Package ‘marr’

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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.

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R topics documented:

- data.frameORSummarizedExperiment-class ........................................... 2
- Marr .................................................. 3
- Marr-class ......................................... 4
- MarrAlpha ........................................... 5
- MarrData ............................................ 6
- MarrFeatures ....................................... 6
- MarrFeaturesfiltered ................................ 7
- MarrFeatureVars .................................... 8
- MarrFilterData ....................................... 8
- MarrPFeatures ....................................... 9
- MarrPlotFeatures .................................... 10
- MarrPlotSamplepairs ................................ 11
- MarrProc ............................................ 11
- MarrPSamplepairs ................................... 12
- MarrSamplepairs ..................................... 13
- MarrSamplepairsfiltered ............................. 14
- msprepCOPD .......................................... 14
- vectorORNull-class .................................. 15

Index  16

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**data.frameORSummarizedExperiment-class**

* S4 Class union

**Description**

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

This function applies an Rcpp-based implementation of a computationally efficient method for assessing reproducibility in high-throughput experiments, called the 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.

**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**


**Examples**

```r
data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
data("msprepCOPD")
data_Marr_COPD <- Marr(object = msprepCOPD, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
```

---

**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
Examples

```r
data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
```

---

**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

```r
MarrAlpha(object)
```

### Arguments

- `object` an object of class Marr.

### Value

Value of alpha argument passed to Marr

### Examples

```r
data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
MarrAlpha(data_Marr)
```
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)

Arguments
object an object of class Marr.

Value
Original data object passed to Marr.

Examples

data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
MarrData(data_Marr)

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)
**MarrFeaturesfiltered**

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.

Examples

```r
data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
MarrFeatures(data_Marr)
```

---

**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

```r
MarrFeaturesfiltered(object)
```

## S4 method for signature 'Marr'

```r
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

```r
data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
MarrFeaturesfiltered(data_Marr)
```
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.

Value

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

Examples

data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
MarrFeatureVars(data_Marr)

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 "features" 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.

Examples

data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
MarrFilterData(data_Marr, by = "both")

---

MarrPFeatures

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

```r
data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
MarrPFeatures(data_Marr)
```

---

**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

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

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

```r
data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
MarrPlotFeatures(data_Marr)
```
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.

Examples

data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
MarrPlotSamplepairs(data_Marr)

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). Default 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

Examples

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

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

```r
data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
MarrSamplepairs(data_Marr)
```

### Description

Given a Marr object, this function returns the Marr sample pairs

Accessors for the 'MarrSamplepairs' slot of a Marr object.

### Usage

```r
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

```r
data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
MarrSamplepairs(data_Marr)
```
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.

Examples

data <- matrix(rnorm(2400), nrow=200, ncol=12)
data_Marr <- Marr(object = data, pSamplepairs=0.75, pFeatures=0.75, alpha=0.05)
MarrSamplepairsfiltered(data_Marr)

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

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 its 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.

Examples
data(msprepCOPD)

---

**vectorORNull-class**  

**S4 Class union**

**Description**
Class union allowing `MarrFeatureVars` slot to be a vector or NULL
Index

* datasets
  msprepCOPD, 14

  data.frameORSummarizedExperiment-class, 2

Marr, 3
Marr-class, 4
MarrAlpha, 5
MarrAlpha,Marr-method (MarrAlpha), 5
MarrData, 6
MarrData,Marr-method (MarrData), 6
MarrFeatures, 6
MarrFeatures,Marr-method
  (MarrFeatures), 6
MarrFeaturesfiltered, 7
MarrFeaturesfiltered,Marr-method
  (MarrFeaturesfiltered), 7
MarrFeatureVars, 8
MarrFeatureVars,Marr-method
  (MarrFeatureVars), 8
MarrFilterData, 8
MarrPFeatures, 9
MarrPFeatures,Marr-method
  (MarrPFeatures), 9
MarrPlotFeatures, 10
MarrPlotSamplepairs, 11
MarrProc, 11
MarrPSamplepairs, 12
MarrPSamplepairs,Marr-method
  (MarrPSamplepairs), 12
MarrSamplepairs, 13
MarrSamplepairs,Marr-method
  (MarrSamplepairs), 13
MarrSamplepairsfiltered, 14
MarrSamplepairsfiltered,Marr-method
  (MarrSamplepairsfiltered), 14
msprepCOPD, 14

vectorORNull-class, 15