

Package ‘XINA’

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Type Package

Title Multiplexes Isobaric Mass Tagged-based Kinetics Data for Network Analysis

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Description The aim of XINA is to determine which proteins exhibit similar patterns within and across experimental conditions, since proteins with co-abundance patterns may have common molecular functions. XINA imports multiple datasets, tags dataset in silico, and combines the data for subsequent subgrouping into multiple clusters. The result is a single output depicting the variation across all conditions. XINA, not only extracts coabundance profiles within and across experiments, but also incorporates protein-protein interaction databases and integrative resources such as KEGG to infer interactors and molecular functions, respectively, and produces intuitive graphical outputs.

Copyright XINA combines multiple quantitative (kinetics) datasets from omics studies into a single input dataset for clustering. Copyright(C)2018 Lang Ho Lee, Arda Halu, Stephanie Morgan, Hiroshi Iwata, Masanori Aikawa, and Sasha A. Singh This program is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, any later version. This program is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details. You should have received a copy of the GNU General Public License along with this program. If not, see <<https://www.gnu.org/licenses/>>. - Contact emails: L. Lee, LHLEE@BWH.HARVARD.EDU S. Singh, SASINGH@BWH.HARVARD.EDU M. Aikawa, MAIKAWA@BWH.HARVARD.EDU - Mailing address: Department

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| | |
|------------|-------------------|
| add_legend | <i>add_legend</i> |
|------------|-------------------|

Description

Add plot legend and locate it outside of a network plot

Usage

```
add_legend(legend_location = "bottomright", ...)
```

Arguments

- legend_location
- Network centrality score matrix
- ... Numeric, complex, or logical vectors.

Value

a legend to a plot

alluvial_enriched *alluvial_enriched*

Description

'alluvial_enriched' draws an alluvial plot and finds comigrated proteins. The comigration is a group of proteins that show the same expression pattern, classified and evaluated by XINA clustering, in at least two conditions. XINA can reduce the dataset complexity by filtering based on the number of comigrated proteins (size, 'comigration_size' parameter) and perform an enrichment test (P-value of Fisher's exact test, 'pval_threshold') to determine significance of enriched comigrations. The Fisher's exact test can only be done for two conditions at a time. The following 2x2 table was used to calculate the P-value from the Fisher's exact test. To evaluate significance of co-migrated proteins from cluster #1 in control to cluster #2 in test group,

| | | | |
|------------------------|---|-----------------------|---------------------------|
| | - | cluster #1 in control | other clusters in control |
| cluster #2 in test | | 65 (TP) | 175 (FP) |
| other clusters in test | | 35 (FN) | 979 (TN) |

Usage

```
alluvial_enriched(clustering_result, selected_conditions,
  comigration_size = 0, pval_threshold = 1, pval_method = "fdr",
  cex = 0.7, alpha = 0.3)
```

Arguments

| | |
|---------------------|--|
| clustering_result | A list containing XINA clustering results. See xina_clustering |
| selected_conditions | A vector of condition names used in XINA clustering results. The number of selected conditions should be at least two. |
| comigration_size | The number of proteins comigrated together in the selected conditions of XINA clustering results. Default is 0 |
| pval_threshold | This option is available only when you selected two conditions for comigration search. |
| pval_method | Method for p-value adjustment. See p.adjust |
| cex | Scaling of fonts of category labels. Default if 0.7. See alluvial |
| alpha | Transparency of the stripes. Default if 0.3. See alluvial |

Value

A data frame containing comigrations and an alluvial plot showing comigrations

Examples

```

# load XINA example data
data(xina_example)

# Get the experimental conditions in the example data
classes <- as.vector(example_clusters$condition)

# Get comigrations without any thresholds
all_comigrations <- alluvial_enriched(example_clusters, classes)

# Get comigrations that have >= 5 size (the number of comigrated proteins)
all_cor_enriched <- alluvial_enriched(example_clusters, classes, comigration_size=5)

# Get all the comigrations between Control and Stimulus1
comigrations_Control_Stimulus1 <- alluvial_enriched(example_clusters,
c(classes[1],classes[2]))

# Get comigrations between Control and Stimulus1, that have >=5 size
comigrations_Control_Stimulus1_over5 <- alluvial_enriched(example_clusters,
c(classes[1],classes[2]), comigration_size=5)

# Get comigrations between Control and Stimulus1,
# that have >= 5 size and enrichment FDR <= 0.01
comigrations_Control_Stimulus1_pval0.01_size5 <- alluvial_enriched(example_clusters,
c(classes[1],classes[2]), comigration_size=5, pval_threshold=0.01)

# Get comigrations between Control and Stimulus1,
# that have >= 5 size and enrichment Benjamini & Yekutieli <= 0.01
comigrations_Control_Stimulus1_BY0.01_size5 <- alluvial_enriched(example_clusters,
c(classes[1],classes[2]), comigration_size=5, pval_threshold=0.01, pval_method="BY")

```

alluvial_enrichment_tests

alluvial_enrichment_tests

Description

Fisher's exact test to calculate the significance over all comigrations. The following 2x2 table was used to calculate p-value from Fisher's exact test. To evaluate significance of comigrated proteins from cluster #1 in control to cluster #2 in test condition,

| | cluster #1 in control | other clusters in control |
|-------------------------------|------------------------------|----------------------------------|
| cluster #2 in test | 65 (TP) | 175 (FP) |
| other clusters in test | 35 (FN) | 979 (TN) |

'alluvial_enrichment_tests' also provides another statistical methods including Hypergeometric test and Chi-square test.

Usage

```

alluvial_enrichment_tests(count_table, c1, c2, non_cluster = 0,
test_type = "fisher")

```

Arguments

| | |
|-------------|--|
| count_table | A data frame generated by using <code>count</code> . |
| c1 | A selected cluster in the first condition. |
| c2 | A selected cluster in the second condition. |
| non_cluster | The cluster number for proteins that were not detected in a specific sample. Default is 0. |
| test_type | Enrichment test type. 'fisher' = Fisher's exact test, 'hyper' = Hypergeometric test, 'chisq' = Chi-square test |

Value

P-value of comigration enrichment test and 2x2 table information

calculate_centrality_scores
calculate_centrality_scores

Description

'calculate_centrality_scores' computes network centrality scores

Usage

```
calculate_centrality_scores(net, centrality_type = "Degree")
```

Arguments

| | |
|-----------------|---|
| net | protein-protein interaction network of igraph |
| centrality_type | the maximum number of clusters |

Value

A vector of network centrality scores

default_size *default_size*

Description

Calculate image size based on the number of clusters

Usage

```
default_size(max_cluster)
```

Arguments

| | |
|-------------|--------------------------------|
| max_cluster | the maximum number of clusters |
|-------------|--------------------------------|

Value

A vector of plot width and height

draw_alluvial_plot *draw_alluvial_plot*

Description

'draw_alluvial_plot' draw a alluvial plot

Usage

```
draw_alluvial_plot(clustering_result, selected_conditions, count_table,  
  alluvia_colors = NULL, cex = 0.7, alpha = 0.3)
```

Arguments

clustering_result A list containing XINA clustering results. See [xina_clustering](#).

selected_conditions A vector of condition names used in XINA clustering results. The number of selected conditions should be at least two.

count_table A data frame generated by using [count](#).

alluvia_colors A vector containing the user-defined colors for each alluvium.

cex Size of cluster number on block axis. Default if 0.7. See [alluvial](#).

alpha Transparency of alluvia colors. Default is 0.3. See [alluvial](#).

Value

An alluvial plot displaying comigrations and the data frame containing the input count_table with colors.

Examples

```
# load XINA example data  
data(xina_example)  
  
# get a vector of experimental conditions analyzed in the clustering results  
classes <- as.vector(example_clusters$condition)  
  
comigrations_size_over5 <- alluvial_enriched(example_clusters, classes, comigration_size=5)  
draw_alluvial_plot(example_clusters, classes, comigrations_size_over5)
```

| | |
|------------------|--|
| example_clusters | <i>Randomly generated example datasets for XINA users. A dataset containing the XINA clustering results.</i> |
|------------------|--|

Description

- aligned. XINA clustering results aligned by conditions
- data_column. Column names for data matrix
- out_dir. Not available in this example dataset
- nClusters. The number of user-desired clusters. It's 30 in the example.
- max_cluster. The number of clusters found in the dataset. It's 21 in the example.
- chosen_model. The chosen covariance model for the example dataset. It's VEI in the example
- optimal_BIC. BIC at the optimized clustering. It's 29473.57 in the example
- condition. The experimental conditions in the dataset.
- color_for_condition. The default color for the conditions that will be used in XINA plot drawing.
- color_for_clusters. The default color for the clusters that will be used in XINA clustering plot.
- norm_method. The used normalization method to standardize the input data. It's "sum_normalization" in the example.

Format

A list with the example XINA clustering result

| | |
|---------------------|----------------------------|
| extract_data_column | <i>extract_data_column</i> |
|---------------------|----------------------------|

Description

Extract data column names from XINA clustering result

Usage

```
extract_data_column(col_head_of_clustering)
```

Arguments

col_head_of_clustering
Column names of XINA clustering result

Value

A vector containing column names of data matrix

find_similar_clusters *find_similar_clusters*

Description

Compare clusters and find similar ones

Usage

```
find_similar_clusters(clustering_result, threshold = 0.95)
```

Arguments

`clustering_result`
A list containing XINA clustering results. See [xina_clustering](#)

`threshold`
Pearson's r threshold to find similar ones

Value

Write a csv file containing similar clustering information based on the given Pearson's R threshold

generate_count_table *generate_count_table*

Description

Count the number of comigrated proteins using [count](#)

Usage

```
generate_count_table(clustering_result, selected_conditions,  
                    comigration_size)
```

Arguments

`clustering_result`
A list containing XINA clustering results. See [xina_clustering](#)

`selected_conditions`
A vector of condition names used in XINA clustering results.

`comigration_size`
The number of proteins comigrated together in the selected conditions of XINA clustering results. Default is 0.

Value

A data frame containing comigrations.

| | |
|-------------------|--------------------------|
| generate_superset | <i>generate_superset</i> |
|-------------------|--------------------------|

Description

Merge input kinetics files

Usage

```
generate_superset(f_names, data_column, delim = ",",
  norm = "sum_normalization")
```

Arguments

| | |
|-------------|--|
| f_names | A vector of .csv file paths containing kinetics data |
| data_column | A vector of column names containing data matrix |
| delim | The delimiter of input file (default is ',') |
| norm | The normalization method. It should be one of c('sum_normalization', 'zs-core'). Default is 'sum_normalization'. |

Value

A data frame containing kinetics data obtained from files in the f_names vector

| | |
|------------|-------------------|
| get_colors | <i>get_colors</i> |
|------------|-------------------|

Description

Generate color series for XINA graphics

Usage

```
get_colors(nClusters, set = "", colorset = NULL)
```

Arguments

| | |
|-----------|------------------------------|
| nClusters | The number of clusters |
| set | Pre-defined color series set |
| colorset | manually defined color codes |

Value

A vector for color code of XINA graphics

```
get_color_for_nodes  get_color_for_nodes
```

Description

Pre-defined 30 colors

Usage

```
get_color_for_nodes()
```

Value

A vector for color code of XINA graphics

```
get_comigrations_by_name
      get_comigrations_by_name
```

Description

'get_comigrations_by_name' finds proteins comigrated with the given proteins

Usage

```
get_comigrations_by_name(clustering_result, selected_conditions,
  protein_list, cex = 0.7, alpha = 0.3)
```

Arguments

clustering_result A list containing XINA clustering results. See [xina_clustering](#)

selected_conditions A vector of condition names used in XINA clustering results. The number of selected conditions should be at least two.

protein_list A vector containing gene names.

cex Size of cluster number on block axis. Default if 0.7. See [alluvial](#)

alpha Transparency of alluvia colors. Default is 0.3. See [alluvial](#)

Value

An alluvial plot displaying comigrations and the data frame containing comigrations of the input proteins

Examples

```
# load XINA example data
data(xina_example)

# the clustering result table
all_proteins <- as.character(example_clusters$aligned$`Gene name`)
# get a vector of experimental conditions analyzed in the clustering results
classes <- as.vector(example_clusters$condition)

comigrated_prots_all <- get_comigrations_by_name(example_clusters, classes, all_proteins[1:3])
```

```
get_condition_biased_comigrations
      get_condition_biased_comigrations
```

Description

get comigrations that at least one biased cluster is involved in. Biased clusters are defined by

Usage

```
get_condition_biased_comigrations(clustering_result, count_table = NULL,
  selected_conditions, condition_composition, threshold_percent = 50,
  color_for_null = "gray", color_for_highly_matched = "red4",
  cex = 0.7, alpha = 0.3)
```

Arguments

clustering_result
A list containing XINA clustering results. See [xina_clustering](#)

count_table
A data frame generated by using [count](#). If count_table is NULL (by default), XINA will consider all the comigrations.

selected_conditions
A vector of condition names used in XINA clustering results. The number of selected conditions should be at least two.

condition_composition
The resulting data frame of 'plot_condition_compositions'. See [plot_condition_compositions](#).

threshold_percent
Default is 50. The percentage threshold for finding condition-biased clusters

color_for_null
A color for non-condition-biased comigrations. Default is 'gray'

color_for_highly_matched
A color for comigrations that are involved with more than two condition-biased clusters. Default is 'red4'

cex
Size of cluster number on block axis. Default if 0.7. See [alluvial](#).

alpha
Transparency of alluvia colors. Default is 0.3. See [alluvial](#).

Value

An alluvial plot displaying comigrations and the data frame containing condition-biased comigrations.

Examples

```
# load XINA example data
data(xina_example)

# get a vector of experimental conditions analyzed in the clustering results
conditions <- as.vector(example_clusters$condition)

# get condition composition information
condition_composition <- plot_condition_compositions(example_clusters)

comigrations_size10 <- alluvial_enriched(example_clusters, conditions, comigration_size=10)
# Finding condition-biased comigrations by 50% threshold
condition_biased_comigrations <-
get_condition_biased_comigrations(clustering_result=example_clusters,
count_table=comigrations_size10, selected_conditions=conditions,
condition_composition=condition_composition)

# Finding condition-biased comigrations by 70% threshold
condition_biased_comigrations <-
get_condition_biased_comigrations(clustering_result=example_clusters,
count_table=comigrations_size10, selected_conditions=conditions,
condition_composition=condition_composition,
threshold_percent=70)
```

get_layout

get_layout

Description

Get igraph layout by the number of nodes

Usage

```
get_layout(subnet_condition)
```

Arguments

```
subnet_condition
  A igraph sub-network
```

Value

igraph network layout

`get_mTOR_proteins` *get_mTOR_proteins*

Description

Get mTOR pathway genes

Usage

```
get_mTOR_proteins(time_points, conditions)
```

Arguments

`time_points` A vector containing time points of the data matrix
`conditions` A vector containing condition information, for example normal, disease and drug treated disease.

Value

A vector containing mTOR pathway gene names

`get_random_data` *get_random_data*

Description

Get randomized time-series data

Usage

```
get_random_data(time_points, conditions, num_total, percent.sign = 0.1,  
equal = TRUE)
```

Arguments

`time_points` A vector containing time points of the data matrix
`conditions` A vector containing condition information, for example normal, disease and drug treated disease.
`num_total` The number of total proteins to be generated
`percent.sign` Percentage of differentially expressed proteins. Ignored when `equal=FALSE`.
`equal` If `equal` is `TRUE`, all the conditions will have numbers between 0 and 1. If it is `FALSE`, the first three conditions will have different ranges. First condition will have numbers from 0.3 to 0.4. Second condition will have numbers from 0.6 to 0.8. Third condition will have numbers from 0.3 to 0.5. Other conditions will have numbers from 0 to 1.

Value

A list containing randomly generated data matrix

| | |
|-----------|------------------|
| get_stats | <i>get_stats</i> |
|-----------|------------------|

Description

Calculate statistics of the given data for XINA network analysis

Usage

```
get_stats(centrality_results, na.rm = FALSE)
```

Arguments

`centrality_results` Network centrality score data frame calculated by XINA network module

`na.rm` If it is FALSE, no exclusion of NA values.

Value

A data frame containing statistics of XINA network centrality scores

| | |
|-----------------|------------------------|
| get_theme_blank | <i>get_theme_blank</i> |
|-----------------|------------------------|

Description

Predefined ggplot theme for removing ticks, titles and labels of X and Y axis

Usage

```
get_theme_blank()
```

Value

A ggplot theme

```
get_unknown_ppi_nodes  get_unknown_ppi_nodes
```

Description

Get proteins with no known interactions within the cluster based on the used protein-protein interaction database source

Usage

```
get_unknown_ppi_nodes(xina_result, cl)
```

Arguments

`xina_result` A list containing XINA network analysis results. See [xina_analysis](#)
`cl` the clustering number of XINA clustering results. See [xina_clustering](#)

Value

A data frame containing proteins with no known interactions within the cluster based on the used protein-protein interaction database source

Examples

```
# load XINA example data
data(xina_example)

# load the previously processed XINA analysis results
# if you want to learn how to run 'xina_analysis', please see \link[XINA]{xina_analysis}
data(xina_result_example)

# Extract unknown PPI nodes in the cluster #1
get_unknown_ppi_nodes(xina_result_example, 1)
```

```
gn A character vector containing 19,396 human genes This is for the ran-
dome data generation of XINA
```

Description

- Characters of human genes

Format

A character vector containing 19,396 human genes

Source

<https://www.ncbi.nlm.nih.gov/gene>

| | |
|---------|--|
| gn_desc | <i>A character vector containing 19,396 human gene descriptions This is for the random data generation of XINA</i> |
|---------|--|

Description

- Human gene description corresponding to 'gn' vector

Format

A character vector containing 19,396 human gene descriptions

Source

<https://www.ncbi.nlm.nih.gov/gene>

| | |
|----------|---|
| hprd_ppi | <i>Protein-protein interaction resource downloaded from HPRD DB A data frame containing HRPD protein-protein interaction data</i> |
|----------|---|

Description

- gene_symbol_1. Gene name interacting with gene name in 'gene_symbol_2'
- gene_symbol_2. Gene name interacting with gene name in 'gene_symbol_1'
- Experiment_type. Experimental or computational methods supporting the interaction

Format

A data frame containing HRPD protein-protein interaction data

Source

<http://www.hprd.org/>

| | |
|---------|----------------|
| length2 | <i>length2</i> |
|---------|----------------|

Description

Customized function for vector length calculation

Usage

```
length2(x, na.rm = FALSE)
```

Arguments

| | |
|-------|--|
| x | A vector |
| na.rm | If it is FALSE, no exclusion of NA values. |

Value

A vector length

load_previous_results *load_previous_results*

Description

Get previous XINA clustering results to R space

Usage

```
load_previous_results(clustering_dir = getwd(), data_column = NULL,  
  fp_clusters = "xina_clusters.csv")
```

Arguments

| | |
|----------------|---|
| clustering_dir | The directory path of XINA clustering results |
| data_column | A vector containing column names of data matrix |
| fp_clusters | File path of XINA clustering results |

Value

Comma-separated file containing aligned XINA clustering results.

Examples

```
# Load XINA's example data  
data(xina_example)  
write.csv(example_clusters$aligned, "xina_clusters_aligned.csv")  
write.csv(example_clusters$clusters, "xina_clusters.csv")  
  
# Reload the clustering result  
example_clusters_reloaded <- load_previous_results(".")
```

make_random_xina_data *make_random_xina_data*

Description

Generate random proteomics dataset for testing XINA 'make_random_xina_data' will make random proteomics data for XINA test. The generated data will have three conditions and seven time points, c("0hr", "2hr", "6hr", "12hr", "24hr", "48hr", "72hr").

Usage

```
make_random_xina_data(n = 500, mtor = TRUE, time_points = c("0hr",  
  "2hr", "6hr", "12hr", "24hr", "48hr", "72hr"),  
  conditions = c("Control", "Stimulus1", "Stimulus2"))
```

Arguments

| | |
|-------------|---|
| n | The number of proteins for one condition. Default is 500. |
| mtor | If it is TRUE (default), mTOR pathway genes will be significant. If it is FALSE, randomly selected genes will be significant in first three conditions. |
| time_points | A vector containing time points of the data matrix |
| conditions | A vector containing condition information, for example normal, disease and drug treated disease. |

Value

Three comma-separated files containing time-series data for XINA

Examples

```
make_random_xina_data()  
g1 <- read.csv("Control.csv", check.names=FALSE,  
  stringsAsFactors = FALSE)  
g2 <- read.csv("Stimulus1.csv", check.names=FALSE,  
  stringsAsFactors = FALSE)  
g3 <- read.csv("Stimulus2.csv", check.names=FALSE,  
  stringsAsFactors = FALSE)  
  
head(g1)  
head(g2)  
head(g3)
```

| | |
|---------------|----------------------|
| mutate_colors | <i>mutate_colors</i> |
|---------------|----------------------|

Description

'mutate_colors' generates new color scheme for XINA clustering plot based on condition composition results ([plot_condition_compositions](#)). If any clusters have higher percentage than the 'threshold_percent', XINA will assign new colors in accordance to 'color_for_condition'. If not, XINA will give 'gray' color or user-defined color via 'null_color' parameter.

Usage

```
mutate_colors(condition_composition, color_for_condition,  
              null_color = "gray", threshold_percent = 50)
```

Arguments

`condition_composition`
A data frame generated by [plot_condition_compositions](#)

`color_for_condition`
A vector like 'color_for_condition' of [xina_clustering](#)

`null_color` Default is 'gray'. This color is for clusters that are not biased to any of experimental conditions

`threshold_percent`
Default is 50. The percentage threshold for giving new colors

Value

A data frame containing statistics of XINA network centrality scores

Examples

```
# load XINA example data  
data(xina_example)  
  
# Plot condition composition pie-chart with default option  
condition_composition <- plot_condition_compositions(example_clusters)  
example_clusters$color_for_clusters <- mutate_colors(condition_composition,  
example_clusters$color_for_condition)  
plot_clusters(example_clusters, xval=c(0,2,6,12,24,48,72), xylab=FALSE)
```

| | |
|-------------------|--------------------------|
| organize_clusters | <i>organize_clusters</i> |
|-------------------|--------------------------|

Description

Organize XINA clustering information by gene name

Usage

```
organize_clusters(clustering_dir = getwd(), super_ds, file_out = TRUE)
```

Arguments

| | |
|----------------|---|
| clustering_dir | The directory path of XINA clustering results |
| super_ds | XINA clusters |
| file_out | If it is TRUE, it writes the aligned clustering informaion to "xina_clusters_aligned.csv" file. |

Value

Comma-separated file containing aligned XINA clustering results.

| | |
|---------------|----------------------|
| plot_clusters | <i>plot_clusters</i> |
|---------------|----------------------|

Description

Draw all the clustering results. 'plot_clusters' draws two plots, scaled and unscaled line graphs. Scaled graphs have same y limits that are 0 to 1 by default, but can be changed via 'y_lim' parameter.

Usage

```
plot_clusters(clustering_result, y_lim = NULL, xval = NULL,
             xtickmark = NULL, xylab = TRUE, ggplot_theme = NULL)
```

Arguments

| | |
|-------------------|--|
| clustering_result | A list containing XINA clustering results. See xina_clustering |
| y_lim | Y axis limit. If you set y_lim=c(0,1), 'plot_clusters' will plot line graphs scaled from 0 to 1 in y-axis Default is NULL, which means unscaled line graphs. |
| xval | XINA basically considers time points as a ordinary variable, like 1,2,3,4...n. You can make the time points as a continuous variable using xval. |
| xtickmark | Change X axis tick marks. Default is data_column of the clustering result list. |
| xylab | If it is FALSE, x and y labels will be blank. If it is TRUE (default), x and y labels will be shown. |
| ggplot_theme | This is ggplot theme to modify XINA clustering plot. |

Value

Line graphs of all the clusters

Examples

```
library(ggplot2)

# load XINA example data
data(xina_example)

# Draw clustering plots
plot_clusters(example_clusters)

# Apply theme to the clustering plot
theme1 <- theme(title=element_text(size=8, face='bold'),
axis.text.x = element_text(size=7),
axis.text.y = element_blank(),
axis.ticks.x = element_blank(),
axis.ticks.y = element_blank(),
axis.title.x = element_blank(),
axis.title.y = element_blank())
plot_clusters(example_clusters, ggplot_theme=theme1)
```

plot_clusters_all *plot_clusters_all*

Description

Draw line graphs of all the proteins in the given dataset

Usage

```
plot_clusters_all(clustering_result, selected_condition = NULL)
```

Arguments

clustering_result

A list containing XINA clustering results. See [xina_clustering](#)

selected_condition

A condition name to draw the kinetics plot

Value

a list containing clustering results and pdf file containing a BIC plot in current working directory.

Examples

```
# load XINA example data
data(xina_example)

# Plot kinetics of all the proteins in Control
plot_clusters_all(example_clusters, selected_condition="Control")
```

```
# Plot kinetics of all the proteins in Stimulus1
plot_clusters_all(example_clusters, selected_condition="Stimulus1")

# Plot kinetics of all the proteins in Stimulus2
plot_clusters_all(example_clusters, selected_condition="Stimulus2")

# Plot kinetics of all the proteins in three data
plot_clusters_all(example_clusters)
```

```
plot_condition_compositions
      plot_condition_compositions
```

Description

computes condition composition of the XINA clustering results and draws pie-charts.

Usage

```
plot_condition_compositions(clustering_result, bullseye = FALSE,
  ggplot_theme = NULL)
```

Arguments

| | |
|-------------------|--|
| clustering_result | A list containing XINA clustering results. See xina_clustering |
| bullseye | If it is TRUE, draw bullseye plot instead of the pie-chart. Default is FALSE |
| ggplot_theme | This is ggplot theme to modify condition composition pie-chart and bulles eye plots. |

Value

A condition composition plot and a data frame containing condition compositions of the clusters

Examples

```
# load XINA example data
data(xina_example)

# Plot condition composition pie-chart with default option
plot_condition_compositions(example_clusters)

# Make a new color code for conditions
condition_colors <- c("tomato", "steelblue1", "gold")
names(condition_colors) <- example_clusters$condition
example_clusters$color_for_condition <- condition_colors

# Draw condition composition pie-chart with the new color code
plot_condition_compositions(example_clusters)

# Draw condition composition bullseye plot
plot_condition_compositions(example_clusters, bullseye = TRUE)
```

```
plot_enrichment_results
      plot_enrichment_results
```

Description

Plot GO and KEGG enrichment results

Usage

```
plot_enrichment_results(enriched_results,
  term_description = "term_description", sig_score = "pvalue",
  num_terms = 0, get_log = TRUE, fill_color = "darkgray")
```

Arguments

| | |
|------------------|--|
| enriched_results | GO or KEGG enrichment results. See xina_enrichment and xina_enrichment |
| term_description | Description of terms to be drawn on Y axis. Default is "term_description" of XINA enrichment results. |
| sig_score | significant score to plot on X axis. Default is "pvalue". |
| num_terms | The number of terms to be plotted. Default is 0, which means no limit. |
| get_log | If this is TRUE, 'plot_enrichment_results' will take -log10 of p-values. |
| fill_color | Default is 'darkgray'. You can change color of bars. |

Value

ggplot bar graph

Examples

```
## Not run:
library(STRINGdb)

# load XINA example data
data(xina_example)

# Get STRING database for protein-protein intereaction information
string_db <- STRINGdb$new( version="10", species=9606,
  score_threshold=0, input_directory="" )
string_db

# XINA analysis with STRING DB
xina_result <- xina_analysis(example_clusters, string_db)

# Select proteins that showed cluster #1 in the Stimulus2 condition
subgroup <- subset(example_clusters$aligned, Stimulus2==1)
protein_list <- as.vector(subgroup$`Gene name`)

# Enrichment test and get significantly enriched functional terms
# that have adjusted p-value less than 0.1
```



```
kegg_enriched <- xina_enrichment(string_db, protein_list,
  enrichment_type = "KEGG", pval_threshold=0.1)
plot_enrichment_results(kegg_enriched$KEGG, num_terms=10)

## End(Not run)
```

plot_NA

plot_NA

Description

Draw NULL plot

Usage

```
plot_NA()
```

Value

a empty plot

rank_centrality

rank_centrality

Description

Give ranks based on network centrality scores

Usage

```
rank_centrality(centrality_score, type, num_breaks = 5)
```

Arguments

centrality_score

Network centrality score matrix

type

Network centrality score type, such as 'Eigenvector'

num_breaks

The number of ranks

Value

A vector containing ranks

| | |
|----------------|---|
| string_example | <i>Protein-protein interaction resource downloaded from STRING DB for XINA's example dataset A data frame containing protein-protein interactions</i> |
|----------------|---|

Description

- gene_symbol_1. Gene name interacting with gene name in 'gene_symbol_2'
- gene_symbol_2. Gene name interacting with gene name in 'gene_symbol_1'
- PPI_Source. Data original source

Format

A data frame containing STRING protein-protein interaction data

Source

<https://string-db.org/>

| | |
|---------------|----------------------|
| xina_analysis | <i>xina_analysis</i> |
|---------------|----------------------|

Description

xina_analysis is to analyze protein-protein interaction(PPI) networks using STRINGdb and igraph R package. This module computes PPI networks within each XINA clusters.

Usage

```
xina_analysis(clustering_result, ppi_db, is_stringdb = TRUE,
              flag_simplify = TRUE, node_shape = "sphere",
              num_clusters_in_row = 5, img_size = NULL, img_qual = 300)
```

Arguments

| | |
|---------------------|--|
| clustering_result | A list containing XINA clustering results. See xina_clustering |
| ppi_db | STRINGdb object |
| is_stringdb | If it is TRUE (default), XINA will process 'ppi_db' as STRINGdb, but if it is FALSE, XINA will accept your 'ppi_db' as it is. You can make your own igraph network using customized PPI information instead of STRINGdb. |
| flag_simplify | If it is TRUE (default), XINA will exclude unconnected proteins |
| node_shape | You can choose node shape. Default is "sphere". See shapes |
| num_clusters_in_row | The number of clusters in a row on the XINA network plot. Default is 5. |
| img_size | Set the image size. For width=1000 and height=1500, it is img_size=c(1000,1500). |
| img_qual | Set the image resolution. Default is 300. |

Value

A PNG file (XINA_Cluster_Networks.png) displaying PPI network plots of all the clusters and a list containing XINA network analysis results.

| Item | Description |
|-------------|--|
| All_network | PPI network of all the input proteins |
| Sub_network | A list containing PPI networks of each clusters |
| Data | XINA clustering results. See xina_clustering |
| Nodes | A list of proteins in each cluster |
| Conditions | A list of experimental condition of proteins in each cluster |
| Titles | A list of plot titles for XINA plotting |
| out_dir | A directory path storing XINA network analysis results |
| is_stringdb | False = different PPI DB and TRUE = STRING DB |

Examples

```
## Not run:
# load XINA example data
data(xina_example)

# use the following code for utilizing up-to-date STRING DB
tax_id <- 9606 # for human
# tax_id <- 10090 # for mouse
library(STRINGdb)
library(igraph)
string_db <- STRINGdb$new( version='10', species=tax_id, score_threshold=0, input_directory='' )
string_db
xina_result <- xina_analysis(example_clusters, string_db, flag_simplify=FALSE)

# Run XINA with a protein-protein interaction edgelist
data(HPRD)
net_all <- simplify(graph_from_data_frame(d=hprd_ppi, directed=FALSE),
remove_multiple = FALSE, remove_loops = TRUE)
xina_result <- xina_analysis(example_clusters, net_all, is_stringdb=FALSE, flag_simplify=FALSE)

## End(Not run)
```

xina_clustering *xina_clustering*

Description

Clustering multiplexed time-series omics data to find co-abundance profiles

Usage

```
xina_clustering(f_names, data_column, out_dir = getwd(),
nClusters = 20, norm = "sum_normalization", chosen_model = "")
```

Arguments

| | |
|--------------|---|
| f_names | A vector containing input file (.csv) paths |
| data_column | A vector containing column names (1st row of the input file) of data matrix |
| out_dir | A directory path for saving clustering results. (default: out_dir=getwd()) |
| nClusters | The number of desired maximum clusters |
| norm | Default is "sum_normalization". Sum-normalization is to divide the data matrix by row sum. If you want to know more about sum-normalization, see https://www.ncbi.nlm.nih.gov/pubmed/19861354 . "zscore" is to calculate Z score for each protein. See scale . |
| chosen_model | You can choose a specific model rather than testing all the models that are available in mclust. mclustModelNames If you want k-means clustering instead of the model-based clustering, use "kmeans" here. |

Value

a plot containing a BIC plot in current working directory and a list containing below information:

| Item | Description |
|---------------------|--|
| clusters | XINA clustering results |
| aligned | XINA clustering results aligned by ID |
| data_column | Data matrix column names |
| out_dir | The directory path containing XINA results |
| nClusters | The number of clusters desired by user |
| max_cluster | The number of clusters optimized by BIC |
| chosen_model | The used covariance model for model-based clustering |
| optimal_BIC | BIC of the optimized covariance model |
| condition | Experimental conditions of the user input data |
| color_for_condition | Colors assigned to each experimental conditions which is used for condition composition plot |
| color_for_clusters | Colors assigned to each clusters which is used for XINA clustering plot |
| norm_method | Used normalization method |

Examples

```
# Generate random multiplexed time-series data
random_data_info <- make_random_xina_data()

# Data files
data_files <- paste(random_data_info$conditions, ".csv", sep='')

# time points of the data matrix
data_column <- random_data_info$time_points

# mclust requires the fixed random seed to get reproduce the clustering results
set.seed(0)

# Run the model-based clustering to find co-abundance profiles
example_clusters <- xina_clustering(data_files, data_column=data_column,
nClusters=30)

# Run k-means clustering to find co-abundance profiles
example_clusters <- xina_clustering(data_files, data_column=data_column,
```

```
nClusters=30,
chosen_model="kmeans")
```

| | |
|-----------------|------------------------|
| xina_enrichment | <i>xina_enrichment</i> |
|-----------------|------------------------|

Description

xina_enrichment conducts functional enrichment tests using gene ontology or KEGG pathway terms for a given protein list

Usage

```
xina_enrichment(string_db, protein_list, enrichment_type = "GO",
  pval_threshold = 0.05, methodMT = "fdr")
```

Arguments

| | |
|-----------------|--|
| string_db | STRINGdb object |
| protein_list | A vector of gene names to draw protein-protein interaction network. |
| enrichment_type | A functional annotation for the enrichment test. 'enrichment_type' should be one of 'GO' and 'KEGG', |
| pval_threshold | P-value threshold to get significantly enriched terms from the given proteins |
| methodMT | Method for p-value adjustment. See get_enrichment . Default is 'fdr'. |

Value

A list of data frames containing enrichment results

Examples

```
## Not run:
library(STRINGdb)
library(Biobase)

# load XINA example data
data(xina_example)

# Get STRING database for protein-protein intereaction information
string_db <- STRINGdb$new( version="10", species=9606, score_threshold=0, input_directory="" )
string_db

# XINA analysis with STRING DB
xina_result <- xina_analysis(example_clusters, string_db)

# Select proteins that showed cluster #1 in the Stimulus2 condition
subgroup <- subset(example_clusters$aligned, Stimulus2==1)
protein_list <- as.vector(subgroup$`Gene name`)

# Enrichment test using KEGG pathway terms that have adjuseted p-value less than 0.1
```

```

kegg_enriched <- xina_enrichment(string_db, protein_list,
enrichment_type = "KEGG", pval_threshold=0.1)
plot_enrichment_results(kegg_enriched$KEGG, num_terms=10)

# Enrichment test using GO terms that have adjusted p-value less than 0.1
go_enriched <- xina_enrichment(string_db, protein_list,
enrichment_type = "GO", pval_threshold=0.1)
plot_enrichment_results(go_enriched$Component, num_terms=10)

## End(Not run)

```

xina_plot_all

xina_plot_all

Description

xina_plot_all is to draw protein-protein interaction network plots of all the clusters

Usage

```

xina_plot_all(xina_result, clustering_result, condition = "all",
centrality_type = NULL, flag_simplify = TRUE, num_breaks = 5,
layout_specified = "", vertex_label_flag = FALSE,
vertex.label.color = "black", vertex.color = "", edge.color = NULL,
vertex.label.dist = 0.6, vertex.label.cex = 0.8,
edge.arrow.size = 0.4, vertex.size = 10, vertex.shape = "sphere",
legend_location = "bottom", num_clusters_in_row = 5,
flag_unknown_only = FALSE, img_size = NULL, img_qual = 300)

```

Arguments

xina_result A list containing XINA network analysis results. See [xina_analysis](#)

clustering_result A list containing XINA clustering results. See [xina_clustering](#)

condition Default is 'all', which means use all the proteins to draw graphs. If you specify the experimental condition name used for XINA clustering, xina_plot_all will draw graphs using specific condition's proteins.

centrality_type 'centrality_type' should be one of c('Degree', 'Eigenvector', 'Hub', 'Authority', 'Closeness', 'Betweenness')

| Centrality score | igraph function |
|------------------|----------------------------------|
| Degree | degree |
| Eigenvector | eigen_centrality |
| Hub | hub_score |
| Authority | authority_score |
| Closeness | closeness |
| Betweenness | betweenness |

flag_simplify If it is TRUE (default), XINA will exclude unconnected proteins

num_breaks 'num_breaks' is the number of ranks based on network centrality. Default is 5.
 layout_specified

This can change network layout. 'layout_specified' should be one of c('sphere', 'star', 'gem', 'tree', 'circle', 'random', 'nicely'). XINA's layouts are based on igraph's layout. See [layout_](#)

| Layout | igraph layout name |
|--------|----------------------------------|
| sphere | layout_on_sphere |
| star | layout_as_star |
| gem | layout_with_gem |
| tree | layout_as_tree |
| circle | layout_in_circle |
| random | layout_randomly |
| nicely | layout_nicely |

Default is 'layout_nicely' of igraph

vertex_label_flag

If vertex_label_flag is TRUE (default), igraph network graphs will be labeled by gene names. If vertex_label_flag is FALSE, igraph network graphs will be drawn without labels.

vertex.label.color

Color of labels. Default is black.

vertex.color Color of nodes. Default is pink.

edge.color Color of edges. Default is pink.

vertex.label.dist

Distance between node and label. Default is 0.6.

vertex.label.cex

Size of labels. Default is 0.8.

edge.arrow.size

Size of edges. Default is 0.4.

vertex.size Size of nodes. Default is 10.

vertex.shape You can choose node shape. Default is 'sphere'. See [shapes](#)

legend_location

If centrality_type is chosen, xina_plot_single add the color legend guiding rank of nodes based on the centrality score. Default is 'bottomright', but you can choose one of these 'bottomright', 'bottom', 'bottomleft', 'left', 'topleft', 'top', 'topright', 'right' and 'center'.

num_clusters_in_row

The number of clusters in a row on the XINA network plot. Default is 5.

flag_unknown_only

If this is TRUE, 'xina_plot_all' will plot proteins that do not have any protein-protein interaction in the given database.

img_size Set the image size. For width=1000 and height=1500, it is img_size=c(1000,1500). Default is c(3000,3000).

img_qual Set the image resolution. Default is 300.

Value

PNG images of PPI network plots of all the clusters

Examples

```
## the following code is to show how it works quickly
## load XINA example data
data(xina_example)

## load the previously processed XINA analysis results
# if you want to learn how to run 'xina_analysis', please see \link[XINA]{xina_analysis}
data(xina_result_example)

# XINA network plots
xina_plot_all(xina_result_example, example_clusters)

# XINA network plots for Control condition
xina_plot_all(xina_result_example, example_clusters, condition='Control')
```

xina_plot_bycluster *xina_plot_bycluster*

Description

xina_plot_bycluster is to draw protein-protein interaction network plots of each cluster

Usage

```
xina_plot_bycluster(xina_result, clustering_result, cl = NULL,
  condition = "all", flag_legend = TRUE, centrality_type = NULL,
  flag_simplify = TRUE, layout_specified = "",
  vertex_label_flag = TRUE, vertex.label.dist = 0.6,
  vertex.label.cex = 0.8, edge.arrow.size = 0.4, vertex.size = 10,
  vertex.shape = "sphere", vertex.color = "",
  edge.color = "darkgray", legend_location = "bottom",
  flag_unknown_only = FALSE)
```

Arguments

| | |
|-------------------|---|
| xina_result | A list containing XINA network analysis results. See xina_analysis |
| clustering_result | A list containing XINA clustering results. See xina_clustering |
| cl | Cluster number in the XINA clustering results |
| condition | Default is 'all', which means use all the proteins to draw graphs. If you specify the experimental condition name used for XINA clustering, |
| flag_legend | If it is TRUE, a legend will be printed out together. |
| centrality_type | 'centrality_type' should be one of c('Degree', 'Eigenvector', 'Hub', 'Authority', 'Closeness', 'Betweenness') |

| Centrality score | igraph function |
|------------------|----------------------------------|
| Degree | degree |
| Eigenvector | eigen_centrality |

| | |
|-------------|---------------------------------|
| Hub | hub_score |
| Authority | authority_score |
| Closeness | closeness |
| Betweenness | betweenness |

`flag_simplify` If it is TRUE (default), XINA will exclude unconnected proteins

`layout_specified`

This can change network layout. 'layout_specified' should be one of c('sphere', 'star', 'gem', 'tree', 'circle', 'random', 'nicely'). XINA's layouts are based on igraph's layout. See [layout_](#)

| Layout | igraph layout name |
|--------|----------------------------------|
| sphere | layout_on_sphere |
| star | layout_as_star |
| gem | layout_with_gem |
| tree | layout_as_tree |
| circle | layout_in_circle |
| random | layout_randomly |
| nicely | layout_nicely |

Default is 'layout_nicely' of igraph

`vertex_label_flag`

If `vertex_label_flag` is TRUE (default), igraph network graphs will be labeled by gene names. If `vertex_label_flag` is FALSE, igraph network graphs will be drawn without labels.

`vertex.label.dist`

Distance between node and label. Default is 0.6

`vertex.label.cex`

Size of labels. Default is 0.8

`edge.arrow.size`

Size of edges. Default is 0.4

`vertex.size` Size of nodes. Default is 10

`vertex.shape` You can choose node shape. Default is 'sphere'. See [shapes](#)

`vertex.color` Color of nodes. Default is pink.

`edge.color` Color of edges. Default is pink.

`legend_location`

If `centrality_type` is chosen, `xina_plot_single` add the color legend guiding rank of nodes based on the centrality score. Default is 'bottomright', but you can choose one of these 'bottomright', 'bottom', 'bottomleft', 'left', 'topleft', 'top', 'topright', 'right' and 'center'.

`flag_unknown_only`

If this is TRUE, 'xina_plot_bycluster' will plot proteins that do not have any protein-protein interaction in the given database

Value

A PNG file (XINA_Cluster_Networks.png) displaying protein-protein interaction network plots of all the clusters and a list containing XINA network analysis results

PNG images of PPI network plots of all the clusters

Examples

```
## the following code is to show how it works quickly
## load XINA example data
data(xina_example)

## load the previously processed XINA analysis results
# if you want to learn how to run 'xina_analysis', please see \link[XINA]{xina_analysis}
data(xina_result_example)

# plot cluster #1
xina_plot_bycluster(xina_result_example, example_clusters, cl=1)

# plot PPI network of Control condition in cluster #1
xina_plot_bycluster(xina_result_example, example_clusters, cl=1, condition='Control')
```

xina_plot_single *xina_plot_single*

Description

xina_plot_single draws protein-protein interaction network plot for given 'protein_list'.

Usage

```
xina_plot_single(xina_result, protein_list, centrality_type = NULL,
  layout_specified = "", vertex_label_flag = TRUE, main = NULL,
  vertex.label.color = "black", vertex.color = NA,
  edge.color = "darkgray", vertex.label.dist = 0.6,
  vertex.label.cex = 0.8, edge.arrow.size = 0.4, vertex.size = 10,
  vertex.shape = "sphere", legend_location = "bottom",
  num_breaks = 5, digits_round_up = 5, flag_simplify = TRUE,
  flag_legend = TRUE)
```

Arguments

xina_result A list containing XINA network analysis results. See [xina_analysis](#)

protein_list A vector of gene names to draw a protein-protein interaction network graph.

centrality_type 'centrality_type' should be one of c('Degree', 'Eigenvector', 'Hub', 'Authority', 'Closeness', 'Betweenness')

| Centrality score | igraph function |
|------------------|----------------------------------|
| Degree | degree |
| Eigenvector | eigen_centrality |
| Hub | hub_score |
| Authority | authority_score |
| Closeness | closeness |
| Betweenness | betweenness |

layout_specified

This can change network layout. 'layout_specified' should be one of c('sphere', 'star', 'gem', 'tree', 'circle', 'random', 'nicely'). XINA's layouts are based on igraph's layout. See [layout_](#)

| Layout | igraph layout name |
|--------|----------------------------------|
| sphere | layout_on_sphere |
| star | layout_as_star |
| gem | layout_with_gem |
| tree | layout_as_tree |
| circle | layout_in_circle |
| random | layout_randomly |
| nicely | layout_nicely |

Default is 'layout_nicely' of igraph

vertex_label_flag

If vertex_label_flag is TRUE (default), igraph network graphs will be labeled by gene names. If vertex_label_flag is FALSE, igraph network graphs will be drawn without labels.

main

Title of network figure. IF it is NULL (default), it will be the number of plotted proteins.

vertex.label.color

Color of labels. Default is black.

vertex.color

Color of nodes. Default is pink.

edge.color

Color of edges. Default is pink.

vertex.label.dist

Distance between node and label. Default is 0.6.

vertex.label.cex

Size of labels. Default is 0.8.

edge.arrow.size

Size of edges. Default is 0.4.

vertex.size

Size of nodes. Default is 10.

vertex.shape

You can choose node shape. Default is 'sphere'. See [shapes](#).

legend_location

If centrality_type is chosen, 'xina_plot_single' adds the color legend guiding rank of nodes based on the centrality score. Default is 'bottomright', but you can choose one of these 'bottomright', 'bottom', 'bottomleft', 'left', 'topleft', 'top', 'topright', 'right' and 'center'.

num_breaks

'num_breaks' is the number of ranks based on network centrality. Default is 5.

digits_round_up

See [Round](#)

flag_simplify

If it is TRUE (default), XINA will exclude unconnected proteins.

flag_legend

If it is TRUE, a legend will be printed out together.

Value

A PNG file (XINA_Cluster_Networks.png) displaying protein-protein interaction network plots of all the clusters and a list containing XINA network analysis results.

Examples

```
## the following code is to show how it works quickly
## load XINA example data
data(xina_example)

## load the previously processed XINA analysis results
# if you want to learn how to run 'xina_analysis', please see \link[XINA]{xina_analysis}
data(xina_result_example)

# get gene names that are clustered to #21 in "Stimulus2" condition
subgroup <- subset(example_clusters$aligned, Stimulus2==21)
protein_list <- subgroup$`Gene name`

# Calculate protein-protein interaction network
xina_plot_single(xina_result_example, protein_list)

# Calculate protein-protein interaction network and Eigenvector centrality
eigen_info <- xina_plot_single(xina_result_example, protein_list, centrality_type='Eigenvector')
```

| | |
|---------------------|--|
| xina_result_example | <i>Previously processed xina analysis using XINA's random example data A list containing 'xina_analysis' results</i> |
|---------------------|--|

Description

- All_network. PPI network of all the input proteins
- Sub_network. A list containing PPI networks of each clusters
- Data. XINA clustering results. See [xina_clustering](#)
- Nodes. A list of proteins in each cluster
- Conditions. A list of experimental condition of proteins in each cluster
- Titles. A list of plot titles for XINA plotting
- out_dir. A directory path storing XINA network analysis results
- is_stringdb. False = different PPI DB and TRUE = STRING DB

Format

A data frame containing STRING protein-protein interaction data

Source

XINA

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