Package 'funOmics'

November 26, 2024

Title Aggregating Omics Data into Higher-Level Functional Representations

Version 1.0.0

Description The 'funOmics' package ggregates or summarizes omics data into higher level functional representations such as GO terms gene sets or KEGG metabolic pathways. The aggregated data matrix represents functional activity scores that facilitate the analysis of functional molecular sets while allowing to reduce dimensionality and provide easier and faster biological interpretations. Coordinated functional activity scores can be as informative as single molecules!

License MIT + file LICENSE

Encoding UTF-8

RoxygenNote 7.3.1

URL https://github.com/elisagdelope/funomics

BugReports https://github.com/elisagdelope/funomics/issues

Depends R (>= 4.4.0), NMF

- **Imports** NMF, pathifier, stats, KEGGREST, AnnotationDbi, org.Hs.eg.db, dplyr, stringr
- **Suggests** knitr, rmarkdown, testthat (>= 3.0.0), MultiAssayExperiment, SummarizedExperiment, airway

VignetteBuilder knitr

VignetteIndexEntry funomics_vignette Vignette

biocViews Software, Transcriptomics, Metabolomics, Proteomics, Pathways, GO, KEGG

Config/testthat/edition 3

git_url https://git.bioconductor.org/packages/funOmics

git_branch RELEASE_3_20

git_last_commit 5b3aeff

git_last_commit_date 2024-10-29

Repository Bioconductor 3.20

Date/Publication 2024-11-25

```
Author Elisa Gomez de Lope [aut, cre]
(<https://orcid.org/0000-0002-7115-7393>),
Enrico Glaab [ctb] (<https://orcid.org/0000-0003-3977-7469>)
```

Maintainer Elisa Gomez de Lope <elisa.gomezdelope@uni.lu>

Contents

funOmics-package	3
short_sets_detail	
	6

Index

funOmics-package

Aggregating Omics Data into Higher-Level Functional Representations

Description

The 'funOmics' package aggregates or summarizes omics data into higher-level functional representations such as GO terms, gene sets, or KEGG metabolic pathways. The aggregated data matrix represents functional activity scores that facilitate the analysis of functional molecular sets while allowing dimensionality reduction and providing easier and faster biological interpretations. Coordinated functional activity scores can be as informative as single molecules!

Details

The package offers functionalities for:

- Data aggregation into functional representations
- · Dimensionality reduction of omics data sets
- · Analysis of coordinated functional activity scores

Use function 'get_kegg_sets' to get KEGG pathway sets for a given organism and geneid type:

get_kegg_sets(organism = "hsa", geneid_type = "entrez")

Use function 'summarize_pathway_level' to summarize omics data into higher-level functional representations that can be interpreted as functional activity scores or measures:

summarize_pathway_level(omicsmat, sets = NULL, type = "mean", minsize = 10)

Author(s)

Elisa Gomez de Lope, Enrico Glaab

Maintainer: Elisa Gomez de Lope (elisa.gomezdelope@uni.lu)

See Also

summarize_pathway_level get_kegg_sets

2

get_kegg_sets Retrieves KEGG pathway gene sets for a specified organism and gene ID type.

Description

This function retrieves KEGG pathway gene sets for a specified organism. It fetches all pathways available for the specified organism from the KEGG database and maps the genes involved in each pathway. Currently, the function only supports choice of gene identifiers (entrez IDs, gene symbols or Ensembl IDs) for Homo sapiens (organism = "hsa") using the org.Hs.eg.db package.

Usage

```
get_kegg_sets(organism = "hsa", geneid_type = "entrez")
```

Arguments

organism	The organism abbreviation for which KEGG pathway gene sets are to be re- trieved (e.g., "ecj" for E. coli). Default is "hsa" (Homo sapiens).
geneid_type	The type of gene IDs to provide. Default is "entrez"; options are "entrez", "symbol", or "ensembl". This parameter is only used when the organism is "hsa" (Homo sapiens).

Value

A list where each element represents a KEGG pathway gene set. The names of the list correspond to the pathway names.

See Also

```
summarize_pathway_level
keggLink,keggList
mapIds
```

Examples

```
# Retrieve KEGG pathway gene sets for Homo sapiens with entrez IDs (default)
hsa_kegg_sets_entrez <- get_kegg_sets()</pre>
```

```
# Retrieve KEGG molecular sets using gene symbols
hsa_kegg_sets_symbol <- get_kegg_sets(geneid_type = "symbol")</pre>
```

```
# Retrieve KEGG molecular sets using Ensembl IDs
hsa_kegg_sets_ensembl <- get_kegg_sets(geneid_type = "ensembl")</pre>
```

```
# Retrieve KEGG pathway gene sets for another organism (e.g., Escherichia coli)
ecoli_kegg_sets <- get_kegg_sets(organism = "ecj")</pre>
```

short_sets_detail Retrieve details and information about short molecular sets

Description

This function identifies molecular sets with sizes less than a specified threshold and returns information about these sets.

Usage

short_sets_detail(sets, minsize)

Arguments

sets	A list of molecular sets.
minsize	The minimum size threshold for sets.

Details

This function identifies molecular sets in the input list that have sizes less than the specified minimum size (minsize). It returns a list containing the names, lengths, and molecules of these short molecular sets.

Value

A list containing information about short molecular sets:

short_sets	Names of the short molecular sets.
lengths	Lengths of the short molecular sets.
genes	Short molecular sets themselves.

Examples

```
ex_sets <- list(set1 = c("mol1", "mol2"), set2 = c("mol3", "mol4", "mol5"))
short_sets_info <- short_sets_detail(ex_sets, minsize = 3)</pre>
```

summarize_pathway_level

Aggregates or summarizes omics data into higher-level functional representations that can be interpreted as functional activity scores or measures.

Description

Given an omics matrix and a list of functional molecular sets, this function aggregates or summarizes the omics data into higher-level functional representations such as GO terms gene sets or KEGG metabolic pathways, facilitating the analysis of functional molecular sets that allow reducing dimensionality and providing easier and faster biological interpretations. Coordinated functional activity scores can be as informative as single molecules.

Usage

```
summarize_pathway_level(omicsmat, sets = NULL, type = "mean", minsize = 10)
```

Arguments

omicsmat	A matrix or data frame representing omics data. Rows correspond to molecular identifiers, and columns correspond to samples.
sets	A list of functional sets. Each element in the list should represent a molecular set, and the elements of the set should match the row names of the omics matrix.
type	The type of pooling operator to be applied for each set. Possible values in- clude "mean" (default), "median", "sd", "min", "max", "pca", "mds", "pathifier", "nmf", "ttest", "wilcox", "kolmogorov".
minsize	The minimum size per molecular set (default is 10).

Details

Notes:

- Different aggregation operators can be used, including summary statistics such as median (de-fault), mean, sd, min, max, dimensionality reduction scores such as pca, mds, pathifier, or nmf, and statistical tests such as ttest, wilcoxon test, kolmogorov test.

- The minimum size per molecular set is by default 10 molecules (e.g. genes or metabolites) and can be changed with the parameter minsize.

- If "pathifier" is chosen as pooling type, the 'aggby_pathifier' function internally generates a log file named 'pathifierlog.txt' during its execution.

This log file may contain additional information that could be useful for troubleshooting or advanced analysis.

Users typically do not need to interact with this file directly, but it is mentioned here for informational purposes. For more details, this function utilizes the Pathifier package.

Value

A matrix-like table with the activity measures for each group or set of molecules, i.e., sxn matrix, for s molecular sets and n samples.

Author(s)

Elisa Gomez de Lope

Examples

```
# Example usage:
g <- 10000
s <- 20
X <- matrix(abs(rnorm(g * s)), nrow = g, dimnames = list(paste0("g", 1:g), paste0("s", 1:s)))
pathways <- as.list(sample(10:100, size = 100, replace = TRUE))
pathways <- lapply(pathways, function(s, g) paste0("g", sample(1:g, size = s, replace = FALSE)), g)
names(pathways) <- paste0("pathway", seq_along(pathways))
pathway_activity <- summarize_pathway_level(X, pathways, type = "mean", minsize = 12)</pre>
```

Index

```
* activity-scores
    funOmics-package, 2
    summarize_pathway_level, 4
* aggregation
    funOmics-package, 2
    summarize_pathway_level, 4
* functional
    funOmics-package, 2
    summarize_pathway_level, 4
* omics
    funOmics-package, 2
    summarize_pathway_level, 4
* package
    funOmics-package, 2
* pathway
    funOmics-package, 2
    summarize_pathway_level, 4
* representation
    funOmics-package, 2
    summarize_pathway_level, 4
* summary
    funOmics-package, 2
    summarize_pathway_level, 4
funOmics(funOmics-package), 2
funOmics-package, 2
get_kegg_sets, 2, 3
keggLink, 3
keggList, 3
mapIds, 3
short_sets_detail, 4
```

summarize_pathway_level, 2, 3, 4