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arrange_row

Sort a data frame

Description

Sort a date frame and keep the row names.

Usage

```
arrange_row(df, ...)
```

batch_shift 3

Arguments

df a data frame.

... further parameters to order.

Details

This function is modified from arrange of R package plyr. arrange deliberately remove rownames, but sometimes it is worth to keep them.

Value

a sorted data frame.

batch_shift

Batch shifting

Description

Remove batch effect withing each block.

Usage

```
batch_shift(x, y, method = "mean", overall_average = TRUE)
```

Arguments

x a data matrix.

y a categorical data for batch/block information.

method method for shifting.

overall_average

a logical value to indicate whether or not an overall average will be added after

shifting.

Value

a shifted data matrix.

References

Silvia Wagner, et.al, Tools in Metabonomics: An Integrated Validation Approach for LC-MS Metabolic Profiling of Mercapturic Acids in Human Urine Anal. Chem., 2007, 79 (7), pp 2918-2926, DOI: 10.1021/ac062153w

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bi_cor_net

Bipartite/two-mode correlation network

Description

Perform bipartite/two-mode correlation network analysis.

Usage

```
bi_cor_net(co_mat, thres = 0.6, dn = NULL)
```

Arguments

co_mat a correlation coefficient matrix.

thres correlation coefficient threshold for network analysis.

dn a character string for correlation name.

Value

```
a list of ggplot2 plots.
```

```
data <- mtExtra:::data
meta <- mtExtra:::meta

## Not run:
## process meta
library(mt)
meta <- mv_filter(meta, thres = 0.3)$dat
meta <- mv.fill(meta, method = "mean")
meta <- preproc(meta, method = "auto")

## End(Not run)

co <- cor(meta, data, use = "pairwise.complete.obs")
heat_dend(co)

res <- bi_cor_net(co, thres = 0.2)
names(res)
res$net1
res$dend2</pre>
```

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blank_filter

MS/NMR data filtering based on "blank" data

Description

MS/NMR data filtering based on "blank" data

Usage

```
blank_filter(
   x,
   y,
   method = c("mean", "median", "max"),
   factor = 1,
   f_mv = TRUE,
   thres_mv = 0.3
)
```

Arguments

```
x a data matrix.

y a character string with contents of "sample", "qc" and "blank".

method method for stats. Support "mean", "median" and "max".

factor multiplier for blank stats

f_mv a flag indicating whether perform missing value filtering on "sample" data.

thres_mv threshold of missing values on QC. Features less than this threshold will be kept.
```

Details

This function provides an option to perform missing value filtering on "sample" data.

Value

a list of with contents:

- · dat the filtered data matrix
- idx a logical vector of index for keeping features.

See Also

```
Other variable filters: locfdr_filter(), mv_filter(), qc_filter(), rsd_filter(), var_filter()
```

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chunk

Split a vector into chunks

Description

Split a vector into chunks.

Usage

```
chunk(x, n)
```

Arguments

```
x an vector.n length of chunk.
```

Details

For details, see https://bit.ly/2SM4m2G

Value

return the split chunk.

Examples

```
x <- 1:10
n <- 3
chunk(x, n)
```

cor_hcl

Correlation hierarchical cluster analysis

Description

Perform hierarchical cluster analysis based on correlation.

Usage

```
cor_hcl(
  mat,
  cutoff = 0.75,
  use = "pairwise.complete.obs",
  method = "pearson",
  fig_title = "Cluster Dendrogram",
  size = 3,
  rotate = FALSE
)
```

cor_net 7

Arguments

mat a data matrix

cutoff a threshold for correlation analysis.

use a string giving a method for computing covariances. For details, see stats::cor().

method method for correlation stats::cor().

fig_title title for plotting

size text font size of ggplot2.

rotate a logical indicating whether to rotate plot.

Value

a list of a ggplot2 object for clustering and a list of cluster centres.

Examples

```
cor_hcl(mtcars)
```

cor_net

Correlation network analysis

Description

Perform network analysis for correlation coefficient.

Usage

```
cor_net(
  mat,
  use = "pairwise.complete.obs",
  method = "pearson",
  thres = 0.6,
  fig_title = "Correlation network"
)
```

Arguments

mat a data matrix for correlation analysis

 $\begin{tabular}{ll} use, method & parameters of stats::cor(). \end{tabular}$

thres correlation coefficient threshold for network analysis. Only keep those with

coefficient larger than thres.

fig_title a character string for figure title.

Value

a list of ggplot2 plots.

8 cor_tab

Examples

```
res <- cor_net(mtcars)
names(res)
res$p1  # or res$p2, res$p3, res$p4
## Not run:
## see https://ggplot2-book.org/arranging-plots.html
library(patchwork)
res$p1 + res$p2 + res$p3 + res$p4
## End(Not run)</pre>
```

cor_tab

Calculate correlation coefficient and p-values

Description

Calculate correlation coefficient and p-values.

Usage

```
cor_tab(
    x,
    cor.method = c("pearson", "kendall", "spearman"),
    adj.method = c("holm", "hochberg", "hommel", "bonferroni", "BH", "BY", "fdr", "none"),
    ...
)
```

Arguments

```
x a data frame or matrix for correlation analysis column-wise.

cor.method method for correlation

adj.method p-value correction method

other parameter for correlation.
```

Details

This file is modified from cor.table of package picante and corr.test of package psych. The original implementation is from Bill Venables, the author of R great book MASS. For details, see https://stat.ethz.ch/pipermail/r-help/2001-November/016201.html

Value

a list with contents:

- r correlation coefficient
- p statistics matrix, in which the lower triangular is p-values and the upper triangular is adjusted p-values

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Examples

```
co <- cor_tab(mtcars, cor.method = "spearman", adj.method = "BH")
names(co)

## Not run:
library(pysch)
co <- corr.test(mtcars, method="spearman",adjust="BH")
# From pysch: For symmetric matrices, p values adjusted for multiple tests
# are reported above the diagonal.
## End(Not run)</pre>
```

dat2long

Melt a numeric data matrix to long format

Description

Reshape a matrix or data frame to long format with row names and column names in two columns.

Usage

```
dat2long(x)
```

Arguments

X

a matrix or data frame

Details

reshape2::melt keeps the rownames when melting a matrix, but not when melting a data frame. This function keeps rownames for both matrix and data frame.

Value

```
a tibble object
```

```
class(mtcars) # data.frame
reshape2::melt(mtcars)
reshape2::melt(as.matrix(mtcars))
dat2long(mtcars)
```

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dat_summ

Data matrix summary

Description

Summarise a data matrix. This is a wrapper function for any summary function on an vector.

Usage

```
dat_summ(x, method = mean, ...)
```

Arguments

```
x a matrix-like object.
```

method summary method for an vector.
... further parameters for method.

Value

a summarised table.

Examples

```
library(dplyr)
library(tidyr)
library(purrr)
iris %>% group_by(Species) %>% group_modify(~ dat_summ(., method = mean))
iris %>% group_by(Species) %>% group_modify(~ dat_summ(., method = vec_stats))
iris %>% group_by(Species) %>% do(dat_summ(., method = vec_segment))
iris %>% dat_summ(method = sd)
```

 ${\tt dat_symb}$

Symbolise data set

Description

Symbolise data values as (-1, 0, 1) based on a range

Usage

```
dat_symb(x, thres)
```

Arguments

x an vector or data matrix.

thres an vector with lower and higher values.

Details

thres can be estimated by locfdr_filter().

dat_trans 11

Value

a symbolic data set.

See Also

locfdr_filter() for estimating threshold and locfdr() for z.2.

dat_trans

Transform data

Description

Perform data set transformation

Usage

```
dat_trans(x, method = "auto", na.rm = TRUE, add = 1)
vec_trans(x, method = "auto", na.rm = TRUE, add = 1)
```

Arguments

x a matrix, data frame or vector.

method transformation method, including: "center", "auto", "range", "pareto", "vast", "level", "log", "log10", "sqrt" and "asinh".

na.rm a logical value indicating whether NA values should be stripped before the com-

putation proceeds.

add a shift value for log transformation.

Value

transformed data

References

Berg, R., Hoefsloot, H., Westerhuis, J., Smilde, A. and Werf, M. (2006), Centering, scaling, and transformations: improving the biological information content of metabolomics data, *BMC Genomics*, 7:142

```
data(iris)
## transform an vector
vec <- iris[, 1]
dat_trans(vec, method = "auto")
vec_trans(vec, method = "auto")
## transform a data frame
mat <- iris[, 1:4]
dat_trans(mat, method = "log")</pre>
```

 $df_{-}t$

```
## transform data frame under different conditions
plyr::ddply(iris, ("Species"), function(x, method) {
    dat_trans(x[, 1:4], method = method)
}, method = "range")

## use 'tidyverse'
library(dplyr)
library(tidyr)
library(purrr)

## transform whole data set
iris %>% mutate(across(where(is.numeric), ~ vec_trans(., method = "range")))

## transform data set within groups
iris %>%
    group_by(Species) %>%
    mutate(across(where(is.numeric), ~ vec_trans(., method = "range")))
```

df_na_idx

Get row index of missing values in data frame

Description

Get row index of missing values in data frame.

Usage

```
df_na_idx(df, vars)
```

Arguments

df data frame being used to check index of missing values.

vars vector of variable names in df for missing values checking.

Value

an vector of missing value index.

df_t

Transpose a numeric data frame (with/without NAs)

Description

Transpose a numeric data frame (with/without NAs)

Usage

```
df_t(x)
```

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Arguments

Χ

a data frame

Details

It is used mostly for numeric data frame with NAs and return a

Value

a transposed data frame.

Examples

```
x \leftarrow data.frame(group = c(1,1,2,NA,2), val = c(6,4,6,3.1,NA))
x \leftarrow df_t(x)
```

dim_mat

Get dimension matrix of a list of data frame

Description

Get a matrix for dimension information of a list of data frame.

Usage

```
dim_mat(mat_list)
```

Arguments

mat_list

a list of data frame.

Value

a data frame.

feat_count

Calculate the count number of features

Description

Calculate the features counts based on the frequency of multiple selectors.

Usage

```
feat\_count(fs.ord, top.k = 30)
```

Arguments

fs.ord data matrix for multiple feature order lists.

top.k top feature number to be processed.

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Value

a data matrix of feature counts.

Examples

```
fs.ord <- mtExtra:::fs.ord
feat_count(fs.ord, top.k = 20)</pre>
```

gg_heat_dend

Heatmap with dendrograms with ggplot2

Description

Plot heatmap of a data matrix using ggplot2. This function is modified from https://bit.ly/2UUnY2L.

Usage

```
gg_heat_dend(
  mat,
  row.dend = T,
  col.dend = T,
  row.dend.right = TRUE,
  colors = c("red", "white", "blue"),
  font.size = 10,
   x.rot = 60,
  legend.title = "value",
  dist.method = "euclidean",
  clust.method = "complete",
  dend.line.size = 0.5
)
```

Arguments

```
a data mstrix to be plotted.
mat
row.dend
                  plot row dendrogram or not.
col.dend
                  plot column dendrogram ot not.
row.dend.right a logical value to indicate the position of row dendrogram.
colors
                  a vector of colours for heatmap.
font.size
                  label font size.
                  plot rotate degree.
x.rot
legend.title
                  legend title.
                  distance method.
dist.method
                  cluster method.
clust.method
dend.line.size dendrogram line size.
```

Value

an object of class ggplot2.

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Examples

```
gg_heat_dend(mtcars)
```

graph_stats

Graph level metrics

Description

Return graph level metrics.

Usage

```
graph_stats(g)
```

Arguments

g

an igraph object.

Value

a vector of graph level metrics.

heat_dend

Heatmap with dendrogram on both sides

Description

Plot heatmap with dendrogram on both sides using lattice

Usage

```
heat_dend(
  mat,
  x.rot = 60,
  col = c("red", "white", "blue"),
  cex = 0.5,
  xlab = "",
  ylab = "",
  main = "",
  ...
)
```

Arguments

```
mat a data matrix for plotting.

x.rot the rotate degree.

col colours for heatmap.

cex font size.

xlab, ylab, main character strings for xlab, ylab and figure title.

... further parameters for lattice.
```

locfdr_filter

Value

an object of class lattice.

Examples

```
heat_dend(mtcars)
```

is_zero

Calculate the zero percentage

Description

Calculate the zero percentage

Usage

```
is_zero(mat)
```

Arguments

mat

a data matrix.

Value

an vector.

locfdr_filter

Filtering variable based on local false discovery rate

Description

Filter data based on local false discovery rate. This function uses z.2 of locfdr.

Usage

```
locfdr_filter(x, plot = 1, thres = NULL, ...)
```

Arguments

X	a	data	matrix

plot an integer for plotting. 0 gives no plots. 1 gives single plot showing the his-

togram of zz and fitted densities f and p0*f0.

thres a user defined threshold for filtering. The default is NULL, which use local FDR

as threshold for filtering.

... other parameters to be passed to locfdr.

locfdr_filter 17

Details

• Keep the variables which have at least one significant element. The significant element is defined as larger than the lower of threshold or less than the upper of threshold.

- Threshold can be given by user or be estimated by locfdr, i.e. the returned z.2 as a threshold. It is not guaranteed that locfdr z.2. If not, user must provide this value.
- From R package locfdr vignette: z.2 is the interval along the zz-axis outside of which fdr(z) < 0.2, the locations of the yellow triangles in the histogram plot. If no elements of zz on the left or right satisfy the criterion, the corresponding element of z.2 is NA, and the corresponding triangle does not appear.

Value

a list of with contents:

- dat the filtered data matrix.
- idx a vector of filtering index.
- thres threshold used for filtering.

See Also

```
locfdr()
```

```
Other variable filters: blank_filter(), mv_filter(), qc_filter(), rsd_filter(), var_filter()
```

```
## Not run:
library(dplyr)
library(tidyr)
library(purrr)
library(readr)
## get ionomics data
dat <- read_csv("https://github.com/wanchanglin/ionflow/raw/master/extra/paper_ko.csv")</pre>
dim(dat)
## missing values filling with mean
dat <- dat %>%
 mutate(across(where(is.numeric), function(x) {
    m \leftarrow mean(x, na.rm = TRUE)
    x[is.na(x)] \leftarrow m
  }))
res <- locfdr_filter(t(dat[, -1]), plot = 1)
res$thres
## filter data
dat <- dat[res$idx, , drop = FALSE]</pre>
## symbolise data
dat_sym <- dat %>%
  mutate(across(where(is.numeric), ~ dat_symb(., thres = res$thres)))
## End(Not run)
```

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mat2df

Convert matrix to df

Description

Convert matrix to df

Usage

```
mat2df(x)
```

Arguments

Х

a matrix

Details

```
from .matrix_to_df of package plyr.
```

Value

a data frame.

mv_filter

Filtering variable based on the percentage of missing values

Description

This function calculates the percentage of missing values and keeps those features with missing values percentage less than the designed threshold.

Usage

```
mv_filter(x, thres = 0.3)
```

Arguments

x a data matrix. The columns are features.

thres threshold of missing values. Features less than this threshold will be kept. Value

has to be between 0 and 1.

Value

a list of with contents:

- dat the filtered data matrix
- idx a logical vector of index for keeping features.

mv_perc 19

See Also

```
mv_perc()
Other variable filters: blank_filter(), locfdr_filter(), qc_filter(), rsd_filter(), var_filter()
```

Examples

```
meta <- mtExtra:::meta
mv_perc(meta)
mv_filter(meta, thres = 0.3)</pre>
```

mv_perc

Missing value percentage

Description

Calculate missing value percentage.

Usage

```
mv_perc(x)
```

Arguments

Х

an vector, matrix or data frame.

Value

missing value percentage.

See Also

```
mv_filter()
```

```
meta <- mtExtra:::meta
mv_perc(meta)
mv_filter(meta, thres = 0.3)</pre>
```

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net_graph

Create an igraph object

Description

Create an igraph object

Usage

```
net_graph(edge_df, node_df = NULL)
```

Arguments

edge_df graph edge matrix.

node_df graph vertex matrix.

Value

an igraph object with some vertex statistics and community detection center.

non_digit

Calculate the percentage of non digits

Description

Calculate the percentage of non digits.

Usage

```
non_digit(mat)
```

Arguments

mat

a data matrix.

Value

an vector.

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non_zero

Calculate the non-zero percentage

Description

Calculate the non-zero percentage.

Usage

```
non_zero(mat)
```

Arguments

mat

a data matrix.

Value

an vector.

 $outl_det_m$

Multivariate outlier detection

Description

Perform multivariate outlier detection.

Usage

```
outl_det_m(x, method = "mcd", conf.level = 0.95)
```

Arguments

x a data matrix.

method methods for resistant estimation of multivariate location and scatter. Only mve,

mcd and classical are supported.

conf.level a confidential level.

Value

a logical vector.

See Also

```
cov.rob() for "Resistant Estimation of Multivariate Location and Scatter"
```

Other outlier detectors: outl_det_u()

outl_det_u

Examples

```
set.seed(134)
x <- cbind(rnorm(80), rnorm(80), rnorm(80))
y <- cbind(rnorm(10, 5, 1), rnorm(10, 5, 1), rnorm(10, 5, 1))
x <- rbind(x, y)
outl <- outl_det_m(x, method = "mcd", conf.level = 0.95)</pre>
```

outl_det_u

Univariate outlier detection

Description

Perform outlier detection using univariate method.

Usage

```
outl_det_u(x, method = c("percentile", "median"))
```

Arguments

x a numeric vector.

method

method for univariate outlier detection. Only percentile and median are supported.

Details

- median: the absolute difference between the observation and the sample median is larger than 2 times of the Median Absolute Deviation divided by 0.6745.
- percentile: either smaller than the 1st quartile minus 1.5 times of IQR, or larger than the 3rd quartile plus 1.5 times of IQR.

Value

a logical vector.

References

Wilcox R R, Fundamentals of Modern Statistical Methods: Substantially Improving Power and Accuracy, Springer 2010 (2nd edition), pages 31-35.

See Also

```
Other outlier detectors: outl_det_m()
```

```
x <- c(2, 3, 4, 5, 6, 7, NA, 9, 50, 50)
outl_det_u(x, "percentile")
```

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pca_plot

PCA plot

Description

Plot PCA of a matrix or data frame with base R function.

Usage

```
pca_plot(x, y = NULL, scale = TRUE, ep.plot = FALSE, ...)
```

Arguments

x a matrix for plotting. Should have row names
 y a factor or character vector specifying the group information of the row.
 scale a logical flag to indicate whether or not scale x.
 ep.plot plot ellipse or not.
 ... further parameters passed to plot

Details

The rownames of x will be shown in the plot. y is used to indicate the group of row of x.

Value

a base R graphics object.

Author(s)

Wanchang Lin

Examples

```
data(iris)
pca_plot(iris[, 1:4], iris[, 5], ep.plot = TRUE)
```

pcor_dat

Partial correlation analysis

Description

Perform partial correlation analysis of two data matrix

Usage

```
pcor_dat(x, y, method = c("pearson", "kendall", "spearman"))
```

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Arguments

x, y two data matrix for correlation analyses.

method correlation method.

Value

a correlation matrix.

See Also

```
ppcor::pcor()
```

Examples

```
library(dplyr)
library(tidyr)
library(purrr)
## 'data' has been processed.
data <- mtExtra:::data
meta <- mtExtra:::meta</pre>
## filtering
meta <- mv_filter(meta, thres = 0.3)$dat</pre>
## missing value filling
meta <- meta %>%
  mutate(across(where(is.numeric), function(x) {
    m <- mean(x, na.rm = TRUE)</pre>
    x[is.na(x)] \leftarrow m
  }))
## normalisation
meta <- meta %>%
  mutate(across(where(is.numeric), ~ {
    .x \leftarrow (.x - mean(.x, na.rm = TRUE)) / sd(.x, na.rm = TRUE)
  }))
co <- pcor_dat(meta, data)</pre>
heat_dend(co)
```

 $plot_aam$

Wrapper function for plotting classification results

Description

This function plots accuracy, AUC and margin (aam) of classification results from package mt.

Usage

```
plot_aam(aam_list, fig_title = "Accuracy, AUC and Margin")
```

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Arguments

aam_list a data matrix of classification results.

fig_title a string of figure title

Value

```
an object of class ggplot2
```

See Also

 ${\tt aam.mcl}$ in R package mt for how to get accuracy, AUC and margin.

Examples

```
aam <- mtExtra:::aam
plot_aam(aam)</pre>
```

plot_pval

Plot adjusted p-values

Description

Plot the adjusted p-values using ggplot2

Usage

```
plot_pval(pval_list)
```

Arguments

pval_list a data matrix or a list of data matrix of p-value correction

Value

```
an object of class ggplot2
```

```
pval <- mtExtra:::pval
plot_pval(pval)</pre>
```

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qc_filter

MS/NMR data filtering based on RSD of "qc" data

Description

MS/NMR data filtering based on RSD of "qc" data

Usage

```
qc_filter(
    x,
    y,
    thres_rsd = 20,
    f_mv = TRUE,
    f_mv_qc_sam = FALSE,
    thres_mv = 0.3
)
```

Arguments

x a data matrix.

y a character string with contents of "sample", "qc" and "blank".

thres_rsd threshold of RSD on QC. Features less than this threshold will be kept.

f_mv a flag indicating whether or not to performance missing value filtering on either "sample" or "qc" data.

f_mv_qc_sam a flag for filtering using percentage of missing values on "qc" or "sample".

TRUE is for "qc".

thres_mv threshold of missing values. Features less than this threshold will be kept.

Details

This filter process takes two steps. First, the missing values filtering is performed on either "qc" or "sample". Then RSD-based filtering is applied to "qc" data.

Value

a list of with contents:

- · dat the filtered data matrix
- idx a logical vector of index for keeping features.

See Also

```
Other variable filters: blank_filter(), locfdr_filter(), mv_filter(), rsd_filter(), var_filter()
```

range_scale 27

range_scale

Scale vector to a defined range

Description

Scale vector to a defined range.

Usage

```
range_scale(x, range = c(0, 1))
```

Arguments

x a numeric vector

range a vector with two values: lower and higher.

Value

a scaled vector.

Examples

```
set.seed(100)
x <- rnorm(10)
range_scale(x, range = c(10, 20))</pre>
```

 $rbind_df$

Row binding of a list of data matrix

Description

Row bind of a list of matrix or data frame with the same dimension.

Usage

```
rbind_df(list)
```

Arguments

list

a list of data matrix.

Value

a data matrix.

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Examples

```
df1 \leftarrow data.frame(x = c(1, 3), y = c(2, 4))
df2 \leftarrow data.frame(x = c(5, 7), y = c(6, 8))
df <- list(df1 = df1, df2 = df2)
rbind_df(df)
tmp <- vector(mode = "list", length = 3)</pre>
for (i in 1:3) {
  tmp[[i]] <- data.frame(</pre>
    a = sample(letters, 5, rep = TRUE),
    b = rnorm(5), c = rnorm(5)
  )
}
names(tmp) \leftarrow c("abc", "def", "ghi")
tmp
do.call("rbind", tmp)
dplyr::bind_rows(tmp, .id = "column_label")
plyr::ldply(tmp, data.frame, .id = "column_label")
rbind_df(tmp)
```

rsd

Relative standard deviation

Description

Calculate Relative Standard Deviation(RSD). RSD is also known as the coefficient of variation (CV)

Usage

```
rsd(x, na.rm = TRUE)
```

Arguments

x an vector, matrix or data frame.

na.rm a logical value indicating whether NA values should be stripped before the computation proceeds.

Details

Some notes:

- The higher the CV, the greater the dispersion in the variable.
- The CV is often presented as the given ratio multiplied by 100
- Basically CV<10 is very good, 10-20 is good, 20-30 is acceptable, and CV>30 is not acceptable.

Value

RSD value multiplied by 100.

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Examples

```
library(ggplot2)
library(dplyr)
library(tidyr)
library(purrr)
data(iris)
rsd(iris[, 1:4])
## group rsd
val <- iris %>%
  group_by(Species) %>%
  group_modify(~ dat_summ(., method = rsd)) %>%
 pivot_longer(cols = !Species) %>% filter(!is.na(value))
ggplot(val, aes(x = value)) +
  geom_histogram(colour = "black", fill = "white") +
  facet_grid(Species ~ .)
ggplot(val, aes(x = Species, y = value)) + geom_boxplot()
## The plotting of missing value is similar like this.
```

rsd_filter

Filtering variable based on relative standard deviation (RSD)

Description

Filtering variable based on relative standard deviation (RSD).

Usage

```
rsd_filter(x, thres = 20)
```

Arguments

x a data frame where columns are features.thres threshold of RSD. Features less than this threshold will be kept.

Value

a list of with contents:

- · dat the filtered data matrix
- idx a logical vector of index for keeping features.

See Also

```
Other variable filters: blank_filter(), locfdr_filter(), mv_filter(), qc_filter(), var_filter()
```

```
x <- matrix(rnorm(20 * 20), ncol = 20)
res <- rsd_filter(x, thres = 30)
dim(res$dat)</pre>
```

30 samp_sub

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Select random sample with stratification

Description

Select random sample with stratification from a binary group.

Usage

```
samp_strat(grp, len, strat = TRUE)
```

Arguments

grp a character string indicating two group information.

len length of random selection.

strat a logical value indicated the sampling should be stratified.

Details

multiple group is not supported at the current stage.

Value

a selected index.

Examples

```
cls <- iris[, 5, drop = TRUE]
cls <- cls[cls == "setosa" | cls == "versicolor"]
cls <- droplevels(cls)
ind <- samp_strat(cls, 6, strat = TRUE)
cls[ind]
ind <- samp_strat(cls, 5, strat = TRUE)
cls[ind]</pre>
```

samp_sub

Select random samples from each group Select random samples from each group.

Description

Select random samples from each group. Select random samples from each group.

Usage

```
samp_sub(x, k, n = 10)
```

sym2long 31

Arguments

x a character string or factor indicating class info.
 k number of samples selected from each class.
 n number of replicates.

Value

a selected index.

Examples

```
cls <- iris[, 5, drop = TRUE]
(tmp <- samp_sub(cls,k = 6, n = 2))
cls[tmp[[1]]]
table(cls[tmp[[1]]])</pre>
```

sym2long

Convert a symmetric table(short format) to long format

Description

Convert a symmetric table(short format) to long format

Usage

```
sym2long(x, tri = c("upper", "lower"))
```

Arguments

x a symmetric matrix-like data set. tri triangular being used.

Value

a data frame of pair-wise comparison.

```
co <- cor_tab(mtcars, cor.method = "spearman", adj.method = "BH")
names(co)
corr <- sym2long(co$r, tri = "upper")
pval <- sym2long(t(co$p), tri = "upper")
padj <- sym2long(co$p, tri = "upper")
tmp <- data.frame(corr, pval, padj)</pre>
```

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trim_str

Trim white spaces

Description

Trim head and hail white spaces of a string.

Usage

```
trim_str(string)
```

Arguments

string

a character string to be processed.

Value

a trimmed string.

upd_data

Update data set by a subset of features

Description

Update data set after feature selection.

Usage

```
upd_data(dat.all, ord)
```

Arguments

dat.all a list of metabolomics data including intensity data, peak data and meta data

ord a subset of selected feature orders

var_filter 33

var_filter Filtering variable based on variability	var_filter	Filtering variable based on variability
--	------------	---

Description

Perform variable filtering based on feature variability measurement such as standard deviation(SD) and inter-quantile range(IQR).

Usage

```
var_filter(x, method = "IQR", na.rm = FALSE, thres = 0.25)
```

Arguments

Х	a matrix or data frame.
method	variability measurement method, such as IQR and sd.
na.rm	a logical value indicating whether NA values should be stripped before the computation proceeds.
thres	a numeric value between 0 and 1 for the threshold of quantile. Features whose variability value is large than this threshold will be kept.

Value

a list of with contents:

- dat the filtered data matrix
- idx a vector of filtering index.

See Also

```
Other variable filters: blank_filter(), locfdr_filter(), mv_filter(), qc_filter(), rsd_filter()
```

```
set.seed(100)
x <- matrix(rnorm(20 * 10), ncol = 10)
res <- var_filter(x, method = "sd", thres = 0.25)
sum(res$idx)</pre>
```

vec_segment vec_segment

vec2dat

Convert a list of unequal vectors to a data frame

Description

Convert a list of unequal vectors to a data frame.

Usage

```
vec2dat(x)
```

Arguments

Х

a list of vector.

Value

a data matrix.

Examples

```
lst <- list(data.frame(a = 1, b = 2), data.frame(a = 2, c = 3, d = 5))
do.call(plyr::rbind.fill, lst)
vec <- list(var1 = c(a = 1, b = 2), var2 = c(a = 2, c = 3, d = 5))
vec2dat(vec)</pre>
```

vec_segment

Vector statistics for error bar plotting

Description

Calculate vector's standard derivation, standard error of mean and confidence interval.

Usage

```
vec_segment(x, bar = c("SD", "SE", "CI"))
```

Arguments

x an vector.

bar a character string, supporting "SD", "SE" and "CI".

Value

an vector including lower, center and upper values.

See Also

```
Other vector stats functions: vec_stats()
```

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Examples

```
library(plyr)
library(reshape2)
library(dplyr)
library(tidyr)
library(purrr)
vec_segment(iris[,1])
## Use 'plyr' and 'reshape2' for group
mat <- melt(iris)</pre>
ddply(mat, .(Species, variable), function(x,bar) {
  vec_segment(x$value, bar = bar)
}, bar = "SD")
## Use 'tidyverse' for group
iris %>%
 pivot_longer(cols = !Species, names_to = "variable") %>%
 group_by(Species, variable) %>%
 nest() %>%
 mutate(map_dfr(.x = data, .f = ~ vec_segment(.x$value))) %>%
  select(!data)
iris %>%
  pivot_longer(cols = !Species, names_to = "variable") %>%
  group_nest(Species, variable) %>%
 mutate(map_dfr(data, ~ vec_segment(.x$value))) %>%
  select(!data)
```

vec_stats

Vector summary

Description

Calculate the statistical summary of a vector.

Usage

```
vec_stats(x, na.rm = FALSE, conf.interval = 0.95)
```

Arguments

```
x a numeric vector.na.rm remove NA or not.conf.interval a numeric value for confidence interval.
```

Details

Can be used for error bar plotting. Modify from https://bit.ly/3onsqot

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Value

a vector of summary consisting:

- number of vector length
- vector mean
- · vector standard derivation
- standard error of mean
- · confidence interval

See Also

Other vector stats functions: vec_segment()

Examples

```
library(dplyr)
library(tidyr)
library(purrr)

iris %>% dat_summ(method = vec_stats)
iris %>% group_by(Species) %>% group_modify(~ dat_summ(., method = vec_stats))
iris %>%
    pivot_longer(cols = !Species, names_to = "var") %>%
    group_nest(Species, var) %>%
    mutate(map_dfr(data, ~ vec_stats(.x$value))) %>%
    select(!data)
```

vertex_stats

Node descriptive metrics

Description

Return node descriptive metrics.

Usage

```
vertex_stats(g)
```

Arguments

g

an igraph object.

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