dcAlgoPredictMain

November 26, 2014

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

Arguments

input.file

an input file containing domain architectures (including individual domains). For example, a file containing UniProt ID and domain architectures for human proteins can be found in 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

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)

2 dcAlgoPredictMain

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.interpro", "Feature2GOBP.interpro", "Feature2GOMF.interpro", "Feature2HPPA.interpro")

weight.method

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

merge.method

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

scale.method

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

feature.mode

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

slim.level

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

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.location

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

dcAlgoPredictMain 3

the runtime). For examples, these files (as a whole or part of them) can be first downloaded into your current working directory, and then set this option as: RData.location = ".". If RData to load is already part of package itself, this parameter can be ignored (since this function will try to load it via function data first)

Value

a term-named vector summarising the predicted scores

Note

When 'output.file' is specified, a tab-delimited text file is output, with the column names: the first two (the same as input file), 3rd for 'Term' (predicted ontology terms), 4th for 'Score' (along with predicted scores)

See Also

dcRDataLoader, dcAlgoPredict

Examples

```
input.file <- "http://dcgor.r-forge.r-project.org/data/Feature/hs.txt"
output <- dcAlgoPredictMain(input.file, RData.HIS="Feature2GOMF.sf")
length(output)
output[1:10]</pre>
```