# 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 attributes 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. These clusters must meet two conditions: clusters must be the most disparate possible among them, and the elements that contain them the most similar. Throughout 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).

A wide variety of frameworks have been presented into the literature based on clustering algorithms such as: 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 allow us 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 attributes are most suitable for clustering. 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 Clustering we have the presentation of clustering, types of clustering and similarity measures. Section Internal and External clustering validation measures presents the definition of the evaluation measures in order to value the distribution of the data in the clusters. Finally Section The Clustering package 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, partitioning, density-based, grid-based and probability distribution. The most commonly used groupings are: hierarchical, part-based and density-based.

• Hierarchical clustering algorithms: create a hierarchical breakdown of data into a dendogram that recursively divides the data set into smaller and smaller data. It can be created in two ways: bottom-up or top-down (Jain et al., 1999a). In bottom-up trees also known as 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. An example of this type of clustering can be found in the Figure 1. 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).

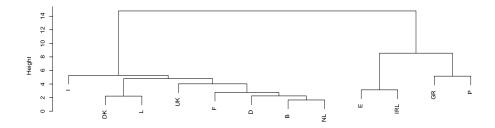


Figure 1: Hierarchical Clustering.

- 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. If we want to observe graphically how this type of clustering works we can see it in the Figure 2. 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).
- 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). These

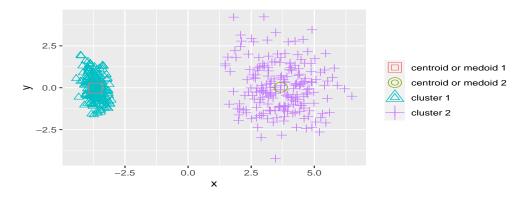


Figure 2: Partitional Clustering.

regions are represented in the Figure 3. Among the density-based algorithms, we highlight the following: Dbscan (Hu, 2019), and Denclue (Khader and Al-Naymat, 2019).

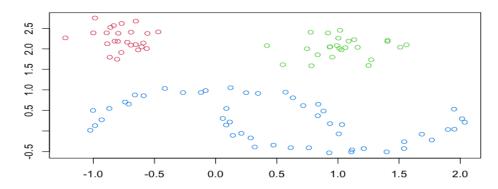


Figure 3: Density Clustering.

- Grid-based clustering algorithms: first quantize the clustering space into a finite number of cells and then perform the required operations on the quantized space (Dang, 2011). 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 we highlight SOM (Thalamuthu et al., 2006). Model-based
  clustering is shown in the Figure 4.

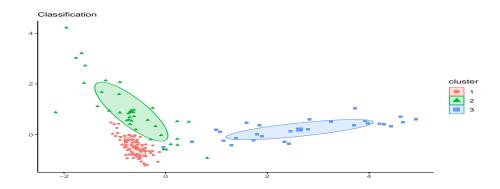


Figure 4: Model-Based Clustering.

#### Dissimilarity measures

Dissimilarity measurements are important to the creation 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  $\infty$ .

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 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: Is a metric in a normed vector space which can be considered as a generalization of both the Euclidean distance and the Manhattan distance (Gan et al., 2007).

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

where m is a positive real number and  $x_i$  and  $y_i$  are two vectors in n-dimensional space.

 Euclidan distance: Is a special case of Minkowski distance. Is a measure of the true straight line distance between two points in Euclidean space. (Jain et al., 1999b).

$$d_{euc} = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}$$
 (2)

Manhattan distance: Also known as the geometry cab driver is defined as the sum of the lengths
of the projections of the line segment between the points onto the coordinate axes (Xu and
Wunsch, 2005).

$$d_{man} = \sum_{i=1}^{n} |x_i - y_i| \tag{3}$$

• Mahalanobis distance: Is a data-driven measure in contrast to Euclidean and Manhattan distances that are independent. It is in charge of measuring the distance in a multivariate space (Xu and Wunsch, 2005).

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

where S is the covariance matrix of the dataset

• Pearson correlation: It's a statistically based metric that measures linear correlation between two variables x and y (Publications et al., 2015).

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

where  $\mu_x$  and  $\mu_y$  are the means for x and y respectively.

• Jaccard Index: Is a classical similarity measure on sets with several practical applications in information retrieval, data mining, machine learning, and many more (Kosub, 2019) (Irani et al., 2016). It measures the similarity of the two data elements as the intersection divided by the union of the data elements as shown below:

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

 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.

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

where  $S_{ij}$  is Gower similarity coefficient (Niakšu, 2013).

$$S_{ij} = \frac{\sum_{k}^{n} w_{ijk} S_{ijk}}{\sum_{n}^{k} w_{ijk}} \tag{8}$$

 $S_{ijk}$  denotes the contribution provided by the k-th variable, and  $w_{ijk}$  is usually 1 or 0 depending if the comparison is valid for the k-th variable.

# 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. When we talk about criteria based on internal measures we must take into account the criteria of compaction and separation (Halkidi et al., 2001) (Berry and Linoff, 2004) as you can see in the Figure 7:

- 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.

These criteria are graphically represented in the image 5.

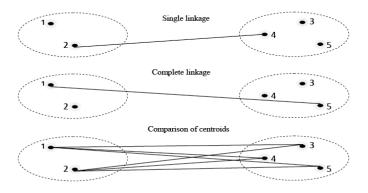


Figure 5: Intercluster distance (Johnson and Wichern, 1998).

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

• Entropy: It evaluates the distribution of categories in a cluster (Kim and Park, 2007).

$$Entropy = \sum_{i=1}^{m} \frac{n_j}{n} E_j \tag{9}$$

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:

$$E_j = \sum_i p_{ij} log(p_{ij}) \tag{10}$$

Where  $p_{ij}$  is the probability of a point in the cluster i of being classified as class j.

 Recall: It indicates the proximity of the measurement results to the true value (Kacprzyk and Farhaoui, 2019).

$$Recall(i,j) = \frac{n_{ij}}{n_i} \tag{11}$$

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

 Precision: It refers to the dispersion of the set of values obtained from repeated measurements of one magnitude (Kacprzyk and Farhaoui, 2019).

$$Precision(i,j) = \frac{n_{ij}}{n_i} \tag{12}$$

 $n_i$  is the number of objects in cluster j.

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

$$F - measure(i, j) = \frac{2 * (Precision(i, j) * Recall(i, j))}{(Precision(i, j) + Recall(i, j))}$$
(13)

• Fowlkes-Mallows Index: 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 ,..., n-1 of the hierarchy (Romano et al., 2016). The measure  $B_i$  is easily generalizable to a measure for clustering of different clusters. 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).

$$Fowlkes = \sqrt{Precision * Recall}$$
 (14)

• Variation information: Variation in information or distance of shared information is a measure of distance between two groups (Romano et al., 2016). This measure is closely related to mutual information (mutual dependence between the two variables). However, in contrast to mutual information (b63, 2008), variation of information is a true metric, in the sense that it is due to the inequality of triangles (for any triangle, the sum of the lengths of any two sides must be greater than or equal to the length of the remaining side).

$$VI = -\sum_{i}^{j} r_{ij} \left[ \log \left( \frac{r_{ij}}{p_i} \right) + \left( \frac{r_{ij}}{q_j} \right) \right]$$
 (15)

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).

$$connectivity = min_{1 \le i \le K} \left( min_{1 \le j \le K, i \ne j} \left( \frac{dist(C_i, C_j)}{max_{1 \le k \le K} \{diam(C_k)\}} \right) \right)$$
 (16)

Where  $dist(C_i, C_j)$  is the distance between two clusters and  $diam(C_k)$  is diameter of a particular cluster (Deborah et al., 2010).

• Dunn: 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 (Ansari et al., 2015).

$$dunn = min_{1 \le i \le k} \left( min_{i+1 \le j \le k} \left( \frac{dist(C_i, C_j)}{max_{1 \le l \le k} diam(C_l)} \right) \right)$$
(17)

Where  $dist(C_i, C_i)$  is distance between clusters  $C_i$  and  $C_i$  and  $diam(C_l)$  is diameter of cluster  $C_l$ .

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

$$S = \frac{1}{N} \sum_{i=0}^{N} \frac{b_i - a_i}{\max(a_i, b_i)}$$
 (18)

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

The above evaluation measures can be grouped into families in order to evaluate the quality of the clusters. If we look at the Figure 6 we can group Entropy, Recall, Precision, F-Measure, Fowlkes-Mallows Index and Variation information into three families (Palacio-Niño and Berzal, 2019):

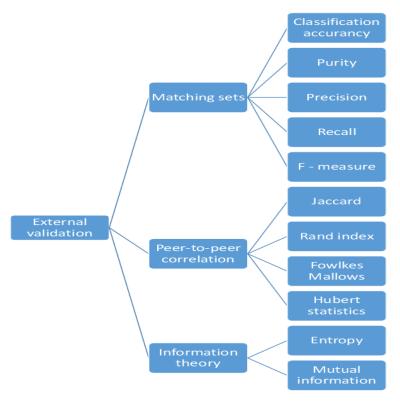


Figure 6: External validation methods (Palacio-Niño and Berzal, 2019).

- Matching Sets: 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 (clustering result prediction) (Palacio-Niño and Berzal, 2019). Several measures can be defined to measure the similarity between the clusters in C, obtained by the clustering algorithm, and the clusters in P, corresponding to our prior (external) knowledge. The metrics included in this method are: Precision, Recall and F-measure.
- Peer-to-peer Correlation: 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 (Palacio-Niño and
  Berzal, 2019). It is assumed that the examples that are in the same cluster in C should be in the
  same class in P, and viceversa. In our package we use the metric: Fowlkes-Mallows Index.
- Measures Based on Information Theory: 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 (Palacio-Niño and Berzal, 2019). This family includes basic measures such as entropy and variation information.

Internal evaluation metrics (see Figure 7) 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).

According to the figure 8, the internal Dunn, Silhouette and Connectivity metrics are based on the concepts mentioned above so we can group them as partitioning methods.

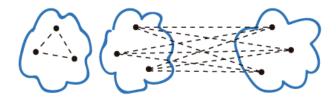


Figure 7: Representation of cohesion and separation in clustering (Palacio-Niño and Berzal, 2019).



Figure 8: Internal validation methods (Palacio-Niño and Berzal, 2019).

# The Clustering package

Clustering package has been written entirely in R language. The package is composed by other packages with hierarchical, partitional and agglometaritve algorithms. The package has been also provided with the abitlity to read data in different formats such as CSV, KEEL, ARFF (Weka) and data.frame objects. This package implements functionality not developed until now. In current implementations, we cannot run several algorithms simultaneously. This option is very useful if you want to compare the results of running several algorithms. Another very useful option not found so far, is the ability to run all the dissimilarity measures implemented for an algorithm in the same run, ie, run for example the K-means algorithm for the measures of dissimilarity Euclidean and Manhattan simultaneously. This perspective is quite interesting when it comes to say what measure to use in the execution of the algorithm. To evaluate the quality of the clusters, we find packages that perform external or internal evaluations, but we do not have implementations that give us a joint evaluation of both. Finishing the review we find that when evaluating the quality of clusters, it is necessary to indicate an attribute of the dataset used in the execution. Depending on the chosen attribute results may vary, so it would be important to have methods that give us the result of running each of the quality measures by attribute, measure of dissimilarity in the case of having, number of clusters and algorithm. With the Clustering package we will be able to execute simultaneously several algorithms for each of the implemented dissimilarity measures. In addition, when evaluating the results of the executions, we have a set of measures that are executed together, which until now was done one execution per measure. It is possible to incorporate new measures quickly in the future. In addition, when running the algorithm, all the attributes of the dataset will be executed for each of the quality metrics. The results of the executions are visually displayed so that you can draw conclusions quickly.

## Algorithms of the package

These are the algorithms available within the package, which we will classify as follows:

- Hierarchical Clustering: agnes, clara, daisy, diana, fanny, fuzzy\_cm, fuzzy\_gk, fuzzy\_gg, hcluster, mona, pam, pvpick and pvclust.
- Partitioning Clustering: gama, gmm, kmeans
- Aglomerative Clustering: aggExCluster, apclusterK

For more information you can check the following links:

- advclust: https://CRAN.R-project.org/package=advclust
- amap: https://CRAN.R-project.org/package=amap
- apcluster: https://CRAN.R-project.org/package=apcluster
- cluster: https://CRAN.R-project.org/package=cluster
- Cluster: https://CRAN.R-project.org/package=ClusterR
- gmp: https://CRAN.R-project.org/package=gmp
- pvclust: https://CRAN.R-project.org/package=pvclust

#### **Package Architecture**

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 correspondence between the evaluation metric calculation and
    the dataset attribute, the measures of similarity 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\_executed. It represents a character vector with the algorithms executed independently of the package.
  - measures\_executed. It represents a vector of characters with the measures of similarity 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 attribute, on the measures of similarity and on the number of clusters. This translates as follows. If we have a dataset with five attributes, using as similarity measures Euclidean and Manhattan and with k partitions the method best\_ranked\_external\_metrics() will return us those attributes that better result return for the indicated algorithms, similarity measures and partitions. If what we want is to group the results by algorithm and similarity measure and obtain the results based on these properties the method we must use is evaluate\_best\_validation\_external\_by\_metrics(). Another method that allows us to obtain the results of the evaluation metrics by algorithm is evaluate\_validation\_external\_by\_metrics(). If we simply want to group the results of the algorithms by number of clusters we must use the result\_external\_algorithm\_by\_metric() method. With this set of methods we manage to group the data obtained and see their behaviour based on the number of partitions, metrics or similarity measures. These methods are used in external evaluation measures.
- 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 attribute, on the measures of similarity and on the number of clusters. The operation is similar to those indicated above for external evaluation measures.
- plot\_clustering(): Method that represents the results of clustering in a bar chart. The graph represents the distribution of the algorithms based on the number of partitions and the evaluation metrics which can be internal or external.
- export\_external\_file(): The results of external metrics can be exported in Latex format, for integration into documents with that format.
- export\_internal\_file(): As indicated above, we have this method to export the results of the internal metrics.

#### 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 (Charte 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 repository 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.

## Analysis of clustering methods using the Clustering package

Once the way to provide the data has been defined the next step is to be able to execute the main method of the application which is clustering. With this method we can compare the clustering algorithms included in the mentioned packages. When comparing we can do it by packages or simply by indicating the algorithms contained in them. In partitional clustering it is necessary to indicate the number of partitions. Apart from indicating the number of partitions, we can evaluate the algorithms by means of a range of partitions, indicating the maximum and minimum of partitions. To evaluate how the data have been distributed in the clusters, it is done through a set of evaluation measures that return numeric values. An improvement built into the package is that in addition to returning the numerical value of the metrics, it can return the dataset attribute corresponding to that value. This means that when evaluating a metric for each of the attributes of a dataset, in addition to returning the value obtained from the calculation it will return the attribute to which it corresponds but in different columns. In addition, the algorithms are executed for all measures of similarity implemented. All this functionality is incorporated into the main method. Therefore the parameters of the clustering method are the following:

- path: The path of file. It is only allowed to use path or df but not both at the same time. Only files in .dat,.csv or arff format are allowed.
- df: data matrix or data frame, or similarity matrix.
- packages: character vector with the packets running the algorithm. The seven packages implemented are: cluster, ClusterR, advclust, amap, apcluster, gama, pvclust. By default runs all packages.
- 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.
- min: An integer with the minimum number of clusters This data is necessary to indicate the minimum number of clusters when grouping the data. The default value is 3.
- max: An integer with the maximum number of clusters. This data is necessary to indicate the maximum number of clusters when grouping the data. The default value is 4.
- metrics: Character vector with the metrics implemented to evaluate the distribution of the data in clusters. The night metrics implemented are: entropy, variation\_information, precision, recall, f\_measure, fowlkes\_mallows\_index, connectivity, dunn, silhouette.

- metricsAttr: Character vector with the metrics implemented to evaluate the distribution of the data in clusters. The night metrics implemented are: entropy, variation\_information, precision, recall, f\_measure, fowlkes\_mallows\_index, connectivity, dunn, silhouette. This column is the same as the previous one, with the difference that shows the dataset attribute.
- attributes: an boolean which indicates that if we want to show as a result the attributes of the datasets. The default value is F.

Once the definition of the attributes of the main method has been completed, we will carry out a test. To do this we will use the data. frame Basketball (this dataset contains five attributes representing the statistics of a set of 96 basketball players. The attributes are: assists per minute, height, time played, age and points per minute) included in the package, and the gmm and fanny algorithms (included in the ClusterR and cluster packages). We will also indicate a range of partitions between 3 and 5 and evaluate entropy as an external evaluation measure and dunn as an internal one.

Algorithm	Distance	Clusters	Dataset	tE 1	entropy	dunn	tI <sup>2</sup>	tEAttr 3	enAttr 4	duAttr 5	tIAttr 6
gmm	gmm_euclidean	3	dataframe	0.0042	0.2374	0.1096	0.0004	5	2	1	1
gmm	gmm_euclidean	3	dataframe	0.0046	0.2120	0.1096	0.0004	1	4	2	2
gmm	gmm_euclidean	3	dataframe	0.0079	0.0064	0.1096	0.0005	3	3	3	3
gmm	gmm_euclidean	3	dataframe	0.0081	0.0032	0.1096	0.0005	2	5	4	4
gmm	gmm_euclidean	3	dataframe	0.0089	0.0000	0.1096	0.0006	4	1	5	5
gmm	gmm_euclidean	4	dataframe	0.0041	0.3734	0.1233	0.0004	5	2	1	4
gmm	gmm_euclidean	4	dataframe	0.0041	0.2983	0.1233	0.0004	2	4	2	5
gmm	gmm_euclidean	4	dataframe	0.0071	0.0064	0.1233	0.0004	4	3	3	1
gmm	gmm_euclidean	4	dataframe	0.0071	0.0032	0.1233	0.0004	1	5	4	2
gmm	gmm_euclidean	4	dataframe	0.0193	0.0000	0.1233	0.0005	3	1	5	3
gmm	gmm_euclidean	5	dataframe	0.0044	0.4175	0.1619	0.0004	3	2	1	1
gmm	gmm_euclidean	5	dataframe	0.0045	0.3857	0.1619	0.0004	1	4	2	4
gmm	gmm_euclidean	5	dataframe	0.0079	0.0064	0.1619	0.0004	4	3	3	5
gmm	gmm_euclidean	5	dataframe	0.0079	0.0032	0.1619	0.0005	2	5	4	3
gmm	gmm_euclidean	5	dataframe	0.0091	0.0000	0.1619	0.0005	5	1	5	2
gmm	gmm_manhattan	3	dataframe	0.0030	0.2498	0.1151	0.0004	3	2	1	4
gmm	gmm_manhattan	3	dataframe	0.0036	0.2201	0.1151	0.0004	2	4	2	1
gmm	gmm_manhattan	3	dataframe	0.0067	0.0064	0.1151	0.0004	5	3	3	5
gmm	gmm_manhattan	3	dataframe	0.0073	0.0032	0.1151	0.0005	1	5	4	2
gmm	gmm_manhattan	3	dataframe	0.0075	0.0000	0.1151	0.0005	4	1	5	3
gmm	gmm_manhattan	4	dataframe	0.0034	0.3563	0.1179	0.0004	4	2	1	4
gmm	gmm_manhattan	4	dataframe	0.0049	0.2919	0.1179	0.0004	2	4	2	1
gmm	gmm_manhattan	4	dataframe	0.0068	0.0064	0.1179	0.0004	5	3	3	2
gmm	gmm_manhattan	4	dataframe	0.0073	0.0032	0.1179	0.0005	1	5	4	5
gmm	gmm_manhattan	4	dataframe	0.0076	0.0000	0.1179	0.0007	3	1	5	3
gmm	gmm_manhattan	5	dataframe	0.0032	0.4290	0.1141	0.0004	4	2	1	1
gmm	gmm_manhattan	5	dataframe	0.0036	0.3887	0.1141	0.0004	1	4	2	5
gmm	gmm_manhattan	5	dataframe	0.0072	0.0064	0.1141	0.0005	3	3	3	4
gmm	gmm_manhattan	5	dataframe	0.0079	0.0032	0.1141	0.0007	2	5	4	2
gmm	gmm_manhattan	5	dataframe	0.0084	0.0000	0.1141	0.0011	5	1	5	3
fanny	fanny_euclidean	3	dataframe	0.0107	0.2069	0.0000	0.0000	5	4	1	1
fanny	fanny_euclidean	3	dataframe	0.0114	0.1675	0.0000	0.0000	2	2	2	2
fanny	fanny_euclidean	3	dataframe	0.0140	0.0032	0.0000	0.0000	4	3	3	3
fanny	fanny_euclidean	3	dataframe	0.0159	0.0032	0.0000	0.0000	1	5	4	4
fanny	fanny_euclidean	3	dataframe	0.0161	0.0000	0.0000	0.0000	3	1	5	5
fanny	fanny_euclidean	4	dataframe	0.0123	0.2069	0.0000	0.0000	3	4	1	1
fanny	fanny_euclidean	4	dataframe	0.0128	0.1675	0.0000	0.0000	1	2	2	2
fanny	fanny_euclidean	4	dataframe	0.0157	0.0032	0.0000	0.0000	4	3	3	3

<sup>&</sup>lt;sup>1</sup>tE - timeExternal

<sup>&</sup>lt;sup>2</sup>tI - timeInternal

 $<sup>^3</sup>$ tEAttr - timeExternalAttr

 $<sup>^4</sup>$ en Attr - entropy Attr

<sup>&</sup>lt;sup>5</sup>duAttr - dunnAttr

 $<sup>^6</sup>$ t<br/>IAttr - timeInternalAttr

fanny	fanny_euclidean	4	dataframe	0.0157	0.0032	0.0000	0.0000	2	5	4	4
fanny	fanny_euclidean	4	dataframe	0.0178	0.0000	0.0000	0.0000	5	1	5	5
fanny	fanny_euclidean	5	dataframe	0.0167	0.2069	0.0000	0.0000	3	4	1	1
fanny	fanny_euclidean	5	dataframe	0.0189	0.1675	0.0000	0.0000	2	2	2	2
fanny	fanny_euclidean	5	dataframe	0.0219	0.0032	0.0000	0.0000	4	3	3	3
fanny	fanny_euclidean	5	dataframe	0.0272	0.0032	0.0000	0.0000	1	5	4	4
fanny	fanny_euclidean	5	dataframe	0.0286	0.0000	0.0000	0.0000	5	1	5	5
fanny	fanny_manhattan	3	dataframe	0.0165	0.2143	0.0000	0.0000	3	4	1	1
fanny	fanny_manhattan	3	dataframe	0.0184	0.1658	0.0000	0.0000	1	2	2	2
fanny	fanny_manhattan	3	dataframe	0.0196	0.0032	0.0000	0.0000	4	3	3	3
fanny	fanny_manhattan	3	dataframe	0.0247	0.0032	0.0000	0.0000	5	5	4	4
fanny	fanny_manhattan	3	dataframe	0.0719	0.0000	0.0000	0.0000	2	1	5	5
fanny	fanny_manhattan	4	dataframe	0.0152	0.2143	0.0000	0.0000	4	4	1	1
fanny	fanny_manhattan	4	dataframe	0.0159	0.1658	0.0000	0.0000	1	2	2	2
fanny	fanny_manhattan	4	dataframe	0.0183	0.0032	0.0000	0.0000	5	3	3	3
fanny	fanny_manhattan	4	dataframe	0.0189	0.0032	0.0000	0.0000	2	5	4	4
fanny	fanny_manhattan	4	dataframe	0.0193	0.0000	0.0000	0.0000	3	1	5	5
fanny	fanny_manhattan	5	dataframe	0.0178	0.2143	0.0000	0.0000	4	4	1	1
fanny	fanny_manhattan	5	dataframe	0.0183	0.1658	0.0000	0.0000	1	2	2	2
fanny	fanny_manhattan	5	dataframe	0.0207	0.0032	0.0000	0.0000	3	3	3	3
fanny	fanny_manhattan	5	dataframe	0.0211	0.0032	0.0000	0.0000	2	5	4	4
fanny	fanny_manhattan	5	dataframe	0.0211	0.0000	0.0000	0.0000	5	1	5	5

**Table 1:** Results of running the main method of the package.

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 similarity used by the algorithm to calculate the similarity between the data.
- Clusters: is the number of clusters used by the algorithm. Used in Partitional Clustering.
- Dataset: is the name of the data. frame. By default appears dataframe 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.
- metrics: each metric indicated in the execution is presented in individual columns. In this case we have both external (entropy) and internal (dunn) metrics. 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.
- metricsAttr: It is the same metrics that instead of showing numerical values are showing the attributes of the dataset..
- timeInternal: time taken to implement internal evaluation measures.

To make it easier to understand the other features implemented in the package, let's focus on a simple example. From the results of the main method, we will take the gmm algorithm, the euclidean dissimilarity measure and three clusters.

Algorithm	Distance	Clusters	Dataset	tE	entropy	dunn	tI	tEAttr	enAttr	duAttr	tIAttr
gmm	gmm_euclidean	3	dataframe	0.0046	0.2120	0.1096	0.0004	1	4	2	2
gmm	gmm_euclidean	3	dataframe	0.0079	0.0064	0.1096	0.0005	3	3	3	3
gmm	gmm_euclidean	3	dataframe	0.0081	0.0032	0.1096	0.0005	2	5	4	4
gmm	gmm_euclidean	3	dataframe	0.0089	0.0000	0.1096	0.0006	4	1	5	5

Table 2: Example of calculation of the attributes of a dataset by algorithm, means and cluster number.

Based on these data, and focusing on the entropy metric, it can be seen that the maximum value in entropy is in row one. To obtain which attribute of the dataset basketball is that it has returned that value, we only need to look at the column enAttr and look at row one. We can see that attribute two of the dataset is the one that is giving me the best value for the gmm algorithm, with euclidean dissimilarity measure and three clusters. In the case of dunn the value is the same for all attributes.

We choose attribute one because it is the one that takes the least time to execute. In the following functions we will see step by step which attribute has the best behaviour based on the algorithm, the measure of dissimilarity or the number of clusters, among others.

> Clustering::best\_ranked\_external\_metrics(result)

Algorithm	Distance	Clusters	Dataset	timeExternal	entropy	timeExternalAttr	entropyAttr
gmm	gmm_euclidean	3	dataframe	0.0104	0.2374	5	2
gmm	gmm_euclidean	4	dataframe	0.0147	0.3734	2	2
gmm	gmm_euclidean	5	dataframe	0.0058	0.4175	5	2
gmm	gmm_manhattan	3	dataframe	0.0066	0.2498	5	2
gmm	gmm_manhattan	4	dataframe	0.0083	0.3563	4	2
gmm	gmm_manhattan	5	dataframe	0.0045	0.4290	5	2
fanny	fanny_euclidean	3	dataframe	0.0177	0.2069	5	4
fanny	fanny_euclidean	4	dataframe	0.0148	0.2069	5	4
fanny	fanny_euclidean	5	dataframe	0.0199	0.2069	1	4
fanny	fanny_manhattan	3	dataframe	0.0311	0.2143	3	4
fanny	fanny_manhattan	4	dataframe	0.0210	0.2143	4	4
fanny	fanny_manhattan	5	dataframe	0.0222	0.2143	2	4

Table 3: Results of the execution of the Clustering::best\_ranked\_external\_metrics().

Clustering::best\_ranked\_external\_metrics method is in charge of selecting from the data set attributes, those that obtain the best result in the evaluation of the measure. In the calculation of the entropy the results are in the interval [0,1]. Being the next to 1 very good. For this example, we have the best attributes in entropy grouped by algorithm, measure of dissimilarity and cluster number. When grouping the data, choose the one with the highest value. We perform the same calculation for internal measurements.

> Clustering::best\_ranked\_internal\_metrics(result)

Algorithm	Distance	Clusters	Dataset	timeInternal	dunn	dunnAttr	timeInternalAttr
gmm	gmm_euclidean	3	dataframe	0.0009	0.1096	1	5
gmm	gmm_euclidean	4	dataframe	0.0008	0.1233	1	4
gmm	gmm_euclidean	5	dataframe	0.0005	0.1619	1	2
gmm	gmm_manhattan	3	dataframe	0.0006	0.1151	1	1
gmm	gmm_manhattan	4	dataframe	0.0005	0.1179	1	2
gmm	gmm_manhattan	5	dataframe	0.0006	0.1141	1	5
fanny	fanny_euclidean	3	dataframe	0.0000	0.0000	1	1
fanny	fanny_euclidean	4	dataframe	0.0000	0.0000	1	1
fanny	fanny_euclidean	5	dataframe	0.0000	0.0000	1	1
fanny	fanny_manhattan	3	dataframe	0.0000	0.0000	1	1
fanny	fanny_manhattan	4	dataframe	0.0000	0.0000	1	1
fanny	fanny_manhattan	5	dataframe	0.0000	0.0000	1	1

Table 4: Results of the execution of the Clustering::best\_ranked\_internal\_metrics().

We already have the best attributes for each execution, we also have methods to group the measures of dissimilarity from the algorithms. When grouping the results by measures of dissimilarity and algorithm, we do not use a specific grouping algorithm, but we keep those values whose value is the maximum depending on the type of metric. In this case we see that for the fanny algorithm with dissimilarity measure euclidean and taking into account the number of clusters, the value closest in entropy to 1 is 0.2090. For the rest of the algorithms the same process is followed.

> Clustering::evaluate\_best\_validation\_external\_by\_metrics(result)

Algorithm	Distance	timeExternal	entropy	timeExternalAttr	entropyAttr
fanny	fanny_euclidean	0.0199	0.2069	5	4
fanny	fanny_manhattan	0.0311	0.2143	4	4
gmm	gmm_euclidean	0.0147	0.4175	5	2
gmm	gmm_manhattan	0.0083	0.429	5	2

Table 5: Results of the execution of the Clustering::evaluate\_best\_validation\_external\_by\_metrics().

With this method we intend to demonstrate whether the choice of measurement of similarity also has an influence. The results obtained in this table are obtained by filtering the values of Clustering::best\_ranked\_external\_metrics() and aggregating them by algorithm and measure of dissimilarity. If we check the Table 3 we see that row three and six give us the highest value for the gmm algorithm and the measures euclidean and manhattan. In the case of fanny all the attributes return the same value, so we choose those whose execution time is lower.

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

> Clustering::evaluate\_validation\_external\_by\_metrics(result)

Algorithm	timeExternal	entropy	timeExternalAttr	entropyAttr
fanny	0.0311	0.2143	5	4
gmm	0.0147	0.4290	5	2

Table 6: Results of the execution of the Clustering::evaluate\_validation\_external\_by\_metrics().

With Clustering::evaluate\_validation\_external\_by\_metrics we can see that the most correct algorithm for the dataset is gmm algorithm, as the value of entropy is closer to 1.

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')

Algorithm	Clusters	timeExte	rnæIntropy	timeExternalAttr	entropyAttr
gmm	3	0.0104	0.2498	5	2
gmm	4	0.0147	0.3734	4	2
gmm	5	0.0058	0.429	5	2

Table 7: Results of the execution of the Clustering::result\_external\_algorithm\_by\_metric().

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 similarity.

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 9 shows this representation. The method that represents the data graphically is Clustering::plot\_clustering which receives as parameter the metric.

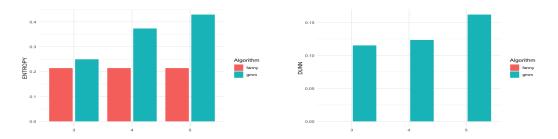


Figure 9: Graphical representation of evaluation measures.

#### 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. Here is an example of how to sort by column.

Algorithm	Distance	Clusters	Dataset	tE	entropy	dunn	tI	tEAttr	enAttr	duAttr	tIAttr
gmm	gmm_euclidean	3	dataframe	0.0780	0.0000	0.1096	0.0040	3	1	5	1
gmm	gmm_manhattan	3	dataframe	0.0342	0.0000	0.1151	0.0026	4	1	5	2
gmm	gmm_euclidean	3	dataframe	0.0428	0.0032	0.1096	0.0015	4	5	4	2
gmm	gmm_manhattan	3	dataframe	0.0319	0.0032	0.1151	0.0020	1	5	4	5
gmm	gmm_euclidean	3	dataframe	0.0323	0.0064	0.1096	0.0010	2	3	3	4
gmm	gmm_manhattan	3	dataframe	0.0131	0.0064	0.1151	0.0013	3	3	3	1
gmm	gmm_euclidean	3	dataframe	0.0159	0.2120	0.1096	0.0008	1	4	2	3
gmm	gmm_manhattan	3	dataframe	0.0088	0.2201	0.1151	0.0009	2	4	2	4
gmm	gmm_euclidean	3	dataframe	0.0146	0.2374	0.1096	0.0005	5	2	1	5
gmm	gmm_manhattan	3	dataframe	0.0067	0.2498	0.1151	0.0008	5	2	1	3

**Table 8:** Sort results by entropy 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]. Example of filtering:

```
> result[entropy > 0.11 & dunn > 0.11 & entropyAttr == 2]
```

Algorithm	Distance	Clusters	Dataset	tE	entropy	dunn	tI	tEAttr	enAttr	duAttr	tIAttr
gmm	gmm_manhattan	3	dataframe	0.0067	0.2498	0.1151	0.0008	5	2	1	3

**Table 9:** Filtering information by different criteria.

- Clustering::export\_file\_external(): exports the results of the clustering object to latex format This method is very useful when working with documents in latex format.
- 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:

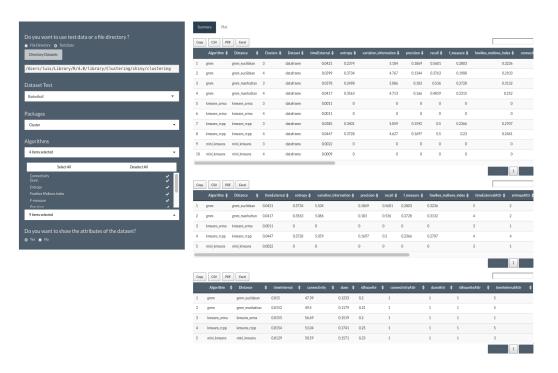
> Clustering::appClustering()

The execution will open our default browser with the interface. As it can be observed in the Figure 10, 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.

The operation of the application is very simple as can be seen in the Figure 11 and we will proceed to explain it step by step.

As you can see in the Figure 11 we have two well differentiated parts:

- 1. In this section we can find the different parameters used by the clustering function 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.



**Figure 10:** Clustering app user interface.

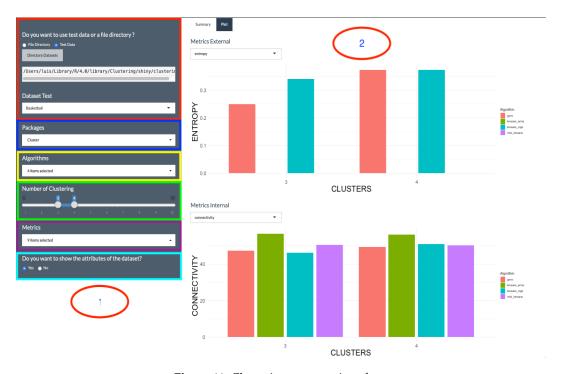


Figure 11: Clustering app user interface.

- 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 to show the attributes of the dataset that corresponds to the values indicated in each of the metrics.
- 2. In main layout we have the options to represent the data.
  - To view the data in graphical mode as shown in the Figure 12, 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.

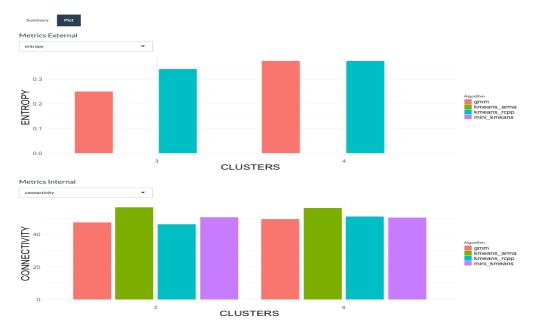


Figure 12: Tab with graphical representation of metrics.

• If we click on the summary tab as shown in the Figure 13, we can see the data represented in tables. If you wish you can export the results in the following formats: csv, pdf and xls. We also have the option of copying the data.

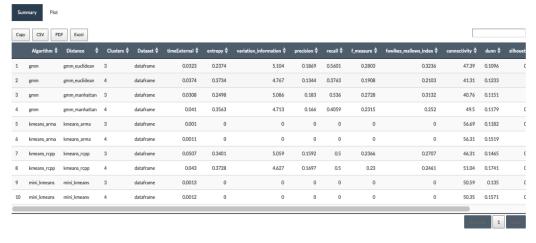


Figure 13: Clustering package execution summary tab.

# 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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