Package ‘simplifyEnrichment’

March 23, 2024

**Type**  Package  
**Title**  Simplify Functional Enrichment Results  
**Version**  1.12.0  
**Date**  2023-04-20  
**Depends**  R (>= 3.6.0), BiocGenerics, grid  
**Imports**  GOSemSim, ComplexHeatmap (>= 2.7.4), circlize, GetoptLong, digest, tm, GO.db, org.Hs.eg.db, AnnotationDbi, slam, methods, clue, grDevices, graphics, stats, utils, proxyC, Matrix, cluster (>= 1.14.2), colorspace, GlobalOptions (>= 0.1.0)  
**Suggests**  knitr, ggplot2, cowplot, mclust, apcluster, MCL, dbscan, igraph, gridExtra, dynamicTreeCut, testthat, gridGraphics, clusterProfiler, msigdbr, DOSE, DO.db, reactome.db, flexclust, BiocManager, InteractiveComplexHeatmap (>= 0.99.11), shiny, shinydashboard, cola, hu6800.db, rmarkdown, genefilter, gridtext, fpc  
**Description**  A new clustering algorithm, "binary cut", for clustering similarity matrices of functional terms is implemented in this package. It also provides functions for visualizing, summarizing and comparing the clusterings.

**biocViews**  Software, Visualization, GO, Clustering, GeneSetEnrichment  
**VignetteBuilder**  knitr  
**License**  MIT + file LICENSE  
**git_url**  https://git.bioconductor.org/packages/simplifyEnrichment  
**git_branch**  RELEASE_3_18  
**git_last_commit**  32b08eb  
**git_last_commit_date**  2023-10-24  
**Repository**  Bioconductor 3.18  
**Date/Publication**  2024-03-22
**R topics documented:**

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all_clustering_methods

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all_clustering_methods

All clustering methods

Description

All clustering methods

Usage

all_clustering_methods()

Details

The default clustering methods are:

kmeans see cluster_by_kmeans.
dynamicTreeCut see cluster_by_dynamicTreeCut.
mclust see cluster_by_mclust.
apcluster see cluster_by_apcluster.
hdbscan see cluster_by_hdbscan.
fast_greedy see cluster_by_igraph.
louvain see cluster_by_igraph.
waktrap see cluster_by_igraph.
MCL see cluster_by_MCL.
binary_cut see binary_cut.

Value

A vector of method names.
See Also

New methods can be added by register_clustering_methods.

Examples

all_clustering_methods()

anno_word_cloud  Word cloud annotations

Description

Word cloud annotations

Usage

anno_word_cloud(align_to, term, exclude_words = NULL, max_words = 10,
word_cloud_grob_param = list(), fontsize_range = c(4, 16), value_range = NULL,
bg_gp = gpar(fill = "#DDDDDD", col = "#AAAAAA"), side = c("right", "left"),
add_new_line = FALSE, count_words_param = list(), ...)

Arguments

align_to  How to align the annotations to the heatmap. Similar as in anno_link, the value of align_to can be a list of row indices or a categorical vector where each vector in the list corresponds to a word cloud. If it is a categorical vector, rows with the same level correspond to a same word cloud. If align_to is a categorical vector and term is a list, names of term should have overlap to the levels in align_to. When align_to is set as a categorical vector, normally the same value is set to row_split in the main heatmap so that each row slice can correspond to a word cloud.

term  The description text used for constructing the word clouds. The value should have the same format as align_to. If align_to is a list, term should also be a list. In this case, the length of vectors in term is not necessarily the same as in align_to. E.g. length(term[[1]]) is not necessarily equal to length(align_to[[1]]). If align_to is a categorical vector, term should also be a character vector with the same length as align_to. To make it more general, when align_to is a list, term can also be a list of data frames where the first column contains keywords and the second column contains numeric values that will be mapped to font sizes in the word clouds.

exclude_words  The words excluded for constructing word cloud.

max_words  Maximal number of words visualized in the word cloud.

word_cloud_grob_param  A list of graphics parameters passed to word_cloud_grob.

fontsize_range  The range of the font size. The value should be a numeric vector with length two. The font size interpolation is linear.
Word cloud annotations from GO

Description

Word cloud annotations from GO

Usage

anno_word_cloud_from_GO(align_to, go_id, stat = c("pvalue", "count"),
    min_stat = ifelse(stat == "count", 5, 0.05),
    term = NULL, exclude_words = NULL, ...)
Arguments
align_to
  The same format as in `anno_word_cloud`.
go_id
  The value should be in the same format as `align_to`. If `go_id` is a vector, it should have the same length as `align_to`, and if `go_id` is a list, note, e.g. `length(go_id[[1]])` is not necessarily equal to `length(align_to[[1]])`. If `align_to` is a categorical vector and `go_id` is a list, names of `go_id` should have overlap to the levels in `align_to`.
min_stat
  Minimal value for `stat` for selecting keywords.
stat
  What type of value to map to font sizes of the keywords. There are two possible values. "pvalue": enrichment is applied to keywords and `-log10(p-value)` is used to map to font size; "count": simply word frequency of keywords.
term
  Alternatively the GO description can be set via the `term` argument. The same format as in `anno_word_cloud`.
exclude_words
  The words excluded for constructing word cloud. Some words are internally excluded: c("via", "protein", "factor", "side", "type", "specific"). ...

All other arguments passed to `anno_word_cloud`.

Examples
# There is no example
NULL

---

area_above_ecdf Area above the eCDF curve

Description
Area above the eCDF curve

Usage
area_above_ecdf(x)

Arguments
  x  A vector of similarity values.

Details
Denote F(x) as the eCDF (empirical Cumulative Distribution Function) of the similarity vector x, this function calculates the area above the eCDF curve, which is $1 - \int_0^1 F(x)dx$.

Value
A numeric value.
**binary_cut**

**Examples**

```r
# There is no example
NULL
```

```r
binary_cut
```

---

**Description**

Cluster functional terms by recursively binary cutting the similarity matrix

**Usage**

```r
binary_cut(mat, value_fun = area_above_ecdf, partition_fun = partition_by_pam,
    cutoff = 0.85, try_all_partition_fun = FALSE, partial = FALSE)
```

**Arguments**

- `mat` A similarity matrix.
- `value_fun` A function that calculates the scores for the four submatrices on a node.
- `partition_fun` A function to split each node into two groups. Pre-defined functions in this package are `partition_by_kmeanspp`, `partition_by_pam` and `partition_by_hclust`.
- `cutoff` The cutoff for splitting the dendrogram.
- `try_all_partition_fun` Different partition_fun gives different clusterings. If the vaule of `try_all_partition_fun` is set to TRUE, the similarity matrix is clustered by three partitioning method: `partition_by_pam`, `partition_by_kmeanspp` and `partition_by_hclust`. The clustering with the highest difference score is finally selected as the final clustering.
- `partial` Whether to generate the complete clustering or the clustering stops when submatrices cannot be split anymore.

**Value**

A vector of cluster labels (in numeric).

**Examples**

```r
mat = readRDS(system.file("extdata", "random_GO_BP_sim_mat.rds",
    package = "simplifyEnrichment"))
binary_cut(mat)
```
cluster_by_apcluster  

Cluster similarity matrix by apcluster

Usage

cluster_by_apcluster(mat, s = apcluster::negDistMat(r = 2), ...)

Arguments

mat  
The similarity matrix.

s  
Passed to the s argument in apcluster.

...  
Other arguments passed to apcluster.

Value

A vector of cluster labels (in numeric).

Examples

# There is no example
NULL

cluster_by_dynamicTreeCut

Cluster similarity matrix by dynamicTreeCut

Description

Cluster similarity matrix by dynamicTreeCut

Usage

cluster_by_dynamicTreeCut(mat, minClusterSize = 5, ...)

Arguments

mat  
The similarity matrix.

minClusterSize  
Minimal number of objects in a cluster. Pass to cutreeDynamic.

...  
Other arguments passed to cutreeDynamic.
cluster_by_hdbscan

Value

A vector of cluster labels (in numeric).

Examples

# There is no example
NULL

cluster_by_hdbscan       Cluster similarity matrix by hdbscan

Description

Cluster similarity matrix by hdbscan

Usage

cluster_by_hdbscan(mat, minPts = 5, ...)

Arguments

mat                The similarity matrix.
minPts             Passed to the minPts argument in hdbscan.
...                Other arguments passed to hdbscan.

Value

A vector of cluster labels (in numeric).

Examples

# There is no example
NULL
cluster_by_igraph

Cluster similarity matrix by graph community detection methods

Description
Cluster similarity matrix by graph community detection methods

Usage
cluster_by_igraph(mat,
                   method = c("fast_greedy",
                               "leading_eigen",
                               "louvain",
                               "walktrap"),
                   ...)

Arguments
- mat: The similarity matrix.
- method: The community detection method.
- ...: Other arguments passed to the corresponding community detection function, see Details.

Details
The symmetric similarity matrix can be treated as an adjacency matrix and constructed as a graph/network with the similarity values as the weight of the edges. Thus, clustering the similarity matrix can be treated as detecting clusters/modules/communities from the graph.

Four methods implemented in igraph package can be used here:

- fast_greedy uses `cluster_fast_greedy`.
- leading_eigen uses `cluster_leading_eigen`.
- louvain uses `cluster_louvain`.
- walktrap uses `cluster_walktrap`.

Value
A vector of cluster labels (in numeric).

Examples

```r
# There is no example
NULL
```
Description

Cluster similarity matrix by k-means clustering

Usage

cluster_by_kmeans(mat, max_k = max(2, min(round(nrow(mat)/5), 100)), ...)

Arguments

- `mat`: The similarity matrix.
- `max_k`: maximal k for k-means clustering.
- `...`: Other arguments passed to `kmeans`.

Details

The best number of k for k-means clustering is identified according to the "elbow" or "knee" method on the distribution of within-cluster sum of squares (WSS) at each k.

Value

A vector of cluster labels (in numeric).

Examples

# There is no example
NULL

Description

Cluster similarity matrix by MCL

Usage

cluster_by_MCL(mat, addLoops = TRUE, ...)

Description

Cluster similarity matrix by MCL
Arguments

- mat: The similarity matrix.
- addLoops: Passed to the addLoops argument in mcl.
- ...: Other arguments passed to mcl.

Value

A vector of cluster labels (in numeric).

Examples

# There is no example
NULL

---

`cluster_by_mclust`  
*Cluster similarity matrix by mclust*

Description

Cluster similarity matrix by mclust

Usage

`cluster_by_mclust(mat, G = seq_len(max(2, min(round(nrow(mat)/5), 100))), ...)`

Arguments

- mat: The similarity matrix.
- G: Passed to the G argument in Mclust.
- ...: Other arguments passed to Mclust.

Value

A vector of cluster labels (in numeric).

Examples

# There is no example
NULL
**cluster_by_pam**

Cluster similarity matrix by pam clustering

**Usage**

```r
cluster_by_pam(mat, max_k = max(2, min(round(nrow(mat)/10), 100)), ...)
```

**Arguments**

- `mat`: The similarity matrix.
- `max_k`: maximal k for pam clustering.
- `...`: Other arguments passed to `pamk`.

**Details**

PAM is applied by `pamk` which can automatically select the best k.

**Value**

A vector of cluster labels (in numeric).

**Examples**

```r
# There is no example
NULL
```

---

**cluster_terms**

Cluster functional terms

**Description**

Cluster functional terms

**Usage**

```r
cluster_terms(mat, method = "binary_cut", control = list(), catch_error = FALSE, verbose = TRUE)
```

---
Arguments

- **mat**: A similarity matrix.
- **method**: Method for clustering the matrix.
- **control**: A list of parameters passed to the corresponding clustering function.
- **catch_error**: Internally used.
- **verbose**: Whether to print messages.

Details

The following methods are the default:

- kmeans see `cluster_by_kmeans`.
- pam see `cluster_by_pam`.
- dynamicTreeCut see `cluster_by_dynamicTreeCut`.
- mclust see `cluster_by_mclust`.
- apcluster see `cluster_by_apcluster`.
- hdbscan see `cluster_by_hdbscan`.
- leading_eigen see `cluster_by_igraph`.
- louvain see `cluster_by_igraph`.
- walktrap see `cluster_by_igraph`.
- MCL see `cluster_by_MCL`.
- binary_cut see `binary_cut`.

Also the user-defined methods in `all_clustering_methods` can be used here.

New clustering methods can be registered by `register_clustering_methods`.

Please note it is better to directly call `cluster_terms` for clustering while not the individual `cluster_by_*` functions because `cluster_terms` does additional cluster label adjustment.

Value

A numeric vector of cluster labels (in numeric).

If `catch_error` is set to TRUE and if the clustering produces an error, the function returns a try-error object.

Examples

# There is no example
NULL
cmp_make_clusters

Description

Apply various clustering methods

Usage

```r
cmp_make_clusters(mat, method = setdiff(all_clustering_methods(), "mclust"),
                    verbose = TRUE)
```

Arguments

- `mat`: The similarity matrix.
- `method`: Which methods to compare. All available methods are in `all_clustering_methods`. A value of all takes all available methods. By default `mclust` is excluded because its long runtime.
- `verbose`: Whether to print messages.

Details

The function compares following default clustering methods by default:

- `kmeans` see `cluster_by_kmeans`.
- `pam` see `cluster_by_pam`.
- `dynamicTreeCut` see `cluster_by_dynamicTreeCut`.
- `mclust` see `cluster_by_mclust`. By default it is not included.
- `apcluster` see `cluster_by_apcluster`.
- `hdbscan` see `cluster_by_hdbscan`.
- `fast_greedy` see `cluster_by_igraph`.
- `louvain` see `cluster_by_igraph`.
- `walktrap` see `cluster_by_igraph`.
- `MCL` see `cluster_by_MCL`.
- `binary_cut` see `binary_cut`.

Also the user-defined methods in `all_clustering_methods` are also compared.

Value

A list of cluster label vectors for different clustering methods.
Examples

```r
## Not run:
mat = readRDS(system.file("extdata", "random_GO_BP_sim_mat.rds", 
    package = "simplifyEnrichment"))
clt = cmp_make_clusters(mat)

## End(Not run)
```

### Description

Make plots for comparing clustering methods

#### Usage

```r
cmp_make_plot(mat, clt, plot_type = c("mixed", "heatmap"), nrow = 3)
```

#### Arguments

- `mat`: A similarity matrix.
- `clt`: A list of clusterings from `cmp_make_clusters`.
- `plot_type`: What type of plots to make. See Details.
- `nrow`: Number of rows of the layout when `plot_type` is set to `heatmap`.

#### Details

If `plot_type` is the default value `mixed`, a figure with three panels generated:

- A heatmap of the similarity matrix with different classifications as row annotations.
- A heatmap of the pair-wise concordance of the classifications of every two clustering methods.
- Barplots of the difference scores for each method (calculated by `difference_score`), the number of clusters (total clusters and the clusters with size $\geq 5$) and the mean similarity of the terms that are in the same clusters.

If `plot_type` is `heatmap`. There are heatmaps for the similarity matrix under clusterings from different methods. The last panel is a table with the number of clusters under different clusterings.

#### Value

No value is returned.
Examples

```r
## Not run:
mat = readRDS(system.file("extdata", "random_GO_BP_sim_mat.rds", 
    package = "simplifyEnrichment"))
clt = cmp_make_clusters(mat)
cmp_make_plot(mat, clt)
cmp_make_plot(mat, clt, plot_type = "heatmap")
## End(Not run)
```

## Compare clustering methods

### Description

Compare clustering methods

### Usage

```r
compare_clustering_methods(mat, method = setdiff(all_clustering_methods(), "mclust"), 
    plot_type = c("mixed", "heatmap"), nrow = 3, verbose = TRUE)
```

### Arguments

- `mat` The similarity matrix.
- `method` Which methods to compare. All available methods are in `all_clustering_methods`. A value of all takes all available methods. By default mclust is excluded because its long runtime.
- `plot_type` See explanation in `cmp_make_plot`.
- `nrow` Number of rows of the layout when `plot_type` is set to heatmap.
- `verbose` Whether to print messages.

### Details

The function compares following clustering methods by default:

- `kmeans` see `cluster_by_kmeans`.
- `pam` see `cluster_by_pam`.
- `dynamicTreeCut` see `cluster_by_dynamicTreeCut`.
- `mclust` see `cluster_by_mclust`. By default it is not included.
- `apcluster` see `cluster_by_apcluster`.
- `hdbscan` see `cluster_by_hdbscan`.
- `fast_greedy` see `cluster_by_igraph`.
louvain see \texttt{cluster\_by\_igraph}.
walktrap see \texttt{cluster\_by\_igraph}.
MCL see \texttt{cluster\_by\_MCL}.
binary\_cut see \texttt{binary\_cut}.

This function is basically a wrapper function. It calls the following two functions:

- \texttt{cmp\_make\_clusters}: applies clustering with different methods.
- \texttt{cmp\_make\_plot}: makes the plots.

\textbf{Value}

No value is returned.

\textbf{Examples}

```r
## Not run:
mat = readRDS(system.file("extdata", "random_GO_BP_sim_mat.rds", package = "simplifyEnrichment"))
compare_clustering_methods(mat)
compare_clustering_methods(mat, plot_type = "heatmap")
## End(Not run)
```

\section*{count\_words}

\textit{Calculate word frequency}

\textbf{Description}

Calculate word frequency

\textbf{Usage}

```r
count\_words(term, 
  exclude\_words = NULL, stop\_words = stopwords(), 
  min\_word\_length = 1, tokenizer = 'words', transform\_case = tolower, 
  remove\_numbers = TRUE, remove\_punctuation = TRUE, custom\_transformer = NULL, 
  stemming = FALSE, dictionary = NULL)
```

\textbf{Arguments}

- \texttt{term} A vector of description texts.
- \texttt{exclude\_words} The words that should be excluded.
- \texttt{stop\_words} The stop words that should be removed.
- \texttt{min\_word\_length} Minimum length of the word to be counted.
tokenizer The tokenizer function, one of the values accepted by `tm::termFreq`.
transform_case The function normalizing lettercase of the words.
remove_numbers Whether to remove numbers.
remove_punctuation Whether to remove punctuation.
custom_transformer Custom function that transforms words.
stemming Whether to only keep the roots of inflected words.
dictionary A vector of words to be counted (if given all other words will be excluded).

Details


Value

A data frame with words and frequencies.

Examples

```r
gm = readRDS(system.file("extdata", "random_GO_BP_sim_mat.rds", package = "simplifyEnrichment"))
go_id = rownames(gm)
go_term = AnnotationDbi::select(GO.db::GO.db, keys = go_id, columns = "TERM")$TERM
count_words(go_term)
```

```r
dend_node_apply(dend, fun)
```

Arguments

dend A dendrogram.
fun A self-defined function.
Details

The function returns a vector or a list as the same length as the number of nodes in the dendrogram. The self-defined function can have one single argument which is the sub-dendrogram at a certain node. E.g. to get the number of members at every node:

```r
dend_node_apply(dend, function(d) attr(d, "members"))
```

The self-defined function can have a second argument, which is the index of current sub-dendrogram in the complete dendrogram. E.g. `dend[[1]]` is the first child node of the complete dendrogram and `dend[[c(1, 2)]]` is the second child node of `dend[[1]]`, et al. This makes that at a certain node, it is possible to get information of its child nodes and parent nodes.

```r
dend_node_apply(dend, function(d, index) {
    dend[[c(index, 1)]] # is the first child node of d, or simply d[[1]]
    dend[[index[-length(index)]]] # is the parent node of d
    ...
})
```

Note for the top node, the value of `index` is `NULL`.

Value

A vector or a list, depends on whether `fun` returns a scalar or more complex values.

Examples

```r
mat = matrix(rnorm(100), 10)
dend = as.dendrogram(hclust(dist(mat)))
# number of members on every node
dend_node_apply(dend, function(d) attr(d, "members"))
# the depth on every node
dend_node_apply(dend, function(d, index) length(index))
```

---

**difference_score**

**Description**

Difference score

**Usage**

difference_score(mat, cl)

**Arguments**

- mat: The similarity matrix.
- cl: Cluster labels.
**Details**

This function measures the different between the similarity values for the terms that belong to the same clusters and in different clusters. The difference score is the Kolmogorov-Smirnov statistic between the two distributions.

**Value**

A numeric scalar.

**Examples**

```r
cmat = readRDS(system.file("extdata", "random_GO_BP_sim_mat.rds", package = "simplifyEnrichment"))
ccl = binary_cut(mmat)
difference_score(mmat, ccl)
```

---

**DO_similarity**

*Calculate Disease Ontology (DO) semantic similarity matrix*

**Description**

Calculate Disease Ontology (DO) semantic similarity matrix

**Usage**

```r
DO_similarity(do_id, measure = "Rel", remove_orphan_terms = FALSE)
```

**Arguments**

- `do_id` A vector of DO IDs.
- `measure` Semantic measure for the DO similarity, pass to `doSim`.
- `remove_orphan_terms` Whether to remove terms that have zero similarity to all other terms?

**Details**

This function is basically a wrapper on `doSim`.

**Value**

A symmetric matrix.

**Examples**

```r
require(DOSE)
do_id = random_DO(10)
DO_similarity(do_id)
```
**Description**

Modify nodes in a dendrogram

**Usage**

```r
edit_node(dend, fun = function(d, index) d)
```

**Arguments**

- **dend**: A dendrogram.
- **fun**: A self-defined function.

**Details**

If `fun` only has one argument, it is basically the same as `dendrapply`, but it can have a second argument which is the index of the node in the dendrogram, which makes it possible to get information of child nodes and parent nodes for a specific node.

As an example, we first assign random values to every node in the dendrogram:

```r
mat = matrix(rnorm(100), 10)
dend = as.dendrogram(hclust(dist(mat)))
dend = edit_node(dend, function(d) {attr(d, 'score') = runif(1); d})
```

Then for every node, we take the maximal absolute difference to all its child nodes and parent node as the attribute `abs_diff`

```r
dend = edit_node(dend, function(d, index) {
  n = length(index)
  s = attr(d, "score")
  if(is.null(index)) { # d is the top node
    s_children = sapply(d, function(x) attr(x, "score"))
    s_parent = NULL
  } else if(is.leaf(d)) { # d is the leaf
    s_children = NULL
    s_parent = attr(dend[[index[-n]]], "score")
  } else {
    s_children = sapply(d, function(x) attr(x, "score"))
    s_parent = attr(dend[[index[-n]]], "score")
  }
  abs_diff = max(abs(s - c(s_children, s_parent)))
  attr(d, "abs_diff") = abs_diff
  return(d)
})
```
Value

A dendrogram object.

Examples

# There is no example
NULL

declare

export_to_shiny_app  Interactively visualize the similarity heatmap

Description

Interactively visualize the similarity heatmap

Usage

export_to_shiny_app(mat, cl = binary_cut(mat))

Arguments

mat  A similarity matrix.
cl   Cluster labels inferred from the similarity matrix, e.g. from cluster_terms or binary_cut.

Examples

if(interactive()) {
  mat = readRDS(system.file("extdata", "random_GO_BP_sim_mat.rds", package = "simplifyEnrichment"))
  cl = binary_cut(mat)
  export_to_shiny_app(mat, cl)
}

declare

GO_similarity  Calculate Gene Ontology (GO) semantic similarity matrix

Description

Calculate Gene Ontology (GO) semantic similarity matrix

Usage

GO_similarity(go_id, ont = NULL, db = 'org.Hs.eg.db', measure = "Rel", remove_orphan_terms = FALSE)
guess_ont

Arguments

- **go_id**: A vector of GO IDs.
- **ont**: GO ontology. Value should be one of "BP", "CC" or "MF". If it is not specified, the function automatically identifies it by random sampling 10 IDs from go_id (see `guess_ont`).
- **db**: Annotation database. It should be from https://bioconductor.org/packages/3.10/BiocViews.html###OrgDb. The value can also directly be a OrgDb object.
- **measure**: Semantic measure for the GO similarity, pass to `termSim`.
- **remove_orphan_terms**: Whether to remove terms that have zero similarity to all other terms?

Details

This function is basically a wrapper on `termSim`.

Value

A symmetric matrix.

Examples

```r
go_id = random_GO(100)
mat = GO_similarity(go_id)
```

---

**guess_ont**

Guess the ontology of the input GO IDs

Description

Guess the ontology of the input GO IDs

Usage

```r
guess_ont(go_id, db = 'org.Hs.eg.db')
```

Arguments

- **go_id**: A vector of GO IDs.
- **db**: Annotation database. It should be from https://bioconductor.org/packages/3.10/BiocViews.html###OrgDb. The value can also directly be a OrgDb object.

Details

10 GO IDs are randomly sampled and checked.
Value

A single character scalar of "BP", "CC" or "MF".

If there are more than one ontologies detected. It returns NULL.

Examples

```r
go_id = random_GO(100)
guess_ont(go_id)
```

---

**Description**

Height for word_cloud grob

**Usage**

```r
## S3 method for class 'word_cloud'
heightDetails(x)
```

**Arguments**

- `x` The word_cloud grob returned by `word_cloud_grob`.

**Value**

A unit object.

**Examples**

```r
# There is no example
NULL
```
ht_clusters  Visualize the similarity matrix and the clustering

Description

Visualize the similarity matrix and the clustering

Usage

ht_clusters(
  mat,
  cl,
  dend = NULL,
  col = c("white", "red"),

  # arguments that control the word cloud annotation
draw_word_cloud = TRUE,
min_term = round(nrow(mat)*0.01),
order_by_size = FALSE,
stat = "pvalue",
min_stat = ifelse(stat == "count", 5, 0.05),
exclude_words = character(0),
max_words = 10,
word_cloud_grob_param = list(),
fontsize_range = c(4, 16),
bg_gp = gpar(fill = "#DDDDDD", col = "#AAAAAA"),

  # arguments that control the heatmaps
column_title = NULL,
ht_list = NULL,
use_raster = TRUE,
run_draw = TRUE,
...)

Arguments

mat  A similarity matrix.
cl   Cluster labels inferred from the similarity matrix, e.g. from cluster_terms or binary_cut.
dend Used internally.
col  A vector of colors that map from 0 to the 97.5\textsuperscript{th} percentile of the similarity values. The value can also be a color mapping function generated by colorRamp2.
draw_word_cloud Whether to draw the word clouds.
min_term Minimal number of functional terms in a cluster. All the clusters with size less than min_term are all merged into one separated cluster in the heatmap.
Keyword enrichment for GO terms

Description

Keyword enrichment for GO terms

Value

A HeatmapList-class object.

Examples

```R
## Not run:
mat = readRDS(system.file("extdata", "random_GO_BP_sim_mat.rds", package = "simplifyEnrichment"))
c1 = binary_cut(mat)
ht_clusters(mat, c1, word_cloud_grob_param = list(max_width = 80))
ht_clusters(mat, c1, word_cloud_grob_param = list(max_width = 80), order_by_size = TRUE)

## End(Not run)
```
Usage

```r
keyword_enrichment_from_GO(go_id, min_bg = 5, min_term = 2)
```

**Arguments**

- `go_id`: A vector of GO IDs.
- `min_bg`: Minimal number of GO terms (in the background, i.e. all GO terms in the GO database) that contain a specific keyword.
- `min_term`: Minimal number of GO terms (GO terms in `go_id`) that contain a specific keyword.

**Details**

The enrichment is applied by Fisher’s exact test. For a keyword, there is the following 2x2 contingency table:

<table>
<thead>
<tr>
<th></th>
<th>contains the keyword</th>
<th>does not contain the keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>In the GO set</td>
<td>s11</td>
<td>s12</td>
</tr>
<tr>
<td>Not in the GO set</td>
<td>s21</td>
<td>s22</td>
</tr>
</tbody>
</table>

where s11, s12, s21 and s22 are number of GO terms in each category.

**Value**

A data frame with keyword enrichment results.

**Examples**

```r
## Not run:
go_id = random_GO(100)
keyword_enrichment_from_GO(go_id)

## End(Not run)
```

---

**partition_by_hclust**  

**Description**

Partition by hclust

**Usage**

```r
partition_by_hclust(mat)
```

**Arguments**

- `mat`: The similarity matrix.
Details

The "ward.D2" clustering method was used.
This function is used to set to the partition_fun argument in `binary_cut`.

Examples

```r
# There is no example
NULL
```

---

**partition_by_kmeans**  
*Partition by kmeans*

Description

Partition by kmeans

Usage

```r
partition_by_kmeans(mat, n_repeats = 10)
```

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>mat</code></td>
<td>The similarity matrix.</td>
</tr>
<tr>
<td><code>n_repeats</code></td>
<td>Number of repeated runs of k-means.</td>
</tr>
</tbody>
</table>

Details

Since k-means clustering brings randomness, this function performs k-means clustering several times (controlled by `n_repeats`) and uses the final consensus partitioning.

This function is used to set to the partition_fun argument in `binary_cut`.

Examples

```r
# There is no example
NULL
```
### partition_by_kmeanspp

**Partition by kmeans++**

**Description**

Partition by kmeans++

**Usage**

```r
partition_by_kmeanspp(mat)
```

**Arguments**

- `mat`: The similarity matrix.

**Details**

This function is used to set to the `partition_fun` argument in `binary_cut`.

**Examples**

```r
# There is no example
NULL
```

---

### partition_by_pam

**Partition by PAM**

**Description**

Partition by PAM

**Usage**

```r
partition_by_pam(mat)
```

**Arguments**

- `mat`: The similarity matrix.

**Details**

The clustering is performed by `pam` with setting `pamonce` argument to 5.

This function is used to set to the `partition_fun` argument in `binary_cut`.

```r
```
**plot_binary_cut**

**Visualize the process of binary cut**

**Description**

Visualize the process of binary cut

**Usage**

```r
plot_binary_cut(mat, value_fun = area_above_ecdf, cutoff = 0.85,
                partition_fun = partition_by_pam, dend = NULL, dend_width = unit(3, "cm"),
                depth = NULL, show_heatmap_legend = TRUE, ...)
```

**Arguments**

- `mat` The similarity matrix.
- `value_fun` A function that calculates the scores for the four submatrices on a node.
- `cutoff` The cutoff for splitting the dendrogram.
- `partition_fun` A function to split each node into two groups. Pre-defined functions in this package are `partition_by_kmeanspp`, `partition_by_pam` and `partition_by_hclust`.
- `dend` A dendrogram object, used internally.
- `depth` Depth of the recursive binary cut process.
- `dend_width` Width of the dendrogram on the plot.
- `show_heatmap_legend` Whether to show the heatmap legend.
- `...` Other arguments.

**Details**

After the functions which perform clustering are executed, such as `simplifyGO` or `binary_cut`, the dendrogram is temporarily saved and `plot_binary_cut` directly uses this dendrogram.

**Examples**

```r
mat = readRDS(system.file("extdata", "random.GO_BP_sim_mat.rds",
                          package = "simplifyEnrichment"))
plot_binary_cut(mat, depth = 1)
plot_binary_cut(mat, depth = 2)
plot_binary_cut(mat)
```
random_DO

Generate random Disease Ontology (DO) IDs

Description
Generate random Disease Ontology (DO) IDs

Usage
random_DO(n)

Arguments
n Number of DO IDs.

details
DO.db package should be installed.

Value
A vector of DO IDs.

Examples
random_DO(100)

random_GO

Generate random GO IDs

Description
Generate random GO IDs

Usage
random_GO(n, ont = "BP", db = 'org.Hs.eg.db')

Arguments
n Number of GO IDs.
ont GO ontology. Value should be one of "BP", "CC" or "MF".
db Annotation database. It should be from https://bioconductor.org/packages/3.10/BiocViews.html#OrgDb
Value
A vector of GO IDs.

Examples
random_GO(100)

Description
Register new clustering methods

Usage
register_clustering_methods(...)

Arguments
... A named list of clustering functions, see Details.

Details
The user-defined functions should accept at least one argument which is the input matrix. The second optional argument should always be ... so that parameters for the clustering function can be passed by control argument from cluster_terms, simplifyGO or simplifyEnrichment. If users forget to add ..., it is added internally.

Please note, the user-defined function should automatically identify the optimized number of clusters.

The function should return a vector of cluster labels. Internally it is converted to numeric labels.

Value
No value is returned.

Examples
register_clustering_methods(
  # assume there are 5 groups
  random = function(mat, ...) sample(5, nrow(mat), replace = TRUE)
)
all_clustering_methods()
remove_clustering_methods("random")
remove_clustering_methods

*Remove clustering methods*

**Description**
Remove clustering methods

**Usage**
remove_clustering_methods(method)

**Arguments**
- **method**
  A vector of method names.

**Value**
No value is returned.

**Examples**
# There is no example
NULL

reset_clustering_methods

*Reset to default clustering methods*

**Description**
Reset to default clustering methods

**Usage**
reset_clustering_methods()

**Details**
The default methods are:
kmeans see `cluster_by_kmeans`
pam see `cluster_by_pam`
dynamicTreeCut see `cluster_by_dynamicTreeCut`
scale_fontsize

mclust see `cluster_by_mclust`.
apcluster see `cluster_by_apcluster`.
hdbscan see `cluster_by_hdbscan`.
fast_greedy see `cluster_by_igraph`.
louvain see `cluster_by_igraph`.
walktrap see `cluster_by_igraph`.
MCL see `cluster_by_MCL`.
binary_cut see `binary_cut`.

Value
No value is returned.

Examples

```
all_clustering_methods()
remove_clustering_methods(c("kmeans", "mclust"))
all_clustering_methods()
reset_clustering_methods()
all_clustering_methods()
```

<table>
<thead>
<tr>
<th>scale_fontsize</th>
<th>Scale font size</th>
</tr>
</thead>
</table>

Description
Scale font size

Usage

```
scale_fontsize(x, rg = c(1, 30), fs = c(4, 16))
```

Arguments

- `x` A numeric vector.
- `rg` The range.
- `fs` Range of the font size.

Value
A numeric vector.

Details
It is a linear interpolation.
Examples

```r
x = runif(10, min = 1, max = 20)
# scale x to fontsize 4 to 16.
scale_fontsize(x)
```

---

select_cutoff  Select the cutoff for binary cut

Description

Select the cutoff for binary cut

Usage

```r
select_cutoff(mat, cutoff = seq(0.6, 0.98, by = 0.01), verbose = TRUE, ...)
```

Arguments

- `mat` A similarity matrix.
- `cutoff` A list of cutoffs to test. Note the range of the cutoff values should be inside [0.5, 1].
- `verbose` Whether to print messages.
- `...` Pass to `binary_cut`.

Details

Binary cut is applied to each of the cutoff and the clustering results are evaluated by following metrics:

- difference score, calculated by `difference_score`.
- number of clusters.
- block mean, which is the mean similarity in the blocks in the diagonal of the heatmap.

Examples

```r
mat = readRDS(system.file("extdata", "random_GO_BP_sim_mat.rds", package = "simplifyEnrichment"))
select_cutoff(mat)
```
**se_opt**  
*Global parameters*

**Description**  
Global parameters

**Usage**  
```r
se_opt(..., RESET = FALSE, READ.ONLY = NULL, LOCAL = FALSE, ADD = FALSE)
```

**Arguments**

- `...` Arguments for the parameters, see "details" section.
- `RESET` Whether to reset to default values.
- `READ.ONLY` Please ignore.
- `LOCAL` Please ignore.
- `ADD` Please ignore.

**Details**
There are the following global options:

- `verbose` Whether to print messages.

**Examples**

```r
# There is no example
NULL
```

---

**simplifyEnrichment**  
*Simplify functional enrichment results*

**Description**
Simplify functional enrichment results

**Usage**
```r
simplifyEnrichment(mat, method = "binary_cut", control = list(),
    plot = TRUE, verbose = TRUE,
    column_title = qq("@{nrow(mat)} terms clustered by '@{method}'"),
    ht_list = NULL, ...)
```
Arguments

mat        A similarity matrix.
method     Method for clustering the matrix. See cluster_terms.
control    A list of parameters for controlling the clustering method, passed to cluster_terms.
plot       Whether to make the heatmap.
column_title Column title for the heatmap.
verbose    Whether to print messages.
ht_list    A list of additional heatmaps added to the left of the similarity heatmap.
...

Details

The usage is the same as simplifyGO.

Examples

# There is no example
NULL

simplifyGO  Simplify Gene Ontology (GO) enrichment results

Description

Simplify Gene Ontology (GO) enrichment results

Usage

simplifyGO(mat, method = "binary_cut", control = list(),
plot = TRUE, verbose = TRUE,
column_title = qq("@{nrow(mat)} GO terms clustered by '@{method}'"),
ht_list = NULL, ...)

Arguments

mat        A GO similarity matrix.
method     Method for clustering the matrix. See cluster_terms.
control    A list of parameters for controlling the clustering method, passed to cluster_terms.
plot       Whether to make the heatmap.
column_title Column title for the heatmap.
verbose    Whether to print messages.
ht_list    A list of additional heatmaps added to the left of the similarity heatmap.
...

Arguments passed to ht_clusters.
Details

This is basically a wrapper function that it first runs `cluster_terms` to cluster GO terms and then runs `ht_clusters` to visualize the clustering.

The arguments in `simplifyGO` passed to `ht_clusters` are:

- `draw_word_cloud` Whether to draw the word clouds.
- `min_term` Minimal number of GO terms in a cluster. All the clusters with size less than `min_term` are all merged into one single cluster in the heatmap.
- `order_by_size` Whether to reorder GO clusters by their sizes. The cluster that is merged from small clusters (size < `min_term`) is always put to the bottom of the heatmap.
- `stat` What values of keywords are used to map to font sizes in the word clouds.
- `exclude_words` Words that are excluded in the word cloud.
- `max_words` Maximal number of words visualized in the word cloud.
- `word_cloud_grob_param` A list of graphic parameters passed to `word_cloud_grob`.
- `fontsize_range` The range of the font size. The value should be a numeric vector with length two. The minimal font size is mapped to word frequency value of 1 and the maximal font size is mapped to the maximal word frequency. The font size interpolation is linear.
- `bg_gp` Graphic parameters for controlling the background of word cloud annotations.

Value

A data frame with two columns: GO IDs and cluster labels.

See Also

- `simplifyGOFromMultipleLists` which performs simplifyGO analysis with multiple lists of GO IDs.

Examples

```r
set.seed(123)
go_id = random_GO(500)
mat = GO_similarity(go_id)
df = simplifyGO(mat, word_cloud_grob_param = list(max_width = 80))
head(df)
```
Perform simplifyGO analysis with multiple lists of GO IDs

**Arguments**

- **lt**
  A data frame, a list of numeric vectors (e.g., adjusted p-values) where each numeric vector has GO IDs as names, or a list of GO IDs.

- **go_id_column**
  Column index of GO ID if `lt` contains a list of data frames.

- **padj_column**
  Column index of adjusted p-values if `lt` contains a list of data frames.

- **padj_cutoff**
  Cut off for adjusted p-values.

- **filter**
  A self-defined function for filtering GO IDs. By default it requires GO IDs should be significant in at least one list.

- **default**
  The default value for the adjusted p-values. See Details.

- **ont**
  GO ontology. Value should be one of "BP", "CC" or "MF". If it is not specified, the function automatically identifies it by random sampling 10 IDs from `go_id` (see `guess_ont`).

- **db**
  Annotation database. It should be from https://bioconductor.org/packages/3.10/BiocViews.html#_OrgDb

- **measure**
  Semantic measure for the GO similarity, pass to `termSim`.

- **heatmap_param**
  Parameters for controlling the heatmap, see Details.

- **show_barplot**
  Whether draw barplots which shows numbers of significant GO terms in clusters.

- **method**
  Pass to `simplifyGO`.

- **control**
  Pass to `simplifyGO`.

- **min_term**
  Pass to `simplifyGO`.

- **verbose**
  Pass to `simplifyGO`.

- **column_title**
  Pass to `simplifyGO`.

- **...**
  Pass to `simplifyGO`.
Details

The input data can have three types of formats:

- A list of numeric vectors of adjusted p-values where each vector has the GO IDs as names.
- A data frame. The column of the GO IDs can be specified with `go_id_column` argument and
  the column of the adjusted p-values can be specified with `padj_column` argument. If these
  columns are not specified, they are automatically identified. The GO ID column is found
  by checking whether a column contains all GO IDs. The adjusted p-value column is found
  by comparing the column names of the data frame to see whether it might be a column for
  adjusted p-values. These two columns are used to construct a numeric vector with GO IDs as
  names.
- A list of character vectors of GO IDs. In this case, each character vector is changed to a
  numeric vector where all values take 1 and the original GO IDs are used as names of the
  vector.

Now let's assume there are \( n \) GO lists, we first construct a global matrix where columns correspond
the \( n \) GO lists and rows correspond to the "union" of all GO IDs in the lists. The value for the \( i \)th
GO ID and in the \( j \)th list are taken from the corresponding numeric vector in \( lt \). If the \( j \)th vector in
\( lt \) does not contain the \( i \)th GO ID, the value defined by `default` argument is taken there (e.g. in
most cases the numeric values are adjusted p-values, `default` is set to 1). Let's call this matrix as
\( M_0 \).

Next step is to filter \( M_0 \) so that we only take a subset of GO IDs of interest. We define a proper
function via argument `filter` to remove GO IDs that are not important for the analysis. Functions
for `filter` is applied to every row in \( M_0 \) and `filter` function needs to return a logical value to
decide whether to remove the current GO ID. For example, if the values in \( lt \) are adjusted p-values,
the `filter` function can be set as `function(x) any(x < padj_cutoff)` so that the GO ID is kept
as long as it is significant in at least one list. After the filter, let's call the filtered matrix \( M_1 \).

GO IDs in \( M_1 \) (row names of \( M_1 \)) are used for clustering. A heatmap of \( M_1 \) is attached to the left of the
GO similarity heatmap so that the group-specific (or list-specific) patterns can be easily observed
and corresponding to GO functions.

Argument `heatmap_param` controls several parameters for heatmap \( M_1 \):

- `transform`: A self-defined function to transform the data for heatmap visualization. The most
typical case is to transform adjusted p-values by \(-\log_{10}(x)\).
- `breaks`: break values for color interpolation.
- `col`: The corresponding values for `breaks`.
- `labels`: The corresponding labels.
- `name`: Legend title.

Examples

```r
# perform functional enrichment on the signatures genes from cola analysis
require(cola)
data(golub_cola)
res = golub_cola["ATC:skmeans"]
require(hu6800.db)
```
x = hug00ENTREZID
mapped_probes = mappedkeys(x)
id_mapping = unlist(as.list(x[mapped_probes]))
lit = functional_enrichment(res, k = 3, id_mapping = id_mapping) # you can check the value of `lit`

# a list of data frames
simplifyGOFromMultipleLists(lit, padj_cutoff = 0.001)

# a list of numeric values
lit2 = lapply(lit, function(x) structure(x$p.adjust, names = x$ID))
simplifyGOFromMultipleLists(lit2, padj_cutoff = 0.001)

# a list of GO IDs
lit3 = lapply(lit, function(x) x$ID[x$p.adjust < 0.001])
simplifyGOFromMultipleLists(lit3)

---

subset_enrichResult  Subset method of the enrichResult class

Description

Subset method of the enrichResult class

Usage

subset_enrichResult(x, i)

Arguments

x  A enrichResult object from 'clusterProfiler' or other related packages.
i  Row indices.

Value

Still a enrichResult object but with the selected subset of rows.

Examples

# There is no example
NULL
term_similarity

Similarity between terms based on the overlap of genes

Description

Similarity between terms based on the overlap of genes

Usage

term_similarity(gl, method = c("kappa", "jaccard", "dice", "overlap"), all = NULL)

Arguments

- **gl**: A list of genes that are in the terms.
- **method**: The similarity measurement.
- **all**: The universe set.

Details

The definition of the four similarity measurements can be found at [https://jokergoo.github.io/simplifyEnrichment_supplementary/supplS01_coefficient_definition/supplS01_coefficient_definition.html](https://jokergoo.github.io/simplifyEnrichment_supplementary/supplS01_coefficient_definition/supplS01_coefficient_definition.html).

Value

A symmetric matrix.

Examples

# There is no example

null

term_similarity_from_enrichResult

Similarity between terms in the enrichResult class

Description

Similarity between terms in the enrichResult class

Usage

term_similarity_from_enrichResult(x, ...)

term_similarity_from_gmt

Arguments

x A enrichResult object from 'clusterProfiler' or other related packages.
...
Pass to term_similarity.

Details

The object is normally from the 'clusterProfiler', 'DOSE', 'meshes' or 'ReactomePA' package.

Value

A symmetric matrix.

Examples

# There is no example
NULL
**term_similarity_from_KEGG**  
*Similarity between KEGG terms*

**Description**  
Similarity between KEGG terms

**Usage**  
```
term_similarity_from_KEGG(term_id, ...)  
```

**Arguments**  
- **term_id**: A vector of KEGG IDs, e.g., hsa001.  
- **...**: Pass to `term_similarity`.

**Value**  
A symmetric matrix.

**Examples**  
```r  
# There is no example  
NULL  
```

---

**term_similarity_from_MSigDB**  
*Similarity between MSigDB terms*

**Description**  
Similarity between MSigDB terms

**Usage**  
```
term_similarity_from_MSigDB(term_id, category = NULL, subcategory = NULL, ...)  
```

**Arguments**  
- **term_id**: A vector of MSigDB gene set names.  
- **category**: E.g., 'C1', 'C2', pass to `msigdbr`.  
- **subcategory**: E.g., 'CGP', 'BP', pass to `msigdbr`.  
- **...**: Pass to `term_similarity`.  

term_similarity_from_Reactome

Similarity between Reactome terms

Description

Similarity between Reactome terms

Usage

term_similarity_from_Reactome(term_id, ...)

Arguments

term_id

A vector of Reactome IDs.

... 

Pass to term_similarity.

Value

A symmetric matrix.

Examples

# There is no example
NULL
widthDetails.word_cloud

*Width for word_cloud grob*

Description

Width for word_cloud grob

Usage

```r
## S3 method for class 'word_cloud'
widthDetails(x)
```

Arguments

- `x` The word_cloud grob returned by `word_cloud_grob`.

Value

A `unit` object.

Examples

```r
# There is no example
NULL
```

word_cloud_grob

*A simple grob for the word cloud*

Description

A simple grob for the word cloud

Usage

```r
word_cloud_grob(text, fontsize, 
    line_space = unit(4, "pt"), word_space = unit(4, "pt"), max_width = unit(80, "mm"), 
    col = function(fs) circlize::rand_color(length(fs), luminosity = "dark"), 
    add_new_line = FALSE, test = FALSE)
```
Arguments

- **text**: A vector of words.
- **fontsize**: The corresponding font size. With the frequency of the words known, `scale_fontsize` can be used to linearly interpolate frequencies to font sizes.
- **line_space**: Space between lines. The value can be a `unit` object or a numeric scalar which is measured in mm.
- **word_space**: Space between words. The value can be a `unit` object or a numeric scalar which is measured in mm.
- **max_width**: The maximal width of the viewport to put the word cloud. The value can be a `unit` object or a numeric scalar which is measured in mm. Note this might be larger than the final width of the returned grob object.
- **col**: Colors for the words. The value can be a vector, in numeric or character, which should have the same length as `text`. Or it is a self-defined function that takes the font size vector as the only argument. The function should return a color vector. See Examples.
- **add_new_line**: Whether to add new line after every word? If `TRUE`, each word will be in a separated line.
- **test**: Internally used. It basically adds borders to the words and the viewport.

Value

A `grob` object. The width and height of the grob can be get by `grobWidth` and `grobHeight`.

Examples

```r
# very old R versions do not have strrep() function
if(!exists("strrep")) {
  strrep = function(x, i) paste(rep(x, i), collapse = "")
}
words = sapply(1:30, function(x) strrep(sample(letters, 1), sample(3:10, 1)))
require(grid)
gb = word_cloud_grob(words, fontsize = runif(30, min = 5, max = 30),
  max_width = 100)
grid.newpage(); grid.draw(gb)

# color as a single scalar
gb = word_cloud_grob(words, fontsize = runif(30, min = 5, max = 30),
  max_width = 100, col = 1)
grid.newpage(); grid.draw(gb)

# color as a vector
require(circlize)
col_fun = colorRamp2(c(5, 17, 30), c("blue", "black", "red"))
gb = word_cloud_grob(words, fontsize = runif(30, min = 5, max = 30),
  max_width = 100, col = col_fun)
grid.newpage(); grid.draw(gb)
```
gb = word_cloud_grob(words, fontsize = runif(30, min = 5, max = 30),
                  max_width = 100, col = function(fs) col_fun(fs))
grid.newpage(); grid.draw(gb)
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