Package 'ontologySimilarity'

March 29, 2024

Type Package Title Calculating Ontological Similarities Version 2.7 **Encoding** UTF-8 Date 2024-03-25 Author Daniel Greene Maintainer Daniel Greene <dg333@cam.ac.uk> Description Calculate similarity between ontological terms and sets of ontological terms based on term information content and assess statistical significance of similarity in the context of a collection of terms sets - Greene et al. 2017 <doi:10.1093/bioinformatics/btw763>. License GPL (>= 2) Imports Rcpp (>= 1.0.0), ontologyIndex (>= 2.0) LinkingTo Rcpp **Depends** R (>= 3.5.0) Suggests knitr, rmarkdown, paintmap VignetteBuilder knitr RoxygenNote 7.3.1 **NeedsCompilation** yes **Repository** CRAN

Date/Publication 2024-03-29 05:50:02 UTC

R topics documented:

ontologySimilarity-package	2
create_sim_index	3
descendants_IC	4
gene_GO_terms	4
get_asym_sim_grid	5
get_profile_sims	5

get_sim	, 6
get_similarity_rank_matrix	. 7
get_sim_grid	. 8
get_sim_p	, 9
get_sim_p_from_ontology	. 10
get_term_set_to_term_sims	. 11
get_term_sim_mat	. 12
GO_IC	. 13
group_term_enrichment	. 13
lin	. 14
resnik	. 15
sample_group_sim	. 15
sample_group_sim_from_ontology	. 17
	18

ontologySimilarity-package

Functions for Calculating Ontological Similarities

Description

Index

Functions for calculating semantic similarities between ontological terms or sets of ontological terms based on term information content and assessing statistical significance of similarity in the context of a collection of sets of ontological terms.

Details

Semantic similarity and similarity significance functions based on Resnik and Lin's measures of similarity. Computationally intensive functions are written in C++ for performance.

Author(s)

Daniel Greene <dg333@cam.ac.uk>

Maintainer: Daniel Greene <dg333@cam.ac.uk>

References

Greene D, Richardson S, Turro E (2017). 'ontologyX: a suite of R packages for working with ontological data. _Bioinformatics_, 33(7), 1104–1106.

Westbury SK, Turro E, Greene D, Lentaigne C, Kelly AM, Bariana TK, Simeoni I, Pillois X, Attwood A, Austin S, Jansen SB, Bakchoul T, Crisp-Hihn A, Erber WN, Favier R, Foad N, Gattens M, Jolley JD, Liesner R, Meacham S, Millar CM, Nurden AT, Peerlinck K, Perry DJ, Poudel P, Schulman S, Schulze H, Stephens JC, Furie B, Robinson PN, Geet Cv, Rendon A, Gomez K, Laffan MA, Lambert MP, Nurden P, Ouwehand WH, Richardson S, Mumford AD and Freson K (2015). 'Human phenotype ontology annotation and cluster analysis to unravel genetic defects in 707 cases with unexplained bleeding and platelet disorders.' _Genome Med_, *7*(1), pp. 36.

Kohler S, Doelken SC, Mungall CJ, Bauer S, Firth HV, Bailleul-Forestier I, Black GC, Brown DL, Brudno M, Campbell J, FitzPatrick DR, Eppig JT, Jackson AP, Freson K, Girdea M, Helbig I, Hurst JA, Jahn J, Jackson LG, Kelly AM, Ledbetter DH, Mansour S, Martin CL, Moss C, Mumford A, Ouwehand WH, Park SM, Riggs ER, Scott RH, Sisodiya S, Van Vooren S, Wapner RJ, Wilkie AO, Wright CF, Vulto-van Silfhout A, de Leeuw N, de Vries B, Washingthon NL, Smith CL, Westerfield M, Schofield P, Ruef BJ, Gkoutos GV, Haendel M, Smedley D, Lewis SE and Robinson PN (2014). 'The Human Phenotype Ontology project: linking molecular biology and disease through phenotype data.' _Nucleic Acids Res._, *42*(Database issue), pp. D966-974.

Resnik, P. (1995). 'Using information content to evaluate semantic similarity in a taxonomy'. Proceedings of the 14th IJCAI 1, 448-453.

Lin D (1998). 'An Information-Theoretic Definition of Similarity.' In Shavlik JW (ed.), _Proceedings of the Fifteenth International Conference on Machine Learning (ICML 1998), Madison, Wisconsin, USA, July 24-27, 1998_, pp. 296-304.

create_sim_index Create similarity index for list of term sets

Description

Create light-weight similarity index for fast lookups of between term set similarity.

Usage

```
create_sim_index(
   ontology,
   term_sets,
   information_content = descendants_IC(ontology),
   term_sim_method = "lin",
   combine = "average"
)
```

Arguments

ontology	ontology_index object.	
term_sets	List of character vectors of ontological term IDs.	
information_com	ntent	
	Numeric vector of information contents of terms (named by term)	
term_sim_method		
	Character string equalling either "lin" or "resnik" to use Lin or Resnik's expres- sion for the similarity of terms.	
combine	Character string - either "average" or "product", indicating whether to use the best-match-product' method, or function accepting two arguments - the first, the similarity matrix obtained by averaging across term sets in term_sets, and the second averaging across those in term_sets2.	

Value

Object of class sim_index.

See Also

link{get_sim} get_sim_p sample_group_sim

descendants_IC	Get information content based on number of descendants each term
	has

Description

Calculate information content of terms based on frequency with which it is an ancestor of other terms. Useful as a default if there is no population frequency information available as it captures the structure of the ontology.

Usage

```
descendants_IC(ontology)
```

Arguments

ontology ontology_index object.

Value

Numeric vector of information contents named by term.

gene_GO_terms

Gene Ontology annotation of genes

Description

list object containing character vectors of term IDs of GO terms annotating each gene, named by gene. Users can select a list of annotations for a subset of the annotated genes using a character vector of gene symbols, e.g. gene_GO_terms[c("ACTN1", "TUBB1")], which can then be used in functions for calculating similarities, e.g. get_sim_grid. Note that these annotation vectors contain annotation from all major branches of the Gene Ontology, however one can simply extract the terms only relevant to one by calling the function in the ontologyIndex package: intersection_with_descendants.

Format

List of character vectors.

References

Annotation downloaded from Gene Ontology consortium website, http://geneontology.org/, dated 20/02/2024.

get_asym_sim_grid Get asymmetrical similarity matrix

Description

Create a numeric matrix of similarities between two lists of term sets, but only averaging over the terms in sets from A the similarities of the best matches in sets from B.

Usage

get_asym_sim_grid(A, B, ...)

Arguments

A	List of term sets.
В	List of term sets.
	Other arguments to be passed to get_sim_grid.

Value

Numeric matrix of similarities

See Also

get_sim_grid get_profile_sims

get_profile_sims Get similarities of term sets to profile

Description

Get numeric vector of similarities between each item in a list of term sets and another 'ontological profile', i.e. a single term set. Similarity averaging over terms in term_sets.

Usage

get_profile_sims(profile, term_sets, ...)

Arguments

profile	Character vector of term IDs.
term_sets	List of character vectors of ontological term IDs.
	Other arguments to pass to get_sim_grid.

Value

Numeric vector of profile similarities.

See Also

get_asym_sim_grid get_sim_grid

get_sim

Calculate the group similarity of a set of row/column indices

Description

Calculates the similarity of a group within a population by applying the function specified by group_sim to the pairwise similarities of group members.

Usage

```
get_sim(pop_sim, ...)
## S3 method for class 'integer'
get_sim(pop_sim, ...)
## S3 method for class 'numeric'
get_sim(pop_sim, group = seq(length(pop_sim)), ...)
## S3 method for class 'matrix'
get_sim(pop_sim, group = seq(nrow(pop_sim)), ...)
## S3 method for class 'sim_index'
get_sim(pop_sim, group = seq(pop_sim[["N"]]), ...)
## Default S3 method:
get_sim(pop_sim, group, type, group_sim = "average", ...)
```

Arguments

pop_sim	An object representing the similarities of an indexed population of objects.
	Other arguments to be passed to get_sim.
group	Character or integer vector specifying names/indices of subgroup for which to calculate a group similarity p-value.

type	Either "matrix", "sim_index" or "numeric" - the type of the pop_sim object.
group_sim	String Either "average" or "min", determining how to calculate the similarity of
	a group of term sets over all pairwise combinations of group members

Value

Numeric value of group similarity

See Also

get_sim_p sample_group_sim

get_similarity_rank_matrix

Get matrix of similarity rank from similarity matrix

Description

Given a lower triangular similarity matrix, construct a distance matrix where the rows are the ranks of the column cases with respect to similarity to the row case. If relative similarity is of interest, this rank-transformation may reduce bias in favour of high similarity scores in downstream analysis.

Usage

```
get_similarity_rank_matrix(similarity_matrix, symmetric = TRUE)
```

Arguments

similarity_matrix	
	Lower triangular numeric matrix of similarities, where the rownames and col- names are identical to the case IDs.
symmetric	Logical value determining whether to 'symmetrify' resultant matrix by averag- ing rank similarity of A -> B and B -> A.

Value

Matrix of rank similarities.

get_sim_grid

Description

Using either an ontology_index object and numeric vector of information content per term or a matrix of between-term similarities (e.g. the output of get_term_sim_mat), create a numeric matrix of 'between-term set' similarities. Either the 'best-match-average' or 'best-matchproduct' approach (i.e. where the 2 scores obtained by applying the asymmetric 'best-match' similarity function to two term sets in each order are combined by taking the average or the product respectively). Either Lin's (default) or Resnik's definition of term similarity can be used. If information_content is not specified, a default value from descendants_IC is generated.

Usage

```
get_sim_grid(
    ontology,
    information_content,
    term_sim_method,
    term_sim_mat,
    term_sets,
    term_sets2 = term_sets,
    combine = "average"
)
```

Arguments

ontology	ontology_index object.
information_con	tent
	Numeric vector of information contents of terms (named by term)
term_sim_method	
	Character string equalling either "lin" or "resnik" to use Lin or Resnik's expres- sion for the similarity of terms.
term_sim_mat	Numeric matrix with rows and columns corresponding to (and named by) term IDs, and cells containing the similarity between the row and column term
term_sets	List of character vectors of ontological term IDs.
term_sets2	Second set of term sets.
combine	Character string - either "average" or "product", indicating whether to use the best-match-product' method, or function accepting two arguments - the first, the similarity matrix obtained by averaging across term sets in term_sets, and the second averaging across those in term_sets2.

Details

Note that if any term set within term_sets has 0 terms associated with it, it will get a similarity of 0 to any other set. If you do not want to compare term sets with no annotation, take care to filter out empty sets first, e.g. by 'term_sets=term_sets[sapply(term_sets, length) > 0]'.

get_sim_p

Value

Numeric matrix of pairwise term set similarities.

See Also

get_term_sim_mat get_sim_p get_asym_sim_grid

Examples

```
library(ontologyIndex)
data(hpo)
term_sets <- list(
`case1`=c("HP:0001873", "HP:0011877"),
`case2`=c("HP:0001872", "HP:0001892"),
`case3`="HP:0001873")
get_sim_grid(ontology=hpo, term_sets=term_sets)</pre>
```

get_sim_p

Get similarity p-value

Description

p-value of group similarity, calculated by estimating the proportion by random sampling of groups the same size as group which have at least as great group similarity than does group.

Usage

```
get_sim_p(pop_sim, ...)
## S3 method for class 'integer'
get_sim_p(pop_sim, ...)
## S3 method for class 'numeric'
get_sim_p(pop_sim, group, ...)
## S3 method for class 'matrix'
get_sim_p(pop_sim, group, ...)
## S3 method for class 'sim_index'
get_sim_p(pop_sim, group, ...)
## Default S3 method:
get_sim_p(
    pop_sim,
    group,
    type,
    min_its = 1000,
```

```
max_its = 1e+05,
signif = 0.05,
log_dismiss = log(1e-06),
group_sim = "average",
...
```

Arguments

pop_sim	An object representing the similarities of an indexed population of objects.
	Arguments for get_sim_p.
group	Character or integer vector specifying names/indices of subgroup for which to calculate a group similarity p-value.
type	Either "matrix", "sim_index" or "numeric" - the type of the pop_sim object.
min_its	Minimum number of simulated group similarities to calculate
max_its	Maximum number of simulated group similarities to calculate
signif	Threshold p-value of statistical significance
log_dismiss	Threshold of log probability, below which to trigger return of current estimated p-value
group_sim	String Either "average" or "min", determining how to calculate the similarity of a group of term sets over all pairwise combinations of group members

Value

p-value.

See Also

get_sim sample_group_sim

get_sim_p_from_ontology

Get similarity p-value for subgroup term sets

Description

Compute a similarity p-value by permutation for subgroup of a list of term sets

Usage

```
get_sim_p_from_ontology(
    ontology,
    term_sets,
    information_content = descendants_IC(ontology),
    term_sim_method = "lin",
    combine = "average",
    ...
)
```

10

Arguments

ontology	ontology_index object.
term_sets	List of character vectors of ontological term IDs.
information_co	ntent
	Numeric vector of information contents of terms (named by term)
term_sim_metho	d
	Character string equalling either "lin" or "resnik" to use Lin or Resnik's expres- sion for the similarity of terms.
combine	Character string - either "average" or "product", indicating whether to use the best-match-product' method, or function accepting two arguments - the first, the similarity matrix obtained by averaging across term sets in term_sets, and the second averaging across those in term_sets2.
•••	Other arguments to be passed to get_sim_p.

Value

Numeric value.

See Also

get_sim_p create_sim_index

```
get_term_set_to_term_sims
```

Get 'term sets to term' similarity matrix

Description

Create a numeric matrix of similarities between term sets and individual terms.

Usage

```
get_term_set_to_term_sims(term_sets, terms, ...)
```

Arguments

term_sets	List of character vectors of ontological term IDs.
terms	Character vector of ontological terms.
	Other arguments to be passed to get_sim_grid.

Value

Numeric matrix of term set-to-term similarities

See Also

get_sim_grid

get_term_sim_mat Get term-term similarity matrix

Description

Get matrix of pairwise similarity of individual terms based on Lin's (default) or Resnik's information content-based expression.

Usage

```
get_term_sim_mat(
    ontology,
    information_content,
    method = "lin",
    row_terms = names(information_content),
    col_terms = names(information_content)
)
```

Arguments

ontology	ontology_index object.	
information_content		
	Numeric vector of information contents of terms (named by term)	
method	Character value equalling either "lin" or "resnik" to use Lin or Resnik's expres- sion for similarity of terms respectively.	
row_terms	Character vector of term IDs to appear as rows of result matrix.	
col_terms	Character vector of term IDs to appear as cols of result matrix.	

Value

Numeric matrix of pairwise term similarities.

See Also

get_sim_grid resnik, lin

GO_IC

Description

Numeric vector containing the information content of Gene Ontology terms based on frequencies of annotation data object gene_GO_terms. The object can be derived using the function get_term_info_content and data object go from the ontologyIndex package.

Format

List of character vectors.

group_term_enrichment Identify enriched terms in subgroup

Description

Create a table of terms ranked by their significance of occurrence in a set of term sets amongst an enclosing set, with p-values computed by permutation. Terms are subselected so that only the minimal set of non-redundant terms at each level of frequency within the group are retained.

Usage

```
group_term_enrichment(
   ontology,
   term_sets,
   group,
   permutations = 1000L,
   min_terms = 2L,
   mc.cores = NULL
)
```

Arguments

ontology	ontology_index object.
term_sets	List of character vectors of ontological term IDs.
group	Integer/logical/character vector specifying indices/positions/names of subgroup for which to calculate a group similarity p-value.
permutations	Number of permutations to test against, or if NULL, perform no permutations and return the unadjusted p-values for the occurrence of each term.
<pre>min_terms</pre>	Minimum number of times a term should occur within the given group to be eligible for inclusion in the results.
mc.cores	If not null and greater than on, the number of cores use calculating permutations (passed to mclapply).

Value

data.frame containing columns: term (with the term ID); name (term readable name); in_term (number of sets in the given group of containing the term); in_no_term (number of sets in the given group not containing the term); out_term and out_no_term (equivalently for the sets not in the given group); p (the p-values calculated by permutation for seeing a term with such a strong association, measured using Fisher's exact test, in a group of term sets the size of the given group among term_sets). Rows ordered by significance (i.e. the p columns).

See Also

sample_group_sim create_sim_index

lin

Calculate Lin similarity score of two term sets

Description

Warning! This function is slow - performing large numbers of 'between term-set' similarity calculations should be done using get_sim_grid.

Usage

lin(ontology, information_content, term_set_1, term_set_2)

Arguments

ontology	ontology_index object.
information_content	
	Numeric vector of information contents of terms (named by term)
term_set_1	Character vector of terms.
term_set_2	Character vector of terms.

Value

Numeric value.

References

Lin D (1998). 'An Information-Theoretic Definition of Similarity.' In Shavlik JW (ed.), _Proceedings of the Fifteenth International Conference on Machine Learning (ICML 1998), Madison, Wisconsin, USA, July 24-27, 1998_, pp. 296-304.

See Also

resnik,get_term_sim_mat

resnik

Description

Warning! This function is slow - performing large numbers of 'between term-set' similarity calculations should be done using get_sim_grid.

Usage

```
resnik(ontology, information_content, term_set_1, term_set_2)
```

Arguments

ontology	ontology_index object.
information_content	
	Numeric vector of information contents of terms (named by term)
term_set_1	Character vector of terms.
term_set_2	Character vector of terms.

Value

Numeric value.

References

Resnik, P. (1995). 'Using information content to evaluate semantic similarity in a taxonomy'. Proceedings of the 14th IJCAI 1, 448-453.

See Also

lin,get_term_sim_mat

sample_group_sim Draw sample of group similarities

Description

Draw sample of group similarities of groups of given size

Usage

```
sample_group_sim(pop_sim, ...)
## S3 method for class 'integer'
sample_group_sim(pop_sim, ...)
## S3 method for class 'numeric'
sample_group_sim(pop_sim, ...)
## S3 method for class 'matrix'
sample_group_sim(pop_sim, ...)
## S3 method for class 'sim_index'
sample_group_sim(pop_sim, ...)
## Default S3 method:
sample_group_sim(
 pop_sim,
  type,
  group_size,
 group_sim = "average",
  sample_size = 10000,
  . . .
)
```

Arguments

pop_sim	An object representing the similarities of an indexed population of objects.
	Other arguments to be passed to sample_group_sim.
type	Either "matrix", "sim_index" or "numeric" - the type of the pop_sim object.
group_size	Integer giving the number of members of a group.
group_sim	String Either "average" or "min", determining how to calculate the similarity of a group of term sets over all pairwise combinations of group members
sample_size	Number of samples to draw.

Value

Numeric vector of random group similarities.

See Also

get_sim get_sim_p

16

Description

ample of group similarities for random groups of given drawn from the given ontology argument

Usage

```
sample_group_sim_from_ontology(
    ontology,
    term_sets,
    information_content = descendants_IC(ontology),
    term_sim_method = "lin",
    combine = "average",
    ...
)
```

Arguments

ontology	ontology_index object.
term_sets	List of character vectors of ontological term IDs.
information_content	
	Numeric vector of information contents of terms (named by term)
term_sim_method	
	Character string equalling either "lin" or "resnik" to use Lin or Resnik's expres- sion for the similarity of terms.
combine	Character string - either "average" or "product", indicating whether to use the best-match-product' method, or function accepting two arguments - the first, the similarity matrix obtained by averaging across term sets in term_sets, and the second averaging across those in term_sets2.
	Other arguments to be passed to get_sim_p.

Value

Numeric vector of group similarities.

See Also

sample_group_sim create_sim_index

Index

* **GO** ontologySimilarity-package, 2 * HPO ontologySimilarity-package, 2 * ontological similarity ontologySimilarity-package, 2 * ontology ontologySimilarity-package, 2 * semantic similarity ontologySimilarity-package, 2 create_sim_index, 3, 11, 14, 17 descendants_IC, 4, 8 gene_GO_terms, 4 get_asym_sim_grid, 5, 6, 9 get_profile_sims, 5, 5 get_sim, 6, 10, 16 get_sim_grid, 4-6, 8, 11, 12, 14, 15 get_sim_p, 4, 7, 9, 9, 11, 16, 17 get_sim_p_from_ontology, 10 get_similarity_rank_matrix,7 get_term_set_to_term_sims, 11 get_term_sim_mat, 8, 9, 12, 14, 15 GO_IC, 13 group_term_enrichment, 13

lin, 12, 14, 15

ontologySimilarity
 (ontologySimilarity-package), 2
ontologySimilarity-package, 2

resnik, *12*, *14*, 15

sample_group_sim, 4, 7, 10, 14, 15, 17
sample_group_sim_from_ontology, 17