Package 'proBatch'

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Type Package

Title Tools for Diagnostics and Corrections of Batch Effects in Proteomics

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Author Jelena Cuklina <chuklina.jelena@gmail.com>, Chloe H. Lee <chloe.h.lee94@gmail.com>, Patrick Pedrioli <pedrioli@gmail.com>

Maintainer Chloe H. Lee <chloe.h.lee94@gmail.com>

Description These tools facilitate batch effects analysis and correction in high-throughput experiments. It was developed primarily for mass-spectrometry proteomics (DIA/SWATH), but could also be applicable to most omic data with minor adaptations. The package contains functions for diagnostics (proteome/genome-wide and feature-level), correction (normalization and batch effects correction) and quality control. Non-linear fitting based approaches were also included to deal with complex, mass spectrometry-specific signal drifts.

biocViews BatchEffect, Normalization, Preprocessing, Software, MassSpectrometry,Proteomics, QualityControl

License GPL-3

URL https://github.com/symbioticMe/proBatch

BugReports https://github.com/symbioticMe/proBatch/issues

Depends R (>= 3.6)

Encoding UTF-8

LazyData true

Imports Biobase, corrplot, dplyr, data.table, ggfortify, ggplot2, grDevices, lazyeval, lubridate, magrittr, pheatmap, preprocessCore, purrr, pvca, RColorBrewer, reshape2, rlang, scales, stats, sva, tidyr, tibble, tools, utils, viridis, wesanderson, WGCNA

Suggests knitr, rmarkdown, devtools, ggpubr, gtable, gridExtra, roxygen2, testthat (>= 2.1.0), spelling

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R topics documented:

`calculate_feature_CV` *Calculate CV distribution for each feature*

Description

Calculate CV distribution for each feature

Usage

```
calculate_feature_CV(
  df_long,
  sample_annotation = NULL,
  feature_id_col = "peptide_group_label",
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  batch_col = NULL,
  biospecimen_id_col = NULL,
  unlog = TRUE,
  log_base = 2,
  offset = 1
)
```

Arguments

`df_long`	data frame where each row is a single feature in a single sample. It minimally has a `sample_id_col`, a `feature_id_col` and a `measure_col`, but usually also an `m_score` (in OpenSWATH output result file). See `help("example_proteome")` for more details.
`sample_annotation`	data frame with: 1. `sample_id_col` (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See `help("example_sample_annotation")`
`feature_id_col`	name of the column with feature/gene/peptide/protein ID used in the long format representation `df_long`. In the wide formatted representation `data_matrix` this corresponds to the row names.

sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).
measure_col	if df_long is among the parameters, it is the column with expression/abundance/intensity; otherwise, it is used internally for consistency.
batch_col	column in sample_annotation that should be used for batch comparison (or other, non-batch factor to be mapped to color in plots).
biospecimen_id_col	column in sample_annotation that defines a unique bio ID, which is usually a combination of conditions or groups. Tip: if such ID is absent, but can be defined from several columns, create new biospecimen_id column
unlog	(logical) whether to reverse log transformation of the original data
log_base	base of the logarithm for transformation
offset	small positive number to prevent 0 conversion to -Inf

Value

data frame with Total CV for each feature & (optionally) per-batch CV

Examples

```
CV_df = calculate_feature_CV(example_proteome,
sample_annotation = example_sample_annotation,
measure_col = 'Intensity',
batch_col = 'MS_batch')
```

---

calculate_peptide_corr_distr

Calculate peptide correlation between and within peptides of one protein

---

Description

Calculate peptide correlation between and within peptides of one protein

Usage

```
calculate_peptide_corr_distr(
  data_matrix,
  peptide_annotation,
  protein_col = "ProteinName",
  feature_id_col = "peptide_group_label"
)
```

Arguments

data_matrix	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use help("example_proteome_matrix"))
peptide_annotation	long format data frame with peptide ID and their corresponding protein and/or gene annotations. See help("example_peptide_annotation").
protein_col	column where protein names are specified
feature_id_col	name of the column with feature/gene/peptide/protein ID used in the long format representation df_long. In the wide formatted representation data_matrix this corresponds to the row names.

Value

dataframe with peptide correlation coefficients that are suggested to use for plotting in plot_peptide_corr_distribution as plot_param:

Examples

```
selected_genes = c('BOVINE_A1ag','BOVINE_FetuinB','Cyfip1')
gene_filter = example_peptide_annotation$Gene %in% selected_genes
peptides_ann = example_peptide_annotation$peptide_group_label
selected_peptides = peptides_ann[gene_filter]
matrix_test = example_proteome_matrix[selected_peptides,]
pep_annotation_sel = example_peptide_annotation[gene_filter, ]
corr_distribution = calculate_peptide_corr_distr(matrix_test,
pep_annotation_sel, protein_col = 'Gene')
```

---

calculate_PVCA *Calculate variance distribution by variable*

Description

Calculate variance distribution by variable

Usage

```
calculate_PVCA(
  data_matrix,
  sample_annotation,
  feature_id_col = "peptide_group_label",
  sample_id_col = "FullRunName",
  factors_for_PVCA = c("MS_batch", "digestion_batch", "Diet", "Sex", "Strain"),
  pca_threshold = 0.6,
  variance_threshold = 0.01,
  fill_the_missing = -1
)
```

Arguments

data_matrix	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use help("example_proteome_matrix"))
sample_annotation	data frame with: 1. sample_id_col (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See help("example_sample_annotation")
feature_id_col	name of the column with feature/gene/peptide/protein ID used in the long format representation df_long. In the wide formatted representation data_matrix this corresponds to the row names.
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).
factors_for_PVCA	vector of factors from sample_annotation, that are used in PVCA analysis
pca_threshold	the percentile value of the minimum amount of the variabilities that the selected principal components need to explain
variance_threshold	the percentile value of weight each of the factors needs to explain (the rest will be lumped together)
fill_the_missing	numeric value determining how missing values should be substituted. If NULL, features with missing values are excluded.

Value

data frame of weights of Principal Variance Components

Examples

```
matrix_test <- example_proteome_matrix[1:150, ]
pvca_df <- calculate_PVCA(matrix_test, example_sample_annotation,
factors_for_PVCA = c('MS_batch', 'digestion_batch',"Diet", "Sex", "Strain"),
pca_threshold = .6, variance_threshold = .01, fill_the_missing = -1)
```

---

calculate_sample_corr_distr

Calculates correlation for all pairs of the samples in data matrix, labels as replicated/same_batch/unrelated in output columns (see "Value").

Description

Calculates correlation for all pairs of the samples in data matrix, labels as replicated/same_batch/unrelated in output columns (see "Value").

Usage

```
calculate_sample_corr_distr(
  data_matrix,
  sample_annotation,
  repeated_samples = NULL,
  biospecimen_id_col = "EarTag",
  sample_id_col = "FullRunName",
  batch_col = "MS_batch"
)
```

Arguments

`data_matrix`	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use `help("example_proteome_matrix")`)
`sample_annotation`	data frame with: 1. `sample_id_col` (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See `help("example_sample_annotation")`
`repeated_samples`	vector of sample IDs to evaluate, if `NULL`, all samples are taken into account for plotting
`biospecimen_id_col`	column in `sample_annotation` that defines a unique bio ID, which is usually a combination of conditions or groups. Tip: if such ID is absent, but can be defined from several columns, create new `biospecimen_id` column
`sample_id_col`	name of the column in `sample_annotation` table, where the filenames (colnames of the `data_matrix` are found).
`batch_col`	column in `sample_annotation` that should be used for batch comparison (or other, non-batch factor to be mapped to color in plots).

Value

dataframe with the following columns, that are suggested to use for plotting in `plot_sample_corr_distribution` as `plot_param`:

1. `replicate`
2. `batch_the_same`
3. `batch_replicate`

4. batches

other columns are:

1. sample_id_1 & sample_id_2, both generated from sample_id_col variable
2. correlation - correlation of two corresponding samples
3. batch_1 & batch_2 or analogous, created the same as sample_id_1

Examples

```
corr_distribution = calculate_sample_corr_distr(data_matrix = example_proteome_matrix,
sample_annotation = example_sample_annotation,
batch_col = 'MS_batch',biospecimen_id_col = "EarTag")
```

---

check_sample_consistency

Check if sample annotation is consistent with data matrix and join the two

---

Description

Check if sample annotation is consistent with data matrix and join the two

Usage

```
check_sample_consistency(
  sample_annotation,
  sample_id_col,
  df_long,
  batch_col = NULL,
  order_col = NULL,
  facet_col = NULL,
  merge = TRUE
)
```

Arguments

sample_annotation	data frame with: 1. sample_id_col (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See help("example_sample_annotation")
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).

df_long	data frame where each row is a single feature in a single sample. It minimally has a sample_id_col, a feature_id_col and a measure_col, but usually also an m_score (in OpenSWATH output result file). See help("example_proteome") for more details.
batch_col	column in sample_annotation that should be used for batch comparison (or other, non-batch factor to be mapped to color in plots).
order_col	column in sample_annotation that determines sample order. It is used for in initial assessment plots (plot_sample_mean_or_boxplot) and feature-level diagnostics (feature_level_diagnostics). Can be 'NULL' if sample order is irrelevant (e.g. in genomic experiments). For more details, order definition/inference, see define_sample_order and date_to_sample_order
facet_col	column in sample_annotation with a batch factor to separate plots into facets; usually 2nd to batch_col. Most meaningful for multi-instrument MS experiments (where each instrument has its own order-associated effects (see order_col) or simultaneous examination of two batch factors (e.g. preparation day and measurement day). For single-instrument case should be set to 'NULL'
merge	(logical) whether to merge df_long with sample_annotation or not

Value

df_long format data frame, merged with sample_annotation using inner_join (samples represented in both)

Examples

```
df_test = check_sample_consistency(sample_annotation = example_sample_annotation,
df_long = example_proteome, sample_id_col = 'FullRunName',
batch_col = NULL, order_col = NULL, facet_col = NULL)
```

---

correct_batch_effects *Batch correction of normalized data*

Description

Batch correction of normalized data. Batch correction brings each feature in each batch to the comparable shape. Currently the following batch correction functions are implemented:

1. Per-feature median centering: center_feature_batch_medians_df(). Median centering of the features (per batch median).
2. correction with ComBat: correct_with_ComBat_df(). Adjusts for discrete batch effects using ComBat. ComBat, described in Johnson et al. 2007. It uses either parametric or non-parametric empirical Bayes frameworks for adjusting data for batch effects. Users are returned an expression matrix that has been corrected for batch effects. The input data are assumed to be free of missing values and normalized before batch effect removal. Please note that missing values are common in proteomics, which is why in some cases corrections like center_peptide_batch_medians_df are more appropriate.

3. Continuous drift correction: `adjust_batch_trend_df()`. Adjust batch signal trend with the custom (continuous) fit. Should be followed by discrete corrections, e.g. `center_feature_batch_medians_df()` or `correct_with_ComBat_df()`.

Alternatively, one can call the correction function with `correct_batch_effects_df()` wrapper. Batch correction method allows correction of continuous signal drift within batch (if required) and adjustment for discrete difference across batches.

Usage

```
center_feature_batch_medians_df(
  df_long,
  sample_annotation = NULL,
  sample_id_col = "FullRunName",
  batch_col = "MS_batch",
  feature_id_col = "peptide_group_label",
  measure_col = "Intensity",
  keep_all = "default",
  no_fit_imputed = TRUE,
  qual_col = NULL,
  qual_value = NULL
)

center_feature_batch_medians_dm(
  data_matrix,
  sample_annotation,
  sample_id_col = "FullRunName",
  batch_col = "MS_batch",
  feature_id_col = "peptide_group_label",
  measure_col = "Intensity"
)

center_feature_batch_means_df(
  df_long,
  sample_annotation = NULL,
  sample_id_col = "FullRunName",
  batch_col = "MS_batch",
  feature_id_col = "peptide_group_label",
  measure_col = "Intensity",
  keep_all = "default",
  no_fit_imputed = TRUE,
  qual_col = NULL,
  qual_value = NULL
)

center_feature_batch_means_dm(
  data_matrix,
  sample_annotation,
  sample_id_col = "FullRunName",
```

```
  batch_col = "MS_batch",
  feature_id_col = "peptide_group_label",
  measure_col = "Intensity"
)

adjust_batch_trend_df(
  df_long,
  sample_annotation = NULL,
  batch_col = "MS_batch",
  feature_id_col = "peptide_group_label",
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  order_col = "order",
  keep_all = "default",
  fit_func = "loess_regression",
  no_fit_imputed = TRUE,
  qual_col = NULL,
  qual_value = NULL,
  min_measurements = 8,
  ...
)

adjust_batch_trend_dm(
  data_matrix,
  sample_annotation,
  batch_col = "MS_batch",
  feature_id_col = "peptide_group_label",
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  order_col = "order",
  fit_func = "loess_regression",
  return_fit_df = TRUE,
  min_measurements = 8,
  ...
)

correct_with_ComBat_df(
  df_long,
  sample_annotation = NULL,
  feature_id_col = "peptide_group_label",
  measure_col = "Intensity",
  sample_id_col = "FullRunName",
  batch_col = "MS_batch",
  par.prior = TRUE,
  no_fit_imputed = TRUE,
  qual_col = NULL,
  qual_value = NULL,
  keep_all = "default"
```

```
)

correct_with_ComBat_dm(
  data_matrix,
  sample_annotation = NULL,
  feature_id_col = "peptide_group_label",
  measure_col = "Intensity",
  sample_id_col = "FullRunName",
  batch_col = "MS_batch",
  par.prior = TRUE
)

correct_batch_effects_df(
  df_long,
  sample_annotation,
  continuous_func = NULL,
  discrete_func = c("MedianCentering", "MeanCentering", "ComBat"),
  batch_col = "MS_batch",
  feature_id_col = "peptide_group_label",
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  order_col = "order",
  keep_all = "default",
  no_fit_imputed = TRUE,
  qual_col = NULL,
  qual_value = NULL,
  min_measurements = 8,
  ...
)

correct_batch_effects_dm(
  data_matrix,
  sample_annotation,
  continuous_func = NULL,
  discrete_func = c("MedianCentering", "ComBat"),
  batch_col = "MS_batch",
  feature_id_col = "peptide_group_label",
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  order_col = "order",
  min_measurements = 8,
  ...
)
```

Arguments

df_long	data frame where each row is a single feature in a single sample. It minimally has a sample_id_col, a feature_id_col and a measure_col, but usually also an m_score (in OpenSWATH output result file). See help("example_proteome")

for more details.

`sample_annotation`
: data frame with:
  1. `sample_id_col` (this can be repeated as row names)
  2. biological covariates
  3. technical covariates (batches etc)

  . See `help("example_sample_annotation")`

`sample_id_col`
: name of the column in `sample_annotation` table, where the filenames (colnames of the `data_matrix` are found).

`batch_col`
: column in `sample_annotation` that should be used for batch comparison (or other, non-batch factor to be mapped to color in plots).

`feature_id_col`
: name of the column with feature/gene/peptide/protein ID used in the long format representation `df_long`. In the wide formatted representation `data_matrix` this corresponds to the row names.

`measure_col`
: if `df_long` is among the parameters, it is the column with expression/abundance/intensity; otherwise, it is used internally for consistency.

`keep_all`
: when transforming the data (normalize, correct) - acceptable values: all/default/minimal (which set of columns be kept).

`no_fit_imputed`
: (logical) whether to use imputed (requant) values, as flagged in `qual_col` by `qual_value` for data transformation

`qual_col`
: column to color point by certain value denoted by `color_by_qual_value`. Design with inferred/requant values in OpenSWATH output data, which means argument value has to be set to `m_score`.

`qual_value`
: value in `qual_col` to color. For OpenSWATH data, this argument value has to be set to 2 (this is an `m_score` value for imputed values (requant values).

`data_matrix`
: features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use `help("example_proteome_matrix")`)

`order_col`
: column in `sample_annotation` that determines sample order. It is used for in initial assessment plots (plot_sample_mean_or_boxplot) and feature-level diagnostics (feature_level_diagnostics). Can be 'NULL' if sample order is irrelevant (e.g. in genomic experiments). For more details, order definition/inference, see define_sample_order and date_to_sample_order

`fit_func`
: function to fit the (non)-linear trend

`min_measurements`
: the number of samples in a batch required for curve fitting.

`...`
: other parameters, usually of `adjust_batch_trend`, and `fit_func`.

`return_fit_df`
: (logical) whether to return the `fit_df` from `adjust_batch_trend_dm` or only the data matrix

`par.prior`
: use parametrical or non-parametrical prior

`continuous_func`
: function to use for the fit (currently only `loess_regression` available); if order-associated fix is not required, should be `NULL`.

`discrete_func`
: function to use for adjustment of discrete batch effects (`MedianCentering` or `ComBat`).

Value

the data in the same format as input (`data_matrix` or `df_long`). For `df_long` the data frame stores the original values of `measure_col` in another column called "preBatchCorr_[measure_col]", and the normalized values in `measure_col` column.

The function `adjust_batch_trend_dm()`, if `return_fit_df` is `TRUE` returns list of two items:

1. `data_matrix`
2. `fit_df`, used to examine the fitting curves

See Also

`fit_nonlinear`

`fit_nonlinear`, `plot_with_fitting_curve`

`fit_nonlinear`, `plot_with_fitting_curve`

Examples

```
#Median centering per feature per batch:
median_centered_df <- center_feature_batch_medians_df(
example_proteome, example_sample_annotation)

#Correct with ComBat:
combat_corrected_df <- correct_with_ComBat_df(example_proteome,
example_sample_annotation)

#Adjust the MS signal drift:
test_peptides = unique(example_proteome$peptide_group_label)[1:3]
test_peptide_filter = example_proteome$peptide_group_label %in% test_peptides
test_proteome = example_proteome[test_peptide_filter,]
adjusted_df <- adjust_batch_trend_df(test_proteome,
example_sample_annotation, span = 0.7,
min_measurements = 8)
plot_fit <- plot_with_fitting_curve(unique(adjusted_df$peptide_group_label),
df_long = adjusted_df, measure_col = 'preTrendFit_Intensity',
fit_df = adjusted_df, sample_annotation = example_sample_annotation)

#Correct the data in one go:
batch_corrected_matrix <- correct_batch_effects_df(example_proteome,
example_sample_annotation,
continuous_func = 'loess_regression',
discrete_func = 'MedianCentering',
batch_col = 'MS_batch',
span = 0.7, min_measurements = 8)
```

create_peptide_annotation *Prepare peptide annotation from long format data frame Create light-weight peptide annotation data frame for selection of illustrative proteins*

Description

Prepare peptide annotation from long format data frame

Create light-weight peptide annotation data frame for selection of illustrative proteins

Usage

```
create_peptide_annotation(
  df_long,
  feature_id_col = "peptide_group_label",
  protein_col = c("ProteinName", "Gene")
)
```

Arguments

df_long	data frame where each row is a single feature in a single sample. It minimally has a sample_id_col, a feature_id_col and a measure_col, but usually also an m_score (in OpenSWATH output result file). See help("example_proteome") for more details.
feature_id_col	name of the column with feature/gene/peptide/protein ID used in the long format representation df_long. In the wide formatted representation data_matrix this corresponds to the row names.
protein_col	column where protein names are specified

Value

data frame containing petpide annotations

See Also

plot_peptides_of_one_protein, plot_protein_corrplot

Examples

```
generated_peptide_annotation <- create_peptide_annotation(
example_proteome, feature_id_col = "peptide_group_label",
protein_col = c("Protein"))
```

`dates_to_posix` *Convert data/time to POSIXct*

Description

convert date/time column of sample_annotation to POSIX format required to keep number-like behavior

Usage

```
dates_to_posix(
  sample_annotation,
  time_column = c("RunDate", "RunTime"),
  new_time_column = "DateTime",
  dateTimeFormat = c("%b_%d", "%H:%M:%S"),
  tz = "GMT"
)
```

Arguments

`sample_annotation`	data frame with: 1. `sample_id_col` (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See `help("example_sample_annotation")`
`time_column`	name of the column(s) where run date & time are specified. These will be used to determine the run order
`new_time_column`	name of the new column to which date&time will be converted to
`dateTimeFormat`	POSIX format of the date and time. See `as.POSIXct` from base R for details
`tz`	for time zone

Value

sample annotation file with a new column `new_time_column` with POSIX-formatted date

Examples

```
date_to_posix <- dates_to_posix(example_sample_annotation,
time_column = c('RunDate','RunTime'),
new_time_column = 'DateTime_new',
dateTimeFormat = c("%b_%d", "%H:%M:%S"))
```

`date_to_sample_order` *Convert date/time to POSIXct and rank samples by it*

Description

Converts date/time columns fo sample_annotation to POSIXct format and calculates sample run rank in order column

Usage

```
date_to_sample_order(
  sample_annotation,
  time_column = c("RunDate", "RunTime"),
  new_time_column = "DateTime",
  dateTimeFormat = c("%b_%d", "%H:%M:%S"),
  new_order_col = "order",
  instrument_col = "instrument"
)
```

Arguments

`sample_annotation`
: data frame with:

  1. `sample_id_col` (this can be repeated as row names)
  2. biological covariates
  3. technical covariates (batches etc)

  . See `help("example_sample_annotation")`

`time_column`
: name of the column(s) where run date & time are specified. These will be used to determine the run order

`new_time_column`
: name of the new column to which date&time will be converted to

`dateTimeFormat`
: POSIX format of the date and time. See `as.POSIXct` from base R for details

`new_order_col`
: name of column with generated the order of sample run based on time columns

`instrument_col`
: column, denoting different instrument used for measurements

Value

sample annotation file with a new column `new_time_column` with POSIX-formatted date & `new_order_col` used in some diagnostic plots (e.g. `plot_iRT`, `plot_sample_mean`)

Examples

```
sample_annotation_wOrder <- date_to_sample_order(
example_sample_annotation,
time_column = c('RunDate','RunTime'),
new_time_column = 'new_DateTime',
dateTimeFormat = c("%b_%d", "%H:%M:%S"),
new_order_col = 'new_order',
instrument_col = NULL)
```

`define_sample_order` *Defining sample order internally*

Description

Defining sample order internally

Usage

```
define_sample_order(
  order_col,
  sample_annotation,
  facet_col,
  batch_col,
  df_long,
  sample_id_col,
  color_by_batch
)
```

Arguments

`order_col`	column in `sample_annotation` that determines sample order. It is used for in initial assessment plots (plot_sample_mean_or_boxplot) and feature-level diagnostics (feature_level_diagnostics). Can be 'NULL' if sample order is irrelevant (e.g. in genomic experiments). For more details, order definition/inference, see define_sample_order and date_to_sample_order
`sample_annotation`	data frame with: 1. `sample_id_col` (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See `help("example_sample_annotation")`
`facet_col`	column in `sample_annotation` with a batch factor to separate plots into facets; usually 2nd to `batch_col`. Most meaningful for multi-instrument MS experiments (where each instrument has its own order-associated effects (see `order_col`) or simultaneous examination of two batch factors (e.g. preparation day and measurement day). For single-instrument case should be set to 'NULL'

batch_col	column in sample_annotation that should be used for batch comparison (or other, non-batch factor to be mapped to color in plots).
df_long	data frame where each row is a single feature in a single sample. It minimally has a sample_id_col, a feature_id_col and a measure_col, but usually also an m_score (in OpenSWATH output result file). See help("example_proteome") for more details.
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).
color_by_batch	(logical) whether to color points and connecting lines by batch factor as defined by batch_col.

Value

list of two items: order_col new name and new df_long

See Also

plot_sample_mean_or_boxplot, feature_level_diagnostics

Examples

```
sample_order = define_sample_order(order_col = 'order',
sample_annotation = example_sample_annotation,
facet_col = NULL, batch_col = 'MS_batch', df_long = example_proteome,
sample_id_col = 'FullRunName', color_by_batch = TRUE)
new_order_col = sample_order$order_col
df_long = sample_order$df_long
```

---

example_peptide_annotation

Peptide annotation data

Description

This is data from Aging study annotated with gene names

Usage

```
example_peptide_annotation
```

Format

A data frame with 535 rows and 10 variables:

peptide_group_label peptide group label ID, identical to peptide_group_label in example_proteome

Gene HUGO gene ID

ProteinName protein group name as specified in example_proteome

example_proteome *Example protein data in long format*

Description

This is OpenSWATH-output data from Aging study with all iRT, spike-in peptides, few representative peptides and proteins for signal improvement demonstration. Using `matrix_to_long` can be converted to `example_proteome_matrix`

Usage

```
example_proteome
```

Format

A data frame with 124655 rows and 7 variables:

peptide_group_label peptide ID, which is regular feature level. This column is mostly used as `feature_id_col`used for merging with `"example_peptide_annotation"`

Intensity peptide group intensity in given sample. Used in function as `measure_col`

Protein Protein group ID, specified as N/UniProtID1|UniProtID2|..., where N is number of protein peptide group maps to. If 1/UniProtID, then this is proteotypic peptide, in functions used as `protein_col`

FullRunName name of the file, in most functions used for `sample_id_col`

m_score column marking the quality of peptide IDs, used as `qual_col` throughout the script; when `qual_value` is 2 in this column, peptide has been imputed (requantified) ...

Source

PRIDE ID will be added upon the publication of the dataset

example_proteome_matrix *Example protein data in matrix*

Description

This is measurement data from Aging study with columns representing samples and rows representing peptides. Generated by `long_to_matrix`

Usage

```
example_proteome_matrix
```

Format

A matrix with 535 rows and 233 columns:

Source

PRIDE ID will be added upon the publication of the dataset

`example_sample_annotation`

Sample annotation data version 1

Description

This is data from BXD mouse population aging study with mock instruments to show how instrument-specific functionality works

Usage

```
example_sample_annotation
```

Format

A data frame with 233 rows and 11 variables:

FullRunName name of the file with the measurement for each sample, referred to as `sample_id_col`

MS_batch mass-spectrometry batch: 4-level factor of manually annotated batches

EarTag mouse ID, i.e. ID of the biological object. Only 14 mice have been replicated, one mouse was profiled 7 times.

Strain mouse strain ID from BXD population set - biological covariate #1, 51 Strain represented

Diet diet, biological covariate #2 - either `HFD` = 'High Fat Diet' or `CD` = 'Chow Diet'

Sex mice sex - biological covariate #3

RunDate mass-spectrometry running date. In combination with `RunTime` used for running order determination. Vector of class `"difftime"` and `"hms"`

RunTime mass-spectrometry running time. In combination with `RunDate` used for running order determination.Vector of class `"POSIXct"` and `"POSIXt"`

DateTime numeric date and time generated by `date_to_sample_order`

order order of samples generated by sorting DateTime in `date_to_sample_order`

digestion_batch peptide digestion batch: 4-level factor of manually annotated batches ...

`feature_level_diagnostics` *Ploting peptide measurements*

Description

Creates a peptide faceted ggplot2 plot of the value in `measure_col` vs `order_col` (if 'NULL', x-axis is simply a sample name order). Additionally, the resulting plot can also be colored either by batch factor, by quality factor (e.g. imputated/non-imputed) and, if needed, faceted by another batch factor, e.g. an instrument. If the non-linear curve was fit, this can also be added to the plot, see functions specific to each case below

Usage

```
plot_single_feature(
  feature_name,
  df_long,
  sample_annotation = NULL,
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  feature_id_col = "peptide_group_label",
  geom = c("point", "line"),
  qual_col = NULL,
  qual_value = NULL,
  batch_col = "MS_batch",
  color_by_batch = FALSE,
  color_scheme = "brewer",
  order_col = "order",
  vline_color = "red",
  facet_col = NULL,
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = NULL,
  theme = "classic",
  ylimits = NULL
)

plot_peptides_of_one_protein(
  protein_name,
  peptide_annotation = NULL,
  protein_col = "ProteinName",
  df_long,
  sample_annotation = NULL,
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
```

```
  feature_id_col = "peptide_group_label",
  geom = c("point", "line"),
  qual_col = NULL,
  qual_value = NULL,
  batch_col = "MS_batch",
  color_by_batch = FALSE,
  color_scheme = "brewer",
  order_col = "order",
  vline_color = "red",
  facet_col = NULL,
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = sprintf("Peptides of %s protein", protein_name),
  theme = "classic"
)

plot_spike_in(
  spike_ins = "BOVIN",
  peptide_annotation = NULL,
  protein_col = "ProteinName",
  df_long,
  sample_annotation = NULL,
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  feature_id_col = "peptide_group_label",
  geom = c("point", "line"),
  qual_col = NULL,
  qual_value = NULL,
  batch_col = "MS_batch",
  color_by_batch = FALSE,
  color_scheme = "brewer",
  order_col = "order",
  vline_color = "red",
  facet_col = NULL,
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = sprintf("Spike-in %s plots", spike_ins),
  theme = "classic"
)

plot_iRT(
  irt_pattern = "iRT",
  peptide_annotation = NULL,
  protein_col = "ProteinName",
```

```
  df_long,
  sample_annotation = NULL,
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  feature_id_col = "peptide_group_label",
  geom = c("point", "line"),
  qual_col = NULL,
  qual_value = NULL,
  batch_col = "MS_batch",
  color_by_batch = FALSE,
  color_scheme = "brewer",
  order_col = "order",
  vline_color = "red",
  facet_col = NULL,
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = "iRT peptide profile",
  theme = "classic"
)

plot_with_fitting_curve(
  feature_name,
  fit_df,
  fit_value_col = "fit",
  df_long,
  sample_annotation = NULL,
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  feature_id_col = "peptide_group_label",
  geom = c("point", "line"),
  qual_col = NULL,
  qual_value = NULL,
  batch_col = "MS_batch",
  color_by_batch = FALSE,
  color_scheme = "brewer",
  order_col = "order",
  vline_color = "grey",
  facet_col = NULL,
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),

  plot_title = sprintf("Fitting curve of %s \n                                peptide",
    paste(feature_name, collapse = " ")),
  theme = "classic"
```

)

Arguments

feature_name	name of the selected feature (e.g. peptide) for diagnostic profiling
df_long	data frame where each row is a single feature in a single sample. It minimally has a sample_id_col, a feature_id_col and a measure_col, but usually also an m_score (in OpenSWATH output result file). See help("example_proteome") for more details.
sample_annotation	data frame with: 1. sample_id_col (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See help("example_sample_annotation")
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).
measure_col	if df_long is among the parameters, it is the column with expression/abundance/intensity; otherwise, it is used internally for consistency.
feature_id_col	name of the column with feature/gene/peptide/protein ID used in the long format representation df_long. In the wide formatted representation data_matrix this corresponds to the row names.
geom	whether to show the feature as points and/or connect by lines (accepted values are: 1. point, line and c('point', 'line'))
qual_col	column to color point by certain value denoted by color_by_qual_value. Design with inferred/requant values in OpenSWATH output data, which means argument value has to be set to m_score.
qual_value	value in qual_col to color. For OpenSWATH data, this argument value has to be set to 2 (this is an m_score value for imputed values (requant values).
batch_col	column in sample_annotation that should be used for batch comparison (or other, non-batch factor to be mapped to color in plots).
color_by_batch	(logical) whether to color points and connecting lines by batch factor as defined by batch_col.
color_scheme	a named vector of colors to map to batch_col, names corresponding to the levels of the factor. For continuous variables, vector doesn't need to be named.
order_col	column in sample_annotation that determines sample order. It is used for in initial assessment plots (plot_sample_mean_or_boxplot) and feature-level diagnostics (feature_level_diagnostics). Can be 'NULL' if sample order is irrelevant (e.g. in genomic experiments). For more details, order definition/inference, see define_sample_order and date_to_sample_order
vline_color	color of vertical lines, typically separating different MS batches in ordered runs; should be 'NULL' for experiments without intrinsic order

facet_col	column in sample_annotation with a batch factor to separate plots into facets; usually 2nd to batch_col. Most meaningful for multi-instrument MS experiments (where each instrument has its own order-associated effects (see order_col) or simultaneous examination of two batch factors (e.g. preparation day and measurement day). For single-instrument case should be set to 'NULL'
filename	path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported
width	option determining the output image width
height	option determining the output image width
units	units: 'cm', 'in' or 'mm'
plot_title	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
theme	ggplot theme, by default classic. Can be easily overriden
ylimits	range of y-axis to plot feature-level trends
protein_name	name of the protein as defined in ProteinName
peptide_annotation	long format data frame with peptide ID and their corresponding protein and/or gene annotations. See help("example_peptide_annotation").
protein_col	column where protein names are specified
spike_ins	name of feature(s), typically proteins that were spiked in for control
irt_pattern	substring used to identify iRT proteins in the column 'ProteinName'
fit_df	data frame output of adjust_batch_trend_df to be plotted with the line
fit_value_col	column in fit_df where the values for fitting trend are found

Value

ggplot2 type plot of measure_col vs order_col, faceted by feature_name and (optionally) by batch_col

Examples

```
single_feature_plot <- plot_single_feature(feature_name = "46213_NVGVSFYADKPEVTQEQK_2",
df_long = example_proteome, example_sample_annotation,
qual_col = NULL)

#color measurements by factor, related to order (MS_batch)
plot_single_feature(feature_name = "46213_NVGVSFYADKPEVTQEQK_2",
df_long = example_proteome, example_sample_annotation,
qual_col = NULL, color_by_batch = TRUE, batch_col = 'MS_batch')

#color measurements by factor, with order-unrelated factor
single_feature_plot <- plot_single_feature(feature_name = "46213_NVGVSFYADKPEVTQEQK_2",
df_long = example_proteome, example_sample_annotation,
qual_col = NULL, color_by_batch = TRUE, batch_col = 'Diet', geom = 'point',
vline_color = NULL)
```

```
#saving the plot
## Not run:
single_feature_plot <- plot_single_feature(feature_name = "46213_NVGVSFYADKPEVTQEQK_2",
df_long = example_proteome, example_sample_annotation,
qual_col = NULL, filename = 'test_peptide.png',
width = 28, height = 18, units = 'cm')

## End(Not run)

#to examine peptides of a single protein:
peptides_of_one_protein_plot <- plot_peptides_of_one_protein (
protein_name = "Haao", peptide_annotation = example_peptide_annotation,
protein_col = "Gene", df_long = example_proteome,
sample_annotation = example_sample_annotation,
order_col = 'order', sample_id_col = 'FullRunName',
batch_col = 'MS_batch')

#saving the peptides of one protein
## Not run:
 peptides_of_one_protein_plot <- plot_peptides_of_one_protein (
protein_name = "Haao", peptide_annotation = example_peptide_annotation,
protein_col = "Gene", df_long = example_proteome,
sample_annotation = example_sample_annotation,
order_col = 'order', sample_id_col = 'FullRunName',
batch_col = 'MS_batch',
filename = 'test_protein.png', width = 14, height = 9, units = 'in')
## End(Not run)

#to illustrate spike-ins:
spike_in_plot <- plot_spike_in(spike_ins = "BOVINE_A1ag",
peptide_annotation = example_peptide_annotation, protein_col = 'Gene',
df_long = example_proteome, sample_annotation = example_sample_annotation,
sample_id_col = 'FullRunName',
plot_title = "Spike-in BOVINE protein peptides")

#to illustrate iRT peptides:
irt_plot <- plot_iRT(irt_pattern = "iRT",
peptide_annotation = example_peptide_annotation,
df_long = example_proteome, sample_annotation = example_sample_annotation,
protein_col = 'Gene')

#illustrate the fitting curve:
special_peptide = example_proteome$peptide_group_label == "10231_QDVDVWLWQQEGSSK_2"
loess_fit_70 <- adjust_batch_trend_df(example_proteome[special_peptide,],
example_sample_annotation, span = 0.7)

fitting_curve_plot <- plot_with_fitting_curve(feature_name = "10231_QDVDVWLWQQEGSSK_2",
df_long = example_proteome, sample_annotation = example_sample_annotation,
fit_df = loess_fit_70, plot_title = "Curve fitting with 70% span")

#with curves colored by the corresponding batch:
fitting_curve_plot <- plot_with_fitting_curve(feature_name = "10231_QDVDVWLWQQEGSSK_2",
```

```
df_long = example_proteome, sample_annotation = example_sample_annotation,
fit_df = loess_fit_70, plot_title = "Curve fitting with 70% span",
color_by_batch = TRUE, batch_col = 'MS_batch')
```

`fit_nonlinear` *Fit a non-linear trend (currently optimized for LOESS)*

Description

Fit a non-linear trend (currently optimized for LOESS)

Usage

```
fit_nonlinear(
  df_feature_batch,
  measure_col = "Intensity",
  order_col = "order",
  feature_id = NULL,
  batch_id = NULL,
  fit_func = "loess_regression",
  optimize_span = FALSE,
  no_fit_imputed = TRUE,
  qual_col = "m_score",
  qual_value = 2,
  min_measurements = 8,
  ...
)
```

Arguments

`df_feature_batch`	data frame containing response variable e.g. samples in order and explanatory variable e.g. measurement for a specific feature (peptide) in a specific batch
`measure_col`	if `df_long` is among the parameters, it is the column with expression/abundance/intensity; otherwise, it is used internally for consistency.
`order_col`	column in `sample_annotation` that determines sample order. It is used for in initial assessment plots (plot_sample_mean_or_boxplot) and feature-level diagnostics (feature_level_diagnostics). Can be 'NULL' if sample order is irrelevant (e.g. in genomic experiments). For more details, order definition/inference, see define_sample_order and date_to_sample_order
`feature_id`	the name of the feature, required for warnings
`batch_id`	the name of the batch, required for warnings
`fit_func`	function to use for the fit, e.g. `loess_regression`
`optimize_span`	logical, whether to specify span or optimize it (specific entirely for LOESS regression)

no_fit_imputed	(logical) whether to fit the imputed (requant) values
qual_col	column to color point by certain value denoted by color_by_qual_value. Design with inferred/requant values in OpenSWATH output data, which means argument value has to be set to m_score.
qual_value	value in qual_col to color. For OpenSWATH data, this argument value has to be set to 2 (this is an m_score value for imputed values (requant values).
min_measurements	the absolute threshold to filter
...	additional parameters to be passed to the fitting function

Value

vector of fitted response values

Examples

```
test_peptide = example_proteome$peptide_group_label[1]
selected_peptide = example_proteome$peptide_group_label == test_peptide
df_selected = example_proteome[selected_peptide,]
selected_batch = example_sample_annotation$MS_batch == 'Batch_1'
batch_selected_df = example_sample_annotation[selected_batch,]
df_for_test = merge(df_selected, batch_selected_df, by = 'FullRunName')
fit_values = fit_nonlinear(df_for_test)

#for the case where are two many missing values, no curve is fit
selected_batch = example_sample_annotation$MS_batch == 'Batch_2'
batch_selected_df = example_sample_annotation[selected_batch,]
df_for_test = merge(df_selected, batch_selected_df, by = 'FullRunName')
fit_values = fit_nonlinear(df_for_test)
missing_values = df_for_test[['m_score']] == 2
all(fit_values[!is.na(fit_values)] == df_for_test[['Intensity']][!missing_values])
```

---

long_to_matrix *Long to wide data format conversion*

Description

Convert from a long data frame representation to a wide matrix representation

Usage

```
long_to_matrix(
  df_long,
  feature_id_col = "peptide_group_label",
  measure_col = "Intensity",
  sample_id_col = "FullRunName",
  qual_col = NULL,
  qual_value = 2
)
```

Arguments

df_long	data frame where each row is a single feature in a single sample. It minimally has a sample_id_col, a feature_id_col and a measure_col, but usually also an m_score (in OpenSWATH output result file). See help("example_proteome") for more details.
feature_id_col	name of the column with feature/gene/peptide/protein ID used in the long format representation df_long. In the wide formatted representation data_matrix this corresponds to the row names.
measure_col	if df_long is among the parameters, it is the column with expression/abundance/intensity; otherwise, it is used internally for consistency.
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).
qual_col	column to color point by certain value denoted by color_by_qual_value. Design with inferred/requant values in OpenSWATH output data, which means argument value has to be set to m_score.
qual_value	value in qual_col to color. For OpenSWATH data, this argument value has to be set to 2 (this is an m_score value for imputed values (requant values).

Value

data_matrix (proBatch) like matrix (features in rows, samples in columns)

See Also

Other matrix manipulation functions: matrix_to_long()

Examples

```
proteome_matrix <- long_to_matrix(example_proteome)
```

---

matrix_to_long *Wide to long conversion*

Description

Convert from wide matrix to a long data frame representation

Usage

```
matrix_to_long(
  data_matrix,
  sample_annotation = NULL,
  feature_id_col = "peptide_group_label",
  measure_col = "Intensity",
  sample_id_col = "FullRunName",
  step = NULL
)
```

Arguments

`data_matrix`	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use `help("example_proteome_matrix")`)
`sample_annotation`	data frame with: 1. `sample_id_col` (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See `help("example_sample_annotation")`
`feature_id_col`	name of the column with feature/gene/peptide/protein ID used in the long format representation `df_long`. In the wide formatted representation `data_matrix` this corresponds to the row names.
`measure_col`	if `df_long` is among the parameters, it is the column with expression/abundance/intensity; otherwise, it is used internally for consistency.
`sample_id_col`	name of the column in `sample_annotation` table, where the filenames (colnames of the `data_matrix` are found).
`step`	normalization step (e.g. `Raw` or `Normalized`. Useful if consecutive steps are compared in plots. Note that in plots these are usually ordered alphabetically, so it's worth naming with numbers, e.g. `1_raw`, `2_quantile`

Value

`df_long` (proBatch) like data frame

See Also

Other matrix manipulation functions: `long_to_matrix()`

Examples

```
proteome_long <- matrix_to_long(example_proteome_matrix,
example_sample_annotation)
```

---

normalize *Data normalization methods*

Description

Normalization of raw (usually log-transformed) data. Normalization brings the samples to the same scale. Currently the following normalization functions are implemented: #'

1. Quantile normalization: 'quantile_normalize_dm()'. Quantile normalization of the data.
2. Median normalization: 'normalize_sample_medians_dm()'. Normalization by centering sample medians to global median of the data

Alternatively, one can call normalization function with 'normalize_data_dm()' wrapper.

Usage

```
quantile_normalize_dm(data_matrix)

quantile_normalize_df(
  df_long,
  feature_id_col = "peptide_group_label",
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  no_fit_imputed = TRUE,
  qual_col = NULL,
  qual_value = 2,
  keep_all = "default"
)

normalize_sample_medians_dm(data_matrix)

normalize_sample_medians_df(
  df_long,
  feature_id_col = "peptide_group_label",
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  no_fit_imputed = FALSE,
  qual_col = NULL,
  qual_value = 2,
  keep_all = "default"
)

normalize_data_dm(
  data_matrix,
  normalize_func = c("quantile", "medianCentering"),
  log_base = NULL,
  offset = 1
)

normalize_data_df(
  df_long,
  normalize_func = c("quantile", "medianCentering"),
  log_base = NULL,
  offset = 1,
  feature_id_col = "peptide_group_label",
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  no_fit_imputed = TRUE,
  qual_col = NULL,
  qual_value = 2,
  keep_all = "default"
)
```

Arguments

data_matrix	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use help("example_proteome_matrix"))
df_long	data frame where each row is a single feature in a single sample. It minimally has a sample_id_col, a feature_id_col and a measure_col, but usually also an m_score (in OpenSWATH output result file). See help("example_proteome") for more details.
feature_id_col	name of the column with feature/gene/peptide/protein ID used in the long format representation df_long. In the wide formatted representation data_matrix this corresponds to the row names.
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).
measure_col	if df_long is among the parameters, it is the column with expression/abundance/intensity; otherwise, it is used internally for consistency.
no_fit_imputed	(logical) whether to use imputed (requant) values, as flagged in qual_col by qual_value for data transformation
qual_col	column to color point by certain value denoted by color_by_qual_value. Design with inferred/requant values in OpenSWATH output data, which means argument value has to be set to m_score.
qual_value	value in qual_col to color. For OpenSWATH data, this argument value has to be set to 2 (this is an m_score value for imputed values (requant values).
keep_all	when transforming the data (normalize, correct) - acceptable values: all/default/minimal (which set of columns be kept).
normalize_func	global batch normalization method (‘quantile‘ or ‘MedianCentering‘)
log_base	whether to log transform data matrix before normalization (e.g. ‘NULL‘, ‘2‘ or ‘10‘)
offset	small positive number to prevent 0 conversion to -Inf

Value

the data in the same format as input (data_matrix or df_long). For df_long the data frame stores the original values of measure_col in another column called "preNorm_intensity" if "intensity", and the normalized values in measure_col column.

Examples

```
#Quantile normalization:
quantile_normalized_matrix <- quantile_normalize_dm(example_proteome_matrix)

#Median centering:
median_normalized_df <- normalize_sample_medians_df(example_proteome)

#Transform the data in one go:
quantile_normalized_matrix <- normalize_data_dm(example_proteome_matrix,
normalize_func = "quantile", log_base = 2, offset = 1)
```

plot_corr_matrix *Visualise correlation matrix*

Description

recommended for heatmap-type visualisation of correlation matrix with <100 items. With >50 samples and ~10 replicate pairs distribution plots may be more informative.

Usage

```
plot_corr_matrix(
  corr_matrix,
  annotation = NULL,
  annotation_id_col = "FullRunName",
  factors_to_plot = NULL,
  cluster_rows = FALSE,
  cluster_cols = FALSE,
  heatmap_color = colorRampPalette(rev(brewer.pal(n = 7, name = "RdYlBu")))(100),
  color_list = NULL,
  filename = NULL,
  width = 7,
  height = 7,
  units = c("cm", "in", "mm"),
  plot_title = NULL,
  ...
)
```

Arguments

corr_matrix	square correlation matrix
annotation	data frame with peptide_annotation for protein correlation heatmap or sample_annotation for sample correlation heatmap
annotation_id_col	feature_id_col for protein correlation heatmap or sample_id_col for sample correlation heatmap
factors_to_plot	vector of technical and biological covariates to be plotted in this diagnostic plot (assumed to be present in sample_annotation)
cluster_rows	boolean values determining if rows should be clustered or hclust object
cluster_cols	boolean values determining if columns should be clustered or hclust object
heatmap_color	vector of colors used in heatmap.
color_list	list, as returned by sample_annotation_to_colors, where each item contains a color vector for each factor to be mapped to the color.

filename	path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported
width	option determining the output image width
height	option determining the output image width
units	units: 'cm', 'in' or 'mm'
plot_title	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
...	parameters for the pheatmap visualisation, for details see examples and help to corresponding functions

Details

Plot correlation of selected samples or peptides

Value

pheatmap object

See Also

pheatmap, plot_sample_corr_distribution, plot_peptide_corr_distribution

Examples

```
peptides <- c("10231_QDVDVWLWQQEGSSK_2", "10768_RLESELDGLR_2")
data_matrix_sub = example_proteome_matrix[peptides,]
corr_matrix = cor(t(data_matrix_sub), use = 'complete.obs')
corr_matrix_plot <- plot_corr_matrix(corr_matrix)
```

---

plot_CV_distr *Plot CV distribution to compare various steps of the analysis*

Description

Plot CV distribution to compare various steps of the analysis

Usage

```
plot_CV_distr(
  df_long,
  sample_annotation = NULL,
  feature_id_col = "peptide_group_label",
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  biospecimen_id_col = "EarTag",
```

```
  batch_col = NULL,
  unlog = TRUE,
  log_base = 2,
  offset = 1,
  plot_title = NULL,
  filename = NULL,
  theme = "classic"
)
```

Arguments

df_long	as in df_long for the rest of the package, but, when it has entries for intensity, represented in measure_col for several steps, e.g. raw, normalized, batch corrected data, as seen in column Step, then multi-step CV comparison can be carried out.
sample_annotation	data frame with: 1. sample_id_col (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See help("example_sample_annotation")
feature_id_col	name of the column with feature/gene/peptide/protein ID used in the long format representation df_long. In the wide formatted representation data_matrix this corresponds to the row names.
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).
measure_col	if df_long is among the parameters, it is the column with expression/abundance/intensity; otherwise, it is used internally for consistency.
biospecimen_id_col	column in sample_annotation that defines a unique bio ID, which is usually a combination of conditions or groups. Tip: if such ID is absent, but can be defined from several columns, create new biospecimen_id column
batch_col	column in sample_annotation that should be used for batch comparison (or other, non-batch factor to be mapped to color in plots).
unlog	(logical) whether to reverse log transformation of the original data
log_base	base of the logarithm for transformation
offset	small positive number to prevent 0 conversion to -Inf
plot_title	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
filename	path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported
theme	ggplot theme, by default classic. Can be easily overriden

Value

ggplot object with the boxplot of CVs on one or several steps

Examples

```
CV_plot = plot_CV_distr(example_proteome,
sample_annotation = example_sample_annotation,
measure_col = 'Intensity', batch_col = 'MS_batch',
plot_title = NULL, filename = NULL, theme = 'classic')
```

---

plot_CV_distr.df *Plot the distribution (boxplots) of per-batch per-step CV of features*

Description

Plot the distribution (boxplots) of per-batch per-step CV of features

Usage

```
plot_CV_distr.df(
  CV_df,
  plot_title = NULL,
  filename = NULL,
  theme = "classic",
  log_y_scale = TRUE
)
```

Arguments

CV_df	data frame with Total CV for each feature & (optionally) per-batch CV
plot_title	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
filename	path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported
theme	ggplot theme, by default classic. Can be easily overriden
log_y_scale	(logical) whether to display the CV on log-scale

Value

ggplot object

plot_heatmap_diagnostic *Plot the heatmap of samples (cols) vs features (rows)*

Description

Plot the heatmap of samples (cols) vs features (rows)

Usage

```
plot_heatmap_diagnostic(
  data_matrix,
  sample_annotation = NULL,
  sample_id_col = "FullRunName",
  factors_to_plot = NULL,
  fill_the_missing = -1,
  color_for_missing = "black",
  heatmap_color = colorRampPalette(rev(brewer.pal(n = 7, name = "RdYlBu")))(100),
  cluster_rows = TRUE,
  cluster_cols = FALSE,
  color_list = NULL,
  peptide_annotation = NULL,
  feature_id_col = "peptide_group_label",
  factors_of_feature_ann = c("KEGG_pathway", "evolutionary_distance"),
  color_list_features = NULL,
  filename = NULL,
  width = 7,
  height = 7,
  units = c("cm", "in", "mm"),
  plot_title = NULL,
  ...
)
```

Arguments

data_matrix	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use help("example_proteome_matrix"))
sample_annotation	data frame with: 1. sample_id_col (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See help("example_sample_annotation")
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).

factors_to_plot
: vector of technical and biological factors to be plotted in this diagnostic plot (assumed to be present in sample_annotation)

fill_the_missing
: numeric value that the missing values are substituted with, or NULL if features with missing values are to be excluded.

color_for_missing
: special color to make missing values. Usually black or white, depending on heatmap_color

heatmap_color
: vector of colors used in heatmap (typicall a gradient)

cluster_rows
: boolean value determining if rows should be clustered

cluster_cols
: boolean value determining if columns should be clustered

color_list
: list, as returned by sample_annotation_to_colors, where each item contains a color vector for each factor to be mapped to the color.

peptide_annotation
: long format data frame with peptide ID and their corresponding protein and/or gene annotations. See help("example_peptide_annotation").

feature_id_col
: name of the column with feature/gene/peptide/protein ID used in the long format representation df_long. In the wide formatted representation data_matrix this corresponds to the row names.

factors_of_feature_ann
: vector of factors that characterize features, as listed in peptide_annotation

color_list_features
: list, as returned by sample_annotation_to_colors, but mapping peptide_annotation where each item contains a color vector for each factor to be mapped to the color.

filename
: path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported

width
: option determining the output image width

height
: option determining the output image width

units
: units: 'cm', 'in' or 'mm'

plot_title
: title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))

...
: other parameters of link[pheatmap]{pheatmap}

Value

object returned by link[pheatmap]{pheatmap}

See Also

sample_annotation_to_colors, pheatmap

Examples

```
log_transformed_matrix = log_transform_dm(example_proteome_matrix)
heatmap_plot <- plot_heatmap_diagnostic(log_transformed_matrix,
example_sample_annotation,
factors_to_plot = c("MS_batch",  "digestion_batch", "Diet", 'DateTime'),
cluster_cols = TRUE, cluster_rows = FALSE,
show_rownames = FALSE, show_colnames = FALSE)

color_list <- sample_annotation_to_colors (example_sample_annotation,
factor_columns = c('MS_batch','EarTag', "Strain",
"Diet", "digestion_batch", "Sex"),
numeric_columns = c('DateTime', 'order'))

log_transformed_matrix = log_transform_dm(example_proteome_matrix)
heatmap_plot <- plot_heatmap_diagnostic(log_transformed_matrix,
example_sample_annotation,
factors_to_plot = c("MS_batch",  "digestion_batch", "Diet", 'DateTime'),
cluster_cols = TRUE, cluster_rows = FALSE,
color_list = color_list,
show_rownames = FALSE, show_colnames = FALSE)
```

---

plot_heatmap_generic *Plot the heatmap*

Description

Plot the heatmap

Usage

```
plot_heatmap_generic(
  data_matrix,
  column_annotation_df = NULL,
  row_annotation_df = NULL,
  col_ann_id_col = "FullRunName",
  row_ann_id_col = "peptide_group_label",
  columns_for_cols = c("MS_batch", "Diet", "DateTime", "order"),
  columns_for_rows = c("KEGG_pathway", "WGCNA_module", "evolutionary_distance"),
  cluster_rows = FALSE,
  cluster_cols = TRUE,
  annotation_color_cols = NULL,
  annotation_color_rows = NULL,
  fill_the_missing = -1,
  color_for_missing = "black",
  heatmap_color = colorRampPalette(rev(brewer.pal(n = 7, name = "RdYlBu")))(100),
  filename = NULL,
  width = 7,
```

```
  height = 7,
  units = c("cm", "in", "mm"),
  plot_title = NULL,
  ...
)
```

Arguments

data_matrix	the matrix of data to be plotted
column_annotation_df	data frame annotating columns of data_matrix
row_annotation_df	data frame annotating rows of data_matrix
col_ann_id_col	column of column_annotation_df whose values are unique identifiers of columns in data_matrix
row_ann_id_col	column of row_annotation_df whose values are unique identifiers of rows in data_matrix
columns_for_cols	vector of factors (columns) of column_annotation_df that will be mapped to color annotation of heatmap columns
columns_for_rows	vector of factors (columns) of row_annotation_df that will be mapped to color annotation of heatmap rows
cluster_rows	boolean: whether the rows should be clustered
cluster_cols	boolean: whether the rows should be clustered
annotation_color_cols	list of color vectors for column annotation, for each factor to be plotted; for factor-like variables a named vector (names should correspond to the levels of factors). Advisable to supply here color list returned by sample_annotation_to_colors
annotation_color_rows	list of color vectors for row annotation, for each factor to be plotted; for factor-like variables a named vector (names should correspond to the levels of factors). Advisable to supply here color list returned by sample_annotation_to_colors
fill_the_missing	numeric value that the missing values are substituted with, or NULL if features with missing values are to be excluded.
color_for_missing	special color to make missing values. Usually black or white, depending on heatmap_color
heatmap_color	vector of colors used in heatmap (typicall a gradient)
filename	path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported
width	option determining the output image width
height	option determining the output image width

units	units: 'cm', 'in' or 'mm'
plot_title	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
...	other parameters of link[pheatmap]{pheatmap}

Value

pheatmap-type object

Examples

```
p <- plot_heatmap_generic(log_transform_dm(example_proteome_matrix),
column_annotation_df = example_sample_annotation,
columns_for_cols = c("MS_batch",  "digestion_batch", "Diet", 'DateTime'),
plot_title = 'test_heatmap',
show_rownames = FALSE, show_colnames = FALSE)
```

---

plot_hierarchical_clustering

cluster the data matrix to visually inspect which confounder dominates

---

Description

cluster the data matrix to visually inspect which confounder dominates

Usage

```
plot_hierarchical_clustering(
  data_matrix,
  sample_annotation,
  sample_id_col = "FullRunName",
  color_list = NULL,
  factors_to_plot = NULL,
  fill_the_missing = 0,
  distance = "euclidean",
  agglomeration = "complete",
  label_samples = TRUE,
  label_font = 0.2,
  filename = NULL,
  width = 38,
  height = 25,
  units = c("cm", "in", "mm"),
  plot_title = NULL,
  ...
)
```

Arguments

data_matrix	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use help("example_proteome_matrix"))
sample_annotation	data frame with: 1. sample_id_col (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See help("example_sample_annotation")
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).
color_list	list, as returned by sample_annotation_to_colors, where each item contains a color vector for each factor to be mapped to the color.
factors_to_plot	vector of technical and biological covariates to be plotted in this diagnostic plot (assumed to be present in sample_annotation)
fill_the_missing	numeric value determining how missing values should be substituted. If NULL, features with missing values are excluded.
distance	distance metric used for clustering
agglomeration	agglomeration methods as used by hclust
label_samples	if TRUE sample IDs (column names of data_matrix) will be printed
label_font	size of the font. Is active if label_samples is TRUE, ignored otherwise
filename	path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported
width	option determining the output image width
height	option determining the output image width
units	units: 'cm', 'in' or 'mm'
plot_title	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
...	other parameters of plotDendroAndColors from WGCNA package

Value

No return

See Also

hclust, sample_annotation_to_colors, plotDendroAndColors

Examples

```
selected_batches = example_sample_annotation$MS_batch %in%
                                                c('Batch_1', 'Batch_2')
selected_samples = example_sample_annotation$FullRunName[selected_batches]
test_matrix = example_proteome_matrix[,selected_samples]

hierarchical_clustering_plot <- plot_hierarchical_clustering(
example_proteome_matrix, example_sample_annotation,
factors_to_plot = c('MS_batch', 'Diet', 'DateTime'),
color_list = NULL,
distance = "euclidean", agglomeration = 'complete',
label_samples = FALSE)

#with defined color scheme:
color_list <- sample_annotation_to_colors (example_sample_annotation,
factor_columns = c('MS_batch', "Strain", "Diet", "digestion_batch"),
numeric_columns = c('DateTime', 'order'))
hierarchical_clustering_plot <- plot_hierarchical_clustering(
example_proteome_matrix, example_sample_annotation,
factors_to_plot = c('MS_batch', "Strain", 'DateTime', "digestion_batch"),
color_list = color_list,
distance = "euclidean", agglomeration = 'complete',
label_samples = FALSE)
```

---

plot_PCA *plot PCA plot*

Description

plot PCA plot

Usage

```
plot_PCA(
  data_matrix,
  sample_annotation,
  feature_id_col = "peptide_group_label",
  sample_id_col = "FullRunName",
  color_by = "MS_batch",
  PC_to_plot = c(1, 2),
  fill_the_missing = -1,
  color_scheme = "brewer",
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = NULL,
  theme = "classic"
)
```

Arguments

data_matrix	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use help("example_proteome_matrix"))
sample_annotation	data frame with: 1. sample_id_col (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See help("example_sample_annotation")
feature_id_col	name of the column with feature/gene/peptide/protein ID used in the long format representation df_long. In the wide formatted representation data_matrix this corresponds to the row names.
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).
color_by	column name (as in sample_annotation) to color by
PC_to_plot	principal component numbers for x and y axis
fill_the_missing	numeric value determining how missing values should be substituted. If NULL, features with missing values are excluded. If NULL, features with missing values are excluded.
color_scheme	a named vector of colors to map to batch_col, names corresponding to the levels of the factor. For continuous variables, vector doesn't need to be named.
filename	path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported
width	option determining the output image width
height	option determining the output image width
units	units: 'cm', 'in' or 'mm'
plot_title	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
theme	ggplot theme, by default classic. Can be easily overriden

Value

ggplot scatterplot colored by factor levels of column specified in factor_to_color

See Also

autoplot.pca_common, ggplot

Examples

```
pca_plot <- plot_PCA(example_proteome_matrix, example_sample_annotation,
color_by = 'MS_batch', plot_title = "PCA colored by MS batch")
pca_plot <- plot_PCA(example_proteome_matrix, example_sample_annotation,
color_by = 'DateTime', plot_title = "PCA colored by DateTime")

color_list <- sample_annotation_to_colors (example_sample_annotation,
factor_columns = c('MS_batch', 'digestion_batch'),
numeric_columns = c('DateTime','order'))
pca_plot <- plot_PCA(example_proteome_matrix, example_sample_annotation,
color_by = 'DateTime', color_scheme = color_list[['DateTime']])

## Not run:
pca_plot <- plot_PCA(example_proteome_matrix, example_sample_annotation,
color_by = 'DateTime', plot_title = "PCA colored by DateTime",
filename = 'test_PCA.png', width = 14, height = 9, units = 'cm')

## End(Not run)
```

`plot_peptide_corr_distribution` *Create violin plot of peptide correlation distribution*

Description

Plot distribution of peptide correlations within one protein and between proteins

Usage

```
plot_peptide_corr_distribution(
  data_matrix,
  peptide_annotation,
  protein_col = "ProteinName",
  feature_id_col = "peptide_group_label",
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = "Distribution of peptide correlation",
  theme = "classic"
)

plot_peptide_corr_distribution.corrDF(
  corr_distribution,
  filename = NULL,
  width = NA,
  height = NA,
```

```
  units = c("cm", "in", "mm"),
  plot_title = "Correlation of peptides",
  theme = "classic"
)
```

Arguments

data_matrix	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use help("example_proteome_matrix"))
peptide_annotation	long format data frame with peptide ID and their corresponding protein and/or gene annotations. See help("example_peptide_annotation").
protein_col	column where protein names are specified
feature_id_col	name of the column with feature/gene/peptide/protein ID used in the long format representation df_long. In the wide formatted representation data_matrix this corresponds to the row names.
filename	path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported
width	option determining the output image width
height	option determining the output image width
units	units: 'cm', 'in' or 'mm'
plot_title	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
theme	ggplot theme, by default classic. Can be easily overriden
corr_distribution	data frame with peptide correlation distribution

Value

ggplot object (violin plot of peptide correlation)

See Also

calculate_peptide_corr_distr, ggplot

Examples

```
peptide_corr_distribution <- plot_peptide_corr_distribution(
example_proteome_matrix,
example_peptide_annotation, protein_col = 'Gene')

selected_genes = c('BOVINE_A1ag','BOVINE_FetuinB','Cyfip1')
gene_filter = example_peptide_annotation$Gene %in% selected_genes
peptides_ann = example_peptide_annotation$peptide_group_label
selected_peptides = peptides_ann[gene_filter]
```

```
matrix_test = example_proteome_matrix[selected_peptides,]
pep_annotation_sel = example_peptide_annotation[gene_filter, ]
corr_distribution = calculate_peptide_corr_distr(matrix_test,
pep_annotation_sel, protein_col = 'Gene')
peptide_corr_distribution <- plot_peptide_corr_distribution.corrDF(corr_distribution)

## Not run:
peptide_corr_distribution <- plot_peptide_corr_distribution.corrDF(corr_distribution,
filename = 'test_peptide.png',
width = 28, height = 28, units = 'cm')

## End(Not run)
```

`plot_protein_corrplot` *Peptide correlation matrix (heatmap)*

Description

Plots correlation plot of peptides from a single protein

Usage

```
plot_protein_corrplot(
  data_matrix,
  protein_name,
  peptide_annotation = NULL,
  protein_col = "ProteinName",
  feature_id_col = "peptide_group_label",
  factors_to_plot = c("ProteinName"),
  cluster_rows = FALSE,
  cluster_cols = FALSE,
  heatmap_color = colorRampPalette(rev(brewer.pal(n = 7, name = "RdYlBu")))(100),
  color_list = NULL,
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = sprintf("Peptide correlation matrix of %s protein", protein_name),
  ...
)
```

Arguments

`data_matrix`	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use `help("example_proteome_matrix")`)
`protein_name`	the name of the protein

peptide_annotation
: long format data frame with peptide ID and their corresponding protein and/or gene annotations. See `help("example_peptide_annotation")`.

protein_col
: column where protein names are specified

feature_id_col
: name of the column with feature/gene/peptide/protein ID used in the long format representation `df_long`. In the wide formatted representation `data_matrix` this corresponds to the row names.

factors_to_plot
: vector of technical and biological covariates to be plotted in this diagnostic plot (assumed to be present in `sample_annotation`)

cluster_rows
: boolean values determining if rows should be clustered or `hclust` object

cluster_cols
: boolean values determining if columns should be clustered or `hclust` object

heatmap_color
: vector of colors used in heatmap.

color_list
: list, as returned by `sample_annotation_to_colors`, where each item contains a color vector for each factor to be mapped to the color.

filename
: path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported

width
: option determining the output image width

height
: option determining the output image width

units
: units: 'cm', 'in' or 'mm'

plot_title
: title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))

...
: parameters for the corrplot visualisation

Value

`pheatmap` object

Examples

```
protein_corrplot_plot <- plot_protein_corrplot(example_proteome_matrix,
protein_name = 'Haao', peptide_annotation = example_peptide_annotation,
protein_col = 'Gene')

protein_corrplot_plot <- plot_protein_corrplot(example_proteome_matrix,
 protein_name = c('Haao', 'Dhtkd1'),
 peptide_annotation = example_peptide_annotation,
 protein_col = 'Gene', factors_to_plot = 'Gene')
```

plot_PVCA *Plot variance distribution by variable*

Description

Plot variance distribution by variable

Usage

```
plot_PVCA(
  data_matrix,
  sample_annotation,
  feature_id_col = "peptide_group_label",
  sample_id_col = "FullRunName",
  technical_factors = c("MS_batch", "instrument"),
  biological_factors = c("cell_line", "drug_dose"),
  fill_the_missing = -1,
  pca_threshold = 0.6,
  variance_threshold = 0.01,
  colors_for_bars = NULL,
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = NULL,
  theme = "classic"
)
```

Arguments

data_matrix	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use help("example_proteome_matrix"))
sample_annotation	data frame with: 1. sample_id_col (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See help("example_sample_annotation")
feature_id_col	name of the column with feature/gene/peptide/protein ID used in the long format representation df_long. In the wide formatted representation data_matrix this corresponds to the row names.
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).

technical_factors
: vector sample_annotation column names that are technical covariates

biological_factors
: vector sample_annotation column names, that are biologically meaningful covariates

fill_the_missing
: numeric value determining how missing values should be substituted. If NULL, features with missing values are excluded. If NULL, features with missing values are excluded.

pca_threshold
: the percentile value of the minimum amount of the variabilities that the selected principal components need to explain

variance_threshold
: the percentile value of weight each of the covariates needs to explain (the rest will be lumped together)

colors_for_bars
: four-item color vector, specifying colors for the following categories: c('residual', 'biological', 'biol:techn', 'technical')

filename
: path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported

width
: option determining the output image width

height
: option determining the output image width

units
: units: 'cm', 'in' or 'mm'

plot_title
: title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))

theme
: ggplot theme, by default classic. Can be easily overriden

Value

ggplot object with the plot

See Also

sample_annotation_to_colors, ggplot

Examples

```
matrix_test <- example_proteome_matrix[1:150, ]
pvca_plot <- plot_PVCA(matrix_test, example_sample_annotation,
technical_factors = c('MS_batch', 'digestion_batch'),
biological_factors = c("Diet", "Sex", "Strain"))

## Not run:
pvca_plot <- plot_PVCA(matrix_test, example_sample_annotation,
technical_factors = c('MS_batch', 'digestion_batch'),
biological_factors = c("Diet", "Sex", "Strain"),
filename = 'test_PVCA.png', width = 28, height = 22, units = 'cm')
```

```
## End(Not run)
```

`plot_PVCA.df` *plot PVCA, when the analysis is completed*

Description

plot PVCA, when the analysis is completed

Usage

```
plot_PVCA.df(
  pvca_res,
  colors_for_bars = NULL,
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = NULL,
  theme = "classic"
)
```

Arguments

`pvca_res`	data frame of weights of Principal Variance Components, result of `calculate_PVCA`
`colors_for_bars`	four-item color vector, specifying colors for the following categories: c('residual', 'biological', 'biol:techn', 'technical')
`filename`	path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported
`width`	option determining the output image width
`height`	option determining the output image width
`units`	units: 'cm', 'in' or 'mm'
`plot_title`	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
`theme`	ggplot theme, by default `classic`. Can be easily overriden

Value

`ggplot` object with bars as weights, colored by bio/tech factors

Examples

```
matrix_test <- example_proteome_matrix[1:150, ]
pvca_df_res <- prepare_PVCA_df(matrix_test, example_sample_annotation,
technical_factors = c('MS_batch', 'digestion_batch'),
biological_factors = c("Diet", "Sex", "Strain"),
pca_threshold = .6, variance_threshold = .01, fill_the_missing = -1)
colors_for_bars = c('grey', 'green','blue','red')
names(colors_for_bars) = c('residual', 'biological','biol:techn','technical')

pvca_plot <- plot_PVCA.df(pvca_df_res, colors_for_bars)
```

---

plot_sample_corr_distribution

Create violin plot of sample correlation distribution

Description

Useful to visualize within batch vs within replicate vs non-related sample correlation

Usage

```
plot_sample_corr_distribution(
  data_matrix,
  sample_annotation,
  repeated_samples = NULL,
  sample_id_col = "FullRunName",
  batch_col = "MS_batch",
  biospecimen_id_col = "EarTag",
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = "Sample correlation distribution",
  plot_param = "batch_replicate",
  theme = "classic"
)

plot_sample_corr_distribution.corrDF(
  corr_distribution,
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = "Sample correlation distribution",
  plot_param = "batch_replicate",
  theme = "classic"
)
```

Arguments

data_matrix	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use help("example_proteome_matrix"))
sample_annotation	data frame with: 1. sample_id_col (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See help("example_sample_annotation")
repeated_samples	if NULL, correlation of all samples is plotted
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).
batch_col	column in sample_annotation that should be used for batch comparison (or other, non-batch factor to be mapped to color in plots).
biospecimen_id_col	column in sample_annotation that captures the biological sample, that (possibly) was profiled several times as technical replicates. Tip: if such ID is absent, but can be defined from several columns, create new biospecimen_id column
filename	path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported
width	option determining the output image width
height	option determining the output image width
units	units: 'cm', 'in' or 'mm'
plot_title	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
plot_param	columns, defined in correlation_df, which is output of calculate_sample_corr_distr, specifically, 1. replicate 2. batch_the_same 3. batch_replicate 4. batches
theme	ggplot theme, by default classic. Can be easily overriden
corr_distribution	data frame with correlation distribution, as returned by calculate_sample_corr_distr

Value

ggplot type object with violin plot for each plot_param

See Also

calculate_sample_corr_distr, ggplot

Examples

```
sample_corr_distribution_plot <- plot_sample_corr_distribution(
example_proteome_matrix,
example_sample_annotation, batch_col = 'MS_batch',
biospecimen_id_col = "EarTag",
plot_param = 'batch_replicate')

corr_distribution = calculate_sample_corr_distr(data_matrix = example_proteome_matrix,
sample_annotation = example_sample_annotation,
batch_col = 'MS_batch',biospecimen_id_col = "EarTag")
sample_corr_distribution_plot <- plot_sample_corr_distribution.corrDF(corr_distribution,
plot_param = 'batch_replicate')

## Not run:
sample_corr_distribution_plot <- plot_sample_corr_distribution.corrDF(corr_distribution,
plot_param = 'batch_replicate',
filename = 'test_sampleCorr.png',
width = 28, height = 28, units = 'cm')

## End(Not run)
```

---

plot_sample_corr_heatmap

Sample correlation matrix (heatmap)

Description

Plot correlation of selected samples

Usage

```
plot_sample_corr_heatmap(
  data_matrix,
  samples_to_plot = NULL,
  sample_annotation = NULL,
  sample_id_col = "FullRunName",
  factors_to_plot = NULL,
  cluster_rows = FALSE,
  cluster_cols = FALSE,
  heatmap_color = colorRampPalette(rev(brewer.pal(n = 7, name = "RdYlBu")))(100),
  color_list = NULL,
  filename = NULL,
  width = NA,
```

```
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = sprintf("Correlation matrix of%s samples",
    ifelse(is.null(samples_to_plot), "", " selected")),
  ...
)
```

Arguments

data_matrix	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use help("example_proteome_matrix"))
samples_to_plot	string vector of samples in data_matrix to be used in the plot
sample_annotation	data frame with: 1. sample_id_col (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See help("example_sample_annotation")
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).
factors_to_plot	vector of technical and biological covariates to be plotted in this diagnostic plot (assumed to be present in sample_annotation)
cluster_rows	boolean values determining if rows should be clustered or hclust object
cluster_cols	boolean values determining if columns should be clustered or hclust object
heatmap_color	vector of colors used in heatmap.
color_list	list, as returned by sample_annotation_to_colors, where each item contains a color vector for each factor to be mapped to the color.
filename	path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported
width	option determining the output image width
height	option determining the output image width
units	units: 'cm', 'in' or 'mm'
plot_title	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
...	parameters for the pheatmap visualisation, for details see examples and help to corresponding functions

Value

pheatmap object

See Also

pheatmap

Examples

```
specified_samples = example_sample_annotation$FullRunName[
which(example_sample_annotation$order %in% 110:115)]

sample_corr_heatmap <- plot_sample_corr_heatmap(example_proteome_matrix,
samples_to_plot = specified_samples,
factors_to_plot = c('MS_batch','Diet', 'DateTime', 'digestion_batch'),
 cluster_rows= FALSE, cluster_cols=FALSE,
 annotation_names_col = TRUE, annotation_legend = FALSE,
 show_colnames = FALSE)


 color_list <- sample_annotation_to_colors (example_sample_annotation,
factor_columns = c('MS_batch','EarTag', "Strain",
"Diet", "digestion_batch", "Sex"),
numeric_columns = c('DateTime', 'order'))
 sample_corr_heatmap_annotated <- plot_sample_corr_heatmap(log_transform_dm(example_proteome_matrix),
 sample_annotation = example_sample_annotation,
 factors_to_plot = c('MS_batch','Diet', 'DateTime', 'digestion_batch'),
 cluster_rows= FALSE, cluster_cols=FALSE,
 annotation_names_col = TRUE,
 show_colnames = FALSE, color_list = color_list)
```

---

plot_sample_mean_or_boxplot

Plot per-sample mean or boxplots for initial assessment

Description

Plot per-sample mean or boxplots (showing median and quantiles). In ordered samples, e.g. consecutive MS runs, order-associated effects are visualised.

Usage

```
plot_sample_mean(
  data_matrix,
  sample_annotation = NULL,
  sample_id_col = "FullRunName",
  batch_col = "MS_batch",
  color_by_batch = FALSE,
  color_scheme = "brewer",
  order_col = "order",
  vline_color = "grey",
```

```
  facet_col = NULL,
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = NULL,
  theme = "classic",
  ylimits = NULL
)

plot_boxplot(
  df_long,
  sample_annotation = NULL,
  sample_id_col = "FullRunName",
  measure_col = "Intensity",
  batch_col = "MS_batch",
  color_by_batch = TRUE,
  color_scheme = "brewer",
  order_col = "order",
  facet_col = NULL,
  filename = NULL,
  width = NA,
  height = NA,
  units = c("cm", "in", "mm"),
  plot_title = NULL,
  theme = "classic",
  ylimits = NULL,
  outliers = TRUE
)
```

Arguments

`data_matrix`	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use `help("example_proteome_matrix")`)
`sample_annotation`	data frame with: 1. `sample_id_col` (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See `help("example_sample_annotation")`
`sample_id_col`	name of the column in `sample_annotation` table, where the filenames (colnames of the `data_matrix` are found).
`batch_col`	column in `sample_annotation` that should be used for batch comparison (or other, non-batch factor to be mapped to color in plots).
`color_by_batch`	(logical) whether to color points and connecting lines by batch factor as defined by `batch_col`.

color_scheme	named vector, names corresponding to unique batch values of batch_col in sample_annotation. Best created with sample_annotation_to_colors
order_col	column in sample_annotation that determines sample order. It is used for in initial assessment plots (plot_sample_mean_or_boxplot) and feature-level diagnostics (feature_level_diagnostics). Can be 'NULL' if sample order is irrelevant (e.g. in genomic experiments). For more details, order definition/inference, see define_sample_order and date_to_sample_order
vline_color	color of vertical lines, typically denoting different MS batches in ordered runs; should be NULL for experiments without intrinsic order
facet_col	column in sample_annotation with a batch factor to separate plots into facets; usually 2nd to batch_col. Most meaningful for multi-instrument MS experiments (where each instrument has its own order-associated effects (see order_col) or simultaneous examination of two batch factors (e.g. preparation day and measurement day). For single-instrument case should be set to 'NULL'
filename	path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported
width	option determining the output image width
height	option determining the output image width
units	units: 'cm', 'in' or 'mm'
plot_title	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
theme	ggplot theme, by default classic. Can be easily overriden
ylimits	range of y-axis to compare two plots side by side, if required.
df_long	data frame where each row is a single feature in a single sample. It minimally has a sample_id_col, a feature_id_col and a measure_col, but usually also an m_score (in OpenSWATH output result file). See help("example_proteome") for more details.
measure_col	if df_long is among the parameters, it is the column with expression/abundance/intensity; otherwise, it is used internally for consistency.
outliers	keep (default) or remove the boxplot outliers

Details

functions for quick visual assessment of trends associated, overall or specific covariate-associated (see batch_col and facet_col)

Value

ggplot2 class object. Thus, all aesthetics can be overridden

See Also

ggplot, date_to_sample_order

Examples

```
mean_plot <- plot_sample_mean(example_proteome_matrix, example_sample_annotation,
order_col = 'order', batch_col = "MS_batch")

color_list <- sample_annotation_to_colors (example_sample_annotation,
factor_columns = c('MS_batch'),
numeric_columns = c('DateTime', 'order'))
plot_sample_mean(example_proteome_matrix, example_sample_annotation,
order_col = 'order', batch_col = "MS_batch", color_by_batch = TRUE,
color_scheme = color_list[["MS_batch"]])

## Not run:
mean_plot <- plot_sample_mean(example_proteome_matrix,
                              example_sample_annotation,
                              order_col = 'order', batch_col = "MS_batch",
                              filename = 'test_meanplot.png',
                              width = 28, height = 18, units = 'cm')

## End(Not run)

boxplot <- plot_boxplot(log_transform_df(example_proteome),
sample_annotation = example_sample_annotation,
batch_col = "MS_batch")

color_list <- sample_annotation_to_colors (example_sample_annotation,
factor_columns = c('MS_batch'),
numeric_columns = c('DateTime', 'order'))
plot_boxplot(log_transform_df(example_proteome),
sample_annotation = example_sample_annotation,
batch_col = "MS_batch", color_scheme = color_list[["MS_batch"]])

## Not run:
boxplot <- plot_boxplot(log_transform_df(example_proteome),
sample_annotation = example_sample_annotation,
batch_col = "MS_batch", filename = 'test_boxplot.png',
width = 14, height = 9, units = 'in')

## End(Not run)
```

---

plot_split_violin_with_boxplot

Plot split violin plot (convenient to compare distribution before and after)

Description

Plot split violin plot (convenient to compare distribution before and after)

Usage

```
plot_split_violin_with_boxplot(
  df,
  y_col = "y",
  col_for_color = "m",
  col_for_box = "x",
  colors_for_plot = c("#8f1811", "#F8C333"),
  hlineintercept = NULL,
  plot_title = NULL,
  theme = "classic"
)
```

Arguments

df	data.frame with y_col, col_for_color, col_for_box
y_col	value to explore the distribution of
col_for_color	column to use to map to two colors
col_for_box	column to use to do group comparison
colors_for_plot	colors to map to col_for_color
hlineintercept	NULL: no intercept line; non-null: intercept value
plot_title	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
theme	ggplot theme, by default classic. Can be easily overriden

Value

ggplot object

---

prepare_PVCA_df *prepare the weights of Principal Variance Components*

Description

prepare the weights of Principal Variance Components

Usage

```
prepare_PVCA_df(
  data_matrix,
  sample_annotation,
  feature_id_col = "peptide_group_label",
  sample_id_col = "FullRunName",
  technical_factors = c("MS_batch", "instrument"),
  biological_factors = c("cell_line", "drug_dose"),
```

```
  fill_the_missing = -1,
  pca_threshold = 0.6,
  variance_threshold = 0.01
)
```

Arguments

data_matrix	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use help("example_proteome_matrix"))
sample_annotation	data frame with: 1. sample_id_col (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See help("example_sample_annotation")
feature_id_col	name of the column with feature/gene/peptide/protein ID used in the long format representation df_long. In the wide formatted representation data_matrix this corresponds to the row names.
sample_id_col	name of the column in sample_annotation table, where the filenames (colnames of the data_matrix are found).
technical_factors	vector sample_annotation column names that are technical covariates
biological_factors	vector sample_annotation column names, that are biologically meaningful covariates
fill_the_missing	numeric value determining how missing values should be substituted. If NULL, features with missing values are excluded. If NULL, features with missing values are excluded.
pca_threshold	the percentile value of the minimum amount of the variabilities that the selected principal components need to explain
variance_threshold	the percentile value of weight each of the covariates needs to explain (the rest will be lumped together)

Value

data frame with weights and factors, combined in a way ready for plotting

Examples

```
matrix_test <- example_proteome_matrix[1:150, ]
pvca_df_res <- prepare_PVCA_df(matrix_test, example_sample_annotation,
technical_factors = c('MS_batch', 'digestion_batch'),
biological_factors = c("Diet", "Sex", "Strain"),
pca_threshold = .6, variance_threshold = .01, fill_the_missing = -1)
```

proBatch *proBatch: A package for diagnostics and correction of batch effects, primarily in proteomics*

Description

The proBatch package contains functions for analyzing and correcting batch effects (unwanted technical variation) from high-thoughput experiments. Although the package has primarily been developed for mass spectrometry proteomics (DIA/SWATH), it has been designed be applicable to most omic data with minor adaptations. It addresses the following needs:

- prepare the data for analysis
- Visualize batch effects in sample-wide and feature-level;
- Normalize and correct for batch effects.

Arguments

`df_long`	data frame where each row is a single feature in a single sample. It minimally has a `sample_id_col`, a `feature_id_col` and a `measure_col`, but usually also an `m_score` (in OpenSWATH output result file). See `help("example_proteome")` for more details.
`data_matrix`	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use `help("example_proteome_matrix")`)
`sample_annotation`	data frame with: 1. `sample_id_col` (this can be repeated as row names) 2. biological covariates 3. technical covariates (batches etc) . See `help("example_sample_annotation")`
`sample_id_col`	name of the column in `sample_annotation` table, where the filenames (colnames of the `data_matrix` are found).
`measure_col`	if `df_long` is among the parameters, it is the column with expression/abundance/intensity; otherwise, it is used internally for consistency.
`feature_id_col`	name of the column with feature/gene/peptide/protein ID used in the long format representation `df_long`. In the wide formatted representation `data_matrix` this corresponds to the row names.
`batch_col`	column in `sample_annotation` that should be used for batch comparison (or other, non-batch factor to be mapped to color in plots).
`order_col`	column in `sample_annotation` that determines sample order. It is used for in initial assessment plots (plot_sample_mean_or_boxplot) and feature-level diagnostics (feature_level_diagnostics). Can be 'NULL' if sample order is irrelevant (e.g. in genomic experiments). For more details, order definition/inference, see define_sample_order and date_to_sample_order

facet_col	column in sample_annotation with a batch factor to separate plots into facets; usually 2nd to batch_col. Most meaningful for multi-instrument MS experiments (where each instrument has its own order-associated effects (see order_col) or simultaneous examination of two batch factors (e.g. preparation day and measurement day). For single-instrument case should be set to 'NULL'
color_by_batch	(logical) whether to color points and connecting lines by batch factor as defined by batch_col.
peptide_annotation	long format data frame with peptide ID and their corresponding protein and/or gene annotations. See help("example_peptide_annotation").
color_scheme	a named vector of colors to map to batch_col, names corresponding to the levels of the factor. For continuous variables, vector doesn't need to be named.
color_list	list, as returned by sample_annotation_to_colors, where each item contains a color vector for each factor to be mapped to the color.
factors_to_plot	vector of technical and biological covariates to be plotted in this diagnostic plot (assumed to be present in sample_annotation)
protein_col	column where protein names are specified
no_fit_imputed	(logical) whether to use imputed (requant) values, as flagged in qual_col by qual_value for data transformation
qual_col	column to color point by certain value denoted by color_by_qual_value. Design with inferred/requant values in OpenSWATH output data, which means argument value has to be set to m_score.
qual_value	value in qual_col to color. For OpenSWATH data, this argument value has to be set to 2 (this is an m_score value for imputed values (requant values).
plot_title	title of the plot (e.g., processing step + representation level (fragments, transitions, proteins) + purpose (meanplot/corrplot etc))
keep_all	when transforming the data (normalize, correct) - acceptable values: all/default/minimal (which set of columns be kept).
theme	ggplot theme, by default classic. Can be easily overriden
filename	path where the results are saved. If null the object is returned to the active window; otherwise, the object is save into the file. Currently only pdf and png format is supported
width	option determining the output image width
height	option determining the output image width
units	units: 'cm', 'in' or 'mm'

Details

To learn more about proBatch, start with the vignettes: browseVignettes(package = "proBatch")

Section

Common arguments to the functions.

`sample_annotation_to_colors` *Generate colors for sample annotation*

Description

Convert the sample annotation data frame to list of colors the list is named as columns included to use in plotting functions

Usage

```
sample_annotation_to_colors(
  sample_annotation,
  sample_id_col = "FullRunName",
  factor_columns = c("MS_batch", "EarTag", "digestion_batch", "Strain", "Diet"),
  numeric_columns = c("DateTime", "order"),
  rare_categories_to_other = TRUE,
  guess_factors = FALSE,
  numeric_palette_type = "brewer"
)
```

Arguments

`sample_annotation`
: data frame with:

  1. `sample_id_col` (this can be repeated as row names)
  2. biological covariates
  3. technical covariates (batches etc)

  . See `help("example_sample_annotation")`

`sample_id_col`
: name of the column in `sample_annotation` table, where the filenames (colnames of the `data_matrix` are found).

`factor_columns`
: columns of `sample_annotation` to be treated as factors. Sometimes categorical variables are depicted as integers (e.g. in column "Batch", values are 1, 2 and 3), specification here allows to map them correctly to qualitative palettes.

`numeric_columns`
: columns of `sample_annotation` to be treated as continuous numeric values.

`rare_categories_to_other`
: if `True` rare categories will be merged into the value `"other"`

`guess_factors`
: whether attempt which of the `factor_columns` are actually numeric

`numeric_palette_type`
: palette to be used for numeric values coloring (can be `'brewer'` and `'viridis'`)

Value

list of three items:

1. list of colors;
2. data frame of colors;
3. new sample annotation (e.g. rare factor levels merged into "other")

Examples

```
color_scheme <- sample_annotation_to_colors (example_sample_annotation,
factor_columns = c('MS_batch','EarTag', "Strain",
"Diet", "digestion_batch", "Sex"),
numeric_columns = c('DateTime', 'order'))
```

---

transform_raw_data *Functions to log transform raw data before normalization and batch correction*

Description

Functions to log transform raw data before normalization and batch correction

Log transformation of the data

"Unlog" transformation of the data to pre-log form (for quantification, forcing log-transform)

Usage

```
log_transform_df(df_long, log_base = 2, offset = 1, measure_col = "Intensity")

unlog_df(df_long, log_base = 2, offset = 1, measure_col = "Intensity")

log_transform_dm(data_matrix, log_base = 2, offset = 1)

unlog_dm(data_matrix, log_base = 2, offset = 1)
```

Arguments

df_long	data frame where each row is a single feature in a single sample. It minimally has a sample_id_col, a feature_id_col and a measure_col, but usually also an m_score (in OpenSWATH output result file). See help("example_proteome") for more details.
log_base	base of the logarithm for transformation
offset	small positive number to prevent 0 conversion to -Inf
measure_col	if df_long is among the parameters, it is the column with expression/abundance/intensity; otherwise, it is used internally for consistency.
data_matrix	features (in rows) vs samples (in columns) matrix, with feature IDs in rownames and file/sample names as colnames. See "example_proteome_matrix" for more details (to call the description, use help("example_proteome_matrix"))

Value

‘log_transform_df()‘ returns `df_long`-size data frame, with `measure_col` log transformed; with old value in another column called "beforeLog_intensity" if "intensity" was the value of `measure_col`; ‘log_transform_dm()‘ returns `data_matrix` format matrix

Examples

```
log_transformed_df <- log_transform_df(example_proteome)

log_transformed_matrix <- log_transform_dm(example_proteome_matrix,
log_base = 10, offset = 1)
```

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