an index
j	an index
	additional parameters

Eoutput-class

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

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
- 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, zscore, pvalue, adjp)

Eoutput-class

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

```
## Not run:
# 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) 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]
## End(Not run)
```

Eoutput-method Methods defined for S4 class Eoutput

Description

Methods defined for S4 class Eoutput.

write(x, file = "Eoutput.txt", verbose = T)

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'
```

Arguments

object	an object of S4 class Eoutput. Usually this is an output from dcEnrichment
х	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
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)

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)
- 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.

Examples

```
data(eTOL)
eT0L
# 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$tip.label) # number of tips</pre>
Nnode <- eTOL$Nnode # number of internal nodes
data <- eTOL$connectivity</pre>
visHeatmapAdv(data, Rowv=FALSE,Colv=FALSE, zlim=c(0,1),
colormap="gray-black",
add.expr=abline(v=c(1,Ntip+1,(Ntip+Nnode+1))-0.5, col="white"),
key=FALSE, labRow=NA, labCol=NA)
```

End(Not run)

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

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>
х
# alternatively, using coerce methods
x <- as(data, "InfoDataFrame")</pre>
х
# 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'
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

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

See Also

InfoDataFrame-class

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.

See Also

InfoDataFrame-class

```
# 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

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 http://www.ebi.ac.uk/interpro/) and ftp://anonymous@ftp.ebi.ac.uk/pub/databases/interpro/Current/interpro2go.

Usage

data(InterPro2GOBP)

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

Anno-class

```
# 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)
```

InterPro2GOCC

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 http://www.ebi.ac.uk/interpro/) and ftp://anonymous@ftp.ebi.ac.uk/pub/databases/interpro/Current/interpro2go.

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

Anno-class

```
# 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)
```

InterPro2GOMF

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 http://www.ebi.ac.uk/interpro/) and ftp://anonymous@ftp.ebi.ac.uk/pub/databases/interpro/Current/interpro2go.

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

Anno-class

```
# 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)
```

Onto-class

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

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

Onto-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>
Х
# 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]
```

Onto-method

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'

Arguments

х	an object of class Onto
object	an object of class Onto

x[i, j, ..., drop = FALSE]

onto.DO

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

See Also

Onto-class

onto.DO

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.D0)

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

onto.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.

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.

onto.GOMF

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)

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.

Examples

data(onto.GOMF)
onto.GOMF

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://purl.obolibrary.org/obo/hp.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

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 pre-pared based on http://purl.obolibrary.org/obo/hp.obo.

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://purl.obolibrary.org/obo/hp.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)

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.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 ftp://ftp.informatics.jax.org/pub/reports/MPheno_OBO.ontology.

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)

Pfam

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

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

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

Anno-class

Pfam2GOCC

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)
```

```
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

Anno-class

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)
```

```
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

Anno-class

Rfam

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)
```

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

Examples

```
# load data
data(Rfam)
Rfam
# retrieve the dimension
dim(Rfam)
# retrieve names of columns
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 http://rfam.xfam.org) and http://geneontology.org/external2go/rfam2go.

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

Rfam2GOCC

Examples

```
# 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)
```

```
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 http://rfam.xfam.org) and http://geneontology.org/external2go/rfam2go.

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

Examples

```
# 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)
```

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 http://rfam.xfam.org) and http://geneontology.org/external2go/rfam2go.

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

SCOP.fa

Examples

```
# 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)
```

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

Examples

```
# 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,]
```

SCOP.fa2DO

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

SCOP.fa2GOBP

Examples

```
# 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)
```

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

Examples

```
# 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)
```

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

SCOP.fa2GOMF

Examples

```
# 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)
```

```
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

```
# 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)
```

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

SCOP.fa2HPON

Examples

```
# 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)
```

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 http://supfam.org/SUPERFAMILY/ dcGO/).

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

```
# 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)
```

SCOP.fa2HPPA

Annotations of SCOP domain families (fa) by Human Phenotype Phenotypic 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

SCOP.fa2MP

Examples

```
# 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)
```

```
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 http://supfam.org/SUPERFAMILY/dcGO/).

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

```
# 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)
```

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

SCOP.sf2DO

Examples

```
# 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,]
```

```
SCOP.sf2DO
```

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

```
# 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)
```

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

SCOP.sf2GOCC

Examples

```
# 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)
```

```
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

```
# 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)
```

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

SCOP.sf2HPMI

Examples

```
# 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)
```

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

```
# 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)
```

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

SCOP.sf2HPPA

Examples

```
# 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)
```

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

```
# 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)
```

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 http://supfam.org/SUPERFAMILY/dcGO/).

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

visEnrichment

Examples

```
# 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)
```

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

е

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 pvalue) will be used. This parameter does not work if the previous 'nodes_query' has been specified
- path.modethe 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" (greenblack-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 topbottom 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

visEnrichment

graph.node.attr	'S
	a list of global node attributes. These node attributes will be changed globally. See 'Note' below for details on the attributes
graph.edge.attr	`S
	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

Examples

```
## Not run:
# 1) load SCOP.sf (as 'InfoDataFrame' object)
SCOP.sf <- dcRDataLoader('SCOP.sf')
# randomly select 20 domains
data <- sample(rowNames(SCOP.sf), 20)</pre>
```

```
# 2) perform enrichment analysis, producing an object of S4 class 'Eoutput'
eoutput <- dcEnrichment(data, domain="SCOP.sf", ontology="GOMF")
eoutput</pre>
```

```
# 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')
```

```
# 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))
```

End(Not run)

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