

# Package ‘evaluomeR’

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**Type** Package

**Title** Evaluation of Bioinformatics Metrics

**URL** <https://github.com/neobernad/evaluomeR>

**Version** 1.4.0

**BugReports** <https://github.com/neobernad/evaluomeR/issues>

**Description** Evaluating the reliability of your own metrics and the measurements done on your own datasets by analysing the stability and goodness of the classifications of such metrics.

**License** GPL-3

**Encoding** UTF-8

**LazyData** true

**Depends** R (>= 3.6), SummarizedExperiment, MultiAssayExperiment, cluster (>= 2.0.7-1), fpc (>= 2.2-3)

**Imports** corrplot (>= 0.84), grDevices, graphics, reshape2, ggplot2, ggdendro, plotrix, stats, matrixStats, Rdpack

**Suggests** BiocStyle, knitr, rmarkdown, kableExtra, magrittr

**VignetteBuilder** knitr

**RdMacros** Rdpack

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**biocViews** Clustering, Classification, FeatureExtraction

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bioMetrics

*Dataset: Metrics for biological pathways*

---

### Description

Metrics for biological pathways, 2 metrics that quantitative characterizations of the importance of regulation in biochemical pathway systems, including systems designed for applications in synthetic biology or metabolic engineering. The metrics are reachability and efficiency

### Usage

```
data("bioMetrics")
```

### Format

An object of class SummarizedExperiment with 15 rows and 3 columns.

### References

Davis JD, Voit EO (2018). “Metrics for regulated biochemical pathway systems.” *Bioinformatics*. doi: [10.1093/bioinformatics/bty942](https://doi.org/10.1093/bioinformatics/bty942).

---

getDataQualityRange     *Dataframe getter for qualityRange function.*

---

### Description

This method is a wrapper to retrieve a specific [SummarizedExperiment](#) given a k value from the object returned by [qualityRange](#) function.

### Usage

```
getDataQualityRange(data, k)
```

### Arguments

|      |   |
|------|---|
| data | The object returned by <a href="#">qualityRange</a> function. |
| k    | The desired k cluster.  |

### Value

The [SummarizedExperiment](#) that contains information about the selected k cluster.

### Examples

```
# Using example data from our package
data("ontMetrics")
qualityRangeData <- qualityRange(ontMetrics, k.range=c(3,5), getImages = FALSE)
# Getting dataframe that contains information about k=5
k5Data = getDataQualityRange(qualityRangeData, 5)
```

---

getOptimalKValue     *Calculating the optimal value of k. getOptimalKValue*

---

### Description

This method finds the optimal value of K per each metric.

### Usage

```
getOptimalKValue(stabData, qualData, k.range = NULL)
```

### Arguments

|          |   |
|----------|---|
| stabData | An output <a href="#">ExperimentList</a> from a <a href="#">stabilityRange</a> execution.     |
| qualData | An output <a href="#">SummarizedExperiment</a> from a <a href="#">qualityRange</a> execution. |
| k.range  | A range of K values to limit the scope of the analysis.                                       |

### Value

It returns a dataframe following the schema: metric, optimal\_k.

## Examples

```
# Using example data from our package
data("rnaMetrics")
stabilityData <- stabilityRange(data=rnaMetrics, k.range=c(2,4), bs=20, getImages = FALSE)
qualityData <- qualityRange(data=rnaMetrics, k.range=c(2,4), getImages = FALSE)
kOptTable = getOptimalKValue(stabilityData, qualityData)
```

---

metricsCorrelations     *Calculation of Pearson correlation coefficient.*

---

## Description

Calculation of Pearson correlation coefficient between every pair of metrics available in order to quantify their interrelationship degree. The score is in the range [-1,1]. Perfect correlations: -1 (inverse), and 1 (direct).

## Usage

```
metricsCorrelations(data, margins = c(0, 10, 9, 11), getImages = TRUE)
```

## Arguments

|           |  |
|-----------|--|
| data      | A <a href="#">SummarizedExperiment</a> . The SummarizedExperiment must contain an assay with the following structure: A valid header with names. The first column of the header is the ID or name of the instance of the dataset (e.g., ontology, pathway, etc.) on which the metrics are measured. The other columns of the header contains the names of the metrics. The rows contains the measurements of the metrics for each instance in the dataset. |
| margins   | See <a href="#">par</a> .  |
| getImages | Boolean. If true, a plot is displayed.   |

## Value

The Pearson correlation matrix as an assay in a [SummarizedExperiment](#) object.

## Examples

```
# Using example data from our package
data("ontMetrics")
cor = metricsCorrelations(ontMetrics, getImages = TRUE, margins = c(1,0,5,11))
```

---

`ontMetrics`*Dataset: Structural ontology metrics*

---

**Description**

Structural ontology metrics, 19 metrics measuring structural aspects of bio-ontologies have been analysed on two different corpora of ontologies: OBO Foundry and AgroPortal

**Usage**

```
data("ontMetrics")
```

**Format**

An object of class `SummarizedExperiment` with 80 rows and 20 columns.

**References**

Franco M, Vivo JM, Quesada-Martínez M, Duque-Ramos A, Fernández-Breis JT (2019-02). "Evaluation of ontology structural metrics based on public repository data." *Bioinformatics*. doi: [10.1093/bib/bbz009](https://doi.org/10.1093/bib/bbz009), <https://dx.doi.org/10.1093/bib/bbz009>.

---

`plotMetricsBoxplot`*Metric values as a boxplot.*

---

**Description**

It plots the value of the metrics in a `SummarizedExperiment` object as a boxplot.

**Usage**

```
plotMetricsBoxplot(data)
```

**Arguments**

`data` A `SummarizedExperiment`. The `SummarizedExperiment` must contain an assay with the following structure: A valid header with names. The first column of the header is the ID or name of the instance of the dataset (e.g., ontology, pathway, etc.) on which the metrics are measured. The other columns of the header contains the names of the metrics. The rows contains the measurements of the metrics for each instance in the dataset.

**Value**

Nothing.

**Examples**

```
# Using example data from our package
data("ontMetrics")
plotMetricsBoxplot(ontMetrics)
```

plotMetricsCluster     *Metric values clustering.*

---

### Description

It clusters the value of the metrics in a [SummarizedExperiment](#) object as a boxplot.

### Usage

```
plotMetricsCluster(data)
```

### Arguments

`data`     A [SummarizedExperiment](#). The SummarizedExperiment must contain an assay with the following structure: A valid header with names. The first column of the header is the ID or name of the instance of the dataset (e.g., ontology, pathway, etc.) on which the metrics are measured. The other columns of the header contains the names of the metrics. The rows contains the measurements of the metrics for each instance in the dataset.

### Value

Nothing.

### Examples

```
# Using example data from our package
data("ontMetrics")
plotMetricsCluster(ontMetrics)
```

---

plotMetricsClusterComparison  
*Comparison between two clusterings as plot. plotMetricsClusterComparison*

---

### Description

It plots a clustering comparison between two different k-cluster vectors for a set of metrics.

### Usage

```
plotMetricsClusterComparison(data, k.vector1, k.vector2, seed = NULL)
```

**Arguments**

|           |  |
|-----------|--|
| data      | A <a href="#">SummarizedExperiment</a> . The SummarizedExperiment must contain an assay with the following structure: A valid header with names. The first column of the header is the ID or name of the instance of the dataset (e.g., ontology, pathway, etc.) on which the metrics are measured. The other columns of the header contains the names of the metrics. The rows contains the measurements of the metrics for each instance in the dataset. |
| k.vector1 | Vector of positive integers representing k clusters. The k values must be contained in [2,15] range.   |
| k.vector2 | Vector of positive integers representing k clusters. The k values must be contained in [2,15] range.   |
| seed      | Positive integer. A seed for internal bootstrap.   |

**Value**

Nothing.

**Examples**

```
# Using example data from our package
data("rnaMetrics")
stabilityData <- stabilityRange(data=rnaMetrics, k.range=c(2,4), bs=20, getImages = FALSE)
qualityData <- qualityRange(data=rnaMetrics, k.range=c(2,4), getImages = FALSE)
kOptTable = getOptimalKValue(stabilityData, qualityData)
```

---

plotMetricsMinMax      *Minimum and maximum metric values plot.*

---

**Description**

It plots the minimum, maximum and standard deviation values of the metrics in a [SummarizedExperiment](#) object.

**Usage**

```
plotMetricsMinMax(data)
```

**Arguments**

|      |  |
|------|--|
| data | A <a href="#">SummarizedExperiment</a> . The SummarizedExperiment must contain an assay with the following structure: A valid header with names. The first column of the header is the ID or name of the instance of the dataset (e.g., ontology, pathway, etc.) on which the metrics are measured. The other columns of the header contains the names of the metrics. The rows contains the measurements of the metrics for each instance in the dataset. |
|------|--|

**Value**

Nothing.

**Examples**

```
# Using example data from our package
data("ontMetrics")
plotMetricsMinMax(ontMetrics)
```

---

plotMetricsViolin      *Metric values as violin plot.*

---

**Description**

It plots the value of the metrics in a [SummarizedExperiment](#) object as a violin plot.

**Usage**

```
plotMetricsViolin(data)
```

**Arguments**

`data`      A [SummarizedExperiment](#). The `SummarizedExperiment` must contain an assay with the following structure: A valid header with names. The first column of the header is the ID or name of the instance of the dataset (e.g., ontology, pathway, etc.) on which the metrics are measured. The other columns of the header contains the names of the metrics. The rows contains the measurements of the metrics for each instance in the dataset.

**Value**

Nothing.

**Examples**

```
# Using example data from our package
data("ontMetrics")
plotMetricsViolin(ontMetrics)
```

---

quality      *Goodness of classifications.*

---

**Description**

The goodness of the classifications are assessed by validating the clusters generated. For this purpose, we use the Silhouette width as validity index. This index computes and compares the quality of the clustering outputs found by the different metrics, thus enabling to measure the goodness of the classification for both instances and metrics. More precisely, this goodness measurement provides an assessment of how similar an instance is to other instances from the same cluster and dissimilar to all the other clusters. The average on all the instances quantifies how appropriately the instances are clustered. Kaufman and Rousseeuw suggested the interpretation of the global Silhouette width score as the effectiveness of the clustering structure. The values are in the range [0,1], having the following meaning:



- There is no substantial clustering structure: [-1, 0.25].
- The clustering structure is weak and could be artificial: ]0.25, 0.50].
- There is a reasonable clustering structure: ]0.50, 0.70].
- A strong clustering structure has been found: ]0.70, 1].

### Usage

```
quality(data, k = 5, getImages = TRUE, seed = NULL)
```

### Arguments

|           |  |
|-----------|--|
| data      | A <a href="#">SummarizedExperiment</a> . The SummarizedExperiment must contain an assay with the following structure: A valid header with names. The first column of the header is the ID or name of the instance of the dataset (e.g., ontology, pathway, etc.) on which the metrics are measured. The other columns of the header contains the names of the metrics. The rows contains the measurements of the metrics for each instance in the dataset. |
| k         | Positive integer. Number of clusters between [2,15] range.   |
| getImages | Boolean. If true, a plot is displayed.   |
| seed      | Positive integer. A seed for internal bootstrap.   |

### Value

A [SummarizedExperiment](#) containing the silhouette width measurements and cluster sizes for cluster k.

### References

Kaufman L, Rousseeuw PJ (2009). *Finding groups in data: an introduction to cluster analysis*, volume 344. John Wiley & Sons.

### Examples

```
# Using example data from our package
data("ontMetrics")
result = quality(ontMetrics, k=4)
```

---

qualityRange

*Goodness of classifications for a range of k clusters.*

---

### Description

The goodness of the classifications are assessed by validating the clusters generated for a range of k values. For this purpose, we use the Silhouette width as validity index. This index computes and compares the quality of the clustering outputs found by the different metrics, thus enabling to measure the goodness of the classification for both instances and metrics. More precisely, this measurement provides an assessment of how similar an instance is to other instances from the same cluster and dissimilar to the rest of clusters. The average on all the instances quantifies how the instances appropriately are clustered. Kaufman and Rousseeuw suggested the interpretation of the global Silhouette width score as the effectiveness of the clustering structure. The values are in the range [0,1], having the following meaning:

- There is no substantial clustering structure: [-1, 0.25].
- The clustering structure is weak and could be artificial: ]0.25, 0.50].
- There is a reasonable clustering structure: ]0.50, 0.70].
- A strong clustering structure has been found: ]0.70, 1].

## Usage

```
qualityRange(data, k.range = c(3, 5), getImages = TRUE, seed = NULL)
```

## Arguments

|           |  |
|-----------|--|
| data      | A <a href="#">SummarizedExperiment</a> . The SummarizedExperiment must contain an assay with the following structure: A valid header with names. The first column of the header is the ID or name of the instance of the dataset (e.g., ontology, pathway, etc.) on which the metrics are measured. The other columns of the header contains the names of the metrics. The rows contains the measurements of the metrics for each instance in the dataset. |
| k.range   | Concatenation of two positive integers. The first value k.range[1] is considered as the lower bound of the range, whilst the second one, k.range[2], as the higher. Both values must be contained in [2,15] range.   |
| getImages | Boolean. If true, a plot is displayed.   |
| seed      | Positive integer. A seed for internal bootstrap.   |

## Value

A list of [SummarizedExperiment](#) containing the silhouette width measurements and cluster sizes from k.range[1] to k.range[2]. The position on the list matches with the k-value used in that dataframe. For instance, position 5 represents the dataframe with k = 5.

## References

Kaufman L, Rousseeuw PJ (2009). *Finding groups in data: an introduction to cluster analysis*, volume 344. John Wiley & Sons.

## Examples

```
# Using example data from our package
data("ontMetrics")
# Without plotting
dataFrameList = qualityRange(ontMetrics, k.range=c(2,3), getImages = FALSE)
```

---

`qualitySet`*Goodness of classifications for a set of k clusters.*

---

### Description

The goodness of the classifications are assessed by validating the clusters generated for a range of k values. For this purpose, we use the Silhouette width as validity index. This index computes and compares the quality of the clustering outputs found by the different metrics, thus enabling to measure the goodness of the classification for both instances and metrics. More precisely, this measurement provides an assessment of how similar an instance is to other instances from the same cluster and dissimilar to the rest of clusters. The average on all the instances quantifies how the instances appropriately are clustered. Kaufman and Rousseeuw suggested the interpretation of the global Silhouette width score as the effectiveness of the clustering structure. The values are in the range [0,1], having the following meaning:

- There is no substantial clustering structure: [-1, 0.25].
- The clustering structure is weak and could be artificial: ]0.25, 0.50].
- There is a reasonable clustering structure: ]0.50, 0.70].
- A strong clustering structure has been found: ]0.70, 1].

### Usage

```
qualitySet(data, k.set = c(2, 4), getImages = TRUE, seed = NULL)
```

### Arguments

|                        |   |
|------------------------|---|
| <code>data</code>      | A <a href="#">SummarizedExperiment</a> . The <code>SummarizedExperiment</code> must contain an assay with the following structure: A valid header with names. The first column of the header is the ID or name of the instance of the dataset (e.g., ontology, pathway, etc.) on which the metrics are measured. The other columns of the header contains the names of the metrics. The rows contains the measurements of the metrics for each instance in the dataset. |
| <code>k.set</code>     | A list of integer values of k, as in <code>c(2,4,8)</code> . The values must be contained in [2,15] range.  |
| <code>getImages</code> | Boolean. If true, a plot is displayed.  |
| <code>seed</code>      | Positive integer. A seed for internal bootstrap.  |

### Value

A list of [SummarizedExperiment](#) containing the silhouette width measurements and cluster sizes from `k.set`.

### References

Kaufman L, Rousseeuw PJ (2009). *Finding groups in data: an introduction to cluster analysis*, volume 344. John Wiley & Sons.

**Examples**

```
# Using example data from our package
data("rnaMetrics")
# Without plotting
dataFrameList = qualitySet(rnaMetrics, k.set=c(2,3), getImages = FALSE)
```

---

|            |                                     |
|------------|-------------------------------------|
| rnaMetrics | <i>Dataset: RNA quality metrics</i> |
|------------|-------------------------------------|

---

**Description**

RNA quality metrics for the assessment of gene expression differences, 2 quality metrics from 16 aliquots of a unique batch of RNA Samples. The metrics are Degradation Factor (DegFact) and RNA Integrity Number (RIN)

**Usage**

```
data("rnaMetrics")
```

**Format**

An object of class SummarizedExperiment with 16 rows and 3 columns.

**References**

Imbeaud S, Graudens E, Boulanger V, Barlet X, Zaborski P, Eveno E, Mueller O, Schroeder A, Auffray C (2005). "Towards standardization of RNA quality assessment using user-independent classifiers of microcapillary electrophoresis traces." *Nucleic acids research*, **33**, e56–e56.

---

|           |                         |
|-----------|-------------------------|
| stability | <i>Stability index.</i> |
|-----------|-------------------------|

---

**Description**

This analysis permits to estimate whether the clustering is meaningfully affected by small variations in the sample. First, a clustering using the k-means algorithm is carried out. The value of k can be provided by the user. Then, the stability index is the mean of the Jaccard coefficient values of a number of bs bootstrap replicates. The values are in the range [0,1], having the following meaning:

- Unstable: [0, 0.60[.
- Doubtful: [0.60, 0.75].
- Stable: ]0.75, 0.85].
- Highly Stable: ]0.85, 1].

**Usage**

```
stability(data, k = 5, bs = 100, getImages = TRUE, seed = NULL)
```

**Arguments**

|           |  |
|-----------|--|
| data      | A <a href="#">SummarizedExperiment</a> . The SummarizedExperiment must contain an assay with the following structure: A valid header with names. The first column of the header is the ID or name of the instance of the dataset (e.g., ontology, pathway, etc.) on which the metrics are measured. The other columns of the header contains the names of the metrics. The rows contains the measurements of the metrics for each instance in the dataset. |
| k         | Positive integer. Number of clusters between [2,15] range.   |
| bs        | Positive integer. Bootstrap value to perform the resampling.   |
| getImages | Boolean. If true, a plot is displayed.   |
| seed      | Positive integer. A seed for internal bootstrap.   |

**Value**

A [ExperimentList](#) containing the stability and cluster measurements for k clusters.

**References**

Milligan GW, Cheng R (1996). “Measuring the influence of individual data points in a cluster analysis.” *Journal of classification*, **13**, 315–335.

Jaccard P (1901). “Distribution de la flore alpine dans le bassin des Dranses et dans quelques regions voisines.” *Bull Soc Vaudoise Sci Nat*, **37**, 241–272.

**Examples**

```
# Using example data from our package
data("ontMetrics")
result <- stability(ontMetrics, k=6, getImages=TRUE)
```

---

|                |   |
|----------------|---|
| stabilityRange | <i>Stability index for a range of k clusters.</i> |
|----------------|---|

---

**Description**

This analysis permits to estimate whether the clustering is meaningfully affected by small variations in the sample. For a range of k values (k.range), a clustering using the k-means algorithm is carried out. Then, the stability index is the mean of the Jaccard coefficient values of a number of bs bootstrap replicates. The values are in the range [0,1], having the following meaning:

- Unstable: [0, 0.60[.
- Doubtful: [0.60, 0.75[.
- Stable: ]0.75, 0.85[.
- Highly Stable: ]0.85, 1[.

**Usage**

```
stabilityRange(data, k.range = c(2, 15), bs = 100, getImages = TRUE,
  seed = NULL)
```

**Arguments**

|           |  |
|-----------|--|
| data      | A <a href="#">SummarizedExperiment</a> . The SummarizedExperiment must contain an assay with the following structure: A valid header with names. The first column of the header is the ID or name of the instance of the dataset (e.g., ontology, pathway, etc.) on which the metrics are measured. The other columns of the header contains the names of the metrics. The rows contains the measurements of the metrics for each instance in the dataset. |
| k.range   | Concatenation of two positive integers. The first value k.range[1] is considered as the lower bound of the range, whilst the second one, k.range[2], as the higher. Both values must be contained in [2,15] range.   |
| bs        | Positive integer. Bootstrap value to perform the resampling.   |
| getImages | Boolean. If true, a plot is displayed.   |
| seed      | Positive integer. A seed for internal bootstrap.   |

**Value**

A [ExperimentList](#) containing the stability and cluster measurements for 2 to k clusters.

**References**

Milligan GW, Cheng R (1996). "Measuring the influence of individual data points in a cluster analysis." *Journal of classification*, **13**, 315–335.

Jaccard P (1901). "Distribution de la flore alpine dans le bassin des Dranses et dans quelques regions voisines." *Bull Soc Vaudoise Sci Nat*, **37**, 241–272.

**Examples**

```
# Using example data from our package
data("ontMetrics")
result <- stabilityRange(ontMetrics, k.range=c(2,3))
```

---

stabilitySet

*Stability index for a set of k clusters.*


---

**Description**

This analysis permits to estimate whether the clustering is meaningfully affected by small variations in the sample. For a set of k values (k.set), a clustering using the k-means algorithm is carried out. Then, the stability index is the mean of the Jaccard coefficient values of a number of bs bootstrap replicates. The values are in the range [0,1], having the following meaning:

- Unstable: [0, 0.60[.
- Doubtful: [0.60, 0.75].
- Stable: ]0.75, 0.85].
- Highly Stable: ]0.85, 1].

**Usage**

```
stabilitySet(data, k.set = c(2, 3), bs = 100, getImages = TRUE,  
seed = NULL)
```

**Arguments**

|           |  |
|-----------|--|
| data      | A <a href="#">SummarizedExperiment</a> . The SummarizedExperiment must contain an assay with the following structure: A valid header with names. The first column of the header is the ID or name of the instance of the dataset (e.g., ontology, pathway, etc.) on which the metrics are measured. The other columns of the header contains the names of the metrics. The rows contains the measurements of the metrics for each instance in the dataset. |
| k.set     | A list of integer values of k, as in <code>c(2,4,8)</code> . The values must be contained in <code>[2,15]</code> range.  |
| bs        | Positive integer. Bootstrap value to perform the resampling.   |
| getImages | Boolean. If true, a plot is displayed.   |
| seed      | Positive integer. A seed for internal bootstrap.   |

**Value**

A [ExperimentList](#) containing the stability and cluster measurements of the list of k clusters.

**References**

Milligan GW, Cheng R (1996). "Measuring the influence of individual data points in a cluster analysis." *Journal of classification*, **13**, 315–335.

Jaccard P (1901). "Distribution de la flore alpine dans le bassin des Dranses et dans quelques regions voisines." *Bull Soc Vaudoise Sci Nat*, **37**, 241–272.

**Examples**

```
# Using example data from our package  
data("rnaMetrics")  
result <- stabilitySet(rnaMetrics, k.set=c(2,3))
```

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