Package 'evaluomeR'

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Type Package

Title Evaluation of Bioinformatics Metrics

URL https://github.com/neobernad/evaluomeR

Version 1.20.0

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 (>= 2.0.9), fpc (>= 2.2-3), randomForest (>= 4.6.14),
flexmix (>= 2.3.15)

Imports corrplot (>= 0.84), grDevices, graphics, reshape2, ggplot2,
ggdendro, plotrix, stats, matrixStats, Rdpack, MASS, class,
prabclus, mclust, kableExtra

Suggests BiocStyle, knitr, rmarkdown, magrittr

VignetteBuilder knitr

RdMacros Rdpack

RoxygenNote 7.0.2

biocViews Clustering, Classification, FeatureExtraction

Collate 'data.R' 'helpers.R' 'internalClusterboot.R'
'internalFunctions.R' 'stabilityIndex.R' 'qualityIndices.R'
'correlation.R' 'metricsAnalysis.R' 'predictions.R'

git_url https://git.bioconductor.org/packages/evaluomeR

git_branch RELEASE_3_19

git_last_commit 02887fc

Contents

---

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.

---

evaluomeRSupportedCBI   *Get supported CBIs in evaluomeR.*

Description

A vector of supported CBIs available in evaluomeR.

Usage

```
evaluomeRSupportedCBI()
```

Value

A String vector.

Examples

```
supportedCBIs <- evaluomeRSupportedCBI
```

---

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 [qualityRange](#) 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 [ExperimentList](#) from a [stabilityRange](#) execution.
qualData	An output [SummarizedExperiment](#) from a [qualityRange](#) 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)
```

---

globalMetric   *Global metric score defined by a prediction.*

Description

This analysis calculates a global metric score based upon a prediction model computed with [flexmix](#) package.

Usage

```
globalMetric(data, k.range = c(2, 15), nrep = 10,
  criterion = c("BIC", "AIC"), PCA = FALSE, seed = NULL)
```

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.

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.

nrep
: Positive integer. Number of random initializations used in adjusting the model.

criterion
: String. Critirion applied in order to select the best model. Possible values: "BIC" or "AIC".

PCA
: Boolean. If true, a PCA is performed on the input dataframe before computing the predictions.

seed
: Positive integer. A seed for internal bootstrap.

Value

A dataframe containing the global metric score for each metric.

Examples

```
# Using example data from our package
data("rnaMetrics")
globalMetric(rnaMetrics, k.range = c(2,3), nrep=10, criterion="AIC", PCA=TRUE)
```

---

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 `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.

margins
: See `par`.

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). "Evaluation of ontology structural metrics based on public repository data." *Bioinformatics*. doi: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, scale = FALSE)
```

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.

scale   Boolean. If true input data is scaled. Default: FALSE.

Value

An hclust object.

Examples

```
# Using example data from our package
data("ontMetrics")
plotMetricsCluster(ontMetrics, scale=TRUE)
```

---

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 [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.

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 [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")
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, cbi = "kmeans", getImages = TRUE, seed = NULL)
```

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.
k	Positive integer. Number of clusters between [2,15] range.
cbi	Clusterboot interface name (default: "kmeans"): "kmeans", "clara", "clara_pam", "hclust", "pamk", "pamk_pam", "pamk". Any CBI appended with '_pam' makes use of pam. The method used in 'hclust' CBI is "ward.D2".
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), cbi = "kmeans",
  getImages = TRUE, seed = NULL)
```

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.

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.

cbi	Clusterboot interface name (default: "kmeans"): "kmeans", "clara", "clara_pam", "hclust", "pamk", "pamk_pam", "pamk". Any CBI appended with '_pam' makes use of [pam](). The method used in 'hclust' CBI is "ward.D2".
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), cbi = "kmeans", getImages = TRUE,
  seed = NULL)
```

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.

k.set   A list of integer values of k, as in c(2,4,8). The values must be contained in
                  [2,15] range.

cbi   Clusterboot interface name (default: "kmeans"): "kmeans", "clara", "clara_pam",
                  "hclust", "pamk", "pamk_pam", "pamk". Any CBI appended with '_pam' makes
                  use of [pam]. The method used in 'hclust' CBI is "ward.D2".

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.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   *Dataset: RNA quality metrics*

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**(6), e56–e56.

---

stability	*Stability index.*

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, cbi = "kmeans", getImages = TRUE,
  seed = NULL)
```

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.
k	Positive integer. Number of clusters between [2,15] range.
bs	Positive integer. Bootstrap value to perform the resampling.
cbi	Clusterboot interface name (default: "kmeans"): "kmeans", "clara", "clara_pam", "hclust", "pamk", "pamk_pam", "pamk". Any CBI appended with '_pam' makes use of [pam](). The method used in 'hclust' CBI is "ward.D2".
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**(2), 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   *Stability index for a range of k clusters.*

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, cbi = "kmeans",
  getImages = TRUE, seed = NULL)
```

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.

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.
cbi	Clusterboot interface name (default: "kmeans"): "kmeans", "clara", "clara_pam", "hclust", "pamk", "pamk_pam", "pamk". Any CBI appended with '_pam' makes use of [pam](). The method used in 'hclust' CBI is "ward.D2".
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**(2), 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, cbi = "kmeans",
  getImages = TRUE, seed = NULL)
```

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.
k.set	A list of integer values of k, as in c(2,4,8). The values must be contained in [2,15] range.
bs	Positive integer. Bootstrap value to perform the resampling.
cbi	Clusterboot interface name (default: "kmeans"): "kmeans", "clara", "clara_pam", "hclust", "pamk", "pamk_pam", "pamk". Any CBI appended with '_pam' makes use of [pam](). The method used in 'hclust' CBI is "ward.D2".
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**(2), 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))
```

Index