Package: metasnf (via r-universe)

March 11, 2025

Title Meta Clustering with Similarity Network Fusion **Version** 2.0.5

Description Framework to facilitate patient subtyping with similarity network fusion and meta clustering. The similarity network fusion (SNF) algorithm was introduced by Wang et al. (2014) in <doi:10.1038/nmeth.2810>. SNF is a data integration approach that can transform high-dimensional and diverse data types into a single similarity network suitable for clustering with minimal loss of information from each initial data source. The meta clustering approach was introduced by Caruana et al. (2006) in <doi:10.1109/ICDM.2006.103>. Meta clustering involves generating a wide range of cluster solutions by adjusting clustering hyperparameters, then clustering the solutions themselves into a manageable number of qualitatively similar solutions, and finally characterizing representative solutions to find ones that are best for the user's specific context. This package provides a framework to easily transform multi-modal data into a wide range of similarity network fusion-derived cluster solutions as well as to visualize, characterize, and validate those solutions. Core package functionality includes easy customization of distance metrics, clustering algorithms, and SNF hyperparameters to generate diverse clustering solutions; calculation and plotting of associations between features, between patients, and between cluster solutions; and standard cluster validation approaches including resampled measures of cluster stability, standard metrics of cluster quality, and label propagation to evaluate generalizability in unseen data. Associated vignettes guide the user through using the package to identify patient subtypes while adhering to best practices for unsupervised learning.

License GPL (>= 3) **Encoding** UTF-8

Roxygen list(markdown = TRUE)

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Imports cli, cluster, data.table, digest, dplyr, ggplot2, grDevices, MASS, mclust, methods, progressr, purrr, RColorBrewer, rlang, SNFtool, stats, tibble, tidyr, utils	
Suggests circlize, ComplexHeatmap, InteractiveComplexHeatmap, clv, future, future.apply, knitr, rmarkdown, testthat (>= 3.0.0), ggalluvial, lifecycle, dbscan	
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abcd_anxiety

Mock ABCD anxiety data

Description

A randomly shuffled and anonymized copy of anxiety data from the NIMH Data archive. The original file used was pdem02.txt. The file was pre-processed by the abcdutils package (https://github.com/BRANCHlab/abcdutils function get_cbcl_anxiety.

Usage

abcd_anxiety

Format

abcd_anxiety:

A data frame with 275 rows and 2 columns:

patient The unique identifier of the ABCD dataset

cbcl_anxiety_r Ordinal value of impairment on CBCL anxiety, either 0 (no impairment), 1 (borderline clinical), or 2 (clinically impaired)

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Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

abcd_colour

Mock ABCD "colour" data

Description

A randomly shuffled and anonymized copy of depression data from the NIMH Data archive. The original file used was pdem02.txt. The file was pre-processed by the abcdutils package (https://github.com/BRANCHlab/abcd function get_cbcl_depress. The data was transformed into categorical colour values to demonstrate the Chi-squared test capabilities of extend_solutions.

Usage

abcd_colour

Format

abcd_colour:

A data frame with 275 rows and 2 columns:

patient The unique identifier of the ABCD dataset **colour** Categorical transformation of cbcl_depress.

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and

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follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

abcd_cort_sa

Mock ABCD cortical surface area data

Description

A randomly shuffled and anonymized copy of cortical surface area data from the NIMH Data archive. The original file used was mrisdp10201.txt The file was pre-processed by the abcdutils package (https://github.com/BRANCHlab/abcdutils) function get_cort_t.

Usage

abcd_cort_sa

Format

abcd_cort_sa:

A data frame with 188 rows and 152 columns:

patient The unique identifier of the ABCD dataset

... Cortical surface areas of various ROIs (mm^2, I think)

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete

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listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

abcd_cort_t

Mock ABCD cortical thickness data

Description

A randomly shuffled and anonymized copy of cortical thickness data from the NIMH Data archive. The original file used was mrisdp10201.txt The file was pre-processed by the abcdutils package (https://github.com/BRANCHlab/abcdutils) function get_cort_t.

Usage

abcd_cort_t

Format

abcd cort t:

A data frame with 188 rows and 152 columns:

patient The unique identifier of the ABCD dataset

... Cortical thicknesses of various ROIs (mm^3, I think)

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

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abcd_depress

Mock ABCD depression data

Description

A randomly shuffled and anonymized copy of depression data from the NIMH Data archive. The original file used was pdem02.txt. The file was pre-processed by the abcdutils package (https://github.com/BRANCHlab/abcdfunction get_cbcl_depress.

Usage

abcd_depress

Format

abcd_depress:

A data frame with 275 rows and 2 columns:

patient The unique identifier of the ABCD dataset

cbcl_depress_r Ordinal value of impairment on CBCL anxiety, either 0 (no impairment), 1 (borderline clinical), or 2 (clinically impaired)

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

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abcd_h_income

Mock ABCD income data

Description

Like abcd_income, but with no NAs in patient column

Usage

abcd_h_income

Format

abcd_income:

A data frame with 300 rows and 2 columns:

patient The unique identifier of the ABCD dataset

household_income Household income in 3 category levels (low = 1, medium = 2, high = 3)

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

abcd_income

Mock ABCD income data

Description

A randomly shuffled and anonymized copy of income data from the NIMH Data archive. The original file used was pdem02.txt The file was pre-processed by the abcdutils package (https://github.com/BRANCHlab/abcdutils) function get_income.

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Usage

abcd_income

Format

abcd_income:

A data frame with 300 rows and 2 columns:

patient The unique identifier of the ABCD dataset

household_income Household income in 3 category levels (low = 1, medium = 2, high = 3)

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

abcd_pubertal

Mock ABCD pubertal status data

Description

A randomly shuffled and anonymized copy of pubertal status data from the NIMH Data archive. The original files used were abcd_ssphp01.txt and abcd_ssphy01.txt. The file was pre-processed by the abcdutils package (https://github.com/BRANCHlab/abcdutils) function get_pubertal_status.

Usage

abcd_pubertal

Format

abcd_pubertal:

A data frame with 275 rows and 2 columns:

patient The unique identifier of the ABCD dataset

pubertal_status Average reported pubertal status between child and parent (1-5 categorical scale)

12 abcd_subc_v

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

abcd_subc_v

Mock ABCD subcortical volumes data

Description

A randomly shuffled and anonymized copy of subcortical volume data from the NIMH Data archive. The original file used was smrip10201.txt The file was pre-processed by the abcdutils package (https://github.com/BRANCHlab/abcdutils) function get_subc_v.

Usage

abcd_subc_v

Format

abcd_subc_v:

A data frame with 174 rows and 31 columns:

patient The unique identifier of the ABCD dataset

... Subcortical volumes of various ROIs (mm³, I think)

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and

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follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

Description

Add rows to a settings_df

Usage

```
add_settings_df_rows(
  sdf,
  n_solutions = 0,
 min_removed_inputs = 0,
 max_removed_inputs = sum(startsWith(colnames(sdf), "inc_")) - 1,
  dropout_dist = "exponential",
 min_alpha = NULL,
 max_alpha = NULL,
 min_k = NULL,
 max_k = NULL,
 min_t = NULL,
 max_t = NULL,
  alpha_values = NULL,
  k_values = NULL,
  t_values = NULL,
  possible_snf_schemes = c(1, 2, 3),
  clustering_algorithms = NULL,
  continuous_distances = NULL,
  discrete_distances = NULL,
  ordinal_distances = NULL,
  categorical_distances = NULL,
 mixed_distances = NULL,
  dfl = NULL,
  snf_input_weights = NULL,
  snf_domain_weights = NULL,
  retry_limit = 10,
```

```
allow_duplicates = FALSE
)
```

Arguments

sdf The existing settings data frame

min_removed_inputs

The smallest number of input data frames that may be randomly removed. By default, 0.

max_removed_inputs

The largest number of input data frames that may be randomly removed. By default, this is 1 less than all the provided input data frames in the data list.

dropout_dist Parameter controlling how the random removal of input data frames should oc-

cur. Can be "none" (no input data frames are randomly removed), "uniform" (uniformly sample between min_removed_inputs and max_removed_inputs to determine number of input data frames to remove), or "exponential" (pick number of input data frames to remove by sampling from min_removed_inputs to

max_removed_inputs with an exponential distribution; the default).

min_alpha The minimum value that the alpha hyperparameter can have. Random assigned

value of alpha for each row will be obtained by uniformly sampling numbers between min_alpha and max_alpha at intervals of 0.1. Cannot be used in con-

junction with the alpha_values parameter.

max_alpha The maximum value that the alpha hyperparameter can have. See min_alpha

parameter. Cannot be used in conjunction with the alpha_values parameter.

min_k The minimum value that the k hyperparameter can have. Random assigned value

of k for each row will be obtained by uniformly sampling numbers between min_k and max_k at intervals of 1. Cannot be used in conjunction with the

k_values parameter.

max_k The maximum value that the k hyperparameter can have. See min_k parameter.

Cannot be used in conjunction with the k_values parameter.

min_t The minimum value that the t hyperparameter can have. Random assigned value

of t for each row will be obtained by uniformly sampling numbers between min_t and max_t at intervals of 1. Cannot be used in conjunction with the

t_values parameter.

max_t The maximum value that the t hyperparameter can have. See min_t parameter.

Cannot be used in conjunction with the t_values parameter.

alpha_values A number or numeric vector of a set of possible values that alpha can take on.

Value will be obtained by uniformly sampling the vector. Cannot be used in

conjunction with the min_alpha or max_alpha parameters.

k_values A number or numeric vector of a set of possible values that k can take on. Value

will be obtained by uniformly sampling the vector. Cannot be used in conjunc-

tion with the min_k or max_k parameters.

t_values A number or numeric vector of a set of possible values that t can take on. Value

will be obtained by uniformly sampling the vector. Cannot be used in conjunc-

tion with the min_t or max_t parameters.

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possible_snf_schemes

A vector containing the possible snf_schemes to uniformly randomly select from. By default, the vector contains all 3 possible schemes: c(1, 2, 3). 1 corresponds to the "individual" scheme, 2 corresponds to the "domain" scheme, and 3 corresponds to the "twostep" scheme.

clustering_algorithms

A list of clustering algorithms to uniformly randomly pick from when clustering. When not specified, randomly select between spectral clustering using the eigen-gap heuristic and spectral clustering using the rotation cost heuristic. See ?clust_fns_list for more details on running custom clustering algorithms.

continuous_distances

A vector of continuous distance metrics to use when a custom dist_fns_list is provided.

discrete_distances

A vector of categorical distance metrics to use when a custom dist_fns_list is provided.

ordinal_distances

A vector of categorical distance metrics to use when a custom dist_fns_list is provided.

categorical_distances

A vector of categorical distance metrics to use when a custom dist_fns_list is provided.

mixed_distances

A vector of mixed distance metrics to use when a custom dist_fns_list is provided.

dfl List containing distance metrics to vary over. See ?generate_dist_fns_list.

snf_input_weights

Nested list containing weights for when SNF is used to merge individual input measures (see ?generate_snf_weights)

snf_domain_weights

Nested list containing weights for when SNF is used to merge domains (see ?generate_snf_weights)

retry_limit

The maximum number of attempts to generate a novel row. This function does not return matrices with identical rows. As the range of requested possible settings tightens and the number of requested rows increases, the risk of randomly generating a row that already exists increases. If a new random row has matched an existing row retry_limit number of times, the function will terminate.

allow_duplicates

If TRUE, enables creation of a settings data frame with duplicate non-feature weighting related hyperparameters. This function should only be used when paired with a custom weights matrix that has non-duplicate rows.

Value

A settings data frame

```
adjusted_rand_index_heatmap
```

Heatmap of pairwise adjusted rand indices between solutions

Description

[Deprecated] Defunct function to create an ARI heatmap. Please use meta_cluster_heatmap() instead.

Usage

```
adjusted_rand_index_heatmap(
    aris,
    order = NULL,
    cluster_rows = FALSE,
    cluster_columns = FALSE,
    log_graph = FALSE,
    scale_diag = "none",
    min_colour = "#282828",
    max_colour = "firebrick2",
    col = circlize::colorRamp2(c(min(aris), max(aris)), c(min_colour, max_colour)),
    ...
)
```

Arguments

aris Matrix of adjusted rand indices from calc_aris()
order Numeric vector containing row order of the heatmap.
cluster_rows Whether rows should be clustered.

cluster_columns

Whether columns should be clustered.

log_graph If TRUE, log transforms the graph.

scale_diag Method of rescaling matrix diagonals. Can be "none" (don't change diagonals),

"mean" (replace diagonals with average value of off-diagonals), or "zero" (re-

place diagonals with 0).

min_colour Colour used for the lowest value in the heatmap.

Colour used for the highest value in the heatmap.

col Colour ramp to use for the heatmap.

... Additional parameters passed to similarity_matrix_heatmap(), the function

that this function wraps.

Value

Returns a heatmap (class "Heatmap" from package ComplexHeatmap) that displays the pairwise adjusted Rand indices (similarities) between the cluster solutions of the provided solutions data frame.

age_df

age_df

Mock age data

Description

Mock age data

Usage

age_df

Format

```
age_df:
```

A data frame with 200 rows and 2 columns:

patient_id Random three-digit number uniquely identifying the patient
age Mock age feature

Source

This data came from the SNFtool package, with slight modifications.

alluvial_cluster_plot Alluvial plot of patients across cluster counts and important features

Description

This alluvial plot shows how observations in a similarity matrix could have been clustered over a set of clustering functions.

Usage

```
alluvial_cluster_plot(
  cluster_sequence,
  similarity_matrix,
  dl = NULL,
  data = NULL,
  key_outcome,
  key_label = key_outcome,
  extra_outcomes = NULL,
  title = NULL
)
```

18 alluvial_cluster_plot

Arguments

Value

title

An alluvial plot (class "gg" and "ggplot") showing distribution of a feature across varying number cluster solutions.

Title of the plot.

Examples

```
input_dl <- data_list(</pre>
    list(gender_df, "gender", "demographics", "categorical"),
    list(diagnosis_df, "diagnosis", "clinical", "categorical"),
    uid = "patient_id"
)
sc <- snf_config(input_dl, n_solutions = 1)</pre>
sol_df <- batch_snf(input_dl, sc, return_sim_mats = TRUE)</pre>
sim_mats <- sim_mats_list(sol_df)</pre>
clust_fn_sequence <- list(spectral_two, spectral_four)</pre>
alluvial_cluster_plot(
    cluster_sequence = clust_fn_sequence,
    similarity_matrix = sim_mats[[1]],
    dl = input_dl,
    key_outcome = "gender", # the name of the feature of interest
    key_label = "Gender", # how the feature of interest should be displayed
    extra_outcomes = "diagnosis", # more features to plot but not colour by
    title = "Gender Across Cluster Counts"
)
```

anxiety 19

anxiety

Mock ABCD anxiety data

Description

Like the mock data frame "abcd_colour", but with "unique_id" as the "uid".

Usage

anxiety

Format

anxiety:

A data frame with 275 rows and 2 columns:

unique_id The unique identifier of the ABCD dataset

cbcl_anxiety_r Ordinal value of impairment on CBCL anxiety, either 0 (no impairment), 1 (borderline clinical), or 2 (clinically impaired)

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

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arrange

Arrange rows in an object

Description

Arrange rows in an object

Usage

```
arrange(.data, ...)
```

Arguments

.data The object to arrange columns from.... Additional arguments for arranging.

Value

Object with arrangeed columns.

```
as.data.frame.data_list
```

Coerce a data_list class object into a data.frame class object

Description

Horizontally joins data frames within a data list into a single data frame, using the uid attribute as the joining key.

Usage

```
## S3 method for class 'data_list'
as.data.frame(x, row.names = NULL, optional = FALSE, ...)
```

Arguments

x A data_list class object.

row.names Additional parameter passed to as.data.frame().

Additional parameter passed to as.data.frame().

Additional parameter passed to as.data.frame().

Value

dl_df A data.frame class object with all the features and observations of dl.

```
as.data.frame.ext_solutions_df  {\it Coerce~a~ \rm ext\_solutions\_df~\it class~object~into~a~ \rm data.frame~\it class~\it object~}
```

Description

Coerce a ext_solutions_df class object into a data.frame class object

Usage

```
## S3 method for class 'ext_solutions_df'
as.data.frame(
    x,
    row.names = NULL,
    optional = FALSE,
    keep_attributes = FALSE,
    ...
)
```

Arguments

```
x A ext_solutions_df class object.

row.names Additional parameter passed to as.data.frame().

optional Additional parameter passed to as.data.frame().

keep_attributes

If TRUE, resulting data frame includes settings data frame and weights matrix.

... Additional parameter passed to as.data.frame().
```

Value

A data. frame class object with all the columns of x and its contained solutions data frame.

```
as.data.frame.solutions_df  {\it Coerce~a~ solutions\_df~ class~object~ into~a~ data.frame~ class~object}
```

Description

Coerce a solutions_df class object into a data.frame class object

22 as.list.clust_fns_list

Usage

```
## S3 method for class 'solutions_df'
as.data.frame(
    X,
    row.names = NULL,
    optional = FALSE,
    keep_attributes = FALSE,
    ...
)
```

Arguments

```
x A solutions_df class object.

row.names Additional parameter passed to as.data.frame().

optional Additional parameter passed to as.data.frame().

keep_attributes

If TRUE, resulting data frame includes settings data frame and weights matrix.

Additional parameter passed to as.data.frame().
```

Value

A data. frame class object with all the columns of x and its contained solutions data frame.

Description

Coerce a clust_fns_list class object into a list class object

Usage

```
## S3 method for class 'clust_fns_list'
as.list(x, ...)
```

Arguments

```
x A clust_fns_list class object.... Additional parameter passed to as.list().
```

Value

A list class object with all the functions of x.

as.list.data_list

as.list.data_list

Coerce a data_list class object into a list class object

Description

Coerce a data_list class object into a list class object

Usage

```
## S3 method for class 'data_list'
as.list(x, ...)
```

Arguments

- x A data_list class object.
- ... Additional parameter passed to as.list().

Value

A list class object with all the objects of x.

Description

Coerce a dist_fns_list class object into a list class object

Usage

```
## S3 method for class 'dist_fns_list'
as.list(x, ...)
```

Arguments

- x A dist_fns_list class object.
- ... Additional parameter passed to as.list().

Value

A list class object with all the functions of x.

24 assemble_data

```
as.matrix.weights_matrix
```

Coerce a weights_matrix class object into a matrix class object

Description

Coerce a weights_matrix class object into a matrix class object

Usage

```
## S3 method for class 'weights_matrix' as.matrix(x, ...)
```

Arguments

x A weights_matrix class object.

... Additional parameter passed to as.matrix().

Value

A matrix and array class object.

assemble_data

Collapse a data frame and/or a data list into a single data frame

Description

Collapse a data frame and/or a data list into a single data frame

Usage

```
assemble_data(data, dl)
```

Arguments

data A data frame.

dl A nested list of input data from data_list().

Value

A class "data.frame" object containing all the features of the provided data frame and/or data list.

assoc_pval_heatmap 25

assoc_pval_heatmap

Heatmap of pairwise associations between features

Description

Heatmap of pairwise associations between features

Usage

```
assoc_pval_heatmap(
  correlation_matrix,
  scale_diag = "max"
  cluster_rows = TRUE,
  cluster_columns = TRUE,
  show_row_names = TRUE,
  show_column_names = TRUE,
  show_heatmap_legend = FALSE,
  confounders = NULL,
  out_of_models = NULL,
  annotation_colours = NULL,
  labels_colour = NULL,
  split_by_domain = FALSE,
  d1 = NULL,
  significance_stars = TRUE,
  slice_font_size = 8,
)
```

Arguments

correlation_matrix

Matrix containing all pairwise association p-values. The recommended way to obtain this matrix is through the calc_assoc_pval function.

scale_diag Parameter that controls how the diagonals of the correlation_matrix are adjusted

in the heatmap. For best viewing, this is set to "max", which will match the

diagonals to whichever pairwise association has the highest p-value.

cluster_rows Parameter for ComplexHeatmap::Heatmap. Will be ignored if split_by_domain

is also provided.

cluster_columns

Parameter for ComplexHeatmap::Heatmap. Will be ignored if split_by_domain is also provided.

show_row_names Parameter for ComplexHeatmap::Heatmap. show_column_names

Parameter for ComplexHeatmap::Heatmap.

show_heatmap_legend

Parameter for ComplexHeatmap::Heatmap.

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confounders A named list where the elements are columns in the correlation_matrix and the names are the corresponding display names. out_of_models Like confounders, but a named list of out of model measures (who are also present as columns in the correlation matrix). annotation_colours Named list of heatmap annotations and their colours. labels_colour Vector of colours to use for the columns and rows of the heatmap. split_by_domain The results of dl_var_summar - a data frame that has the domain of every feature in the plotted data. columns of the correlation matrix. Will be used to "slice" the heatmap into visually separated sections. A nested list of input data from data_list(). significance_stars If TRUE (default), plots significance stars on heatmap cells slice_font_size Font size for domain separating labels.

Value

Returns a heatmap (class "Heatmap" from package ComplexHeatmap) that displays the pairwise associations between features from the provided correlation_matrix.

Additional parameters passed into ComplexHeatmap::Heatmap.

Examples

```
#data_list <- data_list(
# list(income, "household_income", "demographics", "ordinal"),
# list(pubertal, "pubertal_status", "demographics", "continuous"),
# list(fav_colour, "favourite_colour", "demographics", "categorical"),
# list(anxiety, "anxiety", "behaviour", "ordinal"),
# list(depress, "depressed", "behaviour", "ordinal"),
# uid = "unique_id"
#)
#
#assoc_pval_matrix <- calc_assoc_pval_matrix(data_list)
#ap_heatmap <- assoc_pval_heatmap(assoc_pval_matrix)</pre>
```

as_ari_matrix

Convert an object to an ARI matrix

Description

This function coerces non-ari_matrix class objects into ari_matrix class objects.

Usage

```
as_ari_matrix(x)
```

as_data_list 27

Arguments

Х

The object to convert into a weights matrix.

Value

An ari_matrix class object.

as_data_list

Convert an object to a data list

Description

This function coerces non-data_list class objects into data_list class objects.

Usage

```
as_data_list(x)
```

Arguments

Х

The object to convert into a data list.

Value

A data_list class object.

 $as_settings_df$

Convert an object to a settings data frame

Description

This function coerces non-settings_df class objects into settings_df class objects.

Usage

```
as_settings_df(x)
```

Arguments

X

The object to convert into a data list.

Value

A settings_df class object.

28 as_snf_config

as_sim_mats_list

Convert an object to a similarity matrix list

Description

This function converts non-sim_mats_list class objects into sim_mats_list class objects.

Usage

```
as_sim_mats_list(x)
```

Arguments

Χ

The object to convert into a sim_mats_list. Must be a list of square matrices with identical column and row names.

Value

 $A \verb| sim_mats_list| class| object.$

as_snf_config

Convert an object to a snf config

Description

This function coerces non-snf_config class objects into snf_config class objects.

Usage

```
as_snf_config(x)
```

Arguments

Х

The object to convert into a snf config.

Value

A snf_config class object.

as_weights_matrix 29

as_weights_matrix

Convert an object to a weights matrix

Description

This function converts non-weights_matrix objects into weights_matrix class objects.

Usage

```
as_weights_matrix(x)
```

Arguments

Х

The object to convert into a data list.

Value

A weights_matrix class object.

auto_plot

Automatically plot features across clusters

Description

Given a single row of a solutions data frame and data provided through a data list, this function will return a series of bar and/or jitter plots based on feature types.

Usage

```
auto_plot(
    sol_df_row = NULL,
    dl = NULL,
    cluster_df = NULL,
    return_plots = TRUE,
    save = NULL,
    jitter_width = 6,
    jitter_height = 6,
    bar_width = 6,
    verbose = FALSE
)
```

30 bar_plot

Arguments

sol_df_row A single row of a solutions data frame.

dl A data list containing data to plot.

cluster_df Directly provide a cluster_df rather than a solutions matrix. Useful if plotting

data from label propagated results.

instead return the full data frame used for plotting.

save If a string is provided, plots will be saved and this string will be used to prefix

plot names.

jitter_width Width of jitter plots if save is specified.
jitter_height Height of jitter plots if save is specified.
bar_width Width of bar plots if save is specified.
bar_height Height of bar plots if save is specified.
verbose If TRUE, output progress to console.

Value

By default, returns a list of plots (class "gg", "ggplot") with one plot for every feature in the provided data list and/or target list. If return_plots is FALSE, will instead return a single "data.frame" object containing every provided feature for every observation in long format.

bar_plot	Bar plot separating a feature by cluster

Description

Bar plot separating a feature by cluster

Usage

```
bar_plot(df, feature)
```

Arguments

df A data.frame containing cluster column and the feature to plot.

feature The feature to plot.

Value

A bar plot (class "gg", "ggplot") showing the distribution of a feature across clusters.

batch_snf 31

batch_snf	Run variations of SNF.	

Description

This is the core function of the metasnf package. Using the information stored in a settings_df (see ?settings_df) and a data list (see ?data_list), run repeated complete SNF pipelines to generate a broad space of post-SNF cluster solutions.

Usage

```
batch_snf(dl, sc, processes = 1, return_sim_mats = FALSE, sim_mats_dir = NULL)
```

Arguments

dl A nested list of input data from data_list().

sc An snf_config class object which stores all sets of hyperparameters used to

transform data in dl into a cluster solutions. See ?settings_df or https://branchlab.github.io/metasnf/artic

for more details.

processes Specify number of processes used to complete SNF iterations

1 (default) Sequential processing: function will iterate through the settings_df
one row at a time with a for loop. This option will not make use of multiple
CPU cores, but will show a progress bar.

- 2 or higher: Parallel processing will use the future.apply::future_apply to distribute the SNF iterations across the specified number of CPU cores. If higher than the number of available cores, a warning will be raised and the maximum number of cores will be used.
- max: All available cores will be used.

return_sim_mats

If TRUE, function will return a list where the first element is the solutions data frame and the second element is a list of similarity matrices for each row in the sol_df. Default FALSE.

sim_mats_dir If specified, this directory will be used to save all generated similarity matrices.

Value

By default, returns a solutions data frame (class "data.frame"), a a data frame containing one row for every row of the provided settings matrix, all the original columns of that settings data frame, and new columns containing the assigned cluster of each observation from the cluster solution derived by that row's settings. If return_sim_mats is TRUE, the function will instead return a list containing the solutions data frame as well as a list of the final similarity matrices (class "matrix") generated by SNF for each row of the settings data frame. If suppress_clustering is TRUE, the solutions data frame will not be returned in the output.

Examples

```
input_dl <- data_list(
    list(gender_df, "gender", "demographics", "categorical"),
    list(diagnosis_df, "diagnosis", "clinical", "categorical"),
    uid = "patient_id"
)

sc <- snf_config(input_dl, n_solutions = 3)

# A solutions data frame without similarity matrices:
sol_df <- batch_snf(input_dl, sc)

# A solutions data frame with similarity matrices:
# sol_df <- batch_snf(input_dl, sc, return_sim_mats = TRUE)
# sim_mats_list(sol_df)</pre>
```

batch_snf_subsamples Run SNF clustering pipeline on a list of subsampled data lists.

Description

Run SNF clustering pipeline on a list of subsampled data lists.

Usage

```
batch_snf_subsamples(
  dl_subsamples,
  sc,
  processes = 1,
  return_sim_mats = FALSE,
  sim_mats_dir = NULL,
  verbose = TRUE
)
```

Arguments

dl_subsamples

A list of subsampled data lists. This object is generated by the function batch_snf_subsamples().

sc

An snf_config class object which stores all sets of hyperparameters used to

transform data in dl into a cluster solutions. See ?settings_df or https://branchlab.github.io/metasnf/artic for more details.

for more detain

processes

Specify number of processes used to complete SNF iterations

- 1 (default) Sequential processing: function will iterate through the settings_df one row at a time with a for loop. This option will not make use of multiple CPU cores, but will show a progress bar.
- 2 or higher: Parallel processing will use the future.apply::future_apply to distribute the SNF iterations across the specified number of CPU cores. If higher than the number of available cores, a warning will be raised and the maximum number of cores will be used.

calculate_coclustering 33

• max: All available cores will be used.

return_sim_mats

If TRUE, function will return a list where the first element is the solutions data frame and the second element is a list of similarity matrices for each row in the sol_df. Default FALSE.

sim_mats_dir

If specified, this directory will be used to save all generated similarity matrices.

verbose

If TRUE, output progress to console.

Value

By default, returns a one-element list: cluster_solutions, which is itself a list of cluster solution data frames corresponding to each of the provided data list subsamples. Setting the parameters return_sim_mats and return_solutions to TRUE will turn the result of the function to a three-element list containing the corresponding solutions data frames and final fused similarity matrices of those cluster solutions, should you require these objects for your own stability calculations.

Examples

```
# my_dl <- data_list(</pre>
      list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
      list(income, "household_income", "demographics", "continuous"),
#
      list(pubertal, "pubertal_status", "demographics", "continuous"),
#
      uid = "unique_id"
#)
# sc <- snf_config(my_dl, n_solutions = 5, max_k = 40)</pre>
# my_dl_subsamples <- subsample_dl(</pre>
#
      my_dl,
#
      n_subsamples = 20,
#
      subsample_fraction = 0.85
# )
# batch_subsample_results <- batch_snf_subsamples(</pre>
      my_dl_subsamples,
#
      sc,
#
      verbose = TRUE
#)
```

calculate_coclustering

Calculate coclustering data.

Description

Calculate coclustering data.

Usage

```
calculate_coclustering(subsample_solutions, sol_df, verbose = FALSE)
```

Arguments

subsample_solutions

A list of containing cluster solutions from distinct subsamples of the data. This object is generated by the function batch_snf_subsamples(). These solutions should correspond to the ones in the solutions data frame.

sol_df

A solutions data frame. This object is generated by the function batch_snf(). The solutions in the solutions data frame should correspond to those in the subsample solutions.

verbose

If TRUE, output time remaining estimates to console.

Value

A list containing the following components:

- cocluster_dfs: A list of data frames, one per cluster solution, that shows the number of times that every pair of observations in the original cluster solution occurred in the same subsample, the number of times that every pair clustered together in a subsample, and the corresponding fraction of times that every pair clustered together in a subsample.
- cocluster_ss_mats: The number of times every pair of observations occurred in the same subsample, formatted as a pairwise matrix.
- cocluster_sc_mats: The number of times every pair of observations occurred in the same cluster, formatted as a pairwise matrix.
- cocluster_cf_mats: The fraction of times every pair of observations occurred in the same cluster, formatted as a pairwise matrix.
- cocluster_summary: Specifically among pairs of observations that clustered together in the
 original full cluster solution, what fraction of those pairs remained clustered together throughout the subsample solutions. This information is formatted as a data frame with one row per
 cluster solution.

Examples

```
# my_dl <- data_list(
# list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
# list(income, "household_income", "demographics", "continuous"),
# list(pubertal, "pubertal_status", "demographics", "continuous"),
# uid = "unique_id"
# )
#
# sc <- snf_config(my_dl, n_solutions = 5, max_k = 40)
#
# sol_df <- batch_snf(my_dl, sc)
#
# my_dl_subsamples <- subsample_dl(
# my_dl,</pre>
```

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```
n_subsamples = 20,
#
      subsample_fraction = 0.85
#)
#
# batch_subsample_results <- batch_snf_subsamples(</pre>
      my_dl_subsamples,
#
      sc,
      verbose = TRUE
#)
# coclustering_results <- calculate_coclustering(</pre>
      batch_subsample_results,
#
#
      sol_df,
      verbose = TRUE
#)
```

calc_aris

Construct an ARI matrix storing inter-solution similarities

Description

This function constructs an ari_matrix class object from a solutions_df class object. The ARI matrix stores pairwise adjusted Rand indices for all cluster solutions as well as a numeric order for the solutions data frame based on the hierarchical clustering of the ARI matrix.

Usage

```
calc_aris(
  sol_df,
  processes = 1,
  verbose = FALSE,
  dist_method = "euclidean",
  hclust_method = "complete"
)
```

Arguments

sol_df

Solutions data frame containing cluster solutions to calculate pairwise ARIs for.

processes

Specify number of processes used to complete calculations

- 1 (default) Sequential processing
- 2 or higher: Parallel processing will use the future.apply::future_apply to distribute the calculations across the specified number of CPU cores. If higher than the number of available cores, a warning will be raised and the maximum number of cores will be used.
- max: All available cores will be used. Note that no progress indicator is available during multi-core processing.

verbose

If TRUE, output progress to console.

dist_method Distance method to use when calculating sorting order to of the matrix. Ar-

gument is directly passed into stats::dist. Options include "euclidean", "maxi-

mum", "manhattan", "canberra", "binary", or "minkowski".

hclust_method Agglomerative method to use when calculating sorting order by stats::hclust.

Options include "ward.D", "ward.D2", "single", "complete", "average", "mc-

quitty", "median", or "centroid".

Value

om_aris ARIs between clustering solutions of an solutions data frame

Examples

```
dl <- data_list(
    list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
    list(pubertal, "pubertal_status", "demographics", "continuous"),
    uid = "unique_id"
)

sc <- snf_config(dl, n_solutions = 3)
sol_df <- batch_snf(dl, sc)
calc_aris(sol_df)</pre>
```

calc_assoc_pval_matrix

Calculate p-values for all pairwise associations of features in a data list

Description

Calculate p-values for all pairwise associations of features in a data list

Usage

```
calc_assoc_pval_matrix(dl, verbose = FALSE, cat_test = "chi_squared")
```

Arguments

dl A nested list of input data from data_list().

verbose If TRUE, output progress to the console.

cat_test String indicating which statistical test will be used to associate cluster with

a categorical feature. Options are "chi_squared" for the Chi-squared test and

"fisher exact" for Fisher's exact test.

Value

A "matrix" class object containing pairwise association p-values between the features in the provided data list.

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Examples

```
data_list <- data_list(
    list(income, "household_income", "demographics", "ordinal"),
    list(pubertal, "pubertal_status", "demographics", "continuous"),
    list(anxiety, "anxiety", "behaviour", "ordinal"),
    list(depress, "depressed", "behaviour", "ordinal"),
    uid = "unique_id"
)
assoc_pval_matrix <- calc_assoc_pval_matrix(data_list)</pre>
```

calc_nmis

Calculate feature NMIs for a data list and a solutions data frame

Description

Normalized mutual information scores can be used to indirectly measure how important a feature may have been in producing a cluster solution. This function will calculate the normalized mutual information between cluster solutions in a solutions data frame as well as cluster solutions created by including only a single feature from a provided data list, but otherwise using all the same hyperparameters as specified in the original SNF config. Note that NMIs can be calculated between two cluster solutions regardless of what features were actually used to create those cluster solutions. For example, a feature that was not involved in producing a particular cluster solution may still have a high NMI with that cluster solution (typically because it was highly correlated with a different feature that was used).

Usage

```
calc_nmis(
    dl,
    sol_df,
    transpose = TRUE,
    ignore_inclusions = TRUE,
    verbose = FALSE
)
```

Arguments

dl A nested list of input data from data_list().

sol_df Result of batch_snf storing cluster solutions and the settings that were used to

generate them. Use the same value as was used in the original call to batch_snf().

transpose If TRUE, will transpose the output data frame.

ignore_inclusions

If TRUE, will ignore the inclusion columns in the solutions data frame and calculate NMIs for all features. If FALSE, will give NAs for features that were

dropped on a given settings_df row.

verbose If TRUE, output progress to console.

38 cancer_diagnosis_df

Value

A "data.frame" class object containing one row for every feature in the provided data list and one column for every solution in the provided solutions data frame. Populated values show the calculated NMI score for each feature-solution combination.

Examples

```
input_dl <- data_list(
    list(gender_df, "gender", "demographics", "categorical"),
    list(diagnosis_df, "diagnosis", "clinical", "categorical"),
    uid = "patient_id"
)

sc <- snf_config(input_dl, n_solutions = 2)

sol_df <- batch_snf(input_dl, sc)

calc_nmis(input_dl, sol_df)</pre>
```

cancer_diagnosis_df

Mock diagnosis data

Description

This is the same data as diagnosis_df, with renamed features and columns.

Usage

```
cancer_diagnosis_df
```

Format

```
cancer_diagnosis_df:
A data frame with 200 rows and 2 columns:

patient_id Random three-digit number uniquely identifying the patient diagnosis Mock cancer diagnosis feature (1, 2, or 3)
```

Source

This data came from the SNFtool package, with slight modifications.

cell_significance_fn 39

cell_significance_fn Place significance stars on ComplexHeatmap cells.

Description

This is an internal function meant to be used to by the assoc_pval_heatmap function.

Usage

```
cell_significance_fn(data)
```

Arguments

data

The matrix containing the cells to base the significance stars on.

Value

cell_fn Another function that is well-formatted for usage as the cell_fun argument in Complex-Heatmap::Heatmap.

check_dataless_annotations

Helper function to stop annotation building when no data was provided

Description

Helper function to stop annotation building when no data was provided

Usage

```
check_dataless_annotations(annotation_requests, data)
```

Arguments

annotation_requests

A list of requested annotations

data

A data frame with data to build annotations

Value

Does not return any value. This function just raises an error when annotations are requested without any provided data for a heatmap.

Description

Check for ComplexHeatmap and circlize dependencies

Usage

```
check_hm_dependencies()
```

Value

Does not return any value. This function just checks that the ComplexHeatmap and circlize packages are installed.

check_similarity_matrices

Check validity of similarity matrices

Description

Check to see if similarity matrices in a list have the following properties:

- 1. The maximum value in the entire matrix is 0.5
- 2. Every value in the diagonal is 0.5

Usage

```
check_similarity_matrices(similarity_matrices)
```

Arguments

```
similarity_matrices
```

A list of similarity matrices

Value

valid_matrices Boolean indicating if properties are met by all similarity matrices

clust_fns 41

clust_fns

Built-in clustering algorithms

Description

These functions can be used when building a metasnf clustering functions list. Each function converts a similarity matrix (matrix class object) to a cluster solution (numeric vector). Note that these functions (or custom clustering functions) cannot accept number of clusters as a parameter; this value must be built into the function itself if necessary.

Usage

```
spectral_eigen(similarity_matrix)
spectral_rot(similarity_matrix)
spectral_eigen_classic(similarity_matrix)
spectral_rot_classic(similarity_matrix)
spectral_two(similarity_matrix)
spectral_three(similarity_matrix)
spectral_four(similarity_matrix)
spectral_five(similarity_matrix)
spectral_six(similarity_matrix)
spectral_seven(similarity_matrix)
spectral_eight(similarity_matrix)
spectral_eight(similarity_matrix)
spectral_nine(similarity_matrix)
spectral_ten(similarity_matrix)
```

Arguments

```
similarity_matrix
A similarity matrix.
```

Details

 spectral_eigen: Spectral clustering where the number of clusters is based on the eigen-gap heuristic 42 clust_fns_list

 spectral_rot: Spectral clustering where the number of clusters is based on the rotation-cost heuristic

• spectral_(C): Spectral clustering for a C-cluster solution.

Value

solution data A vector of cluster assignments

clust_fns_list

Build a clusteing algorithms list

Description

This function can be used to specify custom clustering algorithms to apply to the final similarity matrices produced by each run of the batch_snf function.

Usage

```
clust_fns_list(clust_fns = NULL, use_default_clust_fns = FALSE)
```

Arguments

If TRUE, prepend the base clustering algorithms (spectral_eigen and spectral_rot, which apply spectral clustering and use the eigen-gap and rotation cost heuristics respectively for determining the number of clusters in the graph) to clust fns.

Value

A list of clustering algorithm functions that can be passed into the batch_snf and generate_settings_list functions.

Examples

cocluster_density 43

cocluster_density

Density plot coclustering stability across subsampled data.

Description

This function creates a density plot that shows, for all pairs of observations that originally clustered together, the distribution of the the fractions that those pairs clustered together across subsampled data.

Usage

```
cocluster_density(cocluster_df)
```

Arguments

cocluster_df A data frame containing coclustering data for a single cluster solution. This object is generated by the calculate_coclustering function.

Value

Density plot (class "gg", "ggplot") of the distribution of coclustering across pairs and subsamples of the data.

Examples

```
# my_dl <- data_list(
# list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
# list(income, "household_income", "demographics", "continuous"),
# list(pubertal, "pubertal_status", "demographics", "continuous"),
# uid = "unique_id"
# )
#</pre>
```

44 cocluster_heatmap

```
# sc <- snf_config(my_dl, n_solutions = 5, max_k = 40)</pre>
# sol_df <- batch_snf(my_dl, sc)</pre>
#
# my_dl_subsamples <- subsample_dl(</pre>
      n_subsamples = 20,
      subsample\_fraction = 0.85
#)
# batch_subsample_results <- batch_snf_subsamples(</pre>
      my_dl_subsamples,
#
      sc,
#
      verbose = TRUE
#)
# coclustering_results <- calculate_coclustering(</pre>
      batch_subsample_results,
#
      sol_df,
      verbose = TRUE
#
#)
# cocluster_density(cocluster_dfs[[1]])
```

cocluster_heatmap

Heatmap of observation co-clustering across resampled data.

Description

Create a heatmap that shows the distribution of observation co-clustering across resampled data.

```
cocluster_heatmap(
  cocluster_df,
  cluster_rows = TRUE,
  cluster_columns = TRUE,
  show_row_names = FALSE,
  show_column_names = FALSE,
  dl = NULL,
  data = NULL,
  left_bar = NULL,
  right_bar = NULL,
  top_bar = NULL,
  bottom_bar = NULL,
  left_hm = NULL,
  right_hm = NULL,
  top_hm = NULL,
  bottom_hm = NULL,
```

cocluster_heatmap 45

```
annotation_colours = NULL,
min_colour = NULL,
max_colour = NULL,
...
)
```

Arguments

```
cocluster_df
                 A data frame containing coclustering data for a single cluster solution. This
                 object is generated by the calculate_coclustering function.
                 Argument passed to ComplexHeatmap::Heatmap().
cluster_rows
cluster_columns
                 Argument passed to ComplexHeatmap::Heatmap().
show_row_names Argument passed to ComplexHeatmap::Heatmap().
show_column_names
                 Argument passed to ComplexHeatmap::Heatmap().
d1
                 See ?similarity_matrix_heatmap.
                 See ?similarity_matrix_heatmap.
data
left_bar
                 See ?similarity_matrix_heatmap.
                 See ?similarity_matrix_heatmap.
right_bar
top_bar
                 See ?similarity_matrix_heatmap.
bottom_bar
                 See ?similarity_matrix_heatmap.
left_hm
                 See ?similarity_matrix_heatmap.
right_hm
                 See ?similarity matrix heatmap.
                 See ?similarity_matrix_heatmap.
top_hm
bottom_hm
                 See ?similarity_matrix_heatmap.
annotation colours
                 See ?similarity_matrix_heatmap.
min_colour
                 See ?similarity_matrix_heatmap.
max_colour
                 See ?similarity_matrix_heatmap.
                 Arguments passed to ComplexHeatmap::Heatmap().
```

Value

Heatmap (class "Heatmap" from ComplexHeatmap) object showing the distribution of observation co-clustering across resampled data.

Examples

```
# my_dl <- data_list(
# list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
# list(income, "household_income", "demographics", "continuous"),
# list(pubertal, "pubertal_status", "demographics", "continuous"),
# uid = "unique_id"</pre>
```

46 collapse_dl

```
#)
# sc <- snf_config(my_dl, n_solutions = 5, max_k = 40)</pre>
# sol_df <- batch_snf(my_dl, sc)</pre>
# my_dl_subsamples <- subsample_dl(</pre>
      my_dl,
      n_subsamples = 20,
#
#
      subsample_fraction = 0.85
# )
# batch_subsample_results <- batch_snf_subsamples(</pre>
      my_dl_subsamples,
#
      sc,
#
      verbose = TRUE
#)
#
# coclustering_results <- calculate_coclustering(</pre>
      batch_subsample_results,
      sol_df,
      verbose = TRUE
#
#)
# cocluster_dfs <- coclustering_results$"cocluster_dfs"</pre>
# cocluster_heatmap(
#
      cocluster_dfs[[1]],
      dl = my_dl,
#
      top_hm = list(
#
          "Income" = "household_income",
          "Pubertal Status" = "pubertal_status"
#
      annotation_colours = list(
          "Pubertal Status" = colour_scale(
              c(1, 4),
              min_colour = "black",
              max_colour = "purple"
          "Income" = colour_scale(
              c(0, 4),
              min_colour = "black",
              max_colour = "red"
#
          )
#
      )
# )
```

colour_scale 47

Description

[Deprecated] Defunct function for converting a data list into a data frame. Please use as.data.frame() instead.

Usage

```
collapse_dl(data_list)
```

Arguments

data_list A nested

A nested list of input data from generate_data_list().

Value

A "data.frame"-formatted version of the provided data list.

colour_scale

Return a colour ramp for a given vector

Description

Given a numeric vector and min and max colour values, return a colour ramp that assigns a colour to each element in the vector. This function is a wrapper for circlize::colorRamp2.'

Usage

```
colour_scale(data, min_colour, max_colour)
```

Arguments

data Vector of numeric values.

min_colour Minimum colour value.

max_colour Maximum colour value.

Value

A "function" class object that can build a circlize-style colour ramp.

48 config_heatmap

config_heatmap

Heatmap for visualizing an SNF config

Description

Create a heatmap where each row corresponds to a different set of hyperparameters in an SNF config object. Numeric parameters are scaled normalized and non-numeric parameters are added as heatmap annotations. Rows can be reordered to match prior meta clustering results.

Usage

```
config_heatmap(
  sc,
  order = NULL,
  hide_fixed = FALSE,
  show_column_names = TRUE,
  show_row_names = TRUE,
  rect_gp = grid::gpar(col = "black"),
  colour\_breaks = c(0, 1),
  colours = c("black", "darkseagreen"),
  column_split_vector = NULL,
  row_split_vector = NULL,
  column_split = NULL,
  row_split = NULL,
  column_title = NULL,
  include_weights = TRUE,
  include_settings = TRUE,
)
```

Arguments

An snf_config class object. sc Numeric vector indicating row ordering of SNF config. order hide_fixed Whether fixed parameters should be removed. show_column_names Whether show column names. show_row_names Whether show row names. Graphic parameters for drawing rectangles (for heatmap body). The value should rect_gp be specified by gpar and fill parameter is ignored. colour_breaks Numeric vector of breaks for the legend. colours Vector of colours to use for the heatmap. Should match the length of colour_breaks. column_split_vector Vector of indices to split columns by.

cort_sa 49

```
row_split_vector

Vector of indices to split rows by.

column_split Split on columns. For heatmap splitting, please refer to https://jokergoo.

github.io/ComplexHeatmap-reference/book/a-single-heatmap.html#heatmap-split

.

row_split Same as split.

column_title Title on the column.

include_weights

If TRUE, includes feature weights of the weights matrix into the config heatmap.

include_settings

If TRUE, includes columns from the settings data frame into the config heatmap.

Additional parameters passed to ComplexHeatmap::Heatmap.
```

Value

Returns a heatmap (class "Heatmap" from package ComplexHeatmap) that displays the scaled values of the provided SNF config.

Examples

```
dl <- data_list(
    list(income, "household_income", "demographics", "ordinal"),
    list(pubertal, "pubertal_status", "demographics", "continuous"),
    list(fav_colour, "favourite_colour", "demographics", "categorical"),
    list(anxiety, "anxiety", "behaviour", "ordinal"),
    list(depress, "depressed", "behaviour", "ordinal"),
    uid = "unique_id"
)

sc <- snf_config(
    dl,
    n_solutions = 10,
    dropout_dist = "uniform"
)</pre>
```

cort_sa

Mock ABCD cortical surface area data

Description

Like the mock data frame "abcd_cort_sa", but with "unique_id" as the "uid".

Usage

cort_sa

50 cort_t

Format

cort_sa:

A data frame with 188 rows and 152 columns:

unique_id The unique identifier of the ABCD dataset

... Cortical surface areas of various ROIs (mm², I think)

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

cort_t

Mock ABCD cortical thickness data

Description

Like the mock data frame "abcd_cort_t", but with "unique_id" as the "uid".

Usage

cort_t

Format

cort_t:

A data frame with 188 rows and 152 columns:

unique id The unique identifier of the ABCD dataset

... Cortical thicknesses of various ROIs (mm³, I think)

data_list 51

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

data_list

Build a data_list class object

Description

data_list() constructs a data list object which inherits from classes data_list and list. This object is the primary way in which features to be used along the metasnf clustering pipeline are stored. The data list is fundamentally a 2-level nested list object where each inner list contains a data frame and associated metadata for that data frame. The metadata includes the name of the data frame, the 'domain' of that data frame (the broader source of information that the input data frame is capturing, determined by user's domain knowledge), and the type of feature stored in the data frame (continuous, discrete, ordinal, categorical, or mixed).

Usage

```
data_list(..., uid)
```

Arguments

```
Any number of lists formatted as (df, "df_name", "df_domain", "df_type") and/or any number of lists of lists formatted as (df, "df_name", "df_domain", "df_type").

(character) the name of the uid column currently used data. data frame.
```

Examples

```
heart_rate_df <- data.frame(
   patient_id = c("1", "2", "3"),
   var1 = c(0.04, 0.1, 0.3),</pre>
```

52 data_list

```
var2 = c(30, 2, 0.3)
)
personality_test_df <- data.frame(</pre>
    patient_id = c("1", "2", "3"),
    var3 = c(900, 1990, 373),
    var4 = c(509, 2209, 83)
survey_response_df <- data.frame(</pre>
    patient_id = c("1", "2", "3"),
    var5 = c(1, 3, 3),
    var6 = c(2, 3, 3)
city_df <- data.frame(</pre>
    patient_id = c("1", "2", "3"),
    var7 = c("toronto", "montreal", "vancouver")
)
# Explicitly (Name each nested list element):
dl <- data_list(</pre>
    list(
        data = heart_rate_df,
        name = "heart_rate",
        domain = "clinical"
        type = "continuous"
    ),
    list(
        data = personality_test_df,
        name = "personality_test",
        domain = "surveys",
        type = "continuous"
    ),
    list(
        data = survey_response_df,
        name = "survey_response",
        domain = "surveys",
        type = "ordinal"
    ),
    list(
        data = city_df,
        name = "city",
        domain = "location",
        type = "categorical"
    ),
    uid = "patient_id"
)
# Compact loading
dl <- data_list(</pre>
    list(heart_rate_df, "heart_rate", "clinical", "continuous"),
    list(personality_test_df, "personality_test", "surveys", "continuous"),
```

depress 53

```
list(survey_response_df, "survey_response", "surveys", "ordinal"),
    list(city_df, "city", "location", "categorical"),
    uid = "patient_id"
)

# Printing data list summaries
summary(dl)

# Alternative loading: providing a single list of lists
list_of_lists <- list(
    list(heart_rate_df, "data1", "domain1", "continuous"),
    list(personality_test_df, "data2", "domain2", "continuous")
)

dl <- data_list(
    list_of_lists,
    uid = "patient_id"
)</pre>
```

depress

Mock ABCD depression data

Description

Like the mock data frame "abcd_depress", but with "unique_id" as the "uid".

Usage

depress

Format

depress:

A data frame with 275 rows and 2 columns:

unique_id The unique identifier of the ABCD dataset

cbcl_depress_r Ordinal value of impairment on CBCL anxiety, either 0 (no impairment), 1 (borderline clinical), or 2 (clinically impaired)

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987,

54 dist_fns

U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

diagnosis_df

Mock diagnosis data

Description

This is the same data as cancer_diagnosis_df, with renamed features and columns.

Usage

diagnosis_df

Format

diagnosis_df:

A data frame with 200 rows and 2 columns:

patient_id Random three-digit number uniquely identifying the patientdiagnosis Mock diagnosis feature

Source

This data came from the SNFtool package, with slight modifications.

dist_fns

Built-in distance functions

Description

These functions can be used when building a metasnf distance functions list. Each function converts a data frame into to a distance matrix.

dist_fns 55

Usage

```
euclidean_distance(df, weights_row)
gower_distance(df, weights_row)
sn_euclidean_distance(df, weights_row)
sew_euclidean_distance(df, weights_row)
hamming_distance(df, weights_row)
```

Arguments

df Data frame containing at least 1 data column

weights_row Single-row data frame where the column names contain the column names in df

and the row contains the corresponding weights_row.

Details

Functions that work for numeric data:

- euclidean_distance: typical Euclidean distance
- sn_euclidean_distance: Data frame is first standardized and normalized before typical Euclidean distance is applied
- siw_euclidean_distance: Squared (including weights) Euclidean distance, where the weights are also squared
- sew_euclidean_distance: Squared (excluding weights) Euclidean distance, where the weights are not also squared

Functions that work for binary data:

• hamming_distance: typical Hamming distance

Functions that work for any type of data:

• gower_distance: Gower distance (cluster::daisy)

Value

A matrix class object containing pairwise distances.

56 dist_fns_list

dist_fns_list

Build a distance metrics list

Description

The distance metrics list object (inherits classes dist_fns_list and list) is a list that stores R functions which can convert a data frame of features into a matrix of pairwise distances. The list is a nested one, where the first layer of the list can hold up to 5 items (one for each of the metasnf recognized feature types, continuous, discrete, ordinal, categorical, and mixed), and the second layer can hold an arbitrary number of distance functions for each of those types.

Usage

```
dist_fns_list(
  cnt_dist_fns = NULL,
  dsc_dist_fns = NULL,
  ord_dist_fns = NULL,
  cat_dist_fns = NULL,
  mix_dist_fns = NULL,
  automatic_standard_normalize = FALSE,
  use_default_dist_fns = FALSE
)
```

Arguments

```
cnt_dist_fns A named list of continuous distance metric functions.

dsc_dist_fns A named list of discrete distance metric functions.

ord_dist_fns A named list of ordinal distance metric functions.

cat_dist_fns A named list of categorical distance metric functions.

mix_dist_fns A named list of mixed distance metric functions.

automatic_standard_normalize
```

If TRUE, will automatically use standard normalization prior to calculation of any numeric distances. This parameter overrides all other distance functions list-related parameters.

```
use_default_dist_fns
```

If TRUE, prepend the base distance metrics (euclidean distance for continuous, discrete, and ordinal data and gower distance for categorical and mixed data) to the resulting distance metrics list.

Details

Call ?distance_metrics to see all distance metric functions provided in metasnf.

Value

A distance metrics list object.

dlapply 57

Examples

```
# Using just the base distance metrics ------
dist_fns_list <- dist_fns_list()</pre>
# Adding your own metrics ------
# This will contain only the and user-provided distance function:
cubed_euclidean <- function(df, weights_row) {</pre>
   # (your code that converts a data frame to a distance metric here...)
   weights <- diag(weights_row, nrow = length(weights_row))</pre>
   weighted_df <- as.matrix(df) %*% weights</pre>
   distance_matrix <- weighted_df |>
       stats::dist(method = "euclidean") |>
       as.matrix()
   distance_matrix <- distance_matrix^3</pre>
   return(distance_matrix)
}
dist_fns_list <- dist_fns_list(</pre>
   cnt_dist_fns = list(
        "my_cubed_euclidean" = cubed_euclidean
   )
)
# Using default base metrics------
# Call ?distance_metrics to see all distance metric functions provided in
# metasnf. The code below will contain a mix of user-provided and built-in
# distance metric functions.
dist_fns_list <- dist_fns_list(</pre>
   cnt_dist_fns = list(
        "my_distance_metric" = cubed_euclidean
   dsc_dist_fns = list(
        "my_distance_metric" = cubed_euclidean
   ),
   ord_dist_fns = list(
        "my_distance_metric" = cubed_euclidean
   ),
   cat_dist_fns = list(
        "my_distance_metric" = gower_distance
   mix_dist_fns = list(
        "my_distance_metric" = gower_distance
   ),
   use_default_dist_fns = TRUE
)
```

Description

This function enables manipulating a data_list class object with lapply syntax without removing that object's data_list class attribute. The function will only preserve this attribute if the result of the apply call has a valid data list structure.

Usage

```
dlapply(X, FUN, ...)
```

Arguments

X A data_list class object.

FUN The function to be applied to each data list component.

... Optional arguments to FUN.

Value

If FUN applied to each component of X yields a valid data list, a data list. Otherwise, a list.

Examples

```
# Convert all UID values to lowercase
dl <- data_list(
    list(abcd_income, "income", "demographics", "discrete"),
    list(abcd_colour, "colour", "likes", "categorical"),
    uid = "patient"
)

dl_lower <- dlapply(
    dl,
    function(x) {
        x$"data"$"uid" <- tolower(x$"data"$"uid")
        return(x)
    }
)</pre>
```

dl_variable_summary

Variable-level summary of a data list

Description

[**Deprecated**] Defunct function to summarize a data list. Please use summary() with argument scope = "feature" instead.

```
dl_variable_summary(dl)
```

Arguments

dl

A nested list of input data from data_list().

Value

variable_level_summary A data frame containing the name, type, and domain of every variable in a data list.

```
dplyr_row_slice.ext_solutions_df
```

Function to extend dplyr to extended solutions data frame objects

Description

Function to extend dplyr to extended solutions data frame objects

Usage

```
dplyr_row_slice.ext_solutions_df(data, i, ...)
```

Arguments

data An extended solutions data frame.

i A vector of row indices.

... Additional arguments.

Value

Row sliced object with appropriately preserved attributes.

```
dplyr_row_slice.solutions_df
```

Function to extend dplyr to solutions data frame objects

Description

Function to extend dplyr to solutions data frame objects

```
dplyr_row_slice.solutions_df(data, i, ...)
```

60 esm_manhattan_plot

Arguments

data A solutions data frame.i A vector of row indices.... Additional arguments.

Value

Row sliced object with appropriately preserved attributes.

esm_manhattan_plot

Manhattan plot of feature-cluster association p-values

Description

Manhattan plot of feature-cluster association p-values

Usage

```
esm_manhattan_plot(
   esm,
   neg_log_pval_thresh = 5,
   threshold = NULL,
   point_size = 5,
   jitter_width = 0.1,
   jitter_height = 0.1,
   text_size = 15,
   plot_title = NULL,
   hide_x_labels = FALSE,
   bonferroni_line = FALSE
)
```

Arguments

Extended solutions data frame storing associations between features and cluster

assignments. See ?extend_solutions.

neg_log_pval_thresh

Threshold for negative log p-values.

threshold P-value threshold to plot dashed line at.

point_size Size of points in the plot.

jitter_width Width of jitter. jitter_height Height of jitter.

text_size Size of text in the plot.

plot_title Title of the plot.

hide_x_labels If TRUE, hides x-axis labels.

bonferroni_line

If TRUE, plots a dashed black line at the Bonferroni-corrected equivalent of the p-value threshold.

Value

A Manhattan plot (class "gg", "ggplot") showing the association p-values of features against each solution in the provided solutions data frame.

Examples

```
# full_dl <- data_list(</pre>
      list(subc\_v, \ "subcortical\_volume", \ "neuroimaging", \ "continuous"),\\
      list(income, "household_income", "demographics", "continuous"),
      list(pubertal, "pubertal_status", "demographics", "continuous"),
      list(anxiety, "anxiety", "behaviour", "ordinal"),
      list(depress, "depressed", "behaviour", "ordinal"),
      uid = "unique_id"
#)
# dl <- full_dl[1:3]
# target_dl <- full_dl[4:5]</pre>
# set.seed(42)
# sc <- snf_config(</pre>
#
      dl = dl,
#
      n_solutions = 20,
#
      min_k = 20,
      max_k = 50
# )
# sol_df <- batch_snf(dl, sc)</pre>
# ext_sol_df <- extend_solutions(</pre>
#
      sol_df,
#
      dl = dl,
      target = target_dl,
      min_pval = 1e-10 # p-values below 1e-10 will be thresholded to 1e-10
#
#)
#
# esm_manhattan <- esm_manhattan_plot(</pre>
      ext_sol_df[1:5, ],
      neg_log_pval_thresh = 5,
     threshold = 0.05,
      point_size = 3,
      jitter_width = 0.1,
      jitter_height = 0.1,
      plot_title = "Feature-Solution Associations",
      text_size = 14,
#
      bonferroni_line = TRUE
# )
```

estimate_nclust_given_graph

Estimate number of clusters for a similarity matrix

62 expression_df

Description

Calculate eigengap and rotation-cost estimates of the number of clusters to use when clustering a similarity matrix. This function was adapted from SNFtool::estimateClustersGivenGraph, but scales up the Laplacian operator prior to eigenvalue calculations to minimize the risk of floating point-related errors.

Usage

```
estimate_nclust_given_graph(W, NUMC = 2:10)
```

Arguments

W Similarity matrix to calculate number of clusters for.

NUMC Range of cluster counts to consider among when picking best number of clus-

ters.

Value

A list containing the top two eigengap and rotation-cost estimates for the number of clusters in a given similarity matrix.

Examples

```
input_dl <- data_list(
    list(gender_df, "gender", "demographics", "categorical"),
    list(diagnosis_df, "diagnosis", "clinical", "categorical"),
    uid = "patient_id"
)

sc <- snf_config(input_dl, n_solutions = 1)
sol_df <- batch_snf(input_dl, sc, return_sim_mats = TRUE)
sim_mat <- sim_mats_list(sol_df)[[1]]
estimate_nclust_given_graph(sim_mat)</pre>
```

expression_df

Modification of SNFtool mock data frame "Data1"

Description

Modification of SNFtool mock data frame "Data1"

```
expression_df
```

extend_solutions 63

Format

```
expression_df:
A data frame with 200 rows and 3 columns:
gene_1_expression Mock gene expression feature
gene_2_expression Mock gene expression feature
patient_id Random three-digit number uniquely identifying the patient
```

Source

This data came from the SNFtool package, with slight modifications.

extend_solutions

Extend a solutions data frame to include outcome evaluations

Description

Extend a solutions data frame to include outcome evaluations

Usage

```
extend_solutions(
  sol_df,
  target_dl = NULL,
  dl = NULL,
  cat_test = "chi_squared",
  min_pval = 1e-10,
  processes = 1,
  verbose = FALSE
)
```

Arguments

sol_df	Result of batch_snf storing cluster solutions and the settings that were used to generate them.
target_dl	A data list with features to calculate p-values for. Features in the target list will be included during p-value summary measure calculations.
dl	A data list with features to calcualte p-values for, but that should not be incorporated into p-value summary measure columns (i.e., min/mean/max p-value columns).
cat_test	String indicating which statistical test will be used to associate cluster with a categorical feature. Options are "chi_squared" for the Chi-squared test and "fisher_exact" for Fisher's exact test.
min_pval	If assigned a value, any p-value less than this will be replaced with this value.
processes	The number of processes to use for parallelization. Progress is only reported for sequential processing (processes $= 1$).
verbose	If TRUE, output progress to console.

64 fav_colour

Value

An extended solutions data frame (ext_sol_df class object) that contains p-value columns for each outcome in the provided data lists

Examples

```
input_dl <- data_list(
    list(gender_df, "gender", "demographics", "categorical"),
    list(diagnosis_df, "diagnosis", "clinical", "categorical"),
    uid = "patient_id"
)

sc <- snf_config(input_dl, n_solutions = 2)

sol_df <- batch_snf(input_dl, sc)

ext_sol_df <- extend_solutions(sol_df, input_dl)</pre>
```

fav_colour

Mock ABCD "colour" data

Description

Like the mock data frame "abcd_colour", but with "unique_id" as the "uid".

Usage

fav_colour

Format

fav_colour:

A data frame with 275 rows and 2 columns:

unique_id The unique identifier of the ABCD dataset
colour Categorical transformation of cbcl_depress.

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988,

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U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

features

Return character vector of features stored in an object

Description

Return character vector of features stored in an object

Usage

features(x)

Arguments

Х

The object to pull features from.

Value

A character vector of features in x.

gender_df

Mock gender data

Description

Mock gender data

Usage

gender_df

Format

```
gender_df:
```

A data frame with 200 rows and 2 columns:

patient_id Random three-digit number uniquely identifying the patient
gender_df Mock gene methylation feature

Source

This data came from the SNFtool package, with slight modifications.

```
generate_clust_algs_list
```

Generate a clustering algorithms list

Description

[**Deprecated**] Deprecated function for building a clustering algorithms list. Please use clust_fns_list() (or better yet, snf_config()) instead.

Usage

```
generate_clust_algs_list(..., disable_base = FALSE)
```

Arguments

... An arbitrary number of named clustering functions

spectral_rot, which apply spectral clustering and use the eigen-gap and rotation cost heuristics respectively for determining the number of clusters in the

graph.

Value

A list of clustering algorithm functions that can be passed into the batch_snf and generate_settings_list functions.

```
generate_distance_metrics_list
```

Generate a list of distance metrics

Description

[**Deprecated**] Deprecated function for building a distance metrics list. Please use dist_fns_list() (or better yet, snf_config()) instead.

```
generate_distance_metrics_list(
  continuous_distances = NULL,
  discrete_distances = NULL,
  ordinal_distances = NULL,
  categorical_distances = NULL,
  mixed_distances = NULL,
  keep_defaults = TRUE
)
```

Arguments

continuous_distances

A named list of distance metric functions

discrete_distances

A named list of distance metric functions

ordinal_distances

A named list of distance metric functions

categorical_distances

A named list of distance metric functions

mixed_distances

A named list of distance metric functions

If TRUE (default), prepend the base distance metrics (euclidean and standard

normalized euclidean)

Value

A nested and named list of distance metrics functions.

```
generate_settings_matrix
```

Build a settings data frame

Description

 $[\textbf{Deprecated}] \ \ \textbf{Deprecated function for building a settings matrix}. \ \ \textbf{Please use settings_df() instead}.$

Usage

```
generate_settings_matrix(...)
```

Arguments

... Arguments used to generate a settings matrix.

Value

Raises a deprecated error.

68 get_cluster_df

	-		
get	cI	uste	rs

Extract cluster membership vector from one solutions data frame row

Description

[**Deprecated**] Deprecated function for building extracting cluster solutions from a solutions data frame. Please use t() instead.

This function takes in a single row of a solutions data frame and returns a vector containing the cluster assignments for each observation. It is similar to get_cluster_df(), which takes a solutions data frame with only one row and returns a data frame with two columns: "cluster" and "uid" '(the UID of the observation) and get_cluster_solutions(), which takes a solutions data frame with any number of rows and returns a data frame indicating the cluster assignments for each of those rows.

Usage

```
get_clusters(sol_df_row)
```

Arguments

sol_df_row Output matrix row.

Value

clusters Vector of assigned clusters.

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get_		ust	C1 _	_uı

Extract cluster membership information from one solutions data frame row

Description

[**Deprecated**] Deprecated function for building extracting cluster solutions from a solutions data frame. Please use t() instead.

This function takes in a single row of a solutions data frame and returns a data frame containing the cluster assignments for each uid. It is similar to get_clusters(), which takes one solutions data frame row and returns a vector of cluster assignments' and get_cluster_solutions(), which takes a solutions data frame with any number of rows and returns a data frame indicating the cluster assignments for each of those rows.

```
get_cluster_df(sol_df_row)
```

get_cluster_solutions 69

Arguments

sol_df_row One row from a solutions data frame.

Value

cluster_df data frame of cluster and uid.

get_cluster_solutions Extract cluster membership information from a sol_df

Description

[**Deprecated**] Deprecated function for building extracting cluster solutions from a solutions data frame. Please use t() instead.

This function takes in a solutions data frame and returns a data frame containing the cluster assignments for each uid. It is similar to 'get_clusters(), which takes one solutions data frame row and returns a vector of cluster assignments' and get_cluster_df(), which takes a solutions matrix with only one row and returns a data frame with two columns: "cluster" and "uid" (the UID of the observation).

Usage

```
get_cluster_solutions(sol_df)
```

Arguments

sol_df A sol df.

Value

A "data.frame" object where each row is an observation and each column (apart from the uid column) indicates the cluster that observation was assigned to for the corresponding solutions data frame row.

get_complete_uids

Pull complete-data UIDs from a list of data frames

Description

This function identifies all observations within a list of data frames that have no missing data across all data frames. This function is useful when constructing data lists of distinct feature sets from the same sample of observations. As data_list() strips away observations with any missing data, distinct sets of observations may be generated by building a data list from the same group of observations over different sets of features. Reducing the pool of observations to only those with complete UIDs first will avoid downstream generation of data lists of differing sizes.

70 get_dl_uids

Usage

```
get_complete_uids(list_of_dfs, uid)
```

Arguments

list_of_dfs List of data frames.

Name of column across data frames containing UIDs

Value

A character vector of the UIDs of observations that have complete data across the provided list of data frames.

Examples

```
complete_uids <- get_complete_uids(</pre>
    list(income, pubertal, anxiety, depress),
    uid = "unique_id"
)
income <- income[income$"unique_id" %in% complete_uids, ]</pre>
pubertal <- pubertal[pubertal$"unique_id" %in% complete_uids, ]</pre>
anxiety <- anxiety[anxiety$"unique_id" %in% complete_uids, ]</pre>
depress <- depress[depress$"unique_id" %in% complete_uids, ]</pre>
input_dl <- data_list(</pre>
    list(income, "income", "demographics", "ordinal"),
   list(pubertal, "pubertal", "demographics", "continuous"),
   uid = "unique_id"
)
target_dl <- data_list(</pre>
   list(anxiety, "anxiety", "behaviour", "ordinal"),
   list(depress, "depressed", "behaviour", "ordinal"),
   uid = "unique_id"
)
```

get_dl_uids

Extract UIDs from a data list

Description

[Deprecated] Deprecated function for extracting UIDs from a data list. Please use uids() instead.

```
get_dl_uids(dl, prefix = FALSE)
```

get_heatmap_order 71

Arguments

dl A nested list of input data from data_list().

prefix If TRUE, preserves the "uid_" prefix added to UIDs when creating a data list.

Value

A character vector of the UID labels contained in a data list.

get_heatmap_order

Return the row or column ordering present in a heatmap

Description

Return the row or column ordering present in a heatmap

Usage

```
get_heatmap_order(heatmap, type = "rows")
```

Arguments

heatmap A heatmap object to collect ordering from.

type The type of ordering to return. Either "rows" or "columns".

Value

A numeric vector of the ordering used within the provided ComplexHeatmap "Heatmap" object.

get_matrix_order

Return the hierarchical clustering order of a matrix

Description

Return the hierarchical clustering order of a matrix

```
get_matrix_order(matrix, dist_method = "euclidean", hclust_method = "complete")
```

72 get_matrix_order

Arguments

matrix Matrix to cluster.

dist_method Distance method to use when calculating sorting order to of the matrix. Argument is directly passed into stats::dist. Options include "euclidean", "maximum", "manhattan", "canberra", "binary", or "minkowski".

hclust_method Agglomerative method to use when calculating sorting order by stats::hclust. Options include "ward.D", "ward.D2", "single", "complete", "average", "mcquitty", "median", or "centroid".

Value

A numeric vector of the ordering derivied by the specified hierarchical clustering method applied to the provided matrix.

Examples

```
# dl <- data_list(</pre>
       list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
       list(income, "household_income", "demographics", "continuous"),
list(pubertal, "pubertal_status", "demographics", "continuous"),
#
       list(anxiety, "anxiety", "behaviour", "ordinal"),
list(depress, "depressed", "behaviour", "ordinal"),
       uid = "unique_id"
# )
#
# sc <- snf_config(</pre>
       dl = dl,
       n_solutions = 20,
       min_k = 20,
       max_k = 50
#)
# sol_df <- batch_snf(dl, sc)</pre>
# ext_sol_df <- extend_solutions(</pre>
#
       sol_df,
#
       dl = dl,
#
       min_pval = 1e-10 # p-values below 1e-10 will be thresholded to 1e-10
#)
# # Calculate pairwise similarities between cluster solutions
# sol_aris <- calc_aris(sol_df)</pre>
# # Extract hierarchical clustering order of the cluster solutions
# meta_cluster_order <- get_matrix_order(sol_aris)</pre>
```

get_pvals 73

get_pvals

Get p-values from an extended solutions data frame

Description

This function can be used to neatly format the p-values associated with an extended solutions data frame. It can also calculate the negative logs of those p-values to make it easier to interpret large-scale differences.

Usage

```
get_pvals(ext_sol_df, negative_log = FALSE, keep_summaries = TRUE)
```

Arguments

ext_sol_df The output of extend_solutions. A data frame that contains at least one p-

value column ending in "_pval".

keep_summaries If FALSE, will remove the mean, min, and max p-value.

Value

A "data.frame" class object Of only the p-value related columns of the provided ext_sol_df.

```
get_representative_solutions
```

Extract representative solutions from a matrix of ARIs

Description

Following clustering with batch_snf, a matrix of pairwise ARIs that show how related each cluster solution is to each other can be generated by the calc_aris function. Partitioning of the ARI matrix can be done by visual inspection of meta_cluster_heatmap() results or by shiny_annotator. Given the indices of meta cluster boundaries, this function will return a single representative solution from each meta cluster based on maximum average ARI to all other solutions within that meta cluster.

Usage

```
get_representative_solutions(aris, sol_df, filter_fn = NULL)
```

Arguments

aris Matrix of adjusted rand indices from calc_aris() sol_df Output of batch_snf containing cluster solutions.

filter_fn Optional function to filter the meta-cluster by prior to maximum average ARI determination. This can be useful if you are explicitly trying to select a solution that meets a certain condition, such as only picking from the 4 cluster solutions within a meta cluster. An example valid function could be $fn <- function(x) \times [x\$"nclust" == 4,].$

Value

The provided solutions data frame reduced to just one row per meta cluster defined by the split vector.

Examples

```
# dl <- data_list(</pre>
      list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
      list(income, "household_income", "demographics", "continuous"),
list(pubertal, "pubertal_status", "demographics", "continuous"),
      list(anxiety, "anxiety", "behaviour", "ordinal"),
#
      list(depress, "depressed", "behaviour", "ordinal"),
#
      uid = "unique_id"
# )
#
# sc <- snf_config(</pre>
      dl = dl,
      n_solutions = 20,
      min_k = 20,
      max_k = 50
# )
# sol_df <- batch_snf(dl, sc)</pre>
# ext_sol_df <- extend_solutions(</pre>
#
      sol_df,
#
      dl = dl,
      min_pval = 1e-10 # p-values below 1e-10 will be thresholded to 1e-10
#
#)
# # Calculate pairwise similarities between cluster solutions
# sol_aris <- calc_aris(sol_df)</pre>
# # Extract hierarchical clustering order of the cluster solutions
# meta_cluster_order <- get_matrix_order(sol_aris)</pre>
# # Identify meta cluster boundaries with shiny app or trial and error
# # ari_hm <- meta_cluster_heatmap(sol_aris, order = meta_cluster_order)
# # shiny_annotator(ari_hm)
# # Result of meta cluster examination
```

income 75

```
# split_vec <- c(2, 5, 12, 17)
#
# ext_sol_df <- label_meta_clusters(ext_sol_df, split_vec, meta_cluster_order)
#
# Extracting representative solutions from each defined meta cluster
# rep_solutions <- get_representative_solutions(sol_aris, ext_sol_df)</pre>
```

income

Mock ABCD income data

Description

Like the mock data frame "abcd_h_income", but with "unique_id" as the "uid".

Like the mock data frame "abcd_cort_sa", but with "unique_id" as the "uid".

Usage

income

income

Format

income:

A data frame with 300 rows and 2 columns:

unique id The unique identifier of the ABCD dataset

household_income Household income in 3 category levels (low = 1, medium = 2, high = 3)

income:

A data frame with 300 rows and 2 columns:

unique_id The unique identifier of the ABCD dataset

household income Household income in 3 category levels (low = 1, medium = 2, high = 3)

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148,

76 is_data_list

U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

is_data_list

Test if the object is a data list

Description

Given an object, returns TRUE if that object inherits from the data_list class.

Usage

is_data_list(x)

Arguments

х

An object.

Value

TRUE if the object inherits from the data_list class.

jitter_plot 77

jitter_plot Jitter plot separating a feature by	cluster
---	---------

Description

Jitter plot separating a feature by cluster

Usage

```
jitter_plot(df, feature)
```

Arguments

df A data.frame containing cluster column and the feature to plot.

feature The feature to plot.

Value

A jitter+violin plot (class "gg", "ggplot") showing the distribution of a feature across clusters.

label_meta_clusters Assign meta cluster labels to rows of a solutions data frame or extended solutions data frame

Description

Given a solutions data frame or extended solutions data frame class object and a numeric vector indicating which rows correspond to which meta clusters, assigns meta clustering information to the "meta_clusters" attribute of the data frame.

Usage

```
label_meta_clusters(sol_df, split_vector, order = NULL)
```

Arguments

sol_df	A solutions data frame or extended solutions data frame to assign meta clus	sters
301_u1		

to.

split_vector A numeric vector indicating which rows of sol_df should be the split points for

meta cluster labeling.

order An optional numeric vector indicating how the solutions data frame should be

reordered prior to meta cluster labeling. This vector can be obtained by running get_matrix_order() on an ARI matrix, which itself can be obtained by calling

calc_aris() on a solutions data frame.

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Value

A solutions data frame with a populated "meta_clusters" attribute.

Examples

```
#dl <- data_list(</pre>
    list(cort_sa, "cortical_surface_area", "neuroimaging", "continuous"),
    list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
    list(income, "household_income", "demographics", "continuous"),
    list(pubertal, "pubertal_status", "demographics", "continuous"),
    uid = "unique_id"
#
#)
#set.seed(42)
#my_sc <- snf_config(</pre>
    dl = dl,
    n_solutions = 20,
    min_k = 20,
#
    max_k = 50
#)
#sol_df <- batch_snf(dl, my_sc)</pre>
#sol_df
#sol_aris <- calc_aris(sol_df)</pre>
#meta_cluster_order <- get_matrix_order(sol_aris)</pre>
## `split_vec` found by iteratively plotting ari_hm or by ?shiny_annotator()
#split_vec <- c(6, 10, 16)
#ari_hm <- meta_cluster_heatmap(</pre>
     sol_aris,
     order = meta_cluster_order,
#
     split_vector = split_vec
#)
#
#mc_sol_df <- label_meta_clusters(</pre>
#
    sol_df,
#
    order = meta_cluster_order,
#
     split_vector = split_vec
#)
#mc_sol_df
```

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Description

Given a solutions data frame containing clustered observations and a data list containing those clustered observations as well as additional to-be-clustered observations, this function will re-run SNF to generate a similarity matrix of all observations and use the label propagation algorithm to assigned predicted clusters to the unclustered observations.

Usage

```
label_propagate(partial_sol_df, full_dl, verbose = FALSE)
```

Arguments

```
partial_sol_df A solutions data frame derived from the training set.

full_dl A data list containing observations from both the training and testing sets.

verbose If TRUE, output progress to console.
```

Value

A data frame with one row per observation containing a column for UIDs, a column for whether the observation was in the train (original) or test (held out) set, and one column per row of the solutions data frame indicating the original and propagated clusters.

Examples

```
## Function to identify obervations with complete data
#uids_with_complete_obs <- get_complete_uids(</pre>
     list(subc_v, income, pubertal, anxiety, depress),
     uid = "unique_id"
#
#)
## Dataframe assigning 80% of observations to train and 20% to test
#train_test_split <- train_test_assign(</pre>
     train_frac = 0.8,
     uids = uids_with_complete_obs
#
#)
## Pulling the training and testing observations specifically
#train_obs <- train_test_split$"train"</pre>
#test_obs <- train_test_split$"test"</pre>
## Partition a training set
#train_subc_v <- subc_v[subc_v$"unique_id" %in% train_obs, ]</pre>
#train_income <- income[income$"unique_id" %in% train_obs, ]</pre>
#train_pubertal <- pubertal[pubertal$"unique_id" %in% train_obs, ]</pre>
#train_anxiety <- anxiety[anxiety$"unique_id" %in% train_obs, ]</pre>
#train_depress <- depress[depress$"unique_id" %in% train_obs, ]</pre>
## Partition a test set
#test_subc_v <- subc_v[subc_v$"unique_id" %in% test_obs, ]</pre>
#test_income <- income[income$"unique_id" %in% test_obs, ]</pre>
```

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```
#test_pubertal <- pubertal[pubertal$"unique_id" %in% test_obs, ]</pre>
#test_anxiety <- anxiety[anxiety$"unique_id" %in% test_obs, ]</pre>
#test_depress <- depress[depress$"unique_id" %in% test_obs, ]</pre>
## Find cluster solutions in the training set
#train_dl <- data_list(</pre>
     list(train_subc_v, "subc_v", "neuroimaging", "continuous"),
     list(train_income, "household_income", "demographics", "continuous"),
    list(train_pubertal, "pubertal_status", "demographics", "continuous"),
     uid = "unique_id"
#)
## We'll pick a solution that has good separation over our target features
#train_target_dl <- data_list(</pre>
    list(train_anxiety, "anxiety", "behaviour", "ordinal"),
#
#
     list(train_depress, "depressed", "behaviour", "ordinal"),
#
    uid = "unique_id"
#)
#
#sc <- snf_config(</pre>
    train_dl,
    n_solutions = 5,
    min_k = 10,
    max_k = 30
#
#)
#train_sol_df <- batch_snf(</pre>
#
    train_dl,
#
    sc,
#
     return_sim_mats = TRUE
#)
#
#ext_sol_df <- extend_solutions(</pre>
    train_sol_df,
     train_target_dl
#)
## Determining solution with the lowest minimum p-value
#lowest_min_pval <- min(ext_sol_df$"min_pval")</pre>
#which(ext_sol_df$"min_pval" == lowest_min_pval)
#top_row <- ext_sol_df[1, ]</pre>
#
## Propagate that solution to the observations in the test set
## data list below has both training and testing observations
#full_dl <- data_list(</pre>
     list(subc_v, "subc_v", "neuroimaging", "continuous"),
     list(income, "household_income", "demographics", "continuous"),
    list(pubertal, "pubertal_status", "demographics", "continuous"),
#
    uid = "unique_id"
#)
## Use the solutions data frame from the training observations and the data list
## from the training and testing observations to propagate labels to the test observations
```

linear_adjust 81

```
#propagated_labels <- label_propagate(top_row, full_dl)
#
#propagated_labels_all <- label_propagate(ext_sol_df, full_dl)
#
#head(propagated_labels_all)
#tail(propagated_labels_all)</pre>
```

linear_adjust

Linearly correct data list by features with unwanted signal

Description

Given a data list to correct and another data list of categorical features to linearly adjust for, corrects the first data list based on the residuals of the linear model relating the numeric features in the first data list to the unwanted signal features in the second data list.

Usage

```
linear_adjust(dl, unwanted_signal_list, sig_digs = NULL)
```

Arguments

dl A nested list of input data from data_list(). unwanted_signal_list

A data list of categorical features that should have their mean differences removed in the first data list.

sig_digs

Number of significant digits to round the residuals to.

Value

A data list ("list") in which each data component has been converted to contain residuals off of the linear model built against the features in the unwanted_signal_list.

Examples

```
has_tutor <- sample(c(1, 0), size = 9, replace = TRUE)
math_score <- 70 + 30 * has_tutor + rnorm(9, mean = 0, sd = 5)

math_df <- data.frame(uid = paste0("id_", 1:9), math = math_score)
tutor_df <- data.frame(uid = paste0("id_", 1:9), tutor = has_tutor)

dl <- data_list(
    list(math_df, "math_score", "school", "continuous"),
    uid = "uid"
)

adjustment_dl <- data_list(
    list(tutor_df, "tutoring", "school", "categorical"),
    uid = "uid"</pre>
```

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```
)
adjusted_dl <- linear_adjust(dl, adjustment_dl)
adjusted_dl[[1]]$"data"$"math"
# Equivalent to:
as.numeric(resid(lm(math_score ~ has_tutor)))</pre>
```

mc_manhattan_plot

Manhattan plot of feature-meta cluster association p-values

Description

Given a data frame of representative meta cluster solutions (see get_representative_solutions(), returns a Manhattan plot for showing feature separation across all features in provided data/target lists.

Usage

```
mc_manhattan_plot(
  ext_sol_df,
  dl = NULL,
  target_dl = NULL,
  variable_order = NULL,
  neg_log_pval_thresh = 5,
  threshold = NULL,
  point_size = 5,
  text_size = 20,
  plot_title = NULL,
  xints = NULL,
  hide_x_labels = FALSE,
  domain_colours = NULL
)
```

Arguments

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```
text_size Size of text in the plot.

plot_title Title of the plot.

xints Either "outcomes" or a vector of numeric values to plot vertical lines at.

hide_x_labels If TRUE, hides x-axis labels.

domain_colours Named vector of colours for domains.
```

Value

A Manhattan plot (class "gg", "ggplot") showing the association p-values of features against each solution in the provided solutions data frame, stratified by meta cluster label.

Examples

```
# dl <- data_list(</pre>
      list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
      list(income, "household_income", "demographics", "continuous"),
      list(pubertal, "pubertal_status", "demographics", "continuous"),
#
      list(anxiety, "anxiety", "behaviour", "ordinal"),
list(depress, "depressed", "behaviour", "ordinal"),
      uid = "unique_id"
# )
#
# sc <- snf_config(</pre>
      dl = dl,
#
      n_solutions = 20,
      min_k = 20,
      max_k = 50
#)
# sol_df <- batch_snf(dl, sc)</pre>
# ext_sol_df <- extend_solutions(</pre>
#
      sol_df,
      dl = dl,
#
#
      min_pval = 1e-10 # p-values below 1e-10 will be thresholded to 1e-10
#)
# # Calculate pairwise similarities between cluster solutions
# sol_aris <- calc_aris(sol_df)</pre>
# # Extract hierarchical clustering order of the cluster solutions
# meta_cluster_order <- get_matrix_order(sol_aris)</pre>
# # Identify meta cluster boundaries with shiny app or trial and error
# # ari_hm <- meta_cluster_heatmap(sol_aris, order = meta_cluster_order)
# # shiny_annotator(ari_hm)
# # Result of meta cluster examination
# split_vec <- c(2, 5, 12, 17)
# ext_sol_df <- label_meta_clusters(ext_sol_df, split_vec, meta_cluster_order)</pre>
```

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```
# # Extracting representative solutions from each defined meta cluster
# rep_solutions <- get_representative_solutions(sol_aris, ext_sol_df)
#
# mc_manhattan <- mc_manhattan_plot(
# rep_solutions,
# dl = dl,
# point_size = 3,
# text_size = 12,
# plot_title = "Feature-Meta Cluster Associations",
# threshold = 0.05,
# neg_log_pval_thresh = 5
# )
#
# mc_manhattan</pre>
```

merge.data_list

Merge observations between two compatible data lists

Description

Join two data lists with the same components (data frames) but separate observations. To instead merge two data lists that have the same observations but different components, simply use c().

Usage

```
## S3 method for class 'data_list'
merge(x, y, ...)
```

Arguments

x The first data list to merge.

y The second data list to merge.

. . . Additional arguments passed into merge function.

Value

A data list ("list"-class object) containing the observations of both provided data lists.

merge.snf_config 85

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merge.	. snt	config

Merge method for SNF config objects

Description

Merge method for SNF config objects

Usage

```
## S3 method for class 'snf_config'
merge(x, y, reset_indices = TRUE, ...)
```

Arguments

x SNF config to merge.y SNF config to merge.

reset_indices If TRUE (default), re-labels the "solutions" indices in the config from 1 to the

number of defined settings.

... Additional arguments passed into merge function.

Value

An SNF config combining the rows of both prior configurations.

merge_df_list

Merge list of data frames into a single data frame

Description

This helper function combines all data frames in a single-level list into a single data frame.

Usage

```
merge_df_list(df_list, join = "inner", uid = "uid", no_na = FALSE)
```

Arguments

df_list list of data frames.

join String indicating if join should be "inner" or "full".

uid Column name to join on. Default is "uid".

no_na Whether to remove NA values from the merged data frame.

Value

Inner join of all data frames in list.

Examples

```
merge_df_list(list(income, pubertal), uid = "unique_id")
```

Description

Heatmap of pairwise adjusted rand indices between solutions

Usage

```
meta_cluster_heatmap(
    aris,
    order = NULL,
    cluster_rows = FALSE,
    cluster_columns = FALSE,
    log_graph = FALSE,
    scale_diag = "none",
    min_colour = "#282828",
    max_colour = "firebrick2",
    col = circlize::colorRamp2(c(min(aris), max(aris)), c(min_colour, max_colour)),
    ...
)
```

Arguments

aris	Matrix of adjusted rand indices from calc_aris()
order	Numeric vector containing row order of the heatmap.
<pre>cluster_rows cluster_column</pre>	Whether rows should be clustered.
	Whether columns should be clustered.
log_graph	If TRUE, log transforms the graph.
scale_diag	Method of rescaling matrix diagonals. Can be "none" (don't change diagonals), "mean" (replace diagonals with average value of off-diagonals), or "zero" (replace diagonals with 0).
min_colour	Colour used for the lowest value in the heatmap.
max_colour	Colour used for the highest value in the heatmap.
col	Colour ramp to use for the heatmap.
•••	Additional parameters passed to similarity_matrix_heatmap(), the function that this function wraps.

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Value

Returns a heatmap (class "Heatmap" from package ComplexHeatmap) that displays the pairwise adjusted Rand indices (similarities) between the cluster solutions of the provided solutions data frame.

Examples

```
#dl <- data_list(</pre>
     list(cort_sa, "cortical_surface_area", "neuroimaging", "continuous"),
     list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
     list(income, "household_income", "demographics", "continuous"),
list(pubertal, "pubertal_status", "demographics", "continuous"),
#
     uid = "unique_id"
#)
#set.seed(42)
#my_sc <- snf_config(</pre>
     dl = dl,
     n_solutions = 20,
     min_k = 20,
     max_k = 50
#)
#sol_df <- batch_snf(dl, my_sc)</pre>
#sol_df
#sol_aris <- calc_aris(sol_df)</pre>
#meta_cluster_order <- get_matrix_order(sol_aris)</pre>
## `split_vec` found by iteratively plotting ari_hm or by ?shiny_annotator()
#split_vec <- c(6, 10, 16)
#ari_hm <- meta_cluster_heatmap(</pre>
     sol_aris,
     order = meta_cluster_order,
     split_vector = split_vec
#)
```

methylation_df

Modification of SNFtool mock data frame "Data2"

Description

Modification of SNFtool mock data frame "Data2"

Usage

```
methylation_df
```

n_features

Format

```
methylation_df:
```

A data frame with 200 rows and 3 columns:

gene_1_expression Mock gene methylation feature
gene_2_expression Mock gene methylation feature

patient_id Random three-digit number uniquely identifying the patient

Source

This data came from the SNFtool package, with slight modifications.

new_solutions_df

Constructor for solutions_df class object

Description

Constructor for solutions_df class object

Usage

```
new_solutions_df(sol_dfl)
```

Arguments

sol_dfl

A solutions data frame-like object to be validated and converted into a solutions data frame.

Value

A solutions_df class object.

n_features

Extract number of features stored in an object

Description

Extract number of features stored in an object

Usage

```
n_features(x)
```

Arguments

Х

The object to extract number of features from.

n_observations 89

Value

The number of features in x.

n_observations

Extract number of observations stored in an object

Description

Extract number of observations stored in an object

Usage

```
n_observations(x)
```

Arguments

Χ

The object to extract number of observations from.

Value

The number of observations in x.

```
print.ari_matrix
```

Print method for class ari_matrix

Description

Custom formatted print for weights matrices that outputs information about feature weights functions to the console.

Usage

```
## S3 method for class 'ari_matrix'
print(x, ...)
```

Arguments

```
x A ari_matrix class object.
```

... Other arguments passed to print (not used in this function)

Value

90 print.data_list

Description

Custom formatted print for clustering functions list objects that outputs information about the contained clustering functions to the console.

Usage

```
## S3 method for class 'clust_fns_list'
print(x, ...)
```

Arguments

- x A clust_fns_list class object.
- ... Other arguments passed to print (not used in this function)

Value

Function prints to console but does not return any value.

Description

Custom formatted print for data list objects that outputs information about the contained observations and components to the console.

Usage

```
## S3 method for class 'data_list'
print(x, ...)
```

Arguments

- x A data_list class object.
- ... Other arguments passed to print (not used in this function)

Value

print.dist_fns_list 91

Description

Custom formatted print for distance metrics list objects that outputs information about the contained distance metrics to the console.

Usage

```
## S3 method for class 'dist_fns_list'
print(x, ...)
```

Arguments

- x A dist_fns_list class object.
- Other arguments passed to print (not used in this function)

Value

Function prints to console but does not return any value.

```
print.ext\_solutions\_df \\ Print\ method\ for\ class\ ext\_solutions\_df
```

Description

Custom formatted print for extended solutions data frame class objects.

Usage

```
## S3 method for class 'ext_solutions_df'
print(x, n = NULL, ...)
```

Arguments

- x A ext_solutions_df class object.n Number of rows to print, passed into tibble::print.tbl_df().
- ... Other arguments passed to print (not used in this function).

Value

92 print.snf_config

print.settings_df

Print method for class settings_df

Description

Custom formatted print for settings data frame that outputs information about SNF hyperparameters to the console.

Usage

```
## S3 method for class 'settings_df'
print(x, ...)
```

Arguments

x A settings_df class object.

Other arguments passed to print (not used in this function)

Value

Function prints to console but does not return any value.

print.snf_config

Print method for class snf_config

Description

Custom formatted print for SNF config

Usage

```
## S3 method for class 'snf_config'
print(x, ...)
```

Arguments

x A snf_config class object.

... Other arguments passed to print (not used in this function)

Value

print.solutions_df 93

print.solutions_df

Print method for class solutions_df

Description

Custom formatted print for weights matrices that outputs information about feature weights functions to the console.

Usage

```
## S3 method for class 'solutions_df'
print(x, n = NULL, tips = TRUE, ...)
```

Arguments

tips

x A weights_matrix class object.

n Number of rows to print, passed into tibble::print.tbl_df().

If TRUE, include lines on how to print more rows / transposed.

Other arguments passed to print (not used in this function).

Value

Function prints to console but does not return any value.

Description

Custom formatted print for transposed solutions data frame class objects.

Usage

```
## S3 method for class 't_ext_solutions_df'
print(x, ...)
```

Arguments

x A t_solutions_df class object.

... Other arguments passed to print (not used in this function)

Value

94 print.weights_matrix

Description

Custom formatted print for transposed solutions data frame class objects.

Usage

```
## S3 method for class 't_solutions_df'
print(x, ...)
```

Arguments

x A t_solutions_df class object.

... Other arguments passed to print (not used in this function)

Value

Function prints to console but does not return any value.

Description

Custom formatted print for weights matrices that outputs information about feature weights functions to the console.

Usage

```
## S3 method for class 'weights_matrix'
print(x, ...)
```

Arguments

x A weights_matrix class object.

... Other arguments passed to print (not used in this function)

Value

pubertal 95

pubertal

Mock ABCD pubertal status data

Description

Like the mock data frame "abcd_pubertal", but with "unique_id" as the "uid".

Usage

pubertal

Format

pubertal:

A data frame with 275 rows and 2 columns:

unique_id The unique identifier of the ABCD dataset

pubertal_status Average reported pubertal status between child and parent (1-5 categorical scale)

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

pval_heatmap

Heatmap of p-values

Description

Heatmap of p-values

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Usage

```
pval_heatmap(
  ext_sol_df,
  order = NULL,
  cluster_columns = TRUE,
  cluster_rows = FALSE,
  show_row_names = FALSE,
  show_column_names = TRUE,
 min_colour = "red2",
 max_colour = "white",
 legend_breaks = c(0, 1),
  col = circlize::colorRamp2(legend_breaks, c(min_colour, max_colour)),
 heatmap\_legend\_param = list(color\_bar = "continuous", title = "p-value", at = c(0, 1)),
  rect_gp = grid::gpar(col = "black"),
  column_split_vector = NULL,
  row_split_vector = NULL,
  column_split = NULL,
  row_split = NULL,
)
```

Arguments

 ${\tt ext_sol_df} \qquad \qquad {\tt An\,ext_solutions_df\,class\,object\,(produced\,from\,the\,function\,extend_solutions.}$

order Numeric vector containing row order of the heatmap.

cluster_columns

Whether columns should be sorted by hierarchical clustering.

cluster_rows Whether rows should be sorted by hierarchical clustering.

show_row_names Whether row names should be shown.

show_column_names

Whether column names should be shown.

min_colour Colour used for the lowest value in the heatmap.

Colour used for the highest value in the heatmap.

legend_breaks Numeric vector of breaks for the legend.

col Colour function for ComplexHeatmap::Heatmap()

heatmap_legend_param

Legend function for ComplexHeatmap()

column_split_vector

Vector of indices to split columns by.

row_split_vector

Vector of indices to split rows by.

column_split Standard parameter of ComplexHeatmap::Heatmap.
row_split Standard parameter of ComplexHeatmap::Heatmap.

... Additional parameters passed to ComplexHeatmap::Heatmap.

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Value

Returns a heatmap (class "Heatmap" from package ComplexHeatmap) that displays the provided p-values.

Examples

```
#dl <- data_list(</pre>
    list(income, "household_income", "demographics", "ordinal"),
    list(pubertal, "pubertal_status", "demographics", "continuous"),
#
    list(fav_colour, "favourite_colour", "demographics", "categorical"),
    list(anxiety, "anxiety", "behaviour", "ordinal"),
#
    list(depress, "depressed", "behaviour", "ordinal"),
    uid = "unique_id"
#)
#sc <- snf_config(
    dl,
    n_solutions = 4,
    dropout_dist = "uniform",
    max_k = 50
#)
#sol_df <- batch_snf(dl, sc)</pre>
#ext_sol_df <- extend_solutions(sol_df, dl)</pre>
#pval_heatmap(ext_sol_df)
```

quality_measures

Quality metrics

Description

These functions calculate conventional metrics of cluster solution quality.

Usage

```
calculate_silhouettes(sol_df)
calculate_dunn_indices(sol_df)
calculate_db_indices(sol_df)
```

Arguments

sol_df A solutions_df class object created by batch_snf() with the parameter return_sim_mats = TRUE.

98 random_removal

Details

calculate_silhouettes: A wrapper for cluster::silhouette that calculates silhouette scores for all cluster solutions in a provided solutions data frame. Silhouette values range from -1 to +1 and indicate an overall ratio of how close together observations within a cluster are to how far apart observations across clusters are. You can learn more about interpreting the results of this function by calling ?cluster::silhouette.

calculate_dunn_indices: A wrapper for clv::clv.Dunn that calculates Dunn indices for all cluster solutions in a provided solutions data frame. Dunn indices, like silhouette scores, similarly reflect similarity within clusters and separation across clusters. You can learn more about interpreting the results of this function by calling ?clv::clv.Dunn.

calculate_db_indices: A wrapper for clv::clv.Davies.Bouldin that calculates Davies-Bouldin indices for all cluster solutions in a provided solutions data frame. These values can be interpreted similarly as those above. You can learn more about interpreting the results of this function by calling ?clv::clv.Davies.Bouldin.

Value

A list of silhouette class objects, a vector of Dunn indices, or a vector of Davies-Bouldin indices depending on which function was used.

Examples

```
input_dl <- data_list(
    list(gender_df, "gender", "demographics", "categorical"),
    list(diagnosis_df, "diagnosis", "clinical", "categorical"),
    uid = "patient_id"
)

sc <- snf_config(input_dl, n_solutions = 5)

sol_df <- batch_snf(input_dl, sc, return_sim_mats = TRUE)

# calculate Davies-Bouldin indices
davies_bouldin_indices <- calculate_db_indices(sol_df)

# calculate Dunn indices
dunn_indices <- calculate_dunn_indices(sol_df)

# calculate silhouette scores
silhouette_scores <- calculate_silhouettes(sol_df)</pre>
```

random_removal

Generate random removal sequence

Description

Helper function to contribute to rows within the settings data frame. Number of columns removed follows a uniform or exponential probability distribution.

rbind.ext_solutions_df

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Usage

```
random_removal(
  columns,
  min_removed_inputs,
  max_removed_inputs,
  dropout_dist = "exponential"
)
```

Arguments

 ${\color{red} \textbf{columns}} \quad {\color{red} \textbf{Columns of the settings_df that are passed in }} \\ {\color{red} \textbf{min_removed_inputs}}$

The smallest number of input data frames that may be randomly removed.

max_removed_inputs

The largest number of input data frames that may be randomly removed.

dropout_dist

Indication of how input data frames should be dropped. can be "none" (no dropout), "uniform" (uniformly draw number between min and max removed inputs), or "exponential" (like uniform, but using an exponential distribution; default).

Value

inclusions_df data frame that can be rbind'ed to the settings_df

```
rbind.ext_solutions_df
```

Row-binding of solutions data frame class objects.

Description

Row-binding of solutions data frame class objects.

Usage

```
## S3 method for class 'ext_solutions_df'
rbind(..., reset_indices = FALSE)
```

Arguments

```
... An arbitrary number of ext_solutions_df class objects.

reset_indices If TRUE, re-labels the "solutions" indices in the solutions data frame from 1 to the number of defined settings.
```

Value

An ext_solutions_df class object.

100 rename_dl

rbind.solutions_df

Row-binding of solutions data frame class objects.

Description

Row-binding of solutions data frame class objects.

Usage

```
## S3 method for class 'solutions_df'
rbind(..., reset_indices = FALSE)
```

Arguments

... An arbitrary number of solutions_df class objects.

the number of defined settings.

Value

A solutions_df class object.

rename_dl

Rename features in a data list

Description

Rename features in a data list

Usage

```
rename_dl(dl, name_mapping)
```

Arguments

dl A nested list of input data from data_list().

name_mapping A named vector where the values are the features to be renamed and the names

are the new names for those features.

Value

A data list ("list"-class object) with adjusted feature names.

resample 101

Examples

```
library(metasnf)

dl <- data_list(
    list(pubertal, "pubertal_status", "demographics", "continuous"),
    list(anxiety, "anxiety", "behaviour", "ordinal"),
    list(depress, "depressed", "behaviour", "ordinal"),
    uid = "unique_id"
)

summary(dl, "feature")

name_changes <- c(
    "anxiety_score" = "cbcl_anxiety_r",
    "depression_score" = "cbcl_depress_r"
)

dl <- rename_dl(dl, name_changes)

summary(dl, "feature")</pre>
```

resample

Helper resample function found in ?sample

Description

Like sample, but when given a single value x, returns back that single value instead of a random value from 1 to x.

Usage

```
resample(x, ...)
```

Arguments

- x Vector or single value to sample from
- ... Remaining arguments for base::sample function

Value

Numeric vector result of running base::sample.

save_heatmap	Save a heatmap object to a file

Description

Save a heatmap object to a file

Usage

```
save_heatmap(heatmap, path, width = 480, height = 480, res = 100)
```

Arguments

heatmap	The heatmap object to save.
path	The path to save the heatmap to.
width	The width of the heatmap.
height	The height of the heatmap.
res	The resolution of the heatmap.

Value

Does not return any value. Saves heatmap to file.

settings_df	Build a settings data frame	

Description

The settings_df is a data frame whose rows completely specify the hyperparameters and decisions required to transform individual input data frames (found in a data list, see ?data_list) into a single similarity matrix through SNF. The format of the settings data frame is as follows:

- A column named "solution": This column is used to keep track of the rows and should have integer values only.
- A column named "alpha": This column contains the value of the alpha hyperparameter that will be used on that run of the SNF pipeline.
- A column named "k": Like above, but for the K (nearest neighbours) hyperparameter.
- A column named "t": Like above, but for the t (number of iterations) hyperparameter.
- A column named "snf_scheme": Which of 3 pre-defined schemes will be used to integrate the data frames of the data list into a final fused network. The purpose of varying these schemes is primarily to increase the diversity of the generated cluster solutions.

 A value of 1 corresponds to the "individual" scheme, in which all data frames are directly merged by SNF into the final fused network. This scheme corresponds to the approach shown in the original SNF paper.

- A value of 2 corresponds to the "two-step" scheme, in which all data frames witin a domain are first merged into a domain-specific fused network. Next, domain-specific networks are fused once more by SNF into the final fused network. This scheme is useful for fairly re-weighting SNF pipelines with unequal numbers of data frames across domains.
- A value of 3 corresponds to the "domain" scheme, in which all data frames within a domain are first concatenated into a single domain- specific data frame before being merged by SNF into the final fused network. This approach serves as an alternative way to reweight SNF pipelines with unequal numbers of data frames across domains. You can learn more about this parameter here: https://branchlab.github.io/metasnf/articles/snf_schemes.html.
- A column named "clust_alg": Specification of which clustering algorithm will be applied to the final similarity matrix. By default, this column can take on the integer values 1 or 2, which correspond to spectral clustering where the number of clusters is determined by the eigengap or rotation cost heuristic respectively. You can learn more about this parameter here: https://branchlab.github.io/metasnf/articles/clustering_algorithms.html.
- A column named "cnt_dist": Specification of which distance metric will be used for data frames of purely continuous data. You can learn about this metric and its defaults here: https://branchlab.github.io/metasnf/articles/distance_metrics.html
- A column named "dsc_dist": Like above, but for discrete data frames.
- A column named "ord_dist": Like above, but for ordinal data frames.
- A column named "cat dist": Like above, but for categorical data frames.
- A column named "mix_dist": Like above, but for mixed-type (e.g., both categorical and discrete) data frames.
- One column for every input data frame in the corresponding data list which can either have the value of 0 or 1. The name of the column should be formatted as "inc_[]" where the square brackets are replaced with the name (as found in dl_summary(dl)\$"name") of each data frame. When 0, that data frame will be excluded from that run of the SNF pipeline. When 1, that data frame will be included.

Usage

```
settings_df(
    dl,
    n_solutions = 0,
    min_removed_inputs = 0,
    max_removed_inputs = length(dl) - 1,
    dropout_dist = "exponential",
    min_alpha = NULL,
    max_alpha = NULL,
    min_k = NULL,
    max_k = NULL,
    min_t = NULL,
    min_t = NULL,
    min_t = NULL,
    min_t = NULL,
    max_t = NULL,
```

```
alpha_values = NULL,
  k_values = NULL,
  t_values = NULL,
  possible_snf_schemes = c(1, 2, 3),
  clustering_algorithms = NULL,
  continuous_distances = NULL,
  discrete_distances = NULL,
  ordinal_distances = NULL,
  categorical_distances = NULL,
 mixed_distances = NULL,
  df1 = NULL,
  snf_input_weights = NULL,
  snf_domain_weights = NULL,
  retry_limit = 10,
  allow_duplicates = FALSE
)
```

Arguments

dl A nested list of input data from data_list().

n_solutions Number of rows to generate for the settings data frame.

min_removed_inputs

The smallest number of input data frames that may be randomly removed. By default, 0.

max_removed_inputs

The largest number of input data frames that may be randomly removed. By default, this is 1 less than all the provided input data frames in the data list.

dropout_dist

Parameter controlling how the random removal of input data frames should occur. Can be "none" (no input data frames are randomly removed), "uniform" (uniformly sample between min removed inputs and max removed inputs to determine number of input data frames to remove), or "exponential" (pick number of input data frames to remove by sampling from min_removed_inputs to max_removed_inputs with an exponential distribution; the default).

min_alpha

The minimum value that the alpha hyperparameter can have. Random assigned value of alpha for each row will be obtained by uniformly sampling numbers between min_alpha and max_alpha at intervals of 0.1. Cannot be used in conjunction with the alpha_values parameter.

max_alpha

The maximum value that the alpha hyperparameter can have. See min_alpha parameter. Cannot be used in conjunction with the alpha_values parameter.

min_k

The minimum value that the k hyperparameter can have. Random assigned value of k for each row will be obtained by uniformly sampling numbers between min_k and max_k at intervals of 1. Cannot be used in conjunction with the k_values parameter.

max_k

The maximum value that the k hyperparameter can have. See min_k parameter. Cannot be used in conjunction with the k_values parameter.

The minimum value that the t hyperparameter can have. Random assigned value of t for each row will be obtained by uniformly sampling numbers between

min_t

min_t and max_t at intervals of 1. Cannot be used in conjunction with the t_values parameter.

max_t The maximum value that the t hyperparameter can have. See min_t parameter.

Cannot be used in conjunction with the t_values parameter.

A number or numeric vector of a set of possible values that alpha can take on. Value will be obtained by uniformly sampling the vector. Cannot be used in conjunction with the min_alpha or max_alpha parameters.

A number or numeric vector of a set of possible values that k can take on. Value will be obtained by uniformly sampling the vector. Cannot be used in conjunction with the min_k or max_k parameters.

t_values A number or numeric vector of a set of possible values that t can take on. Value will be obtained by uniformly sampling the vector. Cannot be used in conjunction with the min_t or max_t parameters.

possible_snf_schemes

alpha_values

k values

A vector containing the possible snf_schemes to uniformly randomly select from. By default, the vector contains all 3 possible schemes: c(1, 2, 3). 1 corresponds to the "individual" scheme, 2 corresponds to the "domain" scheme, and 3 corresponds to the "twostep" scheme.

clustering_algorithms

A list of clustering algorithms to uniformly randomly pick from when clustering. When not specified, randomly select between spectral clustering using the eigen-gap heuristic and spectral clustering using the rotation cost heuristic. See ?clust_fns_list for more details on running custom clustering algorithms.

continuous_distances

A vector of continuous distance metrics to use when a custom dist_fns_list is provided.

discrete_distances

A vector of categorical distance metrics to use when a custom dist_fns_list is provided.

ordinal_distances

A vector of categorical distance metrics to use when a custom dist_fns_list is provided.

categorical_distances

A vector of categorical distance metrics to use when a custom dist_fns_list is provided.

mixed_distances

A vector of mixed distance metrics to use when a custom dist_fns_list is provided

dfl List containing distance metrics to vary over. See ?generate_dist_fns_list.

snf_input_weights

Nested list containing weights for when SNF is used to merge individual input measures (see ?generate_snf_weights)

snf_domain_weights

Nested list containing weights for when SNF is used to merge domains (see ?generate_snf_weights)

shiny_annotator

retry_limit

The maximum number of attempts to generate a novel row. This function does not return matrices with identical rows. As the range of requested possible settings tightens and the number of requested rows increases, the risk of randomly generating a row that already exists increases. If a new random row has matched an existing row retry_limit number of times, the function will terminate.

allow_duplicates

If TRUE, enables creation of a settings data frame with duplicate non-feature weighting related hyperparameters. This function should only be used when paired with a custom weights matrix that has non-duplicate rows.

Value

A settings data frame

shiny_annotator

Launch a shiny app to identify meta cluster boundaries

Description

This function calls the htShiny() function from the package InteractiveComplexHeatmap to assist users in identifying the indices of the boundaries between meta clusters in a meta cluster heatmap. By providing a heatmap of inter-solution similarities (obtained through meta_cluster_heatmap()), users can click on positions within the heatmap that appear to meaningfully separate major sets of similar cluster solutions by visual inspection. The corresponding indices of the clicked positions are printed to the console and also shown within the app. This function can only run from an interactive session of R.

Usage

```
shiny_annotator(ari_heatmap)
```

Arguments

ari_heatmap Heatı

Heatmap of ARIs to divide into meta clusters.

Value

Does not return any value. Launches interactive shiny applet.

Examples

```
#dl <- data_list(
# list(cort_sa, "cortical_surface_area", "neuroimaging", "continuous"),
# list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
# list(income, "household_income", "demographics", "continuous"),
# list(pubertal, "pubertal_status", "demographics", "continuous"),
# uid = "unique_id"
#)</pre>
```

```
#set.seed(42)
#my_sc <- snf_config(</pre>
    dl = dl,
    n_solutions = 20,
    min_k = 20,
    max_k = 50
#)
#sol_df <- batch_snf(dl, my_sc)</pre>
#sol_aris <- calc_aris(sol_df)</pre>
#meta_cluster_order <- get_matrix_order(sol_aris)</pre>
#ari_hm <- meta_cluster_heatmap(sol_aris, order = meta_cluster_order)</pre>
## Click on meta cluster boundaries to obtain `split_vec` values
#shiny_annotator(ari_hm)
#split_vec <- c(6, 10, 16)
#ari_hm <- meta_cluster_heatmap(</pre>
    sol_aris,
    order = meta_cluster_order,
#
#
     split_vector = split_vec
#)
```

similarity_matrix_heatmap

Plot heatmap of similarity matrix

Description

Plot heatmap of similarity matrix

Usage

```
similarity_matrix_heatmap(
    similarity_matrix,
    order = NULL,
    cluster_solution = NULL,
    scale_diag = "mean",
    log_graph = TRUE,
    cluster_rows = FALSE,
    cluster_columns = FALSE,
    show_row_names = FALSE,
    show_column_names = FALSE,
    data = NULL,
```

```
left_bar = NULL,
right_bar = NULL,
top_bar = NULL,
bottom_bar = NULL,
left_hm = NULL,
right_hm = NULL,
top_hm = NULL,
bottom_hm = NULL,
annotation_colours = NULL,
min_colour = NULL,
split_vector = NULL,
row_split = NULL,
column_split = NULL,
...
)
```

Arguments

similarity_matrix

A similarity matrix

order Vector of numbers to reorder the similarity matrix (and data if provided). Over-

writes ordering specified by cluster_solution param.

cluster_solution

Row of a solutions data frame or column of a transposed solutions data frame.

scale_diag Method of rescaling matrix diagonals. Can be "none" (don't change diagonals),

"mean" (replace diagonals with average value of off-diagonals), or "zero" (re-

place diagonals with 0).

log_graph If TRUE, log transforms the graph.

cluster_rows Parameter for ComplexHeatmap::Heatmap.

cluster_columns

Parameter for ComplexHeatmap::Heatmap.

show_row_names Parameter for ComplexHeatmap::Heatmap.

show_column_names

Parameter for ComplexHeatmap::Heatmap.

data A data frame containing elements requested for annotation.

left_bar Named list of strings, where the strings are features in df that should be used for

a barplot annotation on the left of the plot and the names are the names that will

be used to caption the plots and their legends.

right_bar See left_bar.
top_bar See left_bar.
bottom_bar See left_bar.

left_hm Like left_bar, but with a heatmap annotation instead of a barplot annotation.

right_hm See left_hm.

```
top_hm
                 See left_hm.
bottom_hm
                 See left_hm.
annotation_colours
                 Named list of heatmap annotations and their colours.
min_colour
                 Colour used for the lowest value in the heatmap.
                 Colour used for the highest value in the heatmap.
max_colour
split_vector
                 A vector of partition indices.
                 Standard parameter of ComplexHeatmap::Heatmap.
row_split
                 Standard parameter of ComplexHeatmap::Heatmap.
column_split
                 Additional parameters passed into ComplexHeatmap::Heatmap.
. . .
```

Value

Returns a heatmap (class "Heatmap" from package ComplexHeatmap) that displays the similarities between observations in the provided matrix.

```
#my_dl <- data_list(</pre>
     list(
#
         data = expression_df,
#
         name = "expression_data",
#
         domain = "gene_expression",
#
         type = "continuous"
#
     ),
     list(
#
         data = methylation_df,
         name = "methylation_data",
#
         domain = "gene_methylation",
#
         type = "continuous"
#
#
     uid = "patient_id"
#
#)
#sc <- snf_config(my_dl, n_solutions = 10)</pre>
#sol_df <- batch_snf(my_dl, sc, return_sim_mats = TRUE)</pre>
#sim_mats <- sim_mats_list(sol_df)</pre>
#similarity_matrix_heatmap(
     sim_mats[[1]],
     cluster_solution = sol_df[1, ]
#
#)
```

 sim_mats_list

Create or extract a sim_mats_list class object

Description

Create or extract a sim_mats_list class object

Usage

```
sim_mats_list(x)
```

Arguments

Х

The object to create or extract a sim_mats_list from.

Value

A sim_mats_list class object.

```
siw_euclidean_distance
```

Squared (including weights) Euclidean distance

Description

Squared (including weights) Euclidean distance

Usage

```
siw_euclidean_distance(df, weights_row)
```

Arguments

df data frame containing at least 1 data column.

weights_row Single-row data frame where the column names contain the column names in df

and the row contains the corresponding weights.

Value

distance_matrix A distance matrix.

snf_config Define configuration for generating a set of SNF-based cluster solutions

Description

snf_config() constructs an SNF config object which inherits from classes snf_config and list. This object is used to store all settings required to transform data stored in a data_list class object into a space of cluster solutions by SNF. The SNF config object contains the following components:

1. A settings data frame (inherits from settings_df and data.frame). Data frame that stores SNF-specific hyperparameters and information about feature selection and weighting, SNF schemes, clustering algorithms, and distance metrics. Each row of the settings data frame corresponds to a distinct cluster solution.

2. A clustering algorithms list (inherits from clust_fns_list and list), which stores all clustering algorithms that the settings data frame can point to.

3. A distance metrics list (inherits from dist_metrics_list and list), which stores all distance metrics that the settings data frame can point to.

4. A weights matrix (inherits from weights_matrix, matrix, and array'), which stores the feature weights to use prior to distance calculations. Each column of the weights matrix corresponds to a different feature in the data list and each row corresponds to a different row in the settings data frame.

Usage

```
snf_config(
 d1 = NULL,
  sdf = NULL,
 dfl = NULL,
  cfl = NULL,
 wm = NULL,
 n_solutions = 0,
 min_removed_inputs = 0,
 max_removed_inputs = length(dl) - 1,
 dropout_dist = "exponential",
 min_alpha = NULL,
 max_alpha = NULL,
 min_k = NULL,
 max_k = NULL,
 min_t = NULL,
 max_t = NULL,
  alpha_values = NULL,
  k_values = NULL,
  t_values = NULL,
  possible\_snf\_schemes = c(1, 2, 3),
  clustering_algorithms = NULL,
  continuous_distances = NULL,
  discrete_distances = NULL,
  ordinal_distances = NULL,
  categorical_distances = NULL,
```

```
mixed_distances = NULL,
snf_input_weights = NULL,
snf_domain_weights = NULL,
retry_limit = 10,
cnt_dist_fns = NULL,
dsc_dist_fns = NULL,
ord_dist_fns = NULL,
cat_dist_fns = NULL,
mix_dist_fns = NULL,
automatic_standard_normalize = FALSE,
use_default_dist_fns = FALSE,
clust_fns = NULL,
use_default_clust_fns = FALSE,
weights_fill = "ones"
)
```

Arguments

dl A nested list of input data from data_list(A neste	d list of input	data from data	list().
--	---------	-----------------	----------------	---------

sdf A settings_df class object. Overrides settings data frame related parameters.

dfl A dist_fns_list class object. Overrides distance functions list related param-

eters.

cfl A clust_fns_list class object. Overrides clustering functions list related pa-

rameters.

wm A weights_matrix class object. Overrides weights matrix related parameters.

n_solutions Number of rows to generate for the settings data frame.

min_removed_inputs

The smallest number of input data frames that may be randomly removed. By default, 0.

max_removed_inputs

The largest number of input data frames that may be randomly removed. By default, this is 1 less than all the provided input data frames in the data list.

dropout_dist

Parameter controlling how the random removal of input data frames should occur. Can be "none" (no input data frames are randomly removed), "uniform" (uniformly sample between min_removed_inputs and max_removed_inputs to determine number of input data frames to remove), or "exponential" (pick number of input data frames to remove by sampling from min_removed_inputs to max removed inputs with an exponential distribution; the default).

min_alpha

The minimum value that the alpha hyperparameter can have. Random assigned value of alpha for each row will be obtained by uniformly sampling numbers between min_alpha and max_alpha at intervals of 0.1. Cannot be used in conjunction with the alpha_values parameter.

max_alpha

The maximum value that the alpha hyperparameter can have. See min_alpha parameter. Cannot be used in conjunction with the alpha_values parameter.

min_k

The minimum value that the k hyperparameter can have. Random assigned value of k for each row will be obtained by uniformly sampling numbers between

min_k and max_k at intervals of 1. Cannot be used in conjunction with the k_values parameter.

max_k The maximum value that the k hyperparameter can have. See min_k parameter. Cannot be used in conjunction with the k_values parameter.

min_t The minimum value that the t hyperparameter can have. Random assigned value of t for each row will be obtained by uniformly sampling numbers between min_t and max_t at intervals of 1. Cannot be used in conjunction with the t_values parameter.

The maximum value that the t hyperparameter can have. See min_t parameter.

Cannot be used in conjunction with the t_values parameter.

alpha_values A number or numeric vector of a set of possible values that alpha can take on. Value will be obtained by uniformly sampling the vector. Cannot be used in conjunction with the min_alpha or max_alpha parameters.

k_values A number or numeric vector of a set of possible values that k can take on. Value will be obtained by uniformly sampling the vector. Cannot be used in conjunction with the min_k or max_k parameters.

A number or numeric vector of a set of possible values that t can take on. Value will be obtained by uniformly sampling the vector. Cannot be used in conjunction with the min_t or max_t parameters.

possible_snf_schemes

t_values

A vector containing the possible snf_schemes to uniformly randomly select from. By default, the vector contains all 3 possible schemes: c(1, 2, 3). 1 corresponds to the "individual" scheme, 2 corresponds to the "domain" scheme, and 3 corresponds to the "twostep" scheme.

clustering_algorithms

A list of clustering algorithms to uniformly randomly pick from when clustering. When not specified, randomly select between spectral clustering using the eigen-gap heuristic and spectral clustering using the rotation cost heuristic. See ?clust_fns_list for more details on running custom clustering algorithms.

continuous_distances

A vector of continuous distance metrics to use when a custom dist_fns_list is provided.

discrete_distances

A vector of categorical distance metrics to use when a custom dist_fns_list is provided.

ordinal_distances

A vector of categorical distance metrics to use when a custom dist_fns_list is provided.

categorical_distances

A vector of categorical distance metrics to use when a custom dist_fns_list is provided.

mixed distances

A vector of mixed distance metrics to use when a custom dist_fns_list is provided.

snf_input_weights

Nested list containing weights for when SNF is used to merge individual input measures (see ?generate_snf_weights)

snf_domain_weights

Nested list containing weights for when SNF is used to merge domains (see ?generate_snf_weights)

retry_limit

The maximum number of attempts to generate a novel row. This function does not return matrices with identical rows. As the range of requested possible settings tightens and the number of requested rows increases, the risk of randomly generating a row that already exists increases. If a new random row has matched an existing row retry_limit number of times, the function will terminate.

dsc_dist_fns A named list of discrete distance metric functions.

ord_dist_fns A named list of ordinal distance metric functions.

cat_dist_fns A named list of categorical distance metric functions.

mix_dist_fns A named list of mixed distance metric functions.

automatic_standard_normalize

If TRUE, will automatically use standard normalization prior to calculation of any numeric distances. This parameter overrides all other distance functions list-related parameters.

use_default_dist_fns

If TRUE, prepend the base distance metrics (euclidean distance for continuous, discrete, and ordinal data and gower distance for categorical and mixed data) to the resulting distance metrics list.

clust_fns A list of named clustering functions

use_default_clust_fns

If TRUE, prepend the base clustering algorithms (spectral_eigen and spectral_rot, which apply spectral clustering and use the eigen-gap and rotation cost heuristics respectively for determining the number of clusters in the graph) to clust_fns.

weights_fill

String indicating what to populate generate rows with. Can be "ones" (default; fill matrix with 1), "uniform" (fill matrix with uniformly distributed random values), or "exponential" (fill matrix with exponentially distributed random values).

Value

An snf_config class object.

```
# Simple random config for 5 cluster solutions
input_dl <- data_list(
    list(anxiety, "anxiety", "behaviour", "ordinal"),
    list(depress, "depressed", "behaviour", "ordinal"),
    uid = "unique_id"
)
my_sc <- snf_config(</pre>
```

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```
dl = input_dl,
    n_solutions = 5
)
# specifying possible K range
my_sc <- snf_config(</pre>
    dl = input_dl,
    n_solutions = 5,
   min_k = 20,
   max_k = 40
)
# Random feature weights across from uniform distribution
my_sc <- snf_config(</pre>
    dl = input_dl,
   n_solutions = 5,
   min_k = 20,
   max_k = 40,
   weights_fill = "uniform"
)
# Specifying custom pre-built clustering and distance functions
# - Random alternation between 2-cluster and 5-cluster solutions
# - When continuous or discrete data frames are being processed,
   randomly alternate between standardized/normalized Euclidean
   distance vs. regular Euclidean distance
my_sc <- snf_config(</pre>
    dl = input_dl,
   n_solutions = 5,
   min_k = 20,
   max_k = 40,
   weights_fill = "uniform",
    clust_fns = list(
        "two_cluster_spectral" = spectral_two,
        "five_cluster_spectral" = spectral_five
   ),
    cnt_dist_fns = list(
         "euclidean" = euclidean_distance,
         "std_nrm_euc" = sn_euclidean_distance
    ),
    dsc_dist_fns = list(
         "euclidean" = euclidean_distance,
         "std_nrm_euc" = sn_euclidean_distance
    )
)
```

split_parser

Helper function to determine which row and columns to split on

Description

Helper function to determine which row and columns to split on

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Usage

```
split_parser(
  row_split_vector = NULL,
  column_split_vector = NULL,
  row_split = NULL,
  column_split = NULL,
  n_rows,
  n_columns
)
```

Arguments

```
row_split_vector
```

A vector of row indices to split on.

column_split_vector

A vector of column indices to split on.

row_split Standard parameter of ComplexHeatmap::Heatmap.
column_split Standard parameter of ComplexHeatmap::Heatmap.

n_rows The number of rows in the data.n_columns The number of columns in the data.

Value

"list"-class object containing row_split and column_split character vectors to pass into Complex-Heatmap::Heatmap.

subc_v

Mock ABCD subcortical volumes data

Description

Like the mock data frame "abcd_subc_v", but with "unique_id" as the "uid".

Usage

```
subc_v
```

Format

```
subc_v:
```

A data frame with 174 rows and 31 columns:

unique_id The unique identifier of the ABCD dataset

... Subcortical volumes of various ROIs (mm³, I think)

subsample_dl 117

Source

Though this data is no longer "real" ABCD data, the reference for using ABCD as a data source is below:

Data used in the preparation of this article were obtained from the Adolescent Brain Cognitive DevelopmentSM (ABCD) Study (https://abcdstudy.org), held in the NIMH Data Archive (NDA). This is a multisite, longitudinal study designed to recruit more than 10,000 children age 9-10 and follow them over 10 years into early adulthood. The ABCD Study® is supported by the National Institutes of Health and additional federal partners under award numbers U01DA041048, U01DA050989, U01DA051016, U01DA041022, U01DA051018, U01DA051037, U01DA050987, U01DA041174, U01DA041106, U01DA041117, U01DA041028, U01DA041134, U01DA050988, U01DA051039, U01DA041156, U01DA041025, U01DA041120, U01DA051038, U01DA041148, U01DA041093, U01DA041089, U24DA041123, U24DA041147. A full list of supporters is available at https://abcdstudy.org/federal-partners.html. A listing of participating sites and a complete listing of the study investigators can be found at https://abcdstudy.org/consortium_members/. ABCD consortium investigators designed and implemented the study and/or provided data but did not necessarily participate in the analysis or writing of this report. This manuscript reflects the views of the authors and may not reflect the opinions or views of the NIH or ABCD consortium investigators.

subsample_dl

Create subsamples of a data list

Description

Given a data list, return a list of smaller data lists that are generated through random sampling (without replacement). The results of this function can be passed into batch_snf_subsamples() to obtain a list of resampled solutions data frames.

Usage

```
subsample_dl(
   dl,
   n_subsamples,
   subsample_fraction = NULL,
   n_observations = NULL
)
```

Arguments

```
dl A nested list of input data from data_list().

n_subsamples Number of subsamples to create.

subsample_fraction
Percentage of patients to include per subsample.

n_observations Number of patients to include per subsample.
```

Value

A "list" class object containing n_subsamples number of data lists. Each of those data lists contains a random subsample_fraction fraction of the observations of the provided data list.

Examples

```
# my_dl <- data_list(
# list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
# list(income, "household_income", "demographics", "continuous"),
# list(pubertal, "pubertal_status", "demographics", "continuous"),
# uid = "unique_id"
# )
#
# my_dl_subsamples <- subsample_dl(
# my_dl,
# n_subsamples = 20,
# subsample_fraction = 0.85
# )</pre>
```

subsample_pairwise_aris

Calculate pairwise adjusted Rand indices across subsamples of data

Description

Given a list of subsampled solutions data frames from 'batch_snf_subsamples(), this function calculates the adjusted Rand indices across all the subsamples of each solution. ARI calculation between two subsamples only factors in observations that were present in both subsamples.

Usage

```
subsample_pairwise_aris(subsample_solutions, verbose = FALSE)
```

Arguments

```
subsample_solutions
```

A list of solutions data frames from subsamples of the data. This object is generated by the function batch_snf_subsamples().

verbose

If TRUE, output progress to console.

Value

A two-item list: "raw_aris", a list of inter-subsample pairwise ARI matrices (one for each full cluster solution) and "ari_summary", a data frame containing the mean and SD of the inter-subsample ARIs for each original cluster solution.

Examples

```
# my_dl <- data_list(</pre>
      list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
      list(income, "household_income", "demographics", "continuous"),
      list(pubertal, "pubertal_status", "demographics", "continuous"),
#
#
      uid = "unique_id"
# )
# sc <- snf_config(my_dl, n_solutions = 5, max_k = 40)</pre>
# my_dl_subsamples <- subsample_dl(</pre>
#
      my_dl,
#
      n_subsamples = 20,
#
      subsample_fraction = 0.85
#)
# batch_subsample_results <- batch_snf_subsamples(</pre>
      my_dl_subsamples,
#
      sc,
      verbose = TRUE
#
# )
# pairwise_aris <- subsample_pairwise_aris(</pre>
      batch_subsample_results
      verbose = TRUE
#
#)
# # Visualize ARIs
# ComplexHeatmap::Heatmap(
      pairwise_aris[[1]],
      heatmap_legend_param = list(
          color_bar = "continuous",
#
          title = "Inter-Subsample\nARI",
#
          at = c(0, 0.5, 1)
#
#
#
      show_column_names = FALSE,
#
      show\_row\_names = FALSE
#)
```

summarize_clust_fns_list

Summarize a clust_fns_list object

Description

Summarize a clust_fns_list object

Usage

```
summarize_clust_fns_list(cfl)
```

120 summarize_dl

Arguments

cf1

A clust_fns_list class object.

Value

summary_df "data.frame" class object containing the name and index of each clustering algorithm in te provided clust_fns_list.

summarize_dfl

Summarize metrics contained in a dist_fns_list

Description

Summarize metrics contained in a dist_fns_list

Usage

```
summarize_dfl(dist_fns_list)
```

Arguments

```
dist_fns_list A dist_fns_list.
```

Value

"data.frame"-class object summarizing items in a distance metrics list.

summarize_dl

Summarize a data list

Description

[Deprecated] Defunct function for summarizing a data list. Please use summary() instead.

Usage

```
summarize_dl(data_list, scope = "component")
```

Arguments

data_list

A nested list of input data from data_list().

scope

The level of detail for the summary. Options are:

- "component" (default): One row per component (data frame) in the data list
- "feature": One row for each feature in the data list.

summary.data_list 121

Value

data.frame class object summarizing all components (or features if scope == "component").

summary.data_list

Summary method for class data_list

Description

Returns a data list summary (data.frame class object) containing information on components, features, variable types, domains, and component dimensions.

Usage

```
## S3 method for class 'data_list'
summary(object, scope = "component", ...)
```

Arguments

object A data_list class object.

scope The level of detail for the summary. By default, this is set to "component",

which returns a summary of the data list at the component level. Can also be set

to "feature", resulting in a summary at the feature level.

. . . Other arguments passed to summary (not used in this function)

Value

A data frame class object. If scope is "component", each row shows the name, variable type, domain, and dimensions of each component. If scope is "feature", each row shows the name, variable type, and domain of each feature.

summary_features

Pull features used to calculate summary p-values from an object

Description

Pull features used to calculate summary p-values from an object

Usage

```
summary_features(x)
```

Arguments

The object to extract summary features from.

Value

A character vector of summary features.

122 uids

train_test_assign

Training and testing split

Description

Given a vector of uid_id and a threshold, returns a list of which members should be in the training set and which should be in the testing set. The function relies on whether or not the absolute value of the Jenkins's one_at_a_time hash function exceeds the maximum possible value (2147483647) multiplied by the threshold.

Usage

```
train_test_assign(train_frac, uids, seed = 42)
```

Arguments

train_frac The fraction (0 to 1) of observations for training

uids A character vector of UIDs to be distributed into training and test sets.

seed Seed used for Jenkins's one_at_a_time hash function.

Value

A named list containing the training and testing uid_ids.

uids

Pull UIDs from an object

Description

Pull UIDs from an object

Usage

uids(x)

Arguments

Х

The object to extract UIDs from.

Value

A character vector of UIDs.

validate_solutions_df 123

validate_solutions_df Validator for solutions_df class object

Description

Validator for solutions_df class object

Usage

```
validate_solutions_df(sol_dfl)
```

Arguments

sol_dfl

A solutions data frame-like object to be validated and converted into a solutions data frame.

Value

If sol_dfl has a valid structure for a solutions_df class object, returns the input unchanged. Otherwise, raises an error.

var_manhattan_plot

Manhattan plot of feature-feature association p-values

Description

Manhattan plot of feature-feature association p-values

Usage

```
var_manhattan_plot(
   dl,
   key_var,
   neg_log_pval_thresh = 5,
   threshold = NULL,
   point_size = 5,
   text_size = 20,
   plot_title = NULL,
   hide_x_labels = FALSE,
   bonferroni_line = FALSE
)
```

124 weights_matrix

Arguments

dl List of data frames containing data information.

key_var Feature for which the association p-values of all other features are plotted.

neg_log_pval_thresh

Threshold for negative log p-values.

threshold p-value threshold to plot dashed line at.

point_size Size of points in the plot. text_size Size of text in the plot.

plot_title Title of the plot.

hide_x_labels If TRUE, hides x-axis labels.

bonferroni_line

If TRUE, plots a dashed black line at the Bonferroni-corrected equivalent of the p-value threshold.

Value

A Manhattan plot (class "gg", "ggplot") showing the association p-values of features against one key feature in a data list.

```
dl <- data_list(
    list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
    list(income, "household_income", "demographics", "continuous"),
    list(pubertal, "pubertal_status", "demographics", "continuous"),
    list(anxiety, "anxiety", "behaviour", "ordinal"),
    list(depress, "depressed", "behaviour", "ordinal"),
    uid = "unique_id"
)

var_manhattan <- var_manhattan_plot(
    dl,
    key_var = "household_income",
    plot_title = "Correlation of Features with Household Income",
    text_size = 16,
    neg_log_pval_thresh = 3,
    threshold = 0.05
)</pre>
```

weights_matrix 125

Description

Function for building a weights matrix independently of an SNF config. The weights matrix contains one row corresponding to each row of the settings data frame in an SNF config (one row for each resulting cluster solution) and one column for each feature in the data list used for clustering. Values of the weights matrix are passed to distance metrics functions during the conversion of input data frames to distance matrices. Typically, there is no need to use this function directly. Instead, users should provide weights matrix-building parameters to the snf_config() function.

Usage

```
weights_matrix(dl = NULL, n_solutions = 1, weights_fill = "ones")
```

Arguments

dl A nested list of input data from data_list().

weights_fill String indicating what to populate generate rows with. Can be "ones" (default;

fill matrix with 1), "uniform" (fill matrix with uniformly distributed random values), or "exponential" (fill matrix with exponentially distributed random values).

Value

wm A properly formatted matrix containing columns for all the features that require weights and rows.

```
input_dl <- data_list(
    list(subc_v, "subcortical_volume", "neuroimaging", "continuous"),
    list(income, "income", "demographics", "continuous"),
    list(pubertal, "pubertal_status", "demographics", "continuous"),
    uid = "unique_id"
)

sc <- snf_config(input_dl, n_solutions = 5)

wm <- weights_matrix(input_dl, n_solutions = 5, weights_fill = "uniform")

# updating an SNF config in parts
sc$"weights_matrix" <- wm</pre>
```

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