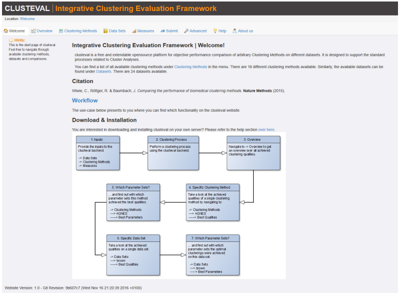
Comparing the Performance of Biomedical Clustering Methods



Hints:
This is the start page of clusteval. Feel free to navigate through available clustering methods, datasets and comparisons.

Integrative Clustering Evaluation Framework | Welcome!

clusteval is a free and extendable opensource platform for objective performance comparison of arbitrary Clustering Methods on different datasets. It is designed to support the standard processes related to Cluster Analyses.

You can find a list of all available clustering methods under Clustering Methods in the menu. There are 18 different clustering methods available. Similarly, the available datasets can be found under Datasets. There are 24 datasets available.

Citation

Wiwie, C., Röttger, R. & Baumbach, J. *Comparing the performance of biomedical clustering methods.* **Nature Methods** (2015).

Workflow

The use-case below presents to you where you can find which functionality on the clusteval website.

Download & Installation

You are interested in downloading and installing clusteval on your own server? Please refer to the help section over here.

1. Inputs
Provide the inputs to the clusteval backend.
-> Data Sets
-> Clustering Methods
-> Measures

2. Clustering Process
Perform a clustering process using the clusteval backend.

3. Overview
Navigate to -> Overview to get an overview over all achieved clustering qualities.

4. Specific Clustering Method
Take a look at the achieved qualities of a single clustering method by navigating to:
-> Clustering Methods
---> AGNES
-----> Best Qualities

5. Which Parameter Sets?
... and find out with which parameter sets this method achieved the best qualities:
-> Clustering Methods
---> AGNES
-----> Best Parameters

6. Specific Data Set
Take a look at the achieved qualities on a single data set.
-> Data Sets
---> brown
-----> Best Qualities

7. Which Parameter Sets?
... and find out with which parameter sets the optimal clusterings were achieved on this data set.
-> Data Sets
---> brown
-----> Best Parameters

Website Version: 1.0 - Git Revision: 9b607c7 (Wed Nov 16 21:20:39 2016 +0100)

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9 January 2018

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C. Wiwie, R. Röttger, J. Baumbach, Comparing the performance of biomedical clustering methods, *Nat. Methods* **12** (2015), 1033–1038.

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- 18 different clustering methods, 24 datasets, 18 common cluster validity indices
- robustness analysis (density reduction, noise addition)
- parameter optimisation (Naïve Grid Optimisation, Adaptive Grid Optimisation)

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Applicable to:

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- the identification of protein complexes using protein-protein interactions

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4. **Standardised evaluation**

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3. **Quality measures/Cluster validity indices** (internal, external)
4. **Standardised evaluation** (poor comparability of clustering results)

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Hierarchical Clustering, Spectral Clustering

Clustering Methods

Density-based

Identifying regions with a locally similar object density.

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Affinity Propagation, clusterONE, Markov Clustering, MCODE, Transitivity Clustering

Datasets

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- Gene expression levels,

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- Language-processing datasets used for word-sense disambiguation

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F_β score, False Discovery rate, False Positive Rate, Fowles-Mallows Index, Jaccard Index, Rand Index, Sensitivity (Recall), Specificity, V-measure

Clustering Validity Indices

Davies-Bouldin Index

$$\boxed{DB = \frac{1}{n} \cdot \sum_{c_i \in C} \max_{c_i \neq c_j \in C} \left(\frac{\sigma_i + \sigma_j}{\|\overline{c_i} - \overline{c_j}\|} \right)},$$

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Dunn Index

$$\boxed{D = \frac{\min\limits_{c_i \neq c_j \in C} \left(\min\limits_{x_i \in c_i, x_j \in c_j} d(x_i, x_j) \right)}{\max\limits_{c_k \in C} \left(\max\limits_{x_i, x_j \in c_k} d(x_i, x_j) \right)}}$$

Clustering Validity Indices

Silhouette Value

$c(x_i)$ – the cluster of object x_i
$o(x_i)$ – the closest cluster to x_i

$$\boxed{S = \frac{1}{n} \sum_i sv_i}$$

$$\begin{aligned} sv_i &= \frac{1}{n} \frac{b(x_i) - a(x_i)}{\max\{a(x_i), b(x_i)\}} \\ a(x_i) &= \frac{1}{|c(x_i)|} \sum_{x_j \in c(x_i)} d(x_i, x_j) \\ b(x_i) &= \frac{1}{|o(x_i)|} \sum_{x_j \in o(x_i)} d(x_i, x_j) \end{aligned}$$

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Correlation among internal and external indices

The silhouette value correlated best (0.71) with the F1 score, F2 score, FM index, Jaccard index and V-measure.

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Remark. The silhouette value is a particularly poor measure for entangled and highly overlapping datasets.