

# Package ‘marr’

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**License** GPL ( $\geq 3$ )

**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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|                                        |
|----------------------------------------|
| data.frameORSummarizedExperiment-class |
| <i>S4 Class union</i>                  |

---

Description

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

---

*Marr**Marr*

---

## 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.

### 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

```
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

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

### Examples

```

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

```

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

```

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 | <i>Generic function that returns the Marr Data</i> |
|----------|----------------------------------------------------|

---

**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 | <i>Generic function that returns the Marr features</i> |
|--------------|--------------------------------------------------------|

---

**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.

**Examples**

```
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**

```
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**

```
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 | <i>Generic function that returns the Marr Feature Vars</i> |
|-----------------|------------------------------------------------------------|

---

### 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 | <i>Filter by Maximum Rank Reproducibility</i> |
|----------------|-----------------------------------------------|

---

### 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**

```
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 | <i>Plot percent reproducible sample pairs per feature for pairwise replicates from Marr function.</i> |
|------------------|-------------------------------------------------------------------------------------------------------|

---

**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"
)
```

**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**

```
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 | <i>Plot percent reproducible features per sample pair for pairwise replicates from Marr function.</i> |
|---------------------|-------------------------------------------------------------------------------------------------------|

---

### 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 | <i>MarrProc</i> |
|----------|-----------------|

---

### 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 | <i>Generic function that returns the Marr P Sample Pairs</i> |
|------------------|--------------------------------------------------------------|

---

**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**

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

---

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**

```
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**

<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 | <i>S4 Class union</i> |
|--------------------|-----------------------|

---

**Description**

Class union allowing MarrFeatureVars slot to be a vector or NULL

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