

Techniques for Evaluating Clustering Data in R. The Clustering Package

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Abstract Clustering is an unsupervised learning technique where the model is adjusted to the observations. This technique is quite common among researchers because they can obtain knowledge quickly and easily. The use of this technique is suitable for automatically classifying data to reveal concentrations of data. This paper presents the **Clustering** package which contains a set of clustering algorithms with two objectives: first grouping data in an homogeneous way by establishing differences between clusters, and second generating a ranking between algorithms and the variables analysed in the dataset. This package contains references to other R packages without using external software. As a complement to the standard execution through the console, it incorporates a GUI through which we can execute the package without having to know the parameters.

Introduction

Exploring the properties of information in order to make groups is an unsupervised learning technique known as clustering (Mann and Kaur, 2013) (Karypis et al., 2000). This technique is a concise data model where a set of data must be partitioned and introduced in groups or clusters of data. These clusters must meet two conditions: clusters must be the most disparate possible among them, and the elements that contain them the most similar. If we review the literature related to clustering we can see that the fields where they can be applied are multiple, among which we highlight the following: Identify tourists and analyze their destination patterns from location-based social media data (Hasnat and Hasan, 2018), Clustering algorithm that maximizes performance on 5G heterogeneous networks (Balevi and Gitlin, 2018), Application of data mining techniques to agriculture data (Ponperiasamy and Thenmozhi, 2017), Weighting of characteristics based on strength between categories and within categories for the analysis of feelings (Wang and Youn, 2018), Music classification, genres and taste patterns (Vlegels and Lievens, 2017), Predict the direction, maximum, minimum and closing prices of the daily exchange rate of bitcoins (Mallqui and Fernandes, 2018) and Clustering of people in a social network based on textual similarity (Singh et al., 2016).

As a rule, the clustering algorithms are based on the optimization of an objective function, which is usually the weighted sum of the distance to the centers, although these functions may vary and in some cases consists of the definition of functions. In the literature we can group the data in different ways among which we highlight (Popat and Emmanuel, 2014): partitional, hierarchical or based on density. One of the best known algorithms that solves the clustering problem is the k-means (Macqueen, 1967)

Throughout the literature we have located a wide variety of frameworks that work with clustering algorithm implementations among which we can cite the following: Weka (Litoriya, 2012), ClustVis (Metsalu T, 2015) and Keel (Fernández et al., 2009) among others. Also within R there is a specific Cluster task view. Inside this section we see two well differentiated parts: on one hand we have the most outstanding packages by functionality and in second place we observe the set of packages that work with cluster ordered. From the set of packages we highlight the following: **ClusterR** (Sculley, 2010), **apcluster** (Frey and Dueck, 2007), **cluster** (Mächler et al., 2017), **advclust** (Farias et al., 2011) as well as alternatives to the traditional implementation of k-means and agglomerative hierarchical clustering.

This contribution presents the **Clustering** package. It is a package that allows you to compare multiple clustering algorithms simultaneously and assess the accuracy of the results. The purpose of this package is to evaluate a set of datasets to determine which variables have the best behavior for a series of clustering algorithms. So we can make evaluations of the clusters created, how they have been distributed, if the distributions are uniform or how they have been categorized from the data.

The distribution of the content of this contribution is as follows: Firstly, in section 2 we have the presentation of clustering, types of clustering and similarity measures is performed. Section 2 presents the definition of the evaluation measures in order to value the distribution of the data in the clusters and finally Section 2.1 describes the structure of the package and it presents a complete example about the use of the package.

Clustering

Cluster analysis is an unsupervised learning method that constitutes a cornerstone of an intelligent data analysis process. It is used for the exploration of inter-relationships among a collection of patterns, by organizing them into homogeneous clusters. It is called unsupervised learning because unlike classification (known as supervised learning), no a priori labeling of some patterns is available to use in categorizing others and inferring the cluster structure of the whole data (Kotsiantis and Pintelas, 2004). The basic concept of clustering should be expressed as follows:

Clustering is the process of identifying natural clusters or clusters within multidimensional data based on some measure of similarity (Euclidean, Manhattan) (Omran et al., 2007).

This is a base definition of the clustering so variations in the problem definition can be significant, depending mostly on the model specified. For example, a generative model should define similarity based on a probabilistic generative mechanism, while a distance-based approach will use a traditional distance function to quantify it. In addition, the types of data specified also have a significant impact on the problem definition.

Clustering types

There are a variety of clustering algorithms that can be classified into: hierarchical (Figure 1), partitioning (Figure 2), density-based (Figure 3), grid-based and probability distribution (Figure 4). The most commonly used groupings are: hierarchical, part-based and density-based.

- Hierarchical clustering algorithms Jain et al. (1999) create a hierarchical breakdown of data into a dendrogram that recursively divides the data set into smaller and smaller data. The tree can be created in two ways: top-down or bottom-up. In bottom-up trees we can also call it agglomerative, as the objects are successively combined according to the measurements, until they are all joined into one or meet a completion condition. In the case of top-down, it is known as divisive, where all the objects are in the same group, and as we iterate they are divided into smaller subsets, until each object is in an individual group or fulfills a condition of completion. Some hierarchical grouping algorithms that belong to this sorting mode are CURE Guha et al. (1998), CHAMELEON Guo et al. (2019), and BIRCH Zhang et al. (1996).

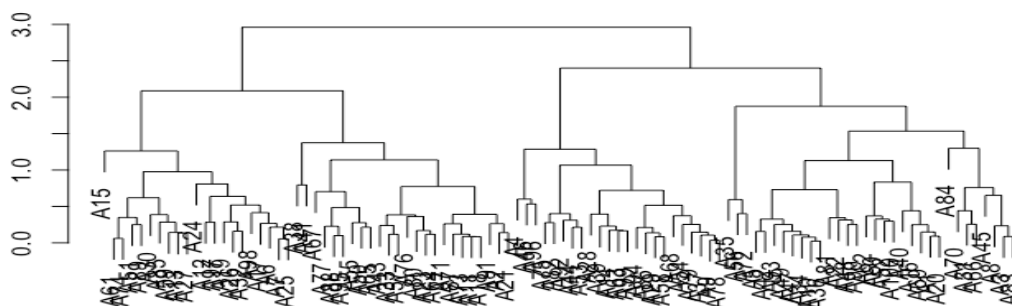


Figure 1: Hierarchical Clustering

- Partial clustering is considered to be the most popular of the clustering algorithms Saxena et al. (2017). Such an algorithm is also known as an iterative relocation algorithm. This algorithm minimizes a given clustering criterion by iteratively relocating data points between clusters until an optimal partition is reached. This type of algorithm divides the data points into a partition k , where each partition represents a cluster. Partial clustering organizes the objects within k clusters so that the total deviation of each object from the center of its cluster or from a cluster distribution is minimal. The deviation of a point can be evaluated differently according to the algorithm, and is generally known as a similarity function. Among the partitioning clustering algorithms we can find CLARANS, CLARA Ramprasanth and Devi (2019), K-prototype Nithya and Prabha (2019), K-mode Huang (1997) and K-means Kushwaha et al. (2020).

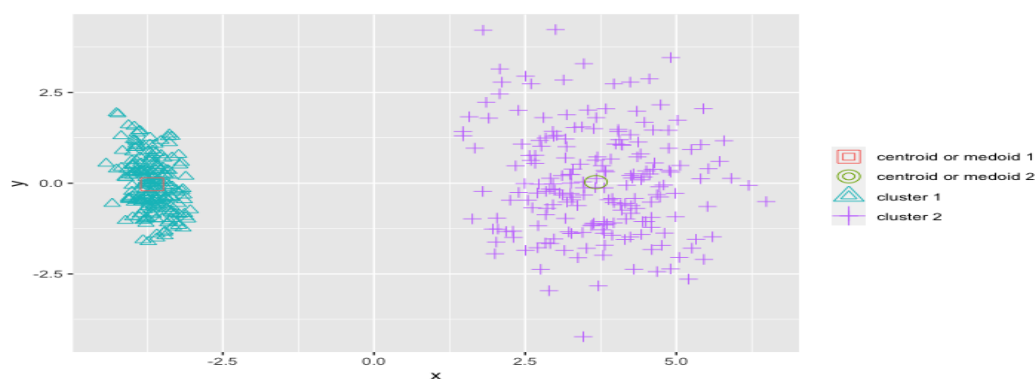


Figure 2: Partitional Clustering

- Density-based algorithms obtain clusters based on dense regions of objects in the data space that are separated by low-density regions (these isolated elements represent noise). Among the density-based algorithms, we highlight the following: Dbscan [Hu \(2019\)](#), and Denclue [Khader and Al-Naymat \(2019\)](#).

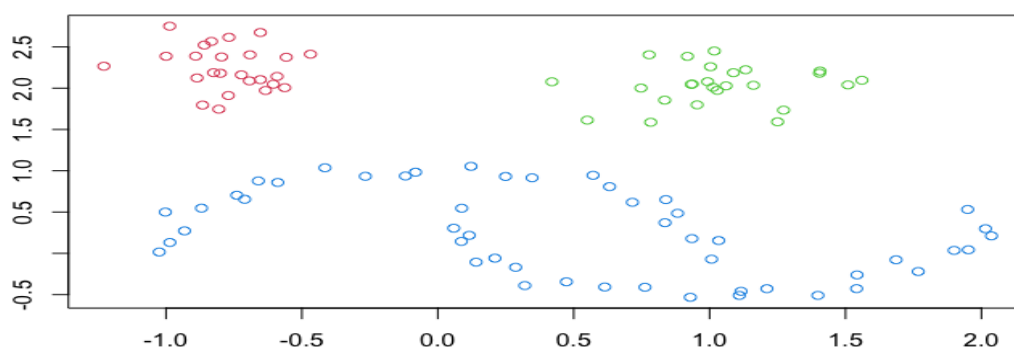


Figure 3: Density Clustering

- Grid-based clustering algorithms [Dang \(2011\)](#) first quantize the clustering space into a finite number of cells and then perform the required operations on the quantized space. Cells that contain more than certain number of points are treated as dense and the dense cells are connected to form the clusters. Some of the grid-based clustering algorithms are: STING [MR and MOHAN \(2010\)](#), Wave Cluster [Xuecheng \(2010\)](#) and CLIQUE [Saini and Rani \(2017\)](#).
- Model-based methods are primarily based on a probability distribution. To be able to measure similarity it is based on the mean values and the algorithm tries to minimize the square error function. Auto Class algorithm uses the Bayesian approach, starting with a random initialization of parameters that is gradually adjusted in order to find the maximum probability estimates. Among the model-based algorithms SOM [Thalamuthu et al. \(2006\)](#)

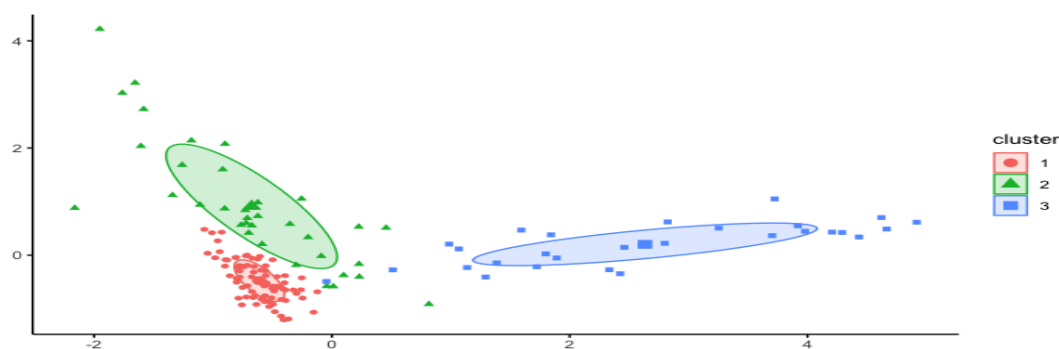


Figure 4: Model-Based Clustering

Dissimilarity measures

Dissimilarity measurements are important because they allow us the creation of clusters with the closest neighbours and the detection of anomalies, and they are also used in a large number of data mining techniques. It is also a measure that determines the degree to which objects are different. We often use the term distance as a synonym for dissimilarity. The values of dissimilarity should be in the range [0,1], but it is common to find in some cases the range 0 to ∞ .

Many distance measures have been proposed in literature for data clustering. The choosing an appropriate similarity measure is also crucial for cluster analysis, especially for a particular type of clustering algorithms. For example, the densit -based clustering algorithms, such as DBScan [Hu \(2019\)](#), rely heavily on the similarity computation. Density-based clustering finds clusters as dense areas in the data set, and the density of a given point is in turn estimated as the closeness of the corresponding data object to its neighboring objects [Pandit et al. \(2011\)](#) [Shirkhorshidi et al. \(2015\)](#).

As measures of dissimilarity in clustering we highlight the following:

- Minkowski: The Minkowski family includes Euclidean distance and Manhattan distance, which are particular cases of the Minkowski distance. The Minkowski distance performs well when the dataset clusters are isolated or compacted; if the dataset does not fulfil this condition, then the large-scale attributes would dominate the others. Another problem with Minkowski metrics is that the largest-scale feature dominates the rest.

$$d_{min} = \left(\sum_{i=1}^n |x_i - y_i|^m \right)^{\frac{1}{m}}, m \geq 1 \quad (1)$$

where m is a positive real number and xi and yi are two vectors in n-dimensional space.

- Euclidan distance: Is a special case of Minkowski distance. It works very well when deployed to datasets that include compact or isolated clusters. Although Euclidean distance is very common in clustering, it has a drawback: if two data vectors have no attribute values in common, they may have a smaller distance than the other pair of data vectors containing the same attribute values. Another problem with Euclidean distance as a family of the Minkowski metric is that the largest-scaled feature would dominate the others. Normalization is the solution to the problem.

$$d_{ij} = \sqrt{\sum_{c=1}^p (X_{ic} - X_{jc})^2} \quad (2)$$

- Manhattan distance: Also known as the geometry cab driver is sensitive to outliers. When this distance measure is used in clustering algorithms, the shape of clusters is hyper-rectangular. This metric was created by Hermann Minkowski in the 19th century and its name refers to the grid pattern of most of the streets on Manhattan Island.

$$d_{ij} = \sum_{c=1}^p |X_{ic} - X_{jc}| \quad (3)$$

- Mahalanobis distance: Is a data-driven measure in contrast to Euclidean and Manhattan distances that are independent of the related dataset to which two data points belong. Also can be used for extracting hyperellipsoidal clusters.

$$d_{mah} = \sqrt{(x - y)S^{-1}(x - y)^T} \quad (4)$$

where S is the covariance matrix of the dataset

- Pearson correlation: It's a statistically based metric, widely used in clustering gene expression data. This similarity measure calculates the similarity between the shapes of two gene expression patterns.

$$Pearson(x, y) = \frac{\sum_{i=1}^n (x_i - \mu_x)(y_i - \mu_y)}{\sqrt{\sum_{i=1}^n (x_i - \mu_x)^2} \sqrt{\sum_{i=1}^n (y_i - \mu_y)^2}} \quad (5)$$

where μ_x and μ_y are the means for x and y respectively.

- Jaccard Index: [Kosub \(2019\)](#) Is a classical similarity measure on sets with a lot of practical applications in information retrieval, data mining, machine learning, and many more. Measuring the relative size of the overlap of two finite sets A and B, the Jaccard index J is formally defined as:

$$J(A, B) = \frac{A \cap B}{A \cup B} \quad (6)$$

- Gower distance: It is a measure of similarity that allows the simultaneous use of quantitative, qualitative and dichotomous variables. By applying this similarity coefficient can be to determine the degree of similarity between individuals; who have been measured qualitative, quantitative characteristics (continuous and discrete) and binary.

$$d_{ij} = \sqrt{(1 - S_{ij})} \quad (7)$$

Internal and External clustering validation measures

Clustering validation is a technique to find a set of clusters that best fits natural partitions (number of clusters) without any class information. The results of a clustering algorithm are known as cluster validity. The following criteria must therefore be taken into account when investigating the validity of clusters. The first criterion is based on external measures, which involves evaluating the results of a base algorithm in a pre-specified structure which is imposed on a data set and reflects our intuition about the structure of clustering of the data set. The second criterion is based on internal measures where it evaluates the results of a clustering algorithm in terms of the quantity involved in the vectors of the dataset itself (e.g. the proximity matrix). And as a third criterion known as relative criterion whose purpose is to compare the results of execution of an algorithm with another using different parameters. There are two proposed criteria for the evaluation and selection of an optimal clustering [Halkidi et al. \(2001\)](#) [Berry and Linoff \(2004\)](#):

1. Compactness, the members of each cluster should be as close to each other as possible. A common measure of compactness is the variance, which should be minimized.
2. Separation, the clusters themselves should be widely spaced. There are three common approaches measuring the distance between two different clusters:
 - Single linkage: It measures the distance between the closest members of the clusters.
 - Complete linkage: It measures the distance between the most distant members.
 - Comparison of centroids: It measures the distance between the centers of the clusters.

The two first approaches are based on statistical tests and their major drawback is their high computational cost. Moreover, the indices related to these approaches aim at measuring the degree to which a data set confirms an a-priori specified scheme. On the other hand, the third approach aims at finding the best clustering scheme that a clustering algorithm can be defined under certain assumptions and parameters.

Inside external tests exits some measures to evalute clustering results. Among which we highlight:

- Entropy: ([Kim and Park, 2007](#)) It evaluates the distribution of categories in a cluster.

$$Entropy = \sum_{j=1}^m \frac{n_j}{n} E_j \quad (8)$$

Where n_j is the cluster size j , n is the number of clusters, and m is the total number of data points. To calculate the entropy of a data set, we need to calculate the class distribution of the objects in each group as follows:

$$E_j = \sum_i p_{ij} \log(p_{ij}) \quad (9)$$

- Recall: [Kacprzyk and Farhaoui \(2019\)](#) It indicates the proximity of the measurement results to the true value.

$$Recall(i, j) = \frac{n_{ij}}{n_i} \quad (10)$$

n_{ij} is the number of objects of class i that are in cluster j , n_j is the number of objects in cluster j and n_i is the number of objects in cluster i .

- Precision: [Kacprzyk and Farhaoui \(2019\)](#) It refers to the dispersion of the set of values obtained from repeated measurements of one magnitude. The lower the dispersion, the higher the accuracy.

$$Precision(i, j) = \frac{n_{ij}}{n_j} \quad (11)$$

n_{ij} is the number of objects in class i that are in cluster j , n_j is the number of objects in cluster j and n_i is the number of objects in class i .

- F-measure: [Rendón et al. \(2011\)](#) It merges the concepts of accuracy and recall of the retrieved information. Therefore, we calculate the cluster accuracy and recall for each class as:

$$F - measure(i, j) = \frac{2 * (Precision(i, j) * Recall(i, j))}{(Precision(i, j) + Recall(i, j))} \quad (12)$$

- Fowlkes-Mallows Index: [Romano et al. \(2016\)](#) It is a measure of comparison of hierarchical clustering, however it can also be used in flat clustering since it consists of the calculation of an index B_i for each level $i = 2, \dots, n-1$ of the hierarchy. The measure B_i is easily generalizable to a measure for clustering of different clusters.

$$Fowlkes = \frac{n_{11}}{\sqrt{(n_{11} + n_{10})(n_{11} + n_{01})}} \quad (13)$$

It can therefore be said that Fowlkes is a measure that can be interpreted as the geometric mean of accuracy (ratio between the number of relevant documents recovered and the total number of documents recovered).

- Variation information: [Romano et al. \(2016\)](#) Variation in information or distance of shared information is a measure of distance between two groups. This measure is closely related to mutual information. However, in contrast to mutual information, variation of information is a true metric, in the sense that it is due to the inequality of triangles.

$$VI = - \sum_i^j r_{ij} \left[\log \left(\frac{r_{ij}}{p_i} \right) + \left(\frac{r_{ij}}{q_j} \right) \right] \quad (14)$$

As with the external measures, we will now list the most relevant internal measures:

- Connectivity: This measure reflects the extent to which items placed in the same group are considered their closest neighbours in the data space, i.e. the degree of connection of the clusters should be minimal [Deborah et al. \(2010\)](#).

$$connectivity = [1 \leq i \leq K] \min\{1 \leq j \leq K, i \neq j\} \min \left\{ \frac{dist(C_i, C_j)}{\max_{1 \leq k \leq K \{diam(C_k)\}}} \right\} \quad (15)$$

- Dunn: [Ansari et al. \(2015\)](#) It represents the relationship of the smallest distance between observations that are not in the same cluster and the largest distance within the same cluster.

$$dunn = \min_{1 \leq i \leq K} \min \left\{ \frac{d(c_i, c_j)}{\max_{1 \leq k \leq c(d(X_k))}} \right\} \quad (16)$$

- Silhouette index: [Starczewski and Krzyzak \(2015\)](#) The silhouette value is a measure of how similar an object is to its own cluster (cohesion) compared to other clusters (separation).

$$S = \frac{1}{N} \sum_{i=0}^N \frac{b_i - a_i}{\max(a_i, b_i)} \quad (17)$$

where

$$a_i = \frac{1}{|C_j| - 1} \sum_{y \in C_j, y \neq x_i} \|y - x_i\|$$

and

$$b_i = \min_{l \in H, l \neq j} \frac{1}{|C_l|} \sum_{y \in C_l} \|y - x_i\|$$

with

$$x_i \in C_j, H = \{h : 1 \leq h \leq K\}$$

The above evaluation measures can be grouped into families in order to evaluate the quality of the clusters. If we look at the Figure 5 we can group Entropy, Recall, Precision, F-Measure, Fowlkes-Mallows Index and Variation information into three families [Palacio-Niño and Berzal \(2019\)](#):

- Matching Sets: [Palacio-Niño and Berzal \(2019\)](#) used to compare two partitions of data consists of those method that identify the relationship between each cluster detected in C and its natural correspondence to the classes in the reference result defined by P. Several measures can be defined to measure the similarity between the clusters in C, obtained by the clustering algorithm, and the clusters if P, corresponding to our prior (external) knowledge. The metrics included in this method are: Precision, Recall and F-measure

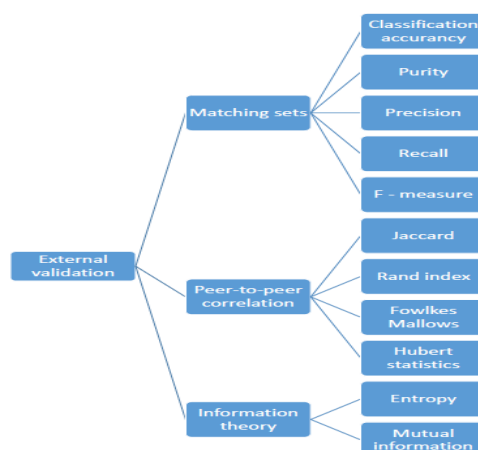


Figure 5: External validation methods [Palacio-Niño and Berzal \(2019\)](#)

- **Peer-to-peer Correlation:** [Palacio-Niño and Berzal \(2019\)](#) are based on the correlation between pairs, i.e. they seek to measure the similarity between two partitions under equal conditions, such as the result of a grouping process for the same set, but by means of two different methods C and P. It is assumed that the examples that are in the same cluster in C should be in the same class in P, and viceversa. We highlight the following metrics: Fowlkes-Mallows Index
- **Measures Based on Information Theory:** [Palacio-Niño and Berzal \(2019\)](#) A third family is based on Information Theory concepts, such as the existing uncertainty in the prediction of the natural classes provided by the partition P. This family includes basic measures such as entropy and variation information.

Internal evaluation metrics (see Figure 6) do not require external information, so they are focused on measuring cohesion (how close the elements are to each other) and separation (they quantify the level of separation between clusters).

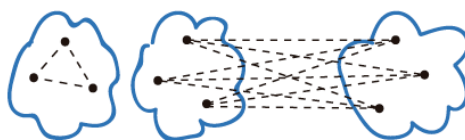


Figure 6: Representation of cohesion and separation in clustering [Palacio-Niño and Berzal \(2019\)](#)

According to the figure 7, the internal Dunn, Silhouette and Connectivity metrics are based on the concepts mentioned above so we can group them as partitioning methods.

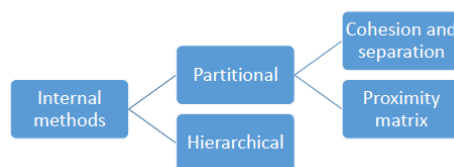


Figure 7: Internal validation methods [Palacio-Niño and Berzal \(2019\)](#)

The Clustering package

Clustering package is a package that has been written entirely in R language. The package contains other **Clustering** packages that run hierarchical, partitional and agglomerative hierarchical algorithms. As an addition to the package it has been provided with the ability to read data in different formats such as CSV, KEEL, ARFF (Weka) and data.frame objects. Most of the methods have been provided

with a set of default parameters, so we can easily run our algorithm without knowing the parameters. Later we will talk about the GUI to make the executions more attractive.

Algorithms of the package

These are the algorithms available within the package: `aggExCluster`, `agnes`, `apclusterK`, `clara`, `daisy`, `diana`, `fanny`, `fuzzy_cm`, `fuzzy_gk`, `fuzzy_gg`, `gama`, `hcluster`, `gmm`, `kmeans`, `mona`, `pam`, `pvpick` and `pvclust`.

Package Architecture

The main advantage of this package is that it allows to compare the most used clustering algorithms in the literature and to be able to compare them to determine which variable is the best behavior for the set of algorithms. With this package we will be able to compare the results based on the best variable and evaluate the results by means of a series of metrics that will indicate how the data has been distributed within our clusters.

The main class of the package is the **Clustering** object.

- `clustering`: This object stores the results of the **Clustering** package execution and contains the following properties:
 - `result`. It represents the data.frame with the results. In each column we have represented the evaluation metrics used to evaluate the clusters. We can also see the execution time of these metrics, datasets, the calculated variables, the measures of dissimilarity and the algorithms.
 - `has_internal_metrics`. It is a boolean operator that indicates if we have used internal evaluation measures in the calculation. It serves to indicate if we have classified the data correctly.
 - `has_external_metrics`. It is a boolean operator that indicates if we have used external evaluation measures in the calculation.
 - `algorithms_execute`. It represents a character vector with the algorithms executed independently of the package.
 - `measures_execute`. It represents a vector of characters with the measures of dissimilarity used by the indicated algorithms.

This class also exports the well-known S3 methods `print()` and `summary()` that show the data structure without codification and a summary with basic information about the dataset respectively. We can also perform sorting and filtering operations for further processing of the results. In any case if we need to perform filtering operations we can overload the operator (`'['`) to perform such operations in an easier way.

- `best_ranked_external_metrics()`, `evaluate_validation_external_by_metrics()`, `evaluate_best_validation_external_by_metrics()`, `result_external_algorithm_by_metric()`: These are methods for working with the results of external metrics. The methods indicated allow us to determine the behaviour of the algorithms based on the best variable, on the measures of dissimilarity and on the number of clusters.
- `best_ranked_internal_metrics()`, `evaluate_validation_internal_by_metrics()`, `evaluate_best_validation_internal_by_metrics()`, `result_internal_algorithm_by_metric()`: Just as we have indicated that there are methods for working with external metrics, we also have them for internal ones. The methods indicated allow us to determine the behaviour of the algorithms based on the best variable, on the measures of dissimilarity and on the number of clusters.

Finally we have the `plot_clustering` methods to graphically represent the evaluation measurements by clusters as well as to export the results of both internal and external measurements in latex format with the `export_external_file` and `export_internal_file` methods

Use of Clustering package

The fastest way to download the **Clustering** package and use it is to use the install instruction.

```
install.packages("Clustering")
```


A development version is also available on the github <https://github.com/laperez/Clustering>. To use the development version you must install the devtools package and use the install_github method.

```
devtools::install_github('laperez/Clustering')
```

The main dependencies of the **Clustering** package are: **advclust**, **amap**, **apcluster**, **cluster**, **ClusterR**, **gmp** and **pvclust**. These are the packages in charge of implementing the clustering algorithms. We can also find dependencies for data processing and GUI, such as shiny and DT among others. Once the package is installed it is necessary to load it in the following way:

```
library("Clustering")
```

Once the installation and loading process has been completed, we proceed with the processing of the data and its execution.

Use and load of datasets

For the execution of the main method of the package we must provide you with data that can be in different formats. The file formats accepted by the package are: KEEL, ARFF and CSV. The data can be loaded in two ways, firstly we can indicate a directory with files in the formats indicated above and load all the available files and secondly we can provide a data.frame with the necessary data for execution. To read the files in ARFF format it has been extracted from the **mldr** package [Vico et al. \(2016\)](#).

If we need to work with test data, we have pre-loaded data. The loaded datasets have been obtained from the KEEL url <https://sci2s.ugr.es/keel/category.php?cat=uns> in csv format.

Note: that the extension is used to determine the type of file format. For reading files in csv format the default values have been used, except for the stringsAsFactors parameter which indicates how to treat the character vector.

Analysis of clustering methods using the Clustering package

Once the way to provide the data to the clustering method has been defined, we can execute it in two ways as we have indicated above. For this example we are going to use a dataset of those provided by the package. The parameters are as follows:

- **df**: is a data.frame type field with the data we are going to use to evaluate.
- **min**: This is a numeric field to indicate the minimum number of clusters.
- **max**: This is a numeric field to indicate the maximum number of clusters.
- **algorithm**: is an array with the list of the algorithms implemented by the packages. The algorithms are: fuzzy_cm, fuzzy_gg, fuzzy_gk, hclust, apclusterK, agnes, clara, daisy, diana, fanny, mona, pam, gmm, kmeans_arma, kmeans_rcpp, mini_kmeans, gama, pvclust.

We go there with the test, we use the basketball dataset, with a range of clusters [3,5], for the gmm algorithm using as external metric (entropy) and as internal metric (dunn).

```
> result <- Clustering::clustering(df = Clustering::basketball, min = 3, max = 5,
  algorithm = c('gmm', 'fanny'), metrics = c('entropy','dunn'))
```

Algorithm	Distance	Clusters	Dataset	timeExternal	entropy	dunn	timeInternal
gmm	gmm_euclidean	3	dataframe	0.0054	0.2374	0.1096	0.0004
gmm	gmm_euclidean	3	dataframe	0.0091	0.2120	0.1096	0.0005
gmm	gmm_euclidean	3	dataframe	0.0093	0.0064	0.1096	0.0005
gmm	gmm_euclidean	3	dataframe	0.0107	0.0032	0.1096	0.0007
gmm	gmm_euclidean	3	dataframe	0.0185	0.0000	0.1096	0.0013
gmm	gmm_euclidean	4	dataframe	0.0053	0.3734	0.1233	0.0004
gmm	gmm_euclidean	4	dataframe	0.0111	0.2983	0.1233	0.0005
gmm	gmm_euclidean	4	dataframe	0.0119	0.0064	0.1233	0.0005
gmm	gmm_euclidean	4	dataframe	0.0122	0.0032	0.1233	0.0006
gmm	gmm_euclidean	4	dataframe	0.0649	0.0000	0.1233	0.0007
gmm	gmm_euclidean	5	dataframe	0.0050	0.4175	0.1619	0.0004
gmm	gmm_euclidean	5	dataframe	0.0051	0.3857	0.1619	0.0004

gmm	gmm_euclidean	5	dataframe	0.0086	0.0064	0.1619	0.0004
gmm	gmm_euclidean	5	dataframe	0.0088	0.0032	0.1619	0.0005
gmm	gmm_euclidean	5	dataframe	0.0100	0.0000	0.1619	0.0005
gmm	gmm_manhattan	3	dataframe	0.0032	0.2498	0.1151	0.0004
gmm	gmm_manhattan	3	dataframe	0.0038	0.2201	0.1151	0.0004
gmm	gmm_manhattan	3	dataframe	0.0070	0.0064	0.1151	0.0005
gmm	gmm_manhattan	3	dataframe	0.0109	0.0032	0.1151	0.0005
gmm	gmm_manhattan	3	dataframe	0.1737	0.0000	0.1151	0.0008
gmm	gmm_manhattan	4	dataframe	0.0031	0.3563	0.1179	0.0004
gmm	gmm_manhattan	4	dataframe	0.0055	0.2919	0.1179	0.0004
gmm	gmm_manhattan	4	dataframe	0.0063	0.0064	0.1179	0.0004
gmm	gmm_manhattan	4	dataframe	0.0071	0.0032	0.1179	0.0006
gmm	gmm_manhattan	4	dataframe	0.0096	0.0000	0.1179	0.0007
gmm	gmm_manhattan	5	dataframe	0.0036	0.4290	0.1141	0.0004
gmm	gmm_manhattan	5	dataframe	0.0040	0.3887	0.1141	0.0004
gmm	gmm_manhattan	5	dataframe	0.0067	0.0064	0.1141	0.0004
gmm	gmm_manhattan	5	dataframe	0.0076	0.0032	0.1141	0.0004
gmm	gmm_manhattan	5	dataframe	0.0083	0.0000	0.1141	0.0005
fanny	fanny_euclidean	3	dataframe	0.0121	0.2069	0.0000	0.0000
fanny	fanny_euclidean	3	dataframe	0.0125	0.1675	0.0000	0.0000
fanny	fanny_euclidean	3	dataframe	0.0152	0.0032	0.0000	0.0000
fanny	fanny_euclidean	3	dataframe	0.0178	0.0032	0.0000	0.0000
fanny	fanny_euclidean	3	dataframe	0.0218	0.0000	0.0000	0.0000
fanny	fanny_euclidean	4	dataframe	0.0161	0.2069	0.0000	0.0000
fanny	fanny_euclidean	4	dataframe	0.0190	0.1675	0.0000	0.0000
fanny	fanny_euclidean	4	dataframe	0.0205	0.0032	0.0000	0.0000
fanny	fanny_euclidean	4	dataframe	0.0208	0.0032	0.0000	0.0000
fanny	fanny_euclidean	4	dataframe	0.0265	0.0000	0.0000	0.0000
fanny	fanny_euclidean	5	dataframe	0.0165	0.2069	0.0000	0.0000
fanny	fanny_euclidean	5	dataframe	0.0171	0.1675	0.0000	0.0000
fanny	fanny_euclidean	5	dataframe	0.0221	0.0032	0.0000	0.0000
fanny	fanny_euclidean	5	dataframe	0.0226	0.0032	0.0000	0.0000
fanny	fanny_euclidean	5	dataframe	0.0250	0.0000	0.0000	0.0000
fanny	fanny_manhattan	3	dataframe	0.0156	0.2143	0.0000	0.0000
fanny	fanny_manhattan	3	dataframe	0.0180	0.1658	0.0000	0.0000
fanny	fanny_manhattan	3	dataframe	0.0201	0.0032	0.0000	0.0000
fanny	fanny_manhattan	3	dataframe	0.0238	0.0032	0.0000	0.0000
fanny	fanny_manhattan	3	dataframe	0.0278	0.0000	0.0000	0.0000
fanny	fanny_manhattan	4	dataframe	0.0171	0.2143	0.0000	0.0000
fanny	fanny_manhattan	4	dataframe	0.0181	0.1658	0.0000	0.0000
fanny	fanny_manhattan	4	dataframe	0.0225	0.0032	0.0000	0.0000
fanny	fanny_manhattan	4	dataframe	0.0266	0.0032	0.0000	0.0000
fanny	fanny_manhattan	4	dataframe	0.0279	0.0000	0.0000	0.0000
fanny	fanny_manhattan	5	dataframe	0.0235	0.2143	0.0000	0.0000
fanny	fanny_manhattan	5	dataframe	0.0242	0.1658	0.0000	0.0000
fanny	fanny_manhattan	5	dataframe	0.0259	0.0032	0.0000	0.0000
fanny	fanny_manhattan	5	dataframe	0.0262	0.0032	0.0000	0.0000
fanny	fanny_manhattan	5	dataframe	0.0271	0.0000	0.0000	0.0000

These are the results of running the clustering method. The meaning and functionality of each column is as follows:

- **Algorithm:** indicates the clustering algorithm used in the data processing.
- **Distance:** is the measure of dissimilarity used by the algorithm to calculate the similarity between the data.
- **Clusters:** is the number of clusters used by the algorithm. When working with clustering it is necessary to indicate the number of clusters.
- **Dataset:** is the name of the data.frame. By default appears data.frame but if instead of using the df parameter in the clustering method we use path (directory with files with extension dat), in the column must appear the names of the processed datasets.
- **timeExternal:** time to implement external evaluation measures.
- **entropy:** as mentioned in the section 2, is the measure in charge of measuring the uncertainty in the prediction of natural classes provided by the P partition.

- dunn: is an internal evaluation measure, it is focused on measuring cohesion (how close the elements are to each other) and separation (they quantify the level of separation between clusters).
 - timeInternal: time taken to implement internal evaluation measures.
- Note: in the metric field we indicate all the measurements we wish to evaluate. The implemented metrics are: entropy, recall, precision, f_measure, fowlkes_mallows_index, connectivity, dunn and silhouette.

The basketball dataset containing five variables. The operation is to execute the same algorithm with the measurement of dissimilarity and the number of clusters for each variable. With this we intend to see if the behaviour is the same for all the variables, or if the choice of a variable influences the quality of the results. From the measures indicated we can start to evaluate the quality of the clusters. Depending on the selected metrics we can evaluate some characteristics or others.

From the data we can see that the value of the variables influences the quality of the results, therefore the next step is to select those variables that provide better quality.

```
> Clustering::best_ranked_external_metrics(result)
```

Result:

Algorithm	Distance	Clusters	Dataset	timeExternal	entropy
gmm	gmm_euclidean	3	dataframe	0.0047	0.2374
gmm	gmm_euclidean	4	dataframe	0.0050	0.3734
gmm	gmm_euclidean	5	dataframe	0.0059	0.4175
gmm	gmm_manhattan	3	dataframe	0.0030	0.2498
gmm	gmm_manhattan	4	dataframe	0.0032	0.3563
gmm	gmm_manhattan	5	dataframe	0.0041	0.4290
fanny	fanny_euclidean	3	dataframe	0.0117	0.2069
fanny	fanny_euclidean	4	dataframe	0.0148	0.2069
fanny	fanny_euclidean	5	dataframe	0.0187	0.2069
fanny	fanny_manhattan	3	dataframe	0.0159	0.2143
fanny	fanny_manhattan	4	dataframe	0.0189	0.2143
fanny	fanny_manhattan	5	dataframe	0.0202	0.2143

The `Clustering::best_ranked_external_metrics` method is responsible for obtaining the best external variables for each execution, i.e. the best results by algorithm, measure of dissimilarity and number of clusters. We perform the same calculation for internal measurements.

```
> Clustering::best_ranked_internal_metrics(result)
```

Result:

Algorithm	Distance	Clusters	Dataset	timeInternal	dunn
gmm	gmm_euclidean	3	dataframe	0.0005	0.1096
gmm	gmm_euclidean	4	dataframe	0.0004	0.1233
gmm	gmm_euclidean	5	dataframe	0.0004	0.1619
gmm	gmm_manhattan	3	dataframe	0.0004	0.1151
gmm	gmm_manhattan	4	dataframe	0.0004	0.1179
gmm	gmm_manhattan	5	dataframe	0.0004	0.1141
fanny	fanny_euclidean	3	dataframe	0.0000	0.0000
fanny	fanny_euclidean	4	dataframe	0.0000	0.0000
fanny	fanny_euclidean	5	dataframe	0.0000	0.0000
fanny	fanny_manhattan	3	dataframe	0.0000	0.0000
fanny	fanny_manhattan	4	dataframe	0.0000	0.0000
fanny	fanny_manhattan	5	dataframe	0.0000	0.0000

We already have the best variables for each execution, we also have methods to group the measures of dissimilarity from the algorithms.

```
> Clustering::evaluate_best_validation_external_by_metrics(result)
```

Result:

Algorithm	Distance	timeExternal	entropy
fanny	fanny_euclidean	0.0163	0.2069
fanny	fanny_manhattan	0.0209	0.2143
gmm	gmm_euclidean	0.0076	0.4175
gmm	gmm_manhattan	0.0039	0.429

If we compare the results of `Clustering::best_ranked_external_metrics` with `Clustering::evaluate_best_validation_external_by_metrics` the functionality it gives us is that of being able to classify the quality of the data based on dissimilarity. This same method is also implemented for internal measures.

If we want to go further and we want to determine the best algorithm from the variables, we can do it in the following way.

```
> Clustering::evaluate_validation_external_by_metrics(result)
```

Result:

Algorithm	timeExternal	entropy
fanny	0.0209	0.2143
gmm	0.0076	0.4290

With `Clustering::evaluate_validation_external_by_metrics` we can see that the most correct algorithm for the dataset is gmm algorithm.

As an addition the `Clustering::result_external_algorithm_by_metric` method has been incorporated to filter the results of the clustering object from an algorithm to be able to choose a suitable cluster.

```
> Clustering::result_external_algorithm_by_metric(result, 'gmm')
```

Result:

Algorithm	Clusters	timeExternal	entropy
gmm	3	0.0045	0.2498
gmm	4	0.0056	0.3734
gmm	5	0.0047	0.429

On the basis of the executions carried out we can state that the gmm algorithm with five clusters is the best distributed data for the measurement of manhattan dissimilarity.

All these operations that we have carried out to evaluate the external measures can be extrapolated to the internal ones and obtain the necessary information for the appropriate choice of the algorithm as well as the number of clusters. Another feature incorporated in the package is the possibility of being able to represent the evaluation metrics according to the number of clusters, so that in some cases you can be quite quick in choosing the best results. Figure 8 shows this representation

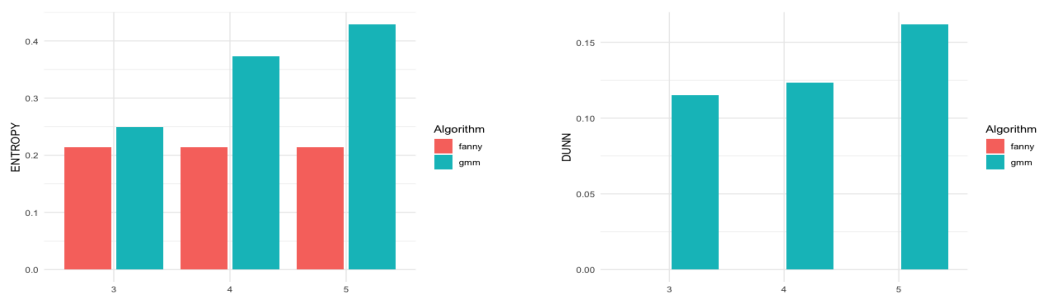


Figure 8: Graphical representation of evaluation measures

Post-processing of data

To conclude the definition of the methods of the package it is always necessary to have a functionality that allows us to sort, filter the information or export the data set. To do this we will detail the methods used:

- `sort(clustering_object, column_name)`: Sometimes it is necessary to determine what the maximum or minimum value of a column is and the easiest way to do this is by sorting the column.
- `"[.clustering"`: There are times when we need to apply filters on a series of columns for a set of values. This process can be done using third party packages, but due to its great usefulness we have incorporated this functionality. To filter we must do it in the following way: `clustering_object [column_1 operator value_1 conditional_1 column_n operator value_n]`. For more detailed information you can find it in the help of the package itself.

- `Clustering::export_file_external()`: exporting the result of the clustering object to the latex format is rare and very necessary when working with table in Latex.
- `Clustering::export_file_internal()`: this method is similar to the previous one, but only exports the internal metrics.

Graphical User Interface of the Clustering package

As mentioned throughout this paper, the **Clustering** package provides a GUI to work with clustering algorithms and to be able to evaluate and run the results more comfortable. The way to run the user interface is to execute the following instruction:

```
> appClustering()
```

The execution will open our default browser with the interface. As it can be observed in the Figure 9, we have a layout with header, side menu and main. In the header menu we can choose to see the numerical results or in graphical mode. In the left menu we can see the different parameters with which we can run our algorithm and finally in the central menu you can see the result of running the clustering algorithm.

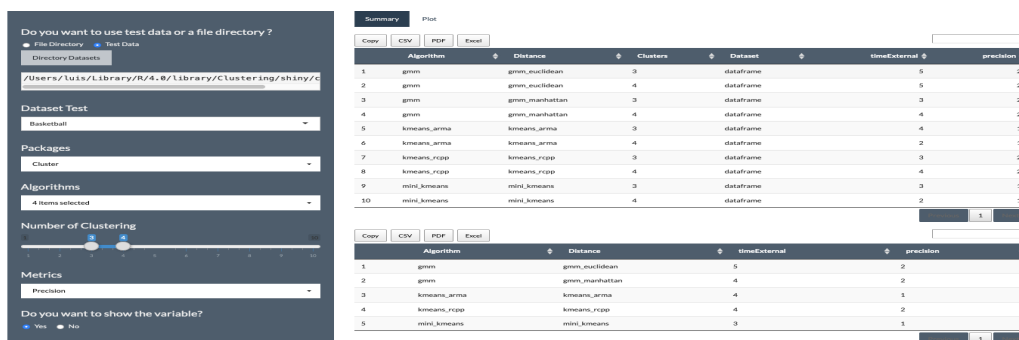


Figure 9: Clustering app user interface

The operation of the application is very simple as can be seen in the Figure 10 and we will proceed to explain it step by step.

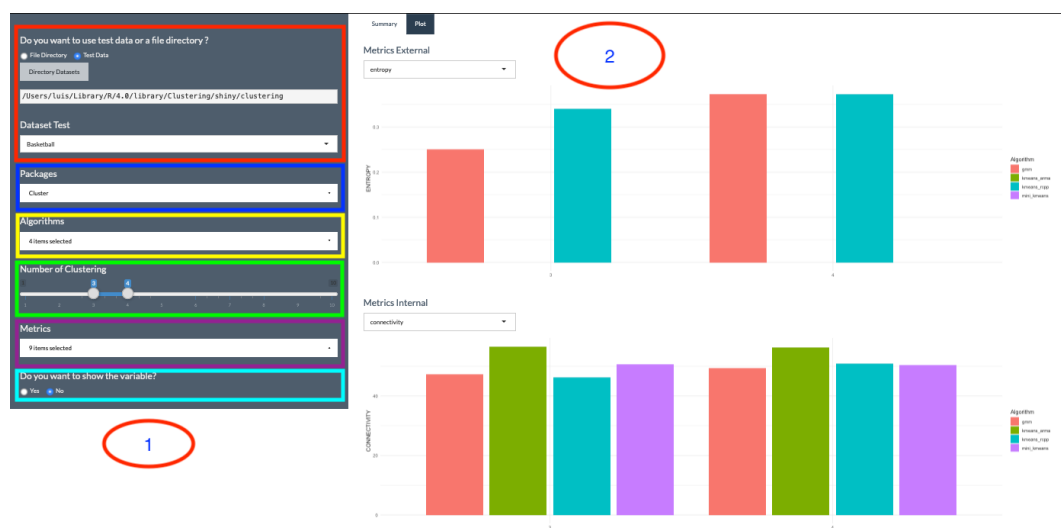


Figure 10: Clustering app user interface

As you can see in the Figure 10 we have two well differentiated parts:

1. In this section we can find the different parameters used by the clustering algorithm to filter the information.

- Marked in red, we can indicate if we want to work with test datasets or indicate a directory of dataset files to be processed.
- In blue we have the packages that implement the clustering algorithms mentioned throughout the paper. We can mark all the packages or individually. When a package is marked, all the algorithms implemented within the selected package are also marked.
- In yellow we have the algorithms implemented by the packages. If we mark an algorithm it will automatically mark its corresponding package in the package combo.
- In green we have the number of clusters. We can indicate ranges or select only one cluster by positioning the max and minimum on the same value.
- In violet we indicate the evaluation metrics used when validating the clusters.
- Finally we have a check through which instead of showing the metric values we can show the variable number. In the image we have an example of execution with default variables.

	Algorithm	Distance	Clusters	Dataset	Ranking	timeExternal	entropy	dunn	timeInternal
height	gmm	gmm_euclidean	3	dataframe	1	0.0061	0.2374	0.1096	0.0007

Figure 11: Execution of the default clustering method

In the Figure 12 it is the execution of the same method with variable to true.

	Algorithm	Distance	Clusters	Dataset	Ranking	timeExternal	entropy	dunn	timeInternal
height	gmm	gmm_euclidean	3	dataframe	1	4	2	1	5

Figure 12: Execution of the clustering method with variable to true

Note: the variables represent the dataset variables.

2. In main layout we have the options to represent the data.
- To view the data in graphical mode as shown in the Figure 13, we mark the Plot tab. In the figure we can see represented the internal and external evaluation metrics and depending on the type of evaluation we can filter individually by metrics to see the data represented graphically.

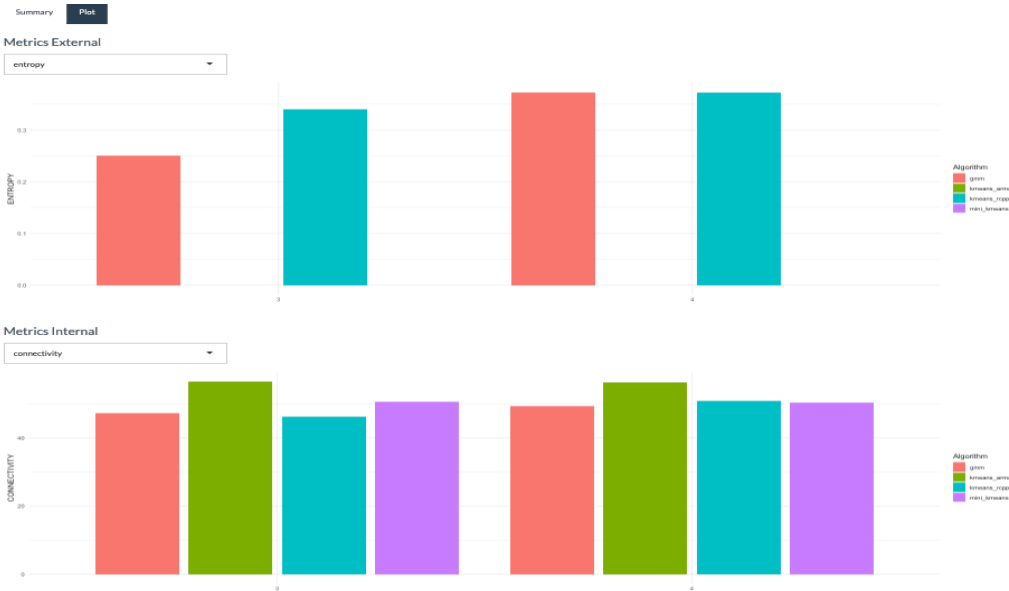


Figure 13: Tab with graphical representation of metrics

- If we click on the summary tab as shown in the Figure 14, we can see the data represented in tables. If you wish you can export the results in the following formats: csv,pdf and xls. If you wish you can copy the results.

Summary		Plot													
Copy	CSV	PDF	Excel												
Algorithm	Distance	Clusters	Dataset	timeExternal	entropy	variation_information	precision	recall	f_measure	feature_selection_index	connectivity	dens	silhouette		
1	gmm	gmm_euclidean	3	dataframe	0.0323	0.2374	5.004	0.1869	0.5601	0.2803	0.3236	47.39	0.1096	C	
2	gmm	gmm_euclidean	4	dataframe	0.0374	0.3734	4.767	0.1344	0.3763	0.1908	0.2103	41.31	0.1233	C	
3	gmm	gmm_manhattan	3	dataframe	0.0308	0.2498	5.086	0.183	0.536	0.2728	0.3132	40.76	0.1151	C	
4	gmm	gmm_manhattan	4	dataframe	0.041	0.3563	4.713	0.166	0.4059	0.2315	0.252	49.5	0.1179	C	
5	kmeans_arma	kmeans_arma	3	dataframe	0.001	0	0	0	0	0	0	56.69	0.1182	C	
6	kmeans_arma	kmeans_arma	4	dataframe	0.0011	0	0	0	0	0	0	56.31	0.1519	C	
7	kmeans_rcpp	kmeans_rcpp	3	dataframe	0.0507	0.3601	5.059	0.1592	0.5	0.2366	0.2707	46.31	0.1465	C	
8	kmeans_rcpp	kmeans_rcpp	4	dataframe	0.043	0.3728	4.627	0.1697	0.5	0.23	0.2441	51.04	0.1741	C	
9	mini_kmeans	mini_kmeans	3	dataframe	0.0012	0	0	0	0	0	0	50.59	0.135	C	
10	mini_kmeans	mini_kmeans	4	dataframe	0.0012	0	0	0	0	0	0	50.35	0.1571	C	

Figure 14: Clustering package execution summary tab

Conclusion

In this paper we have made an introduction to the **Clustering** package. The package has dependencies with other packages as seen throughout the paper. It allows the reading and loading of datasets in KEEL, CSV or ARFF format. We also offer the functionality of loading a data.frame in memory or using test datasets. As a complement the package has been enhanced with the inclusion of a graphical interface that allows the user to run the package in a simple way without the need to know the parameters. The development of the package will be continued with the inclusion of new algorithms, functionalities and improvement of the interface, therefore we encourage developers to contribute to the improvement of the package with the inclusion of new algorithms or functionalities or the inclusion of new proposals that complement the package.

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