

Package ‘omicsViewer’

October 18, 2022

Title Interactive and explorative visualization of SummarizedExpressionSet or ExpressionSet using omicsViewer

Version 1.0.1

Description omicsViewer visualizes ExpressionSet (or SummarizedExperiment) in an interactive way. The omicsViewer has a separate back- and front-end. In the back-end, users need to prepare an ExpressionSet that contains all the necessary information for the downstream data interpretation. Some extra requirements on the headers of phenotype data or feature data are imposed so that the provided information can be clearly recognized by the front-end, at the same time, keep a minimum modification on the existing ExpressionSet object. The pure dependency on R/Bioconductor guarantees maximum flexibility in the statistical analysis in the back-end. Once the ExpressionSet is prepared, it can be visualized using the front-end, implemented by shiny and plotly. Both features and samples could be selected from (data) tables or graphs (scatter plot/heatmap). Different types of analyses, such as enrichment analysis (using Bioconductor package fgsea or fisher's exact test) and STRING network analysis, will be performed on the fly and the results are visualized simultaneously. When a subset of samples and a phenotype variable is selected, a significance test on means (t-test or ranked based test; when phenotype variable is quantitative) or test of independence (chi-square or fisher's exact test; when phenotype data is categorical) will be performed to test the association between the phenotype of interest with the selected samples. Additionally, other analyses can be easily added as extra shiny modules. Therefore, omicsViewer will greatly facilitate data exploration, many different hypotheses can be explored in a short time without the need for knowledge of R. In addition, the resulting data could be easily shared using a shiny server. Otherwise, a standalone version of omicsViewer together with designated omics data could be easily created by integrating it with portable R, which can be shared with collaborators or submitted as supplementary data together with a manuscript.

Depends R (>= 4.2)

License GPL-2

Imports survminer, survival, fastmatch, reshape2, stringr, beeswarm, grDevices, DT, shiny, shinythemes, shinyWidgets, plotly, networkD3, httr, matrixStats, RColorBrewer, Biobase, fgsea, openxlsx, psych, shinybusy, ggseqlogo, htmlwidgets, graphics, grid, stats, utils, methods, shinyjs, curl, flatxml, ggplot2, S4Vectors, SummarizedExperiment, RSQLite, Matrix, shinycssloaders

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biocViews Software, Visualization, GeneSetEnrichment,
DifferentialExpression, MotifDiscovery, Network,
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BugReports <https://github.com/mengchen18/omicsViewer>

URL <https://github.com/mengchen18/omicsViewer>

Video <https://www.youtube.com/watch?v=0nirB-exquY&list=PLo2m88IJf-RRoLKMY8UEGqCpraKYrX5lk>

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app_module	<i>Application level 0 module</i>
------------	-----------------------------------

Description

Function should only be used for the developers

Usage

```
app_module(
  input,
  output,
  session,
  .dir,
  filePattern = ".(RDS|db|sqlite|sqlite3)$",
  additionalTabs = NULL,
  ESVObj = reactive(NULL),
  esetLoader = readESVObj,
  exprsGetter = getExprs,
  pDataGetter = getPData,
  fDataGetter = getFData,
  imputeGetter = getExprsImpute,
  defaultAxisGetter = getAx,
```

```

  appName = "omicsViewer",
  appVersion = packageVersion("omicsViewer")
)

```

Arguments

input	input
output	output
session	session
.dir	reactive; directory containing the .RDS file of ExpressionSet or SummarizedExperiment
filePattern	file pattern to be displayed.
additionalTabs	additional tabs added to "Analyst" panel
ESVobj	the ESV object given, the drop down list should be disable in the "ui" component.
esetLoader	function to load the eset object, if an RDS file, should be "readRDS"
exprsGetter	function to get the expression matrix from eset
pDataGetter	function to get the phenotype data from eset
fDataGetter	function to get the feature data from eset
imputeGetter	function to get the imputed expression matrix from eset, only used when exporting imputed data to excel
defaultAxisGetter	function to get the default axes to be visualized. It should be a function with two arguments: x - the object loaded to the viewer; what - one of "sx", "sy", "fx" and "fy", representing the sample space x-axis, sample space y-axis, feature space x-axis and feature space y-axis respectively.
appName	name of the application
appVersion	version of the application

Value

do not return any values

Examples

```

if (interactive()) {
  dir <- system.file("extdata", package = "omicsViewer")
  server <- function(input, output, session) {
    callModule(app_module, id = "app", dir = reactive(dir))
  }
  ui <- fluidPage(
    app_ui("app")
  )
  shinyApp(ui = ui, server = server)
}

```

app_ui	<i>Application level 0 UI</i>
--------	-------------------------------

Description

Function should only be used for the developers

Usage

```
app_ui(id, showDropList = TRUE, activeTab = "Feature")
```

Arguments

id	id
showDropList	logical; whether to show the dropdown list to select RDS file, if the ESVObj is given, this should be set to "FALSE"
activeTab	one of "Feature", "Feature table", "Sample", "Sample table", "Heatmap"

Value

a list of UI components

Examples

```
if (interactive()) {
  dir <- system.file("extdata", package = "omicsViewer")
  server <- function(input, output, session) {
    callModule(app_module, id = "app", dir = reactive(dir))
  }
  ui <- fluidPage(
    app_ui("app")
  )
  shinyApp(ui = ui, server = server)
}
```

asEsetWithAttr	<i>Convert SummarizedExperiment to ExpressionSet retaining all attributes</i>
----------------	---

Description

Convert SummarizedExperiment to ExpressionSet retaining all attributes

Usage

```
asEsetWithAttr(x)
```

Arguments

x an object of class SummarizedExperiment

Value

an object of class ExpressionSet

correlationAnalysis *Correlating a expression matrix with phenotypical variables*

Description

This is a convenience function to perform correlation analysis, the output is in a format ready to be incorporated into object to be visualized by omicsViewer.

Usage

```
correlationAnalysis(x, pheno, min.value = 12, prefix = "Cor")
```

Arguments

x an expression matrix, rows are the features (e.g. proteins), columns are the samples

pheno a data.frame storing the numerical phenotypical variable to be correlated with the rows (features) in expression matrix.

min.value the minimum number of samples required in the correlation analysis, if lower than this number, NA will be returned.

prefix prefix of the names. Usually don't need to be changed by the user. When changes are needed, the prefix should be in a format like [analysis name][subset] so the "analysis name" and "subset" can be selected in the omicsViewer.

Value

Every correlation analysis returns a data.frame with five columns: R - pearson correlation coefficient N - number of values used in the analysis P - p-values returned by pearson correlation analysis logP - log transformed p-values range - the range of values in expression matrix used in the analysis

Examples

```
e1 <- matrix(rnorm(500), 50, 10)
rownames(e1) <- paste0("FT", 1:50)
p1 <- matrix(rnorm(50), 10, 5)
colnames(p1) <- paste0("PH", 1:5)
colnames(e1) <- rownames(p1) <- paste0("S", 1:10)
correlationAnalysis(x = e1, pheno = p1, min.value = 8)
```

csc2list	<i>convert a column compressed sparse matrix to a list</i>
----------	--

Description

convert a column compressed sparse matrix to a list

Usage

```
csc2list(x)
```

Arguments

x a matrix or CsparseMatrix object

Value

a sparse frame in data.frame

exprspca	<i>Perform PCA and prepare results for omicsViewer</i>
----------	--

Description

This is a convenience function to perform PCA on expression matrix, the output of PCA will be in a format ready to be incorporated into object to be visualized by omicsViewer.

Usage

```
exprspca(x, n = min(8, ncol(x) - 1), prefix = "PCA|All", fillNA = FALSE, ...)
```

Arguments

x an expression matrix, where rows are features and samples are on columns.

n number of components to keep

prefix prefix of the names. Usually don't need to be changed by the user. When changes are needed, the prefix should be in a format like [analysis name][subset] so the "analysis name" and "subset" can be selected in the omicsViewer.

fillNA logical; whether NA should be filled? If FALSE (default), na.omit will be called before PCA. If TRUE, the missing value will be replaced using [fillNA](#).

... other parameters passed to [prcomp](#)

Value

a data.frame storing the PCA results

Examples

```
# reading expression
packdir <- system.file("extdata", package = "omicsViewer")
expr <- read.delim(file.path(packdir, "expressionMatrix.tsv"), stringsAsFactors = FALSE)
# call PCA
pc <- exprspca(expr)
head(pc$samples)
head(pc$features)
```

extendMetaData	<i>Add extra columns to the phenoData/colData or featureData/rowData in ExpressionSet/SummarizedExperiment</i>
----------------	--

Description

Add extra columns to the phenoData/colData or featureData/rowData in ExpressionSet/SummarizedExperiment

Add extra columns to the phenoData/colData or featureData/rowData in ExpressionSet/SummarizedExperiment

Add extra columns to the phenoData/colData or featureData/rowData in ExpressionSet/SummarizedExperiment

Usage

```
extendMetaData(object, newData, where)

## S4 method for signature 'ExpressionSet,data.frame'
extendMetaData(
  object,
  newData,
  where = c("pData", "fData", "colData", "rowData")[1]
)

## S4 method for signature 'SummarizedExperiment,data.frame'
extendMetaData(
  object,
  newData,
  where = c("pData", "fData", "colData", "rowData")[1]
)

## S4 method for signature 'SummarizedExperiment,DFrame'
extendMetaData(
  object,
  newData,
  where = c("pData", "fData", "colData", "rowData")[1]
)
```


Arguments

object	an object of ExpressionSet-class
newData	a data.frame containing the data to be added
where	where to add the extra columns, should be one of "pData", "fData", "rowData" and "colData".

Value

an object of ExpressionSet-class

Note

The attributes in the pheno data and feature data will be preserved

Examples

```
est <- Biobase::ExpressionSet(assayData=matrix(runif(1000), nrow=100, ncol=10))
Biobase::pData(est)
est <- extendMetaData(est, data.frame(letter = letters[1:10]), where = "pData")
Biobase::pData(est)
```

fgsea1	<i>Wrapper of fgseaMultilevel function to take binary gene set matrix as input</i>
--------	--

Description

Wrapper of fgseaMultilevel function to take binary gene set matrix as input

Usage

```
fgsea1(gs, stats, gs_desc = NULL, ...)
```

Arguments

gs	either a data.frame or a (sparse) matrix input. If a data.frame object is given, it should have at least three columns named as "featureId", "gsId" and "weight". If a matrix is given, the matrix is binary matrix where rows are features and columns are gene sets. The values in the matrix should be either 1 or 0 representing the presence and absence of a feature in the genesets, respectively.
stats	ranking stats
gs_desc	description of gene sets, it should be a named vector and the names should be the same as colnames(gs)
...	other parameters passed to fgseaMultilevel

Value

a data.frame of fgsea results

Examples

```
## not for users
# library(fgsea)
# library(Biobase)
# dat <- readRDS(system.file(package = "omicsViewer", "extdata/demo.RDS"))
# fd <- fData(dat)
# fdgs <- fd[, grep("^GS\\|", colnames(fd))]
# res <- fgsea1(fdgs, stats = fd$t-test|OV_BR|md`, minSize = 5, maxSize = 500)
# res <- fgsea1(
#   fdgs, stats = fd$t-test|OV_BR|md`,
#   minSize = 5, maxSize = 500, gs_desc = colnames(fdgs))
```

fillNA	<i>Filling NAs in a matrix using constants calculated from user the defined function</i>
--------	--

Description

This function is usually use to impute missing values in expression matrix, where the rows are feature and columns are samples. This function impute the missing values on the row-wise, that is, every row will be imputed using different constant.

Usage

```
fillNA(
  x,
  maxfill = quantile(x, probs = 0.15, na.rm = TRUE),
  fillingFun = function(x) min(x, na.rm = TRUE) - log10(2)
)
```

Arguments

x	a matrix with NA values
maxfill	the maximum filled value, if the value calculated by fillingFun is greater than maxfill, then maxfill will the used to replace NAs.
fillingFun	function to calculate the filling values. It should be a function accept at least one argument "x", which is a row of input expression matrix. The default is $\text{function}(x) \min(x, \text{na.rm} = \text{TRUE}) - \log_{10}(2)$ corresponds to the "half of lowest detected values" if the expression matrix is log10 transformed. More examples:#' $\text{function}(x) \min(x, \text{na.rm} = \text{TRUE}) - 1$ # half of lowest detected value when expression matrix is in log2 scale $\text{function}(x) 0$ # replace NA by 0

Value

a matrix without NAs

Note

The returned matrix may have -Inf, which may need to be filtered/replaced additionally

Examples

```
m <- matrix(rnorm(200), 20, 10)
m[sample(1:200, size = 20)] <- NA
mf <- fillNA(m)
```

 filterRow

Filter out rows of expression matrix

Description

The function is used to filter rows with values of low intensities or do not reproducible presented in replicates.

Usage

```
filterRow(x, max.quantile = NULL, max.value = NULL, var = NULL, min.rep = 2)
```

Arguments

x	an expression matrix
max.quantile	a single numerical value between (0, 1), if the row maximum is smaller than this quantile (calculated from the whole matrix), the row will be removed.
max.value	a single numerical value, if the the maximum value of a row is smaller than this value, the row will be removed. Only used if max.quantile is set to "NULL".
var	variables has the same length as the column number in x to indicate which sample is from which group
min.rep	the minimum number of replicate in at least one of the groups, if less than this value, the row will be removed.

Value

a logical vector where the TRUE means row to keep

Examples

```
e1 <- matrix(rnorm(5000, sd = 0.3), 500, 10) + rnorm(500)
f <- filterRow(x = e1, max.quantile = 0.25)
table(f)
```

`getAutoRIF`*Get genes associated with search terms and AutoRIF annotations*

Description

Get genes associated with search terms and AutoRIF annotations

Usage

```
getAutoRIF(term, rif = c("generif", "autorif")[1], filter = TRUE)
```

Arguments

<code>term</code>	a character vector of terms want to search
<code>rif</code>	either autorif or generif, see " https://maayanlab.cloud/geneshot/ "
<code>filter</code>	whether the result should be filtered. The least frequently mentioned genes (most like 1 or 2 times) will be removed.

Value

a `data.frame` of 4 columns: gene, n, perc, rank.

Note

<https://amp.pharm.mssm.edu/geneshot/>

References

Alexander Lachmann, Brian M Schilder, Megan L Wojciechowicz, Denis Torre, Maxim V Kuleshov, Alexandra B Keenan, Avi Ma'ayan, Geneshot: search engine for ranking genes from arbitrary text queries, *Nucleic Acids Research*, Volume 47, Issue W1, 02 July 2019, Pages W571–W577, <https://doi.org/10.1093/nar/gkz393>

Alexander Lachmann, Brian M Schilder, Megan L Wojciechowicz, Denis Torre, Maxim V Kuleshov, Alexandra B Keenan, Avi Ma'ayan, Geneshot: search engine for ranking genes from arbitrary text queries, *Nucleic Acids Research*, Volume 47, Issue W1, 02 July 2019, Pages W571–W577, <https://doi.org/10.1093/nar/gkz393>

Examples

```
a <- getAutoRIF("mtor signaling")
```

getMQParams	<i>Parse mqpar.xml file</i>
-------------	-----------------------------

Description

Getting the experimental informatione (TMT or label free) from mqpar.xml file.

Usage

```
getMQParams(x)
```

Arguments

x	the path to mqpar.xml file
---	----------------------------

Value

a list of MQ paramters

getUPRefProteomeID	<i>get uniprot reference proteome IDs</i>
--------------------	---

Description

get uniprot reference proteome IDs

get uniprot reference proteome IDs

Usage

```
getUPRefProteomeID(
  domain = c("Eukaryota", "Archaea", "Bacteria", "Viruses")[1]
)
```

```
downloadUPRefProteome(
  id,
  domain = c("Eukaryota", "Archaea", "Bacteria", "Viruses")[1],
  destdir = "./"
)
```

Arguments

domain	the domain, one of "Eukaryota", "Archaea", "Bacteria" or "Viruses"
id	the UP id to download
destdir	destination directory

Value

a character vector of UP ids
 a character vector of UP ids

Functions

- getUPRefProteomeID: get uniprot reference protein IDs

<code>gsAnnotIdList</code>	<i>Annotation of gene/protein function using multiple IDs.</i>
----------------------------	--

Description

Annotation of gene/protein function using multiple IDs.

Usage

```
gsAnnotIdList(
  idList,
  gsIdMap,
  minSize = 5,
  maxSize = 500,
  data.frame = FALSE,
  sparse = TRUE
)
```

Arguments

<code>idList</code>	list of protein IDs, e.g. <code>list(c("ID1", "ID2"), c("ID13"), c("ID4", "ID8", "ID10"))</code>
<code>gsIdMap</code>	a data frame for geneset to id map, it has two columns - id: the ID column - term: annotation terms e.g. <code>gsIdMap <- data.frame(id = c("ID1", "ID2", "ID1", "ID2", "ID8", "ID10"), term = c("T1", "T1", "T2", "T2", "T2", "T2"), stringsAsFactors = FALSE)</code>
<code>minSize</code>	minimum size of gene sets
<code>maxSize</code>	maximum size of gene sets
<code>data.frame</code>	logical; whether to organize the result into data.frame format, see "Value" section.
<code>sparse</code>	logical; whether to return a sparse matrix, only used when <code>data.frame=FALSE</code>

Value

A binary matrix (if `data.frame = FALSE`), the number of rows is the same with length of `idList`, the columns are the annotated gene set; or a data.frame (if `data.frame = TRUE`) with three columns: `featureId`, `gsId`, `weight`.

Examples

```

terms <- data.frame(
  id = c("ID1", "ID2", "ID1", "ID2", "ID8", "ID10"),
  term = c("T1", "T1", "T2", "T2", "T2", "T2"),
  stringsAsFactors = FALSE
)
features <- list(c("ID1", "ID2"), c("ID13"), c("ID4", "ID8", "ID10"))
gsAnnotIdList(idList = features, gsIdMap = terms, minSize = 1, maxSize = 500)

terms <- data.frame(
  id = c("ID1", "ID2", "ID1", "ID2", "ID8", "ID10", "ID4", "ID4"),
  term = c("T1", "T1", "T2", "T2", "T2", "T2", "T1", "T2"),
  stringsAsFactors = FALSE
)
features <- list(F1 = c("ID1", "ID2", "ID4"), F2 = c("ID13"), F3 = c("ID4", "ID8", "ID10"))
gsAnnotIdList(features, gsIdMap = terms, data.frame = TRUE, minSize = 1)
gsAnnotIdList(features, gsIdMap = terms, data.frame = FALSE, minSize = 1)

```

hasAttr

Check whether an object has an attribute

Description

Check whether an object has an attribute

Usage

```
hasAttr(x, attr.name)
```

Arguments

x	the object
attr.name	a character vector containing the name of attributes to be checked

Value

a logical value/vector has the same length as attr.name

hclust2str	<i>Convert hclust object to/from single character</i>
------------	---

Description

Convert hclust object to/from single character

Usage

```
hclust2str(x)
```

```
str2hclust(x)
```

Arguments

x a character of length one or an hclust object

Value

a character stores the hclust object

a hclust object

Note

The \$call element in hclust will not be retained in the conversion. The conversion decreases the precision in the \$height element.

Examples

```
# not for end users
# m <- matrix(rnorm(50), 25)
# hc <- hclust(dist(m))
# plot(hc)
# te <- hclust2str(hc)
# hc2 <- str2hclust(te)
# plot(hc2)
```

list2csc	<i>convert a list to column compressed sparse matrix</i>
----------	--

Description

convert a list to column compressed sparse matrix

Usage

```
list2csc(l, dimnames)
```

Arguments

l	a data.frame with at least two columns - featureId, gsId; optionally a "weight" column.
dimnames	a list of dimnames, should contain at least one element for the row names.

Value

a sparse matrix, CsparseMatrix, column compressed

multi.t.test	<i>Function to perform multiple t-tests on an expression matrix</i>
--------------	---

Description

This is a convenience function to perform multiple student's t-test. The output is in a format ready to be incorporated into object to be visualized by omicsViewer. This function use [t.test](#).

Usage

```
multi.t.test(x, pheno, compare = NULL, fillNA = FALSE, ...)
```

Arguments

x	an expression matrix, usually log10 transformed.
pheno	phenotype data of x, the number of rows in pheno must equal the number of columns of x. Please refer to examples for more details.
compare	NULL or a matrix with three columns to define the comparisons to do. When a matrix is given, the first column should be one of the column headers in pheno; then the second and third columns should be two values presented (more than once) in the columns of pheno selected by the values in the first column. The samples mapped to the two values are compared. If paired comparisons to be done, the orders of samples should be mapped

fillNA logical; whether NA should be filled? If FALSE (default), t test will be performed whenever possible. If not possible, then NA will be returned. If TRUE, the missing value will be replaced using `fillNA`.

... other parameters passed to `t.test`

Value

a data.frame stores the t-test results with the follow columns: mean|[selected header in pheno]|[group 1 in test] - The mean value of group 1 n value|[selected header in pheno]|[group 1 in test] - The number of value used in the test for group 1 quantile|[selected header in pheno]|[group 1 in test] - The quantile of means values in group 1 mean|[selected header in pheno]|[group 2 in test] - The mean value of group 2 n value|[selected header in pheno]|[group 2 in test] - The number of value used in the test for group 2 quantile|[selected header in pheno]|[group 2 in test] - The quantile of means values in group 2 ttest|[group 1 in test]_vs_[group 2 in test]|pvalue - The p-value return by `t.test` ttest|[group 1 in test]_vs_[group 2 in test]|log.pvalue - The -log10 transformed p-value ttest|[group 1 in test]_vs_[group 2 in test]|fdr - The BH method corrected p-values, e.g. FDR ttest|[group 1 in test]_vs_[group 2 in test]|log.fdr - The -log10 transformed FDR ttest|[group 1 in test]_vs_[group 2 in test]|mean.diff - The difference between the means of the two groups, e.g. fold change

Examples

```
# reading expression
packdir <- system.file("extdata", package = "omicsViewer")
expr <- read.delim(file.path(packdir, "expressionMatrix.tsv"), stringsAsFactors = FALSE)
# reading phenotype data
pd <- read.delim(file.path(packdir, "sampleGeneral.tsv"), stringsAsFactors = FALSE)

## Single t-test
head(pd)
# define comparisons
tests <- c("Origin", "RE", "ME")
tres <- multi.t.test(x = expr, pheno = pd, compare = tests)

## multiple t-test
head(pd)
# define comparisons
tests <- rbind(
  c("Origin", "RE", "ME"),
  c("Origin", "RE", "LE"),
  c('TP53.Status', "MT", "WT")
)
tres <- multi.t.test(x = expr, pheno = pd, compare = tests)
```

Description

Mainly used in the shiny app to generate reproducible k distinct colors.

Usage

```
nColors(k, stop = FALSE)
```

Arguments

k	a number between 1 to 60 tells how many distinct colors to use
stop	logical; whether the function should return an error message if k is not in the range of 2 to 60. Default FALSE, the function will return NULL.

Value

a vector of hex code for k colors or NULL

Examples

```
nColors(5)
nColors(1, stop = FALSE)
```

normalize.nQuantiles *Normalization using n quantiles*

Description

Normalization using n quantiles

Usage

```
normalize.nQuantiles(x, probs = 0.5, shareFeature = FALSE, ref = 1)
```

Arguments

x	an expression matrix, usually log transformed
probs	the quantiles to be aligned across samples. If probs is a length 1 numerical vector, the quantiles will aligned. As a special case, probs = 0.5 equals the median centering. If probs' length is > 1, a shift and scaling factor of samples will be calculating by fitting linear models using quantiles of samples, the median and variance of samples will be corrected using the intersect and slope of the fitted model.
shareFeature	logical; if TRUE, the normalization will be based on the shared features between samples
ref	the columns name or index to specify the reference sample, only used when shareFeature = TRUE

Value

a normalized matrix

Examples

```
e1 <- matrix(rnorm(5000), 500, 10)
e1[, 6:10] <- 0.3 * e1[, 6:10] + 3
boxplot(e1)
# median centering, no variance correction
e2 <- normalize.nQuantiles(x = e1, probs = 0.5)
boxplot(e2)
# median centering + variance stablization
e3 <- normalize.nQuantiles(x = e1, probs = seq(0.25, 0.75, by = 0.1))
boxplot(e3)
```

normalize.totsum	<i>Normalize total sum</i>
------------------	----------------------------

Description

Normalize total sum

Usage

```
normalize.totsum(x)
```

Arguments

x a log10 transformed expression matrix

Value

a normalized matrix

Examples

```
e1 <- matrix(rnorm(5000), 500, 10)
e1[, 6:10] <- e1[, 6:10]+3
boxplot(e1)
e2 <- normalize.totsum(x = e1)
boxplot(e2)
```

normalizeColWise	<i>Column-wise normalization of expression matrix</i>
------------------	---

Description

A wrapper function of all column-wise normalization methods

Usage

```
normalizeColWise(
  x,
  method = c("Median centering", "Median centering (shared ID)", "Total sum",
    "median centering + variance stablization")[1]
)
```

Arguments

x	an expression matrix where rows are features and columns are samples, usually log transformed.
method	normalization method to use "Median centering" - median centering, see normalize.nQuantiles "Median centering (shared ID)" - median centering using shared features, see normalize.nQuantiles "Total sum" - total sum normalization "median centering + variance stablization" - 10 quantile normalization using 0.25, 0.3, ..., 0.75, see normalize.nQuantiles

Value

a normalized matrix

Examples

```
e1 <- matrix(rnorm(5000), 100, 50)+10
boxplot(e1)
e2 <- normalizeColWise(x = e1, method = "Median centering")
boxplot(e2)
```

normalizeData	<i>Normalized expression matrix</i>
---------------	-------------------------------------

Description

A wrapper function of all normalization methods, including row-wise or column-wise normalization.

Usage

```
normalizeData(
  x,
  colWise = c("None", "Median centering", "Median centering (shared ID)", "Total sum",
    "median centering + variance stablization")[1],
  rowWise = c("None", "Reference", "Batch mean", "Batch reference")[1],
  ref = NULL,
  batch = NULL
)
```

Arguments

x	an expression matrix where rows are features and columns are samples, usually log transformed.
colWise	column-wise normalization method to use, see normalizeColWise
rowWise	row-wise normalization method to used Reference - using removeVarQC method Batch mean - using rowshift method without reference samples Batch reference - using rowshift method with reference samples
ref	index of reference samples
batch	batch factor

Value

a normalized matrix

Examples

```
e1 <- matrix(rnorm(5000), 100, 50)+10
boxplot(e1)
e2 <- normalizeData(x = e1, ref = seq(5, 45, by = 10), rowWise = "Reference")
boxplot(e2)
```

omicsViewer

Start omicsViewer

Description

Start omicsViewer

Usage

```
omicsViewer(
  dir,
  additionalTabs = NULL,
  filePattern = ".(RDS|DB|SQLITE|SQLITE3)$",
```

```

    ESVObj = NULL,
    esetLoader = readESVObj,
    exprsGetter = getExprs,
    pDataGetter = getPData,
    fDataGetter = getFData,
    defaultAxisGetter = getAx,
    appName = "omicsViewer",
    appVersion = packageVersion("omicsViewer")
  )

```

Arguments

<code>dir</code>	directory to the ExpressionSet or SummarizedExperiment object. Only give the directory in this argument, not the .rds file.
<code>additionalTabs</code>	additional tabs added to "Analyst" panel
<code>filePattern</code>	file pattern to be displayed.
<code>ESVObj</code>	the ESV object
<code>esetLoader</code>	function to load the eset object, if an RDS file, should be "readRDS"
<code>exprsGetter</code>	function to get the expression matrix from eset
<code>pDataGetter</code>	function to get the phenotype data from eset
<code>fDataGetter</code>	function to get the feature data from eset
<code>defaultAxisGetter</code>	function to get the default axes to be visualized. It should be a function with two arguments: x - the object loaded to the viewer; what - one of "sx", "sy", "fx" and "fy", representing the sample space x-axis, sample space y-axis, feature space x-axis and feature space y-axis respectively.
<code>appName</code>	name of the application
<code>appVersion</code>	version of the application

Value

do not return values

Examples

```

1
## To start the shiny app:
# omicsViewer(
#   system.file("extdata", package = "omicsViewer")
# )

```

parseDatTerm *Extract function annotation from uniprot .dat file*

Description

Extract function annotation from uniprot .dat file

Usage

```
parseDatTerm(file, outputDir = NULL, ...)
```

Arguments

file	the .dat or .dat.gz file
outputDir	dir of output file
...	other parameters passed to readLines

Value

a data.frame parse from .dat file

plotly_boxplot_module *Shiny module for boxplot using plotly - Module*

Description

Shiny module for boxplot using plotly - Module

Usage

```
plotly_boxplot_module(
  input,
  output,
  session,
  reactive_param_plotly_boxplot,
  reactive_checkpoint = reactive(TRUE)
)
```

Arguments

input	input
output	output
session	session
reactive_param_plotly_boxplot	reactive value; argument passed to plotly_boxplot
reactive_checkpoint	reactive_value; check this value before render any plot/executing any calculation

Value

do not return any values

Examples

```
if (interactive()) {  
  
  library(shiny)  
  
  ui <- fluidPage(  
    plotly_boxplot_ui("testplotly")  
  )  
  
  server <- function(input, output, session) {  
  
    x <- cbind(matrix(rnorm(10000, mean = 3), 1000, 10), matrix(rnorm(20000), 1000, 20))  
    x[sample(1:length(x), size = 0.3*length(x))] <- NA  
    rownames(x) <- paste("R", 1:nrow(x), sep = "")  
    colnames(x) <- paste("C", 1:ncol(x), sep = "")  
    callModule(plotly_boxplot_module, id = "testplotly",  
      reactive_param_plotly_boxplot = reactive(list(  
        x = x# , i = c(4, 20, 80)# , highlight = c(1, 4, 5, 20), extvar = 1:30  
      ))  
    )  
  }  
  
  shinyApp(ui, server)  
}
```

plotly_boxplot_ui

Shiny module for boxplot using plotly - UI

Description

Function should only be used for the developers

Usage

```
plotly_boxplot_ui(id)
```

Arguments

id id

Value

a tagList of UI components

a tagList of UI components

Examples

```

if (interactive()) {

  library(shiny)

  ui <- fluidPage(
    plotly_boxplot_ui("testplotly")
  )

  server <- function(input, output, session) {

    x <- cbind(matrix(rnorm(10000, mean = 3), 1000, 10), matrix(rnorm(20000), 1000, 20))
    x[sample(1:length(x), size = 0.3*length(x))] <- NA
    rownames(x) <- paste("R", 1:nrow(x), sep = "")
    colnames(x) <- paste("C", 1:ncol(x), sep = "")
    callModule(plotly_boxplot_module, id = "testplotly",
               reactive_param_plotly_boxplot = reactive(list(
                 x = x# , i = c(4, 20, 80)# , highlight = c(1, 4, 5, 20), extvar = 1:30
               ))
    )
  }

  shinyApp(ui, server)
}

```

plotly_scatter_module *Shiny module for scatter plot using plotly - Module*

Description

Function should only be used for the developers

Usage

```

plotly_scatter_module(
  input,
  output,
  session,
  reactive_param_plotly_scatter,
  reactive_regLine = reactive(FALSE),
  reactive_checkpoint = reactive(TRUE),
  htest_var1 = reactive(NULL),
  htest_var2 = reactive(NULL)
)

```

Arguments

input input

output	output
session	session
reactive_param_plotly_scatter	reactive parameters for plotly_scatter
reactive_regLine	logical show or hide the regression line
reactive_checkpoint	checkpoint
htest_var1	when the plot is a beeswarmplot, two groups could be selected for two group comparison, this argument gives the default value. Mainly used for restoring the saved session.
htest_var2	see above

Value

a list containing the information about the selected data points
 an reactive object containing the information of selected, brushed points.

Examples

```
if (interactive()) {
  library(shiny)

  # two random variables
  x <- rnorm(30)
  y <- x + rnorm(30, sd = 0.5)

  # variables mapped to color, shape and size
  cc <- sample(letters[1:4], replace = TRUE, size = 30)
  shape <- sample(c("S1", "S2", "S3"), replace = TRUE, size = 30)
  sz <- sample(c(10, 20, 30), replace = TRUE, size = 30))

  ui <- fluidPage(
    plotly_scatter_ui("test_scatter")
  )

  server <- function(input, output, session) {
    v <- callModule(plotly_scatter_module, id = "test_scatter",
      # reactive_checkpoint = reactive(FALSE),
      reactive_param_plotly_scatter = reactive(list(
        x = x, y = y,
        color = cc,
        shape = shape,
        size = sz,
        tooltips = paste("A", 1:30)
      )))
    observe(print(v()))
  }
  shinyApp(ui, server)
```

```
# example beeswarm horizontal
x <- rnorm(30)
y <- sample(c("x", "y", "z"), size = 30, replace = TRUE)
shinyApp(ui, server)

# example beeswarm vertical
x <- sample(c("x", "y", "z"), size = 30, replace = TRUE)
y <- rnorm(30)
shinyApp(ui, server)

# return values
x <- c(5, 6, 3, 4, 1, 2)
y <- c(5, 6, 3, 4, 1, 2)
ui <- fluidPage(
  plotly_scatter_ui("test_scatter")
)
server <- function(input, output, session) {
  v <- callModule(plotly_scatter_module, id = "test_scatter",
    reactive_param_plotly_scatter = reactive(list(
      x = x, y = y, tooltips = paste("A", 1:6), highlight = 2:4
    )))

  observe(print(v()))
}
shinyApp(ui, server)
}
```

plotly_scatter_ui *Shiny module for scatter plot using plotly - UI*

Description

Function should only be used for the developers

Usage

```
plotly_scatter_ui(id, height = "400px")
```

Arguments

id	id
height	figure height

Value

a tagList of UI components

Examples

```

if (interactive()) {
  library(shiny)

  # two random variables
  x <- rnorm(30)
  y <- x + rnorm(30, sd = 0.5)

  # variables mapped to color, shape and size
  cc <- sample(letters[1:4], replace = TRUE, size = 30)
  shape <- sample(c("S1", "S2", "S3"), replace = TRUE, size = 30)
  sz <- sample(c(10, 20, 30), replace = TRUE, size = 30)

  ui <- fluidPage(
    plotly_scatter_ui("test_scatter")
  )

  server <- function(input, output, session) {
    v <- callModule(plotly_scatter_module, id = "test_scatter",
      # reactive_checkpoint = reactive(FALSE),
      reactive_param_plotly_scatter = reactive(list(
        x = x, y = y,
        color = cc,
        shape = shape,
        size = sz,
        tooltips = paste("A", 1:30)
      )))
    observe(print(v()))
  }
  shinyApp(ui, server)

  # example beeswarm horizontal
  x <- rnorm(30)
  y <- sample(c("x", "y", "z"), size = 30, replace = TRUE)
  shinyApp(ui, server)

  # example beeswarm vertical
  x <- sample(c("x", "y", "z"), size = 30, replace = TRUE)
  y <- rnorm(30)
  shinyApp(ui, server)

  # return values
  x <- c(5, 6, 3, 4, 1, 2)
  y <- c(5, 6, 3, 4, 1, 2)
  ui <- fluidPage(
    plotly_scatter_ui("test_scatter")
  )
  server <- function(input, output, session) {
    v <- callModule(plotly_scatter_module, id = "test_scatter",
      reactive_param_plotly_scatter = reactive(list(

```

```

        x = x, y = y, tooltips = paste("A", 1:6), highlight = 2:4
    )))

    observe(print(v()))
  }
  shinyApp(ui, server)
}

```

```
prepOmicsViewer
```

```
Prepare object to be viewed by omicsViewer
```

Description

This is a convenience function to prepare the data to be visualized using [omicsViewer](#). The result of PCA and t-test could be included directly.

Usage

```

prepOmicsViewer(
  expr,
  pData,
  fData,
  PCA = TRUE,
  ncomp = min(8, ncol(expr)),
  pca.fillNA = TRUE,
  t.test = NULL,
  ttest.fillNA = FALSE,
  ...,
  gs = NULL,
  stringDB = NULL,
  surv = NULL,
  SummarizedExperiment = TRUE
)

```

Arguments

<code>expr</code>	expression matrix where the rows are feature and columns are samples, matrix should be log10 transformed and have unique row and column names
<code>pData</code>	phenotype data
<code>fData</code>	feature data
<code>PCA</code>	pca
<code>ncomp</code>	number of components to keep
<code>pca.fillNA</code>	logical, whether the NA should be filled with a constant in PCA.
<code>t.test</code>	will be passed to the compare argument in multi.t.test
<code>ttest.fillNA</code>	logical, whether the NA should be filled with a constant in t-test.

... arguments passed to `t.test`, such as paired.

gs gene-set data, please refer to examples for more details about the format

stringDB the IDs that can be used in the STRING database (<https://string-db.org/>) query.

surv survival data, please refer to examples for more details about the format

SummarizedExperiment logical; whether to return an object of class SummarizedExperiment. If set to FALSE, the function will return an ExpressionSet object.

Value

an object of ExpressionSet or SummarizedExperiment that can be visualized using omicsViewer

Examples

```
packdir <- system.file("extdata", package = "omicsViewer")
# reading expression
expr <- read.delim(file.path(packdir, "expressionMatrix.tsv"), stringsAsFactors = FALSE)
colnames(expr) <- make.names(colnames(expr))
rownames(expr) <- make.names(rownames(expr))
# reading feature data
fd <- read.delim(file.path(packdir, "featureGeneral.tsv"), stringsAsFactors = FALSE)
# reading phenotype data
pd <- read.delim(file.path(packdir, "sampleGeneral.tsv"), stringsAsFactors = FALSE)

# reading other datasets
drugData <- read.delim(file.path(packdir, "sampleDrug.tsv"))
# survival data
# this data is from cell line, the survival data are fake data to
# show how to use the survival data in #' omicsViewer
surv <- read.delim(file.path(packdir, "sampleSurv.tsv"))
# gene set information
genesets <- read_gmt(file.path(packdir, "geneset.gmt"), data.frame = TRUE)
gsannot <- gsAnnotIdList(idList = rownames(fd), gsIdMap = genesets, data.frame = TRUE)

# Define t-test to be done, a matrix nx3
# every row define a t-test, the format
# [column header] [group 1 in the test] [group 2 in the test]
tests <- rbind(
  c("Origin", "RE", "ME"),
  c("Origin", "RE", "LE"),
  c('TP53.Status', "MT", "WT")
)
# prepare column for stringDB query
strid <- sapply(strsplit(fd$Protein.ID, ";|-"), "[", 1)
###
d <- prepOmicsViewer(
  expr = expr, pData = pd, fData = fd,
  PCA = TRUE, pca.fillNA = TRUE,
  t.test = tests, tttest.fillNA = FALSE,
  gs = gsannot, stringDB = strid, surv = surv)
# feature space - default x axis
```

```

attr(d, "fx") <- "ttest|RE_vs_ME|mean.diff"
# feature space - default y axis
attr(d, "fy") <- "ttest|RE_vs_ME|log.fdr"
# sample space - default x axis
attr(d, "sx") <- "PCA|All|PC1("
# sample space - default y axis
attr(d, "sy") <- "PCA|All|PC2("
# Save object and view
# saveRDS(d, file = "dtest.RDS")
## to open the viewer
# omicsViewer("./")

```

read.proteinGroups *Reading proteinGroup table of MaxQuant output*

Description

A convenience function to read the proteinGroups table of MaxQuant output. The function organize the result into different tables, e.g. iBAQ.

Usage

```
read.proteinGroups(x, quant = c("LF", "TMT")[1])
```

Arguments

x	the proteinGroup.txt file returned by MaxQuant search
quant	the quantification method, LF or TMT

Value

a list of tables extracted from proteinGroups.txt file

read.proteinGroups.lf *Read protein groups output of maxquant output and split it to columns*

Description

Read protein groups output of maxquant output and split it to columns

Usage

```
read.proteinGroups.lf(file)
```

Arguments

file	Maxquant proteinGroup.txt file path
------	-------------------------------------

Value

a list of tables extracted from proteinGroups.txt file

readESVObj	<i>Read the object of SummarizedExperiment or ExpressionSet to be visualized using omicsViewer</i>
------------	--

Description

This function accept a path to a sqlite database or RDS object. If an RDS file to be read, The function is similar to readRDS. It reads the object to R working environment and perform extra two things.

1. If the loaded data an class of SummarizedExperiment, it will be converted to ExpressionSet;
2. If the gene set annotation is in matrix format, the gene set annotation is converted to data.frame format.

Usage

```
readESVObj(x)
```

Arguments

x	the path of an object of SummarizedExperiment or ExpressionSet, passed to readRDS
---	---

Value

an object of class ExpressionSet or SummarizedExperiment to be visualized.

Examples

```
file <- system.file("extdata/demo.RDS", package = "omicsViewer")
obj <- readESVObj(file)
```

read_gmt	<i>Reading gene set .gmt file</i>
----------	-----------------------------------

Description

Frequently the .gmt files are downloaded from MSigDB database

Usage

```
read_gmt(x, id = NA, data.frame = FALSE)
```

Arguments

x	the name/path of the gmt file to be read
id	the id used in gene sets, if is not NA, it should be either "SYMBOL" or "ENTREZ". Usually only used when reading the .gmt file downloaded from MSigDB.
data.frame	logical; whether to organize the data in data.frame format. Default is FALSE, a list will be returned.

Value

a list or data frame of gene set. When data.frame = TRUE, the returned object is a data.frame with two columns: id and term.

Examples

```
file <- system.file("extdata", package = "omicsViewer")
file <- file.path(file, "geneset.gmt")
gs <- read_gmt(file)
```

removeVarQC

Removing variance of reference samples

Description

This normalization removes the variance in reference samples. The method do not need to specific the batch assignment but cannot work with data contains less than five common reference samples. A typical use of this normalization is to correct some drifting effect in mass spec based label free proteomics or untargeted metabolomics experiment. Usually, this is a very strong normalization should only be used with good reasons.

Usage

```
removeVarQC(x, ref, positive = TRUE, ...)
```

Arguments

x	an expression matrix
ref	the index of reference samples
positive	logical; force only positive values in the resulted matrix
...	if given, normalize.nQuantiles will be called first, the arguments here will be passed to normalize.nQuantiles

Value

a normalized matrix

Examples

```
e1 <- matrix(rnorm(5000), 100, 50)+10
e2 <- removeVarQC(x = e1, ref = seq(5, 45, by = 10))
boxplot(e2)
```

rowshift	<i>Row-wise normalization of expression matrix with or without reference sample</i>
----------	---

Description

Row-wise normalization of expression matrix with or without reference sample

Usage

```
rowshift(x, batch, ref = NULL, useMean = FALSE)
```

Arguments

x	an expression matrix where rows are features, e.g. genes, proteins and columns are samples. The values in the matrix are usually log transformed.
batch	a factor or vector has the same length as <code>ncol(x)</code> to indicate the batch assignment of samples.
ref	a logical vector has the same length as <code>ncol(x)</code> to indicated which columns are the common references among batches. If it is <code>NULL</code> (by default), the mean of all channels will be used as batch reference. When <code>NA</code> present in the reference channels, the mean values will be used in correction.
useMean	logical; whether to use means of batches, usually set to <code>TRUE</code> when no reference available

Value

a matrix (hopefully without/with less batch effect)

Examples

```
e1 <- matrix(rnorm(5000), 500, 10)
e1[, 6:10] <- e1[, 6:10] + 3
boxplot(e1)
f <- rep(c("a", "b"), each = 5)
e2 <- rowshift(x = e1, batch = f)
boxplot(e2)
```

saveOmicViewerDb *Save the xcmsViewer result object as sqlite database*

Description

Save the xcmsViewer result object as sqlite database

Usage

```
saveOmicViewerDb(obj, db.file, overwrite = TRUE)

## S4 method for signature 'SummarizedExperiment,character'
saveOmicViewerDb(obj, db.file, overwrite = TRUE)

## S4 method for signature 'ExpressionSet,character'
saveOmicViewerDb(obj, db.file, overwrite = TRUE)
```

Arguments

obj an object of class ExpressionSet or SummarizedExperiment
db.file a character indicate file name of the database file
overwrite logical. whether the database should be overwritten if exist already.

Value

the directory where the database saved

Examples

```
f <- system.file("extdata", "demo.RDS", package = "omicsViewer")
es <- readRDS(f)
# The following line will write a database file on your disk
# saveOmicViewerDb(es, db.file = "./omicsViewerData.db")
```

triselector_module *The three-step selector - the module function*

Description

The selector is used to select columns of phenotype and feature data. Function should only be used for the developers.

Usage

```
triselector_module(
  input,
  output,
  session,
  reactive_x,
  reactive_selector1 = reactive(NULL),
  reactive_selector2 = reactive(NULL),
  reactive_selector3 = reactive(NULL),
  label = "Group Label:"
)
```

Arguments

input	input
output	output
session	session
reactive_x	an nx3 matrix
reactive_selector1	default value for selector 1
reactive_selector2	default value for selector 2
reactive_selector3	default value for selector 3
label	of the triselector

Value

an reactive object containing the selected values

Examples

```
if (interactive()) {
  library(shiny)
  library(Biobase)

  file <- system.file("extdata/demo.RDS", package = "omicsViewer")
  dat <- readRDS(file)
  fData <- fData(dat)
  triset <- stringr::str_split_fixed(colnames(fData), '\\\\|', n= 3)

  ui <- fluidPage(
    triselector_ui("tres"),
    triselector_ui("tres2")
  )
  server <- function(input, output, session) {
    v1 <- callModule(triselector_module, id = "tres", reactive_x = reactive(triset),
                    reactive_selector1 = reactive("ttest"),
                    reactive_selector2 = reactive("RE_vs_ME"),
```

```

        reactive_selector3 = reactive("mean.diff")
    )
    v2 <- callModule(triselector_module, id = "tres2", reactive_x = reactive(triset),
        reactive_selector1 = reactive("ttest"),
        reactive_selector2 = reactive("RE_vs_ME"),
        reactive_selector3 = reactive("log.fdr"))

    observe({
      print("////////////////////////////////////")
      print(v1())
    })
  }

  shinyApp(ui, server)
}

```

triselector_ui	<i>The three-step selector - the ui function</i>
----------------	--

Description

Function should only be used for the developers

Usage

```
triselector_ui(id)
```

Arguments

```
id          id
```

Value

a tagList of UI components

Examples

```

if (interactive()) {
  library(shiny)
  library(Biobase)

  file <- system.file("extdata/demo.RDS", package = "omicsViewer")
  dat <- readRDS(file)
  fData <- fData(dat)
  triset <- stringr::str_split_fixed(colnames(fData), '\\\\|', n= 3)

  ui <- fluidPage(
    triselector_ui("tres"),
    triselector_ui("tres2")
  )
  server <- function(input, output, session) {

```

```

v1 <- callModule(triselector_module, id = "tres", reactive_x = reactive(triset),
  reactive_selector1 = reactive("ttest"),
  reactive_selector2 = reactive("RE_vs_ME"),
  reactive_selector3 = reactive("mean.diff")
)
v2 <- callModule(triselector_module, id = "tres2", reactive_x = reactive(triset),
  reactive_selector1 = reactive("ttest"),
  reactive_selector2 = reactive("RE_vs_ME"),
  reactive_selector3 = reactive("log.fdr"))

observe({
  print("////////////////////////////////////")
  print(v1())
})
}

shinyApp(ui, server)
}

```

trisetter

Create a nx3 matrix that can be use for triselector given a meta and expression table

Description

only used inside reactive

Usage

```
trisetter(meta, expr = NULL, combine)
```

Arguments

meta	a meta data, usually either phenotype data or feature data
expr	expression matrix, optional.
combine	how the meta and expression to be combined. Should be either "pheno" or "feature" or "none".

Value

a nx3 matrix
a data.frame with 3 columns

validMQFolder	<i>MQ folder validator</i> Validate whether a folder is a MQ output folder
---------------	--

Description

MQ folder validator Validate whether a folder is a MQ output folder

Usage

```
validMQFolder(dir)
```

Arguments

dir	the directory to check
-----	------------------------

Details

from the root level, these files exist: mqpar.xml [[combined/]txt/]proteinGroups.txt

Value

a list containing the info about MQ folder check

varSelector	<i>variable selector</i>
-------------	--------------------------

Description

variable selector

Usage

```
varSelector(x, expr, meta, alternative = NULL)
```

Arguments

x	variable return by triselector, a list of length three named as "analysis", "subset" and "variable"
expr	the expression matrix
meta	a meta matrix
alternative	alternative value to be returned when nothing to select

Value

the selected values in input argument x

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