Package 'countsimQC'

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```
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Description countsimQC provides functionality to create a comprehensive report
      comparing a broad range of characteristics across a collection of count
      matrices. One important use case is the comparison of one or more synthetic
     count matrices to a real count matrix, possibly the one underlying the
     simulations. However, any collection of count matrices can be compared.
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Title Compare Characteristic Features of Count Data Sets

Type Package

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Description

countsimQC

Author(s)

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See Also

Useful links:

- https://github.com/csoneson/countsimQC
- Report bugs at https://github.com/csoneson/countsimQC/issues

 ${\tt calculateDispersionsddsList}$

Calculate dispersions

Description

Calculate the dispersions for each data set in a list of DESeqDataSets, using both edgeR and DESeq2.

Usage

calculateDispersionsddsList(ddsList, maxNForDisp)

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Arguments

ddsList A list of DESeqDataSets

maxNForDisp If any data set contains more than maxNForDisp samples, maxNForDisp of them

will be randomly sampled before the dispersions are calculated, in order to speed

up calculations

Value

A list of the same length as the input list. Each element in the list is itself a list, containing a DGEList and a DESeqDataSet with calculated dispersions.

Author(s)

Charlotte Soneson

calculateFeatureCorrs Calculate Spearman correlation between feature pairs

Description

Calculate Spearman correlation between feature pairs

Usage

calculateFeatureCorrs(ddsList, maxNForCorr)

Arguments

ddsList List of lists, with one element per data set. Each element is a list containing

a DGEList and a DESeqDataSet, with calculated dispersions (e.g., output from

 $calculate {\tt DispersionsddsList}).$

maxNForCorr Maximal number of features to use for calculation of correlations. If the number

of features in a data set exceeds maxNForCorr, maxNForCorr features will be

randomly selected for calculation of correlations.

Value

A data frame with pairwise feature correlations for each data set

Author(s)

Charlotte Soneson

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calculateSampleCorrs Calculate Spearman correlation between sample pairs

Description

Calculate Spearman correlation between sample pairs

Usage

```
calculateSampleCorrs(ddsList, maxNForCorr)
```

Arguments

ddsList List of lists, with one element per data set. Each element is a list containing

a DGEList and a DESeqDataSet, with calculated dispersions (e.g., output from

calculateDispersionsddsList).

maxNForCorr Maximal number of samples to use for correlation calculation. If the number

of samples in a data set exceeds maxNForCorr, maxNForCorr samples will be

randomly selected for calculation of correlations.

Value

A data frame with pairwise sample correlations for each data set

Author(s)

Charlotte Soneson

calculateStats

Calculate statistics for pairwise comparison of data sets

Description

Calculate a range of statistics and p-values for comparison of two data sets.

```
calculateStats(
  df,
  ds1,
  ds2,
  column,
  subsampleSize,
  permute = FALSE,
  kmin,
  kfrac,
  xmin,
  xmax
)
```

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Arguments

df The input data frame. Must contain at least a column named 'dataset' and an

additional column with values to use as the basis for the comparison.

ds1, ds2 The names of the two data sets to be compared.

column The name of the column(s) of df to be used as the basis for the comparison.

subsampleSize The number of observations for which certain time-consuming statistics will be

calculated. The observations will be selected randomly among the rows of df.

permute Whether to permute the dataset column of df before calculating the statistics.

kmin, kfrac For statistics that require the extraction of k nearest neighbors of a given point,

the number of neighbors will be max(kmin, kfrac * nrow(df)).

xmin, xmax Smallest and largest value of column, used to normalize the x-axis when calcu-

lating the area between the eCDFs.

Value

A vector with statistics and p-values

Author(s)

Charlotte Soneson

countsimExample Example list with three count data sets

Description

A named list with three elements, each corresponding to a (real or simulated) count data set.

Usage

```
data("countsimExample")
```

Format

A named list with three elements, each corresponding to a (real or simulated) count data set.

Details

The Original data set represents a subset of 10,000 genes and 11 cells from the GSE74596 single-cell RNA-seq data set, obtained from the conquer repository (http://imlspenticton.uzh.ch:3838/conquer/). The Sim1 and Sim2 data sets similarly represent subsets of scRNA-seq data sets simulated with two different simulation methods, using the real GSE74596 data set as the basis for parameter estimation. Each data set is represented as a DESeqDataSet object.

Value

A named list with three elements, each corresponding to a (real or simulated) count data set.

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countsimExample_dfmat Example list with three count data sets in different formats

Description

A named list with three elements, each corresponding to a (real or simulated) count data set. One of them is provided as a DESeqDataset, one as a count data frame and one as a count matrix.

Usage

```
data("countsimExample_dfmat")
```

Format

A named list with three elements, each corresponding to a (real or simulated) count data set.

Details

The Original data set represents a subset of 10,000 genes and 11 cells from the GSE74596 single-cell RNA-seq data set, obtained from the conquer repository (http://imlspenticton.uzh.ch:3838/conquer/). The Sim1 and Sim2 data sets similarly represent subsets of scRNA-seq data sets simulated with two different simulation methods, using the real GSE74596 data set as the basis for parameter estimation.

Value

A named list with three elements, each corresponding to a (real or simulated) count data set.

countsimQCReport

Generate countsimQC report

Description

Generate a report comparing a range of characteristics across a collection of one or more count data sets.

```
countsimQCReport(
  ddsList,
  outputFile,
  outputDir = "./",
  outputFormat = NULL,
  showCode = FALSE,
  rmdTemplate = NULL,
  forceOverwrite = FALSE,
  savePlots = FALSE,
  description = NULL,
  maxNForCorr = 500,
  maxNForDisp = Inf,
```

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```
calculateStatistics = TRUE,
subsampleSize = 500,
kfrac = 0.01,
kmin = 5,
permutationPvalues = FALSE,
nPermutations = NULL,
knitrProgress = FALSE,
quiet = FALSE,
ignorePandoc = FALSE,
useRAGG = FALSE,
dpi = 96,
...
)
```

Arguments

ddsList Named list of DESeqDataSets or count matrices to compare. See the DESeq2

Bioconductor package (http://bioconductor.org/packages/release/bioc/html/DESeq2.html) for more information about the DESeqDataSet class. Each DESeqDataSet object in the list should contain a count matrix, a data frame with sample information and a design formula. The sample information and design formula will be used to calculate dispersions appropriately. If count matrices are provided, it is assumed that all columns represent replicate samples, and the design formula ~1

will be used.

outputFile The file name of the final report. The extension must match the selected outputFormat

(i.e., either .html or .pdf).

outputDir The directory where the final report should be saved.

outputFormat The output format of the report. If set to NULL or "html_document", an html

report will be generated. If set to "pdf_document", a pdf report will be gener-

ated.

showCode Whether or not to include the code in the final report.

rmdTemplate The Rmarkdown (.Rmd) file that will be used as the template for generating the

report. If set to NULL (default), the template provided with the countsimQC

package will be used. See Details for more information.

forceOverwrite Whether to force overwrite existing output files when saving the generated re-

port and figures.

savePlots Whether to save the ggplot objects for all the output figures, to allow additional

fine-tuning and generation of individual plots. Note that the resulting file can be

quite large, especially when many and/or large data sets are compared.

description A string (of arbitrary length) describing the content of the generated report. This

will be included in the beginning of the report. If set to NULL, a default descrip-

tion listing the number and names of the included data sets will be used.

maxNForCorr The maximal number of samples (features) for which pairwise correlation co-

efficients will be calculated. If the number of samples (features) exceeds this number, they will be randomly subsampled.

maxNForDisp The maximal number of samples that will be used to estimate dispersions. By

default, all samples are used. This can be lowered to speed up calculations (and

obtain approximate results) for large data sets.

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calculateStatistics

Whether to calculate quantitative pairwise statistics for comparing data sets in

addition to generating the plots.

subsampleSize The number of randomly selected observations (samples, features or pairs of

samples or features) for which certain (time-consuming) statistics will be calcu-

lated. Only used if calculateStatistics = TRUE.

kmin, kfrac For statistics that require the extraction of the k nearest neighbors of a given

point, the number of neighbors will be max(kmin, kfrac * nrow(df))

permutationPvalues

Whether to calculate permutation p-values for selected pairwise data set com-

parison statistics.

nPermutations The number of permutations to perform when calculating permutation p-values

for data set comparison statistics. Only used if permutationPvalues = TRUE.

knitrProgress Whether to show the progress bar when the report is generated.

quiet Whether to suppress warnings and progress messages when the report is gener-

ated.

ignorePandoc Determines what to do if pandoc or pandoc-citeproc is missing (if Sys.which("pandoc")

or Sys.which("pandoc-citeproc") is ""). If ignorePandoc is TRUE, only a warning is given. The figures will be generated, but not the final report. If ignorePan-

doc is FALSE (default), the execution stops immediately.

useRAGG Logical scalar, indicating whether to use ragg_png as the graphics device in the

report rather than the default png.

dpi Numeric scalar, setting the dpi of the generated plots. Only used if useRAGG is

TRUE.

... Other arguments that will be passed to rmarkdown::render.

Details

When the function is called, the template file (specified by rmdTemplate) will be copied into the output folder, and rmarkdown::render will be called to generate the final report. If there is already a .Rmd file with the same name in the output folder, the function will raise an error and stop, to avoid overwriting the existing file. The reason for this behaviour is that the copied template in the output folder will be deleted once the report is generated.

Value

No value is returned, but a report is generated in the outputDir directory.

Author(s)

Charlotte Soneson

Examples

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defaultStats

Return a vector of NA scores

Description

Return a vector of NA scores

Usage

```
defaultStats(n, withP = FALSE)
```

Arguments

Number of columns to use for the comparisonwithPWhether or not to include p-value columns

Value

A vector with NA values for all applicable statistics

Author(s)

Charlotte Soneson

defineTableDesc

Define table descriptions

Description

Generate the text that describes the content of the tables generated by makeDF.

```
defineTableDesc(
   calculateStatistics,
   subsampleSize,
   kfrac,
   kmin,
   obstype,
   aspect,
   minvalue,
   maxvalue,
   permutationPvalues,
   nPermutations,
   nDatasets
)
```

Arguments

calculateStatistics

Whether or not statistics and p-values are calculated

subsampleSize The number of observations for which certain (time-consuming) statistics will

be calculated

kmin, kfrac For statistics that require the extraction of k nearest neighbors of a given point,

the number of neighbors will be max(kmin, kfrac * nrow(df))

obstype The type of observation (e.g., sample, feature, sample pair)

aspect The name of the aspect of interest

minvalue, maxvalue

The minimal and maximal value of the aspect of interest, used for scaling of the

x axis when calculating the area between the eCDFs

permutationPvalues

Whether or not to calculate p-values of statistics via permutation

nPermutations The number of permutations (only used if permutationPvalues = TRUE)

nDatasets The number of data sets that are being compared

Value

A list with two text strings in markdown format: one for tables based on a single data column, and one for tables based on two data columns

Author(s)

Charlotte Soneson

generateIndividualPlots

Generate individual plots from countsimQCReport output

Description

Generate separate plots for all evaluation criteria using the collection of ggplot objects that can be saved when generating a countsimQC report (by setting savePlots = TRUE).

```
generateIndividualPlots(
  ggplotsRds,
  device = "png",
  outputDir = "./",
  nDatasets = 2
)
```

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Arguments

The path to a .rds file generated by countsimQCReport by setting savePlots =
TRUE, or the list of plots stored in this file.

device One of "eps", "ps", "tex" (pictex), "pdf", "jpeg", "tiff", "png", "bmp", "svg"
or "wmf" (windows only) (will be provided to the ggsave function from the
ggplot2 package).

outputDir The output directory where the plots should be generated.

nDatasets The number of data sets that are compared in the figures. This is needed to set

the size of the plots correctly.

Value

Nothing is returned, but plots are generated in the designated output directory.

Author(s)

Charlotte Soneson

Examples

makeDF

Construct data frame with pairwise statistics

Description

Construct a data frame containing statistics and p-values for pairwise comparison of data sets.

```
makeDF(
   df,
   column,
   permutationPvalues,
   nPermutations,
   subsampleSize,
   kmin,
   kfrac
)
```

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Arguments

df The input data frame. Must contain at least a column named 'dataset' and an

additional column with values

column The name of the column(s) of df to be used as the basis for the comparison

permutationPvalues

Whether or not to calculate p-values of statistics via permutation

nPermutations The number of permutations (only used if permutationPvalues = TRUE)

subsampleSize The number of observations for which certain (time-consuming) statistics will

be calculated. The observations will be selected randomly among the rows of

df

kmin, kfrac For statistics that require the extraction of k nearest neighbors of a given point,

the number of neighbors will be max(kmin, kfrac * nrow(df))

Value

A data table with statistics and p-values for pairwise comparisons of data sets, based on the provided column

Author(s)

Charlotte Soneson

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