Package 'marr'

October 22, 2025

Type Package

Title Maximum rank reproducibility

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License GPL (>= 3)

Description marr (Maximum Rank Reproducibility) is a nonparametric approach that detects reproducible signals using a maximal

rank statistic for high-dimensional biological data.

In this R package, we implement functions that measures the reproducibility of features per sample

pair and sample pairs per feature in high-dimensional biological replicate experiments. The

user-friendly plot functions in this package also plot

histograms of the reproducibility of

features per sample pair and sample pairs per feature.

Furthermore, our approach also allows the users to select

optimal filtering threshold values for the

identification of reproducible features and sample pairs based on output visualization checks (histograms). This package also provides the subset of data filtered by

reproducible features and/or sample pairs.

biocViews QualityControl, Metabolomics, MassSpectrometry, RNASeq, ChIPSeq

BugReports https://github.com/Ghoshlab/marr/issues

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 ${\tt data.frameORSummarizedExperiment-class} \\ {\tt S4~Class~union}$

Description

Class union allowing MarrData slot to be a data.frame or Summarized Experiment

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| | |

Description

This function applies an Rcpp-based implementation of a computationally efficient method for assessing reproducibility in high-throughput experiments, called the Marr procedure. This function also defines the Marr class and constructor.

Usage

```
Marr(
  object,
  pSamplepairs = 0.75,
  pFeatures = 0.75,
  alpha = 0.05,
  featureVars = NULL
)
```

Arguments

| object | an object which is a matrix or data.frame with features (e.g. metabolites or genes) on the rows and samples as the columns. Alternatively, a user can provide a SummarizedExperiment object and the assay(object) will be used as input for the Marr procedure. |
|--------------|---|
| pSamplepairs | (Optional) a threshold value that lies between 0 and 1, used to assign a feature to be reproducible based on the reproducibility output of the sample pairs per feature. Default is 0.75. |
| pFeatures | (Optional) a threshold value that lies between 0 and 1, used to assign a sample pair to be reproducible based on the reproducibility output of the features per sample pair. Default is 0.75. |
| alpha | (Optional) level of significance to control the False Discovery Rate (FDR). Default is 0.05 . |
| featureVars | (Optional) Vector of the columns which identify features. If a 'SummarizedExperiment' is used for 'data', row variables will be used. |

Details

marr (Maximum Rank Reproducibility) is a nonparametric approach, which assesses reproducibility in high-dimensional biological replicate experiments. Although it was originally developed for RNASeq data it can be applied across many different high-dimensional biological data including MassSpectrometry based Metabolomics and ChIPSeq. The Marr procedure uses a maximum rank statistic to identify reproducible signals from noise without making any distributional assumptions of reproducible signals. This procedure can be easily applied to a variety of measurement types since it employs a rank scale.

This function computes the distributions of percent reproducible sample pairs (row-wise) per feature and percent reproducible features (column-wise) per sample pair, respectively. Additionally, it also computes the percent of reproducible sample pairs and features based on a threshold value. See the vignette for more details.

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Value

A object of the class Marr that contains a numeric vector of the Marr sample pairs in the MarrSamplepairs slot, a numeric vector of the Marr features in the MarrFeatures slot, a numeric value of the Marr filtered features in the MarrSamplepairsfiltered slot, and a numeric value of the Marr filtered sample pairs in the MarrFeaturesfiltered slot.

References

Philtron, D., Lyu, Y., Li, Q. and Ghosh, D., 2018. Maximum Rank Reproducibility: A Nonparametric Approach to Assessing Reproducibility in Replicate Experiments. Journal of the American Statistical Association, 113(523), pp.1028-1039.

Examples

Marr-class

the Marr class

Description

Objects of this class store needed information to work with a Marr object

Value

MarrSamplepairs returns the distribution of percent reproducible features (column-wise) per sample pair, MarrFeatures returns the distribution of percent reproducible sample pairs (row-wise) per feature, MarrSamplepairsfiltered returns the percent of reproducible features based on a threshold value and MarrFeaturesfiltered returns the percent of reproducible sample pairs based on a threshold value

Slots

MarrSamplepairs Marr sample pairs

MarrFeatures Marr features

MarrSamplepairsfiltered Marr sample pairs post filtering

MarrFeaturesfiltered Marr metabolites post filtering

MarrData Original data object passed to Marr

MarrPSamplepairs Value of pSamplepairs argument passed to Marr

MarrPFeatures Value of pFeatures argument passed to Marr

MarrAlpha Value of alpha argument passed to Marr

MarrFeatureVars Value of featureVars passed to Marr. NULL if featureVars was left blank

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Examples

MarrAlpha

Generic function that returns the Marr Alpha

Description

Given a Marr object, this function returns the Marr Alpha Accessors for the 'MarrAlpha' slot of a Marr object.

Usage

```
MarrAlpha(object)
## S4 method for signature 'Marr'
MarrAlpha(object)
```

Arguments

object

an object of class Marr.

Value

Value of alpha argument passed to Marr

Examples

MarrData

Generic function that returns the Marr Data

Description

Given a Marr object, this function returns the Marr Data Accessors for the 'MarrData' slot of a Marr object.

Usage

```
MarrData(object)
## S4 method for signature 'Marr'
MarrData(object)
```

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Arguments

object an object of class Marr.

Value

Original data object passed to Marr

Examples

MarrFeatures

Generic function that returns the Marr features

Description

Given a Marr object, this function returns the Marr features Accessors for the 'MarrFeatures' slot of a Marr object.

Usage

```
MarrFeatures(object)
## S4 method for signature 'Marr'
MarrFeatures(object)
```

Arguments

object an object of class Marr.

Value

The distribution of percent reproducible sample pairs (row-wise) per feature after applying the maximum rank reproducibility.

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MarrFeaturesfiltered Generic function that returns the Marr filtered features

Description

Given a Marr object, this function returns the Marr filtered features Accessors for the 'MarrFeaturesfiltered' slot of a Marr object.

Usage

```
MarrFeaturesfiltered(object)
## S4 method for signature 'Marr'
MarrFeaturesfiltered(object)
```

Arguments

object an object of class Marr.

Value

The percent of reproducible sample pairs based on a threshold value after applying maximum rank reproducibility.

Examples

MarrFeatureVars

Generic function that returns the Marr Feature Vars

Description

Given a Marr object, this function returns the Marr Feature Vars Accessors for the 'MarrFeatureVars' slot of a Marr object.

Usage

```
MarrFeatureVars(object)
## S4 method for signature 'Marr'
MarrFeatureVars(object)
```

Arguments

object an object of class Marr.

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Value

Value of featureVars passed to Marr. NULL if featureVars was left blank

Examples

MarrFilterData

Filter by Maximum Rank Reproducibility

Description

Filters Marr object according to the Maximum Rank Reproducibility of the features, samples pairs, or both. Features are removed if their reproducibility per sample pair is less than pFeatures. Samples are removed if their sample pair reproducibility per feature is less than pSamplepairs for all pairings of that sample and the other samples in the set.

Usage

```
MarrFilterData(object, by = c("both", "features", "samplePairs"))
```

Arguments

object a Marr object from Marr

by String specifying which reproducibility values to filter by. Options include "fea-

tures" to filter features according to their reproducibility, "samplePairs" to filter samples according to the reproducibility of sample pairs, or "both" to filter both features and sample pairs according to their respective reproducibility. Default

is "both".

Value

A list of data. frame's or a SummarizedExperiment. If a data. frame was originally input into the Marr function, a list with three elements, filteredData, removedSamples, and removedFeatures, will be returned. If a SummarizedExperiment was originally input, output will be a SummarizedExperiment with the assay filtered and with two metadata objects, removedSamples and removedFeatures added.

MarrPFeatures 9

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Generic function that returns the Marr P Features

Description

Given a Marr object, this function returns the Marr P Features Accessors for the 'MarrPFeatures' slot of a Marr object.

Usage

```
MarrPFeatures(object)
## S4 method for signature 'Marr'
MarrPFeatures(object)
```

Arguments

object

an object of class Marr.

Value

Value of MarrPFeatures argument passed to Marr

Examples

 ${\tt MarrPlotFeatures}$

Plot percent reproducible sample pairs per feature for pairwise replicates from Marr function.

Description

This function plots a histogram showing the features along the y-axis and percent reproducible sample pairs per feature on the x-axis.

Usage

```
MarrPlotFeatures(
  object,
  xLab = "Percent reproducible sample pairs per feature",
  yLab = "Feature"
)
```

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Arguments

object a Marr object from Marr

xLab label for x-axis. Default is 'Percent reproducible sample pairs per feature for

pairwise replicates'.

yLab label for y-axis. Default is 'Feature'

Value

A histogram will be created showing the features along the y-axis and percent reproducible sample pairs per feature on the x-axis.

Examples

MarrPlotSamplepairs

Plot percent reproducible features per sample pair for pairwise replicates from Marr function.

Description

This function plots a histogram showing the sample pairs along the y-axis and percent reproducible features per sample pair on the x-axis.

Usage

```
MarrPlotSamplepairs(
  object,
  xLab = "Percent reproducible features per sample pair",
  yLab = "Sample pair"
)
```

Arguments

object a Marr object from Marr

xLab label for x-axis. Default is 'Percent reproducible features per sample pair for

pairwise replicates'.

yLab label for y-axis. Default is 'Sample pair'

Value

A histogram will be created showing the sample pairs along the y-axis and percent reproducible features per sample pair on the x-axis.

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Examples

MarrProc

MarrProc

Description

This function is a helper function that computes distributions of reproducible sample pairs per feature and reproducible features per sample pair for the function Marr.

Usage

```
MarrProc(object, alpha = 0.05)
```

Arguments

object an object which is a matrix or data.frame with features (e.g. metabolites or

genes) on the rows and samples as the columns. Alternatively, a user can provide a SummarizedExperiment object and the assay(object) will be used as input

for the Marr procedure.

alpha (Optional) level of significance to control the False Discovery Rate (FDR). De-

fault is 0.05.

Value

A list of percent reproducible statistics including

samplepairs the distribution of percent reproducible features (column-wise) per sample pair features the distribution of percent reproducible sample pairs (row-wise) per feature

```
data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_MarrProc <- MarrProc(object=data, alpha = 0.05)</pre>
```

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MarrPSamplepairs

Generic function that returns the Marr P Sample Pairs

Description

Given a Marr object, this function returns the Marr P Sample Pairs Accessors for the 'MarrPSamplepairs' slot of a Marr object.

Usage

```
MarrPSamplepairs(object)
## S4 method for signature 'Marr'
MarrPSamplepairs(object)
```

Arguments

object an object of class Marr.

Value

Value of pSamplepairs argument passed to Marr

Examples

MarrSamplepairs

Generic function that returns the Marr sample pairs

Description

Given a Marr object, this function returns the Marr sample pairs Accessors for the 'MarrSamplepairs' slot of a Marr object.

Usage

```
MarrSamplepairs(object)
## S4 method for signature 'Marr'
MarrSamplepairs(object)
```

Arguments

object an object of class Marr.

Value

The distribution of percent reproducible features (column-wise) per sample pair after applying the maximum rank reproducibility.

Examples

MarrSamplepairsfiltered

Generic function that returns the Marr filtered sample pairs

Description

Given a Marr object, this function returns the Marr filtered sample pairs Accessors for the 'MarrSamplepairsfiltered' slot of a Marr object.

Usage

```
MarrSamplepairsfiltered(object)
## S4 method for signature 'Marr'
MarrSamplepairsfiltered(object)
```

Arguments

```
object an object of class Marr.
```

Value

The percent of reproducible features based on a threshold value after applying maximum rank reproducibility.

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msprepCOPD

Example of processed mass spectrometry dataset

Description

Data contains LC-MS metabolite analysis for samples from 20 subjects. and 662 metabolites. The raw data was pre-processed using MSPrep method. The raw data pre-processing include 3 steps- Filtering, Missing Value Imputation and Normalization. Filtering- the metabolites(columns) in the raw data were removed if they were missing more than 80 percent of the samples. Missing Value Imputation- The Bayesian Principal Component Analysis (BPCA) was applied to impute the missing values. Normalization- median normalization was applied to remove unwanted variation appears from various sources in metabolomics studies. The first three columns indicate "Mass" indicating the mass-to-charge ratio, "Retention.Time", and "Compound.Name" for each present metabolite. The remaining columns indicate abundance for each of the 645 mass/retention-time combination for each subject combination.

Usage

data(msprepCOPD)

Format

SummarizedExperiment assay object containing 645 metabolites (features) of 20 subjects (samples).

Mass Mass-to-charge ratio

Retention.Time Retention-time

Compound.Name Compound name for each mass/retention time combination

X10062C The columns indicate metabolite abundances found in each subject combination. Each column begins with an 'X', followed by the subject ID.

Source

https://www.metabolomicsworkbench.org/data/DRCCMetadata.php?Mode=Project&ProjectID=PR000438

The raw data is available at the NIH Common Fund's National Metabolomics Data Repository (NMDR) website, the Metabolomics Workbench, https://www.metabolomicsworkbench.org, where it has been assigned Project ID PR000438. The raw data can be accessed directly via it's Project DOI: 10.21228/M8FC7C This work is supported by NIH grant, U2C- DK119886.

References

Nichole Reisdorph. Untargeted LC-MS metabolomics analysis of human COPD plasma, HILIC & C18, metabolomics_workbench, V1.

Hughes, G., Cruickshank-Quinn, C., Reisdorph, R., Lutz, S., Petrache, I., Reisdorph, N., Bowler, R. and Kechris, K., 2014. MSPrep—Summarization, normalization and diagnostics for processing of mass spectrometry—based metabolomic data. Bioinformatics, 30(1), pp.133-134.

Examples

data(msprepCOPD)

vectorORNull-class 15

Description

Class union allowing MarrFeatureVars slot to be a vector or NULL $\,$

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