

Package ‘evaluomeR’

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Type Package

Title Evaluation of Bioinformatics Metrics

URL <http://sele.inf.um.es/evaluome/index.html>

Version 1.0.0

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

Imports cluster (>= 2.0.7-1), corrplot (>= 0.84), grDevices, graphics, stats, Rdpack

Suggests BiocStyle, knitr, rmarkdown, kableExtra, magrittr

VignetteBuilder knitr

RdMacros Rdpack

RoxygenNote 6.1.1

biocViews Clustering, Classification, FeatureExtraction

Collate 'data.R' 'helpers.R' 'internalFunctions.R' 'stabilityIndex.R' 'qualityIndices.R' 'correlation.R'

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bioMetrics	<i>Dataset: Metrics for biological pathways</i>
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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	<i>Dataframe getter for qualityRange function.</i>
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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 <code>qualityRange</code> 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)
```

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://doi.org/10.1093/bib/bbz009), <https://dx.doi.org/10.1093/bib/bbz009>.

`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)
```

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.
getImages	Boolean. If true, a plot is displayed.

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 dissimilarly 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)
```

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.
getImages	Boolean. If true, a plot is displayed.

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(2,6), 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	<i>Stability index.</i>
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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)
```

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.
getImages	Boolean. If true, a plot is displayed.

Value

A [SummarizedExperiment](#), containing an assay with the stability measurements and means for 1 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 régions 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, getImages = TRUE)
```

Arguments

<code>data</code>	A SummarizedExperiment . 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.range</code>	Concatenation of two positive integers. The first value <code>k.range[1]</code> is considered as the lower bound of the range, whilst the second one, <code>k.range[2]</code> , as the higher. Both values must be contained in [2,15] range.
<code>bs</code>	Positive integer. Bootstrap value to perform the resampling.
<code>getImages</code>	Boolean. If true, a plot is displayed.

Value

A [SummarizedExperiment](#) containing the stability measurements and means for 1 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 régions 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))
```


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