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Performance Evaluation of Some Clustering Algorithms under Different Validity Indices

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ABSTRACT

Clustering, a pivotal technique in statistics, enables the summarisation of data sets through the identification of related object groups. A prevalent question in clustering literature pertains to the precise number of partitions present within a data set. An array of clustering methods and indices has been proposed to discern the optimal number of clusters within a data set, each following its own set of rules. However, none of these methods universally excel in capturing the true components across all types of data structures. Particularly, they tend to grapple with uniquely shaped data sets or instances where objects from different groups are in close proximity. In this study, the performance of several clustering methods (Single Linkage, Complete Linkage, Average Linkage, Centroid Linkage, Ward.2D Linkage, Median Linkage) is evaluated in conjunction with different internal validity indices (KL, CH, Sil, Gap). This evaluation utilises simulated data, encompassing varied models, sample sizes, and distance measures, and is conducted using R software 3.1. Furthermore, several external indices (Rand, F-M, Purity) are employed to ascertain the degree of agreement between the true clusters of data points and the partitions computed through the clustering methods.

1. INTRODUCTION

Clustering is a common technique in statistics, which is addressed in many disciplines such as image analysis [1], machine learning [2], bioinformatics [3], pattern recognition [4], and data mining [5]. There are many available algorithms which attempt to select the optimal number of clusters in terms of their own rules; however, with a high performance no one capture the true clusters of all types of data structure [6]. In other words, clustering is the process of grouping items into groups (clusters) such that objects in the same cluster are more similar than those in other clusters. One of the well-known clustering algorithms is called hierarchical clustering which is a common methodology in statistics (more details can be found in studies [7] and [8]. There are two different hierarchical clustering approaches: agglomerative and divisive hierarchical methods. Our main interest in this paper is the agglomerative hierarchical method, which starts with the distance matrix and each object being in a separate cluster, then in each agglomeration step, we merge the closest clusters. Our goal is to select the clustering algorithms which have the ability to capture the true clusters with high performance under different models and different sample sizes, where this technique could use to evaluate the performance of the new suggested approaches. Therefore, in this paper, different models and different distance measures are used to evaluate the performance of some clustering methods (single linkage, complete linkage, average linkage, centroid linkage, ward.2D linkage, median linkage) under different validity indices (KL, CH, Sil, Gap), different simulated data and different sample sizes using R software 3.1. Also, some external indices (Rand, F-M, Purity) will be used to get the rate of agreement between the true clusters of the data points and the partitions that we have computed using clustering methods. The results of all models show that the clustering method average linkage results with CH index match the true clusters about more that 90% with different distance measure and different sample sizes. There are three main possible linkage procedures in hierarchical clustering which are: single linkage (closest neighbour), complete linkage (furthest-neighbour) and average linkage. When we merge two clusters, we have to update the distance matrix depending on the choice of linkage method. For example, suppose we have a data set, $\{x_1, x_2 \ldots x_5\}$, and assume the distance between the observations x_2 and x_4, d_{24}, is the smallest. Thus, x_2 and x_4 are merged together in the first agglomeration step, and we denote this new cluster with x_6 [9]. The distance between x_6 and x_1 is

$$d_{61} = \min\{d_{21}, d_{41}\} \tag{1}$$

and in the same way distances between the new cluster and other data points are updated. If we use the complete linkage or average linkage, the distance between x_6 and x_1 will be calculated respectively as follows [10]:

$$d_{61} = \max\{d_{21}, d_{41}\} \text{ or } \frac{1}{2}(d_{21} + d_{41}) \tag{2}$$

Simulated Data: For illustrative purposes, two-component data from $N(\mu, \sigma 2)$ in R_2 is generated and shown in Table 1, where each component includes three observations. The tree for the simulated data is hierarchically build using Euclidean distances with average linkage, where the Euclidean distance is given by:

$$d(x,y) = \sqrt{\sum_{j=1}^{d}(x_j - y_j)^2} \qquad (3)$$

The Euclidean distance matrix for the simulated data in Table 1 is computed and is shown in Table 2, and objects is clustered hierarchically using the stats package (R Core Team, 2017) in R. The dendrogram corresponding to the generated data is given in Figure 1. Blue labels for the internal nodes represent the agglomeration order, and internal nodes are labelled starting from n + 1, where n is the number of objects in the data, so n = 9, and the possible clustering schemes for this dendrogram are given in Table 3.

Table 1. Generated data from $N(\mu, \sigma^2)$ in R^2

Index	Component	1st Dimension	2nd Dimension
1	1	0.356	1.637
2	1	0.826	1.912
3	1	0.739	0.244
4	2	3.138	3.343
5	2	2.049	1.721
6	2	2.163	0.726
7	3	3.998	5.403
8	3	4.911	4.971
9	3	6.320	4.213

Table 2. Euclidean distance matrix for the generated data in Table 1

	1	2	3	4	5	6	7	8
2	0.545							
3	1.444	1.670						
4	3.264	2.719	3.919					
5	1.695	1.238	1.974	1.954				
6	2.024	1.787	1.503	2.793	1.002			
7	5.239	4.717	6.102	2.232	4.166	5.024		
8	5.645	5.103	6.304	2.407	4.330	5.057	1010	
9	6.497	5.956	6.848	3.299	4.945	5.426	2.609	1.6

Table 3. Clustering scheme for the data in Table 1

q	D_j where $j \in \{1, 2, \ldots, q\}$
1	{1,2,3,4,5,6,7,8,9}
2	{1,2,3,5,6}, {4,7,8,9}
3	{1,2,3,5,6},{4}, {7,8,9}
4	{1,2,3,5,6},{4}, {7,8},{9}
5	{1,2,3},{4}, {5,6}, {7,8},{9}
6	{1,2},{3},{4}, {5,6}, {7,8},{9}
7	{1,2},{3},{4},{5},{6},{7},{8},{9}
8	{1},{2},{3},{4},{5},{6},{7},{8},{9}

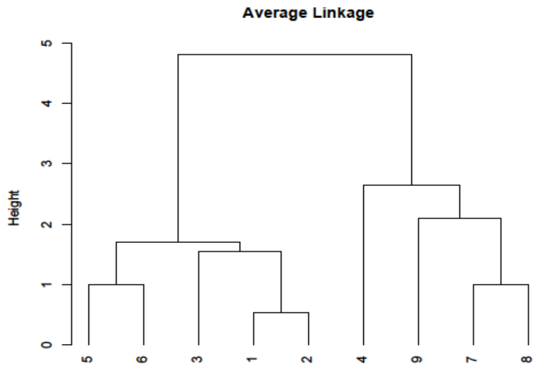


Figure 1. The dendrogram of the data in Table 1

After a dendrogram is building, it is not easy to know where to cut the tree in order to determine how many clusters we have. Thus, we need some algorithms which help us to select a partition represents the data better. To address this question, in the literature some indices which is called internal cluster validity indices are proposed. In the next section, we will discuss these indices in detail.

2. CLUSTER VALIDITY INDICES

Cluster validity indices can be divided into two types: internal indices and external scores. Internal indices are used to choose the best partitioning after applying the clustering algorithm. While, the external scores can be used to measure the agreement between the true partition and the results of clustering if the true partition of the data is known [11]. In the following sections we will discuss these indices in detail.

2.1 Internal indices

In the literature, there are many internal indices, so we pick four different internal indices from the most commonly referenced indices: Calinski and Harabasz index (CH index) [12], Silhouette index (Sil index) [13], Krzanowski and Lai index (KL index) [14] and Gap index [15]. All these internal indices are available in the NbClust package [16] in R. Internal index calculations are based on two quantities which are between-cluster sum of squares (BSS) and within-cluster sum of squares (WSS). So, we have to define BSS and WSS with some notation which are used in the discussion of various indices. We define:

- Data points, xi, $i = 1, 2, \ldots, m$, where $x_i \in R^p$.
- Number of objects, m.
- Mean of all objects, $\overline{x}$.
- Number of clusters, q.
- Number of variables, p.
- Cluster j, C_j, $j = 1, 2, \ldots, q$.
- Number of elements in cluster C_j, m_j.
- The distance between x_i and $x_{i'}$ data points, $d(x_i, x_i')$, $i, i' \in \{1, 2, \ldots, m\}$.
- The centroid of the cluster C_j which is defined by

$$c_j = \frac{1}{m_j} \sum_{i \in C_j} x_i \qquad (4)$$

Depending on the above notations, BSS and WSS are defined by the following equations:

$$BSS(q) = \sum_{j=1}^{q} m_j (c_j - \overline{x})(c_j - \overline{x})^T \qquad (5)$$

$$WSS(q) = \sum_{j=1}^{q} \sum_{i \in C_j} (x_j - c_j)(x_j - c_j)^T \qquad (6)$$

- **CH Index**

The CH index (Calinski and Harabasz index) was proposed in the study [12] and this index is defined by:

$$CHI(q) = \frac{tr(BSS(q)/(q-1)}{tr(WSS(q)/(m-q)}, q > 1 \qquad (7)$$

If we cluster the similar objects together, BSS(q) will be high, and WSS(q) will be small and we can take the proportion of BSS(q) and WSS(q). Then, the optimal number of clusters is the value of q which maximizes CHI, because CHI will take the maximum value when large distances will be occur between clusters.

- **KL Index**

The KL index (Krzanowski and Lai index) was suggested in the study [15] and this index is given by:

$$KLI(q) = \left|\frac{DIFF(q)}{DIFF(q+1)}\right|, q \geq 2 \tag{8}$$

where, DIFF(q) = (q − 1)$^{2/p}$ tr (WSS(q−1)) − q$^{2/p}$ tr (WSS(q)). The optimal number of clusters will be the value of q which maximizes KLI(q).

- **Silhouette Index**

Silhouette index (Sil Index) is introduced [13], this index is defined by:

$$Sil(q) = \frac{1}{m}\sum_{i=1}^{m} S(i), Sil \in [-1,1], q \neq 1 \tag{9}$$

where,

$$S(i) = \frac{b(i) - a(i)}{max\{\, a(i), b(i)\}},$$
$$a(i) = \frac{1}{n_j - 1}\sum_{r \in C_j} d(x_i\,, x_r)$$
$$b(i) = min_{s \neq r}\{\, d(x_i, x_r)\}$$

Here, $a(i)$ represents the average of the distance between the ith point and other points in the same cluster. While $b(i)$ represents the average of the distance between the ith point and the points from the nearest cluster. The optimal number of clusters in the data will be equal to the maximum value of the index.

- **Gap Index**

The Gap index was proposed [15]. It computes using the following equation:

$$Gap_m(q) = E_m^*(\log(WSS(q))) - \log(WSS(q)) \tag{10}$$

where, $E_m^*(log(WSS(q)))$ is the expectation of a sample which is generated from the reference distribution. We can summarise how to compute the Gap index as follows:

- For each clustering scheme, WSS(q) is computed, where q∈ $\{1, \dots, (n-1)\}$.
- Generate B reference data sets. Each data set is clustered, then for each possible partitioning.

WSS_b^* is calculated where b∈{1,...,B}. After that, we can calculate the Gap statistic, given in Eq. (10).

- Compute the standard deviation of log(WSS_b^*),b=1,…,B, which is defined by:

$$sd_q = \left[\tfrac{1}{B}\textstyle\sum_{b\in\{1,\dots,B\}}\left[log(\,WSS * (q)) - \textstyle\sum_{b\in\{1,\dots,B\}} log(\,WSS_b^*(q))\right]^2\right]^{(1/2)}$$

- Choose the smallest q, which represents the optimal number of clusters, such that $Gap(k) \geq Gap(k+1) - s_{q+1}$, where, $s_q = sd_q\sqrt{1 + 1/B}$

2.2 External scores

In order to evaluate the performance of the internal indices, which have been illustrated above, we pick the following external scores: Rand index [17] which is available in the mclust package, FM index, and Purity index [18] which is available in the IntNMF package [19].

- **Rand Index**

The Rand measure, which is suggested [17] is a measure of the agreement between two partitions. Let $P^{(1)} = \{C_1^{(1)}, \dots, C_u^{(1)}\}$ and $P^{(2)} = \{C_1^{(2)}, \dots, C_u^{(2)}\}$ be two partitions where n$_{ij}$ represents the number of observations allocated in the cluster $C_i^{(1)}$ in P$^{(1)}$ and to cluster $C_j^{(2)}$ in P$^{(2)}$ (see Table 4), then the Rand index is defined by the following formula:

$$RI = \frac{\binom{m}{2} + \sum_{i,j} n_{ij}^2 - \frac{1}{2}(\sum_{i=1}^{u} n_i^2 + \sum_{j=1}^{v} n_j^2}{\binom{m}{2}}, RI \in [0,1]$$

As we can see RI 2 [0; 1], the value 0 indicates that the two data clustering do not agree on any pair of points, while the value 1 indicates that the two parathions are exactly the same.

Table 4. The general form of contingency table between two partitions $P^{(1)} = \{C_1^{(1)}, \dots, C_u^{1}\}$ and $P^{(2)} = \{C_1^{(2)}, \dots, C_v^{(2)}\}$

		$P^{(2)}$				sums
		$C_1^{(2)}$	$C_2^{(2)}$	....	$C_v^{(2)}$	
	$C_1^{(1)}$	n_{11}	n_{12}	....	n_{1v}	$n_{1.}$
	$C_2^{(1)}$	n_{21}	n_{22}	....	n_{2v}	$n_{2.}$
$P^{(1)}$	.	.. …..				
	.	.. …..				
	.	.. …..				
	$C_u^{(1)}$	n_{u1}	n_{u2}	....	n_{uv}	$n_{u.}$
Sums		$n_{.1}$	$n_{.2}$	....	$n_{.v}$	

- **Fowlkes and Mallows Index (FMI)**

This index was introduced [20] as an external score to check the similarity between two partitions of a data points, and this index is defined by:

$$FMI = \frac{T_k}{\sqrt{P_k Q_K}}, FMI \in [0,1]$$

where,

$$T_k = \textstyle\sum_{i=1}^{u}\sum_{j=1}^{v} n_{ij}^2 - m, P_k \sum_{i=1}^{u}(\sum_{j=1}^{v} n_{ij})^2 - m, Q_k = \sum_{j=1}^{v}(\sum_{i=1}^{u} n_{ij})^2 - m.$$

- **Purity Index**

The purity index [18] takes the average purity for each cluster C_i from the same partition, C_j, and the maximum number of elements clustered together will be defined as purity. Hence, the purity measure is defined by:

$$PUI = \frac{1}{m}\sum_{i=1}^{u}\max_j \left|C_i^{(1)} \cap C_j^{(2)}\right|_j \tag{11}$$

where, PUI $\in$ [-1, 1], if PUI is close to one, this means the similarity between the clustering and the true clusters is high.

3. PERFORMANCE EVALUATION

In this section, we evaluate the performance of some linkage clustering methods (single, complete, average, centroid, ward.2D, median) with different internal validity indices (KL, CH, Sil, Gap) using simulated data with different models, different sample sizes, and different distance measures (Euclidean and Manhattan) using R software 3.1. The purpose of the suggested algorithm is three folds. First, which clustering algorithm able to detect the true clusters. Second, which internal validity index is able to cut the tree correctly to get the true number of clusters. Third, which external validity measure is able to get the high agreement between the results of clustering methods and the true clusters. For

this purpose, we generate groups of data from various models with different parameters and we measure the performance of clustering algorithms with the data that we have generated. We consider different models in which each of the above varies:

1. Model 1: five groups of size 100 observations are generated from:

$$N_2\left(\mu_i, \sum\right), i = 1, 2, \dots, 5$$

where,

$$\mu_i \in \left\{\begin{bmatrix}0.25\\0.25\end{bmatrix}, \begin{bmatrix}4.5\\4.5\end{bmatrix}, \begin{bmatrix}7\\7\end{bmatrix}, \begin{bmatrix}11\\11\end{bmatrix}, \begin{bmatrix}15\\15\end{bmatrix}\right\}, \sum = \begin{bmatrix}1.25 & 0\\0 & 1.25\end{bmatrix}$$

2. Model 2: nine groups are generated from:

$$N_2(\mu_i, \textstyle\sum_i), i = 1, 2, \dots., 9$$

where,

$$\mu_i \in \left\{\begin{bmatrix}-2\\0\end{bmatrix}, \begin{bmatrix}2\\0\end{bmatrix}, \begin{bmatrix}4\\2\end{bmatrix}, \begin{bmatrix}0\\1\end{bmatrix}, \begin{bmatrix}-3\\2\end{bmatrix}, \begin{bmatrix}0\\4\end{bmatrix}\begin{bmatrix}4\\-2\end{bmatrix}, \begin{bmatrix}0\\-3\end{bmatrix}, \begin{bmatrix}-3\\3\end{bmatrix}\right\}$$

and

$$\textstyle\sum_i \in \left\{\begin{bmatrix}0.25 & 0\\0 & 0.25\end{bmatrix}, \begin{bmatrix}0.5 & 0\\0 & 0.5\end{bmatrix}, \begin{bmatrix}0.7 & 0\\0 & 0.7\end{bmatrix}, \begin{bmatrix}0.1 & 0\\0 & 0.1\end{bmatrix}, \begin{bmatrix}0.6 & 0\\0 & 0.6\end{bmatrix}, \begin{bmatrix}0.3 & 0\\0 & 0.3\end{bmatrix}, \begin{bmatrix}0.4 & 0\\0 & 0.4\end{bmatrix}, \begin{bmatrix}0.2 & 0\\0 & 0.2\end{bmatrix}\right\}$$

3. Model 3: eight groups of size 60 observations are generated from $N_2(\mu_i, \sum_i), i = 1, \dots, 8$

where,

$$\mu_i \in \left\{\begin{bmatrix}8\\8\end{bmatrix}, \begin{bmatrix}3\\8\end{bmatrix}, \begin{bmatrix}8\\2\end{bmatrix}, \begin{bmatrix}2\\2\end{bmatrix}, \begin{bmatrix}2\\5\end{bmatrix}, \begin{bmatrix}5\\2\end{bmatrix}\begin{bmatrix}5\\5\end{bmatrix}, \begin{bmatrix}8\\5\end{bmatrix}\right\},$$

and

$$\textstyle\sum_i \in \left\{\begin{bmatrix}0.75 & 0\\0 & 0.75\end{bmatrix}, \begin{bmatrix}0.6 & 0\\0 & 0.6\end{bmatrix}, \begin{bmatrix}0.8 & 0\\0 & 0.8\end{bmatrix}, \begin{bmatrix}0.4 & 0\\0 & 0.4\end{bmatrix}, \begin{bmatrix}0.2 & 0\\0 & 0.2\end{bmatrix}, \begin{bmatrix}0.5 & 0\\0 & 0.5\end{bmatrix}, \begin{bmatrix}0.9 & 0\\0 & 0.9\end{bmatrix}, \begin{bmatrix}0.25 & 0\\0 & 0.25\end{bmatrix}\right\}$$

4. Model 4: ten groups are generated from $N_2(\mu_i, \sum), i = 1, \dots., 10$ with sizes which are 40 for groups $\{G_i, i = 1, \dots., 5\}$ and 55 for groups $\{G_i, i = 6, \dots., 10\}$, where, $\mu_i \in \left\{\begin{bmatrix}2\\12\end{bmatrix}, \begin{bmatrix}12\\8\end{bmatrix}, \begin{bmatrix}6\\6\end{bmatrix}, \begin{bmatrix}13\\3\end{bmatrix}, \begin{bmatrix}4\\3\end{bmatrix}, \begin{bmatrix}7\\3\end{bmatrix}\begin{bmatrix}2\\8\end{bmatrix}, \begin{bmatrix}12\\13\end{bmatrix}, \begin{bmatrix}1\\3\end{bmatrix}, \begin{bmatrix}7\\11\end{bmatrix}\right\}$, and $\sum \in \left\{\begin{bmatrix}0.75 & 0\\0 & 0.75\end{bmatrix}\right\}$.

We evaluate the performance of some clustering methods and some validity indices using the following algorithm.

Algorithm 1

1. Generate data points {(x_1, y_1); (x_2, y_2), …, (x_m, y_m)} from different models $N_2(\mu_i, \sum_i)$ as described above, where these data points consist of k true clusters.

2. Calculate the distance matrices, M_1 and M_2, between these observations using Euclidean distance and Manhattan distance which are defined by:

$$d((x_i, y_i), (y_j, y_j)) = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} \qquad (12)$$

$$d((x_i, y_i), (y_j, y_j)) = \left|x_i - x_j\right| + \left|y_i - y_j\right|, i = 1, \dots, m; j = 1, \dots, m \qquad (13)$$

3. Build the tree for the data points using some distance-based clustering methods (single linkage, complete linkage, average linkage, centroid, ward.2D, median) with distance matrices M_1 and M_2.

4. Use internal validity indices (KL, CH, Sil, Gap) to get the optimal number of clusters, q.

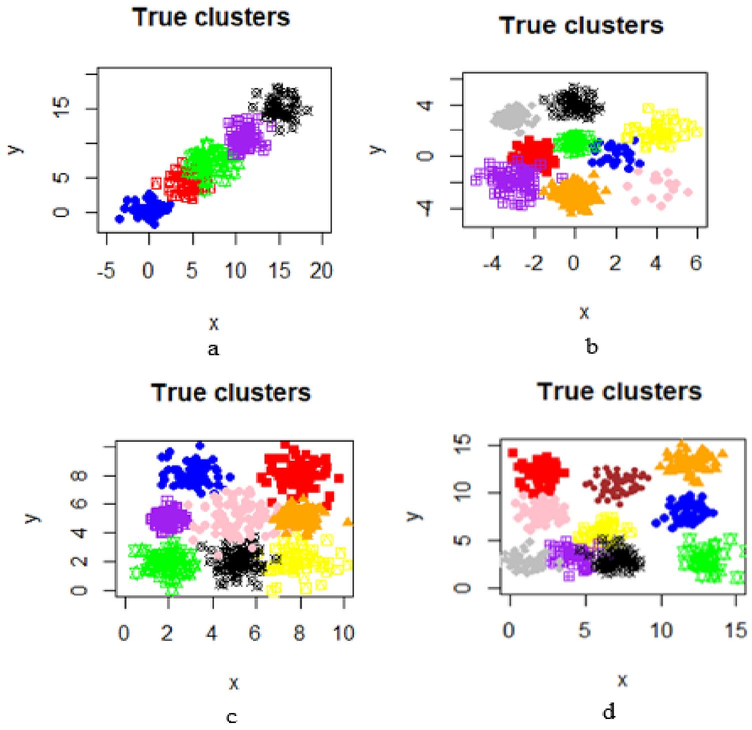
5. Use external validity indices (Rand, FM, Purity) to get the agreement between the true clusters and the partitions that we have computer from step (4).

The results of Algorithm 1 are presented in the next section.

4. RESULTS

The results of the simulation are presented in Tables 5 to 12 and Figures 2 to 5. Figure 2 shows the true clusters for the models (Model 1, _ve groups), (Model 2, nine groups), (Model 3, eight groups), (Model 4, ten groups). Tables 5, 7, 9, 11 show the number of clusters for the simulated models by using some clustering methods with some indices, while Tables 6, 8, 10, 12 illustrate the rate of agreement between the true clusters and the results of the clustering methods with internal similarity indices using some external indices (Rand, F-M, Purity). In these results we can see the following:

- The results of clustering method (single linkage) with all internal indices (KL, CH, Sil, Gap) and different distance measure doesn't match the true clusters.
- The results of average linkage and ward. D2 clustering methods with CH index match the true clusters under different distance measure (Euclidean and Manhattan) and different models.
- In Model 1, we can see that the Median clustering method with Euclidean distance match the true clusters with three indices (KL, CH, Gap).
- In Model 2, we notice that the complete linkage clustering method with different distance measure (Euclidean and Manhattan) match the true clustering with CH index.



a

b

c

d

Figure 2. (a) True clusters for (Model 1, number of clusters is 5); (b) True clusters for (Model 2, number of clusters is 9); (c) True clusters for (Model 3, number of clusters is 8); (d) True clusters for (Model 4, number of clusters is 10)

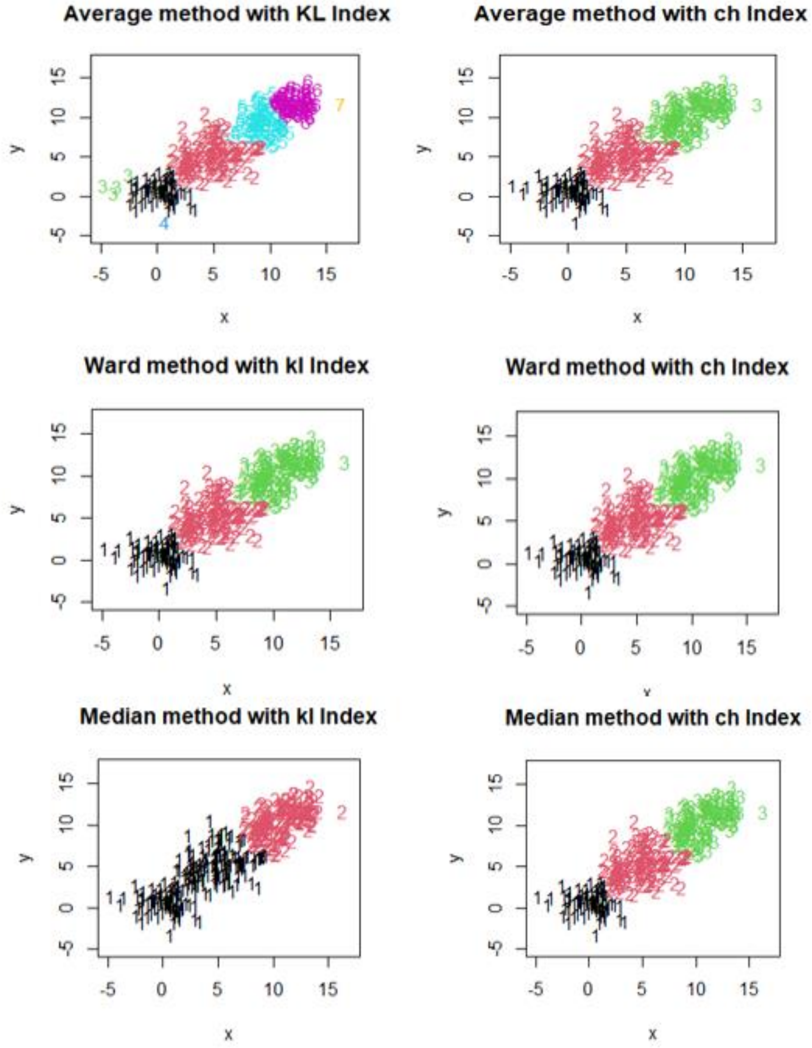
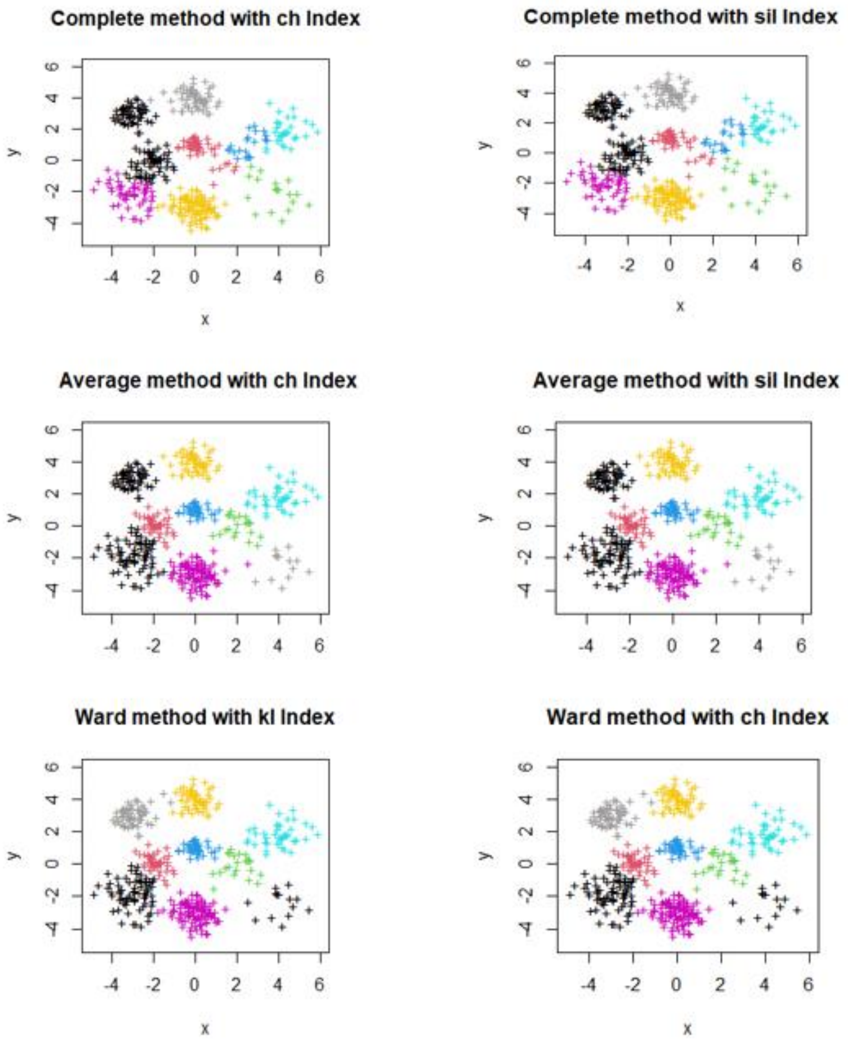


Figure 3. Clustering methods (average, ward.D2, median) with some internal indices (KL, CH)



Complete method with ch Index

Complete method with sil Index

Average method with ch Index

Average method with sil Index

Ward method with kl Index

Ward method with ch Index

Figure 4. Clustering methods (complete, average, Ward.D2) with some internal indices (KL, CH, Sil)

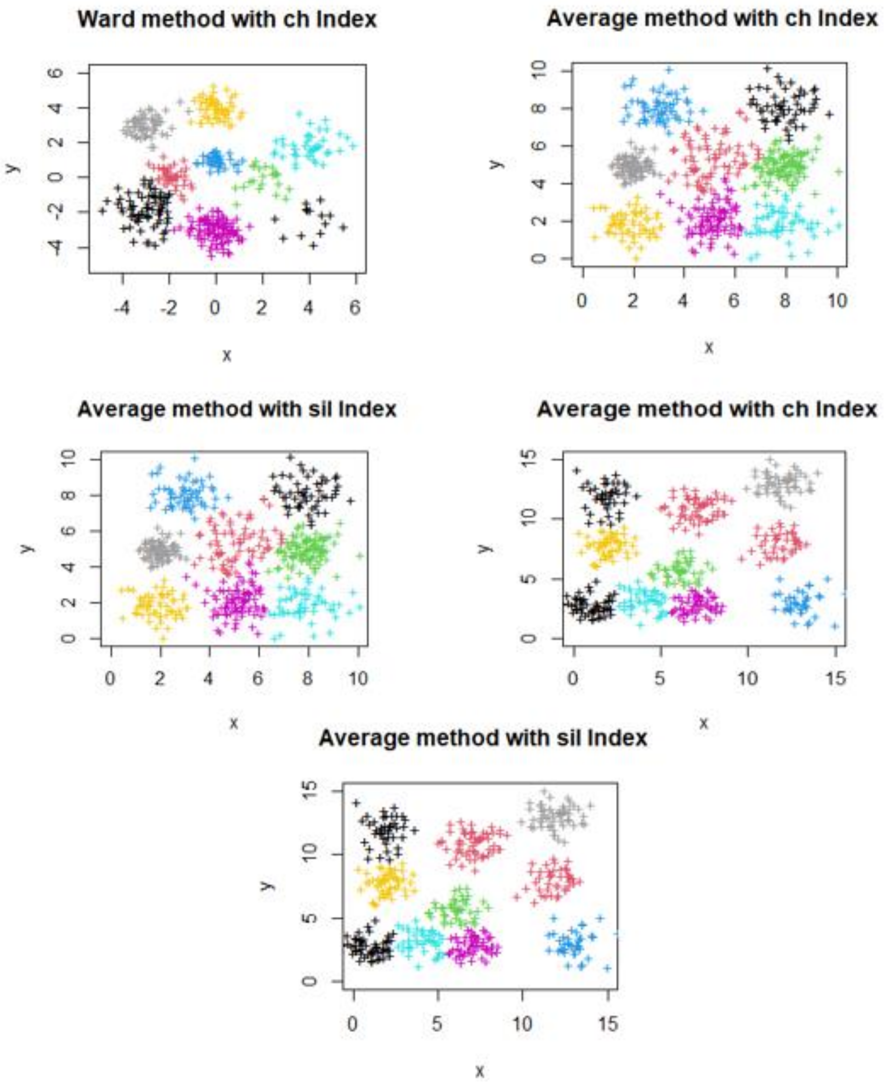
Table 5. Number of clusters for data points (Model 1) using clustering methods with internal indices and two types of distance measures (Euclidean and Manhattan)

	Euclidean Distance				**Manhattan Distance**			
	KL	CH	Sil	Gap	KL	CH	Sil	Gap
Single	8	8	2	2	6	6	2	2
Complete	4	4	2	2	4	4	2	2
Average	4	5	2	2	4	5	4	2
Centroid	2	4	2	2	8	4	2	2
Ward.D2	4	5	2	4	4	5	2	4
Median	5	5	3	5	7	7	4	7

Table 6. The rate of agreement between the true clusters and the partitions that we have computed for (Model 1) using external similarity indices under Euclidean distance and Manhattan distance

	Euclidean Distance			**Manhattan Distance**		
Clustering methods	Rand	F-M	Purity	Rand	F-M	Purity
Single, KL	0.759	0.646	0.608	0.529	0.527	0.416
Single, CH	0.759	0.646	0.608	0.529	0.527	0.416
Single, Sil	0.201	0.441	0.204	0.201	0.441	0.204
Single, Gap	0.201	0.441	0.204	0201	0.441	0.204
Complete, KL	0.899	0.791	0.776	0.886	0.767	0.760
Complete, CH	0.899	0.791	0.776	0.886	0.767	0.760
Complete, Sil	0.672	0.601	0.400	0.672	0.601	0.400
Complete, Gap	0.672	0.601	0.400	0.672	0.601	0.400
Average, KL	0.907	0.813	0.792	0.894	0.775	0.792
Average, CH	0.944	0.859	0.920	0.918	0.809	0.856
Average, Sil	0.672	0.601	0.400	0.894	0.775	0.792
Average, Gap	0.672	0.601	0.400	0.511	0.529	0.396

Centroid, KL	0.672	0.601	0.400	0.917	0.800	0.864
Centroid, CH	0.906	0.808	0.788	0.899	0.803	0.780
Centroid, Sil	0.672	0.601	0.400	0.664	0.599	0.400
Centroid, Gap	0.672	0.601	0.400	0.664	0.599	0.400
Ward.D2, KL	0.910	0.819	0.796	0.910	0.819	0.796
Ward.D2, CH	0.949	0.872	0.928	0.947	0.867	0.924
Ward.D2, Sil	0.672	0.601	0.400	0.672	0.601	0.400
Ward.D2, Gap	0.910	0.819	0.796	0.910	0.819	0.796
Median, KL	0.908	0.818	0.792	0.865	0.690	0.772
Median, CH	0.908	0.818	0.792	0.865	0.690	0.772
Median, Sil	0.759	0.661	0.600	0.755	0.642	0.596
Median, Gap	0.908	0.818	0.792	0.865	0.690	0.772



Ward method with ch Index

Average method with ch Index

Average method with sil Index

Average method with ch Index

Average method with sil Index

Figure 5. Clustering methods (average, ward.D2, median) with some internal indices (CH, Sil) .These methods show an equality between the number of clusters and the number of true clusters

Table 7. Number of clusters for data points (Model 2) using clustering methods with internal indices and two types of distance measures (Euclidean and Manhattan)

	Euclidean Distance				**Manhattan Distance**			
	KL	CH	Sil	Gap	KL	CH	Sil	Gap
Single	12	12	12	2	4	7	7	2
Complete	12	9	9	3	9	8	8	2
Average	10	9	9	2	10	9	9	2
Centroid	7	10	7	2	7	8	7	2
Ward.D2	9	9	9	2	9	9	9	2
Median	12	12	12	12	6	7	8	6

Table 8. The rate of agreement between the true clusters and the partitions that we have computed for (Model 2) using external similarity indices under Euclidean distance and Manhattan distance

	Euclidean Distance			**Manhattan Distance**		
Clustering methods	Rand	F-M	Purity	Rand	F-M	Purity
Single, KL	0.710	0.556	0.604	0.198	0.377	0.258
Single, CH	0.710	0.556	0.604	0.598	0.498	0.516
Single, Sil	0.710	0.556	0.604	0.598	0.498	0.516
Single, Gap	0.138	0.367	0.226	0138	0.367	0.226
Complete, KL	0.958	0.837	0.914	0.973	0.906	0.910
Complete, CH	0.972	0.896	0.914	0.974	0.907	0.910
Complete, Sil	0.972	0.896	0.914	0.974	0.907	0.910
Complete, Gap	0.767	0.602	0.447	0.363	0.415	0.314
Average, KL	0.981	0.932	0.959	0.979	0.922	0.955
Average, CH	0.982	0.936	0.959	0.981	0.932	0.955
Average, Sil	0.982	0.936	0.959	0.981	0.932	0.955
Average, Gap	0.413	0.429	0.314	0.416	0.430	0.314
Centroid, KL	0.952	0.856	0.822	0.951	0.850	0.817
Centroid, CH	0.986	0.950	0.968	0.957	0.865	0.862
Centroid, Sil	0.952	0.856	0.822	0.951	0.850	0.817
Centroid, Gap	0.350	0.413	0.314	0.195	0.378	0.256
Ward.D2, KL	0.980	0.928	0.955	0.982	0.935	0.957
Ward.D2, CH	0.980	0.928	0.955	0.982	0.935	0.957
Ward.D2, Sil	0.980	0.928	0.955	0.982	0.935	0.957
Ward.D2, Gap	0.632	0.515	0.357	0.632	0.515	0.357
Median, KL	0.959	0.850	0.928	0.875	0.680	0.635
Median, CH	0.959	0.850	0.928	0.901	0.722	0.714
Median, Sil	0.959	0.850	0.928	0.904	0.726	0.746
Median, Gap	0.959	0.850	0.928	0.875	0.680	0.635

Table 9. Number of clusters for data points (Model 3) using clustering methods with internal indices and two types of distance measures (Euclidean and Manhattan)

	Euclidean Distance				**Manhattan Distance**			
	KL	CH	Sil	Gap	KL	CH	Sil	Gap
Single	9	9	2	2	5	6	2	2
Complete	4	8	8	2	10	8	8	2
Average	4	8	8	2	12	8	8	2
Centroid	5	9	9	2	4	10	10	2
Ward.D2	8	10	8	2	8	8	8	2
Median	2	7	7	2	3	10	10	2

Table 10. The rate of agreement between the true clusters and the partitions that we have computed for (Model 3) using external similarity indices under Euclidean distance and Manhattan distance

	Euclidean Distance			**Manhattan Distance**		
Clustering methods	Rand	F-M	Purity	Rand	F-M	Purity
Single, KL	0.150	0.350	0.158	0.136	0.352	0.150
Single, CH	0.339	0.390	0.266	0.327	0.392	0.257
Single, Sil	0.128	0.354	0.144	0.128	0.354	0.144
Single, Gap	0.128	0.354	0.144	0128	0.354	0.144
Complete, KL	0.810	0.584	0.514	0.961	0.839	0.935
Complete, CH	0.942	0.784	0.880	0.967	0.873	0.935
Complete, Sil	0.942	0.784	0.880	0.967	0.873	0.935
Complete, Gap	0.583	0.452	0.286	0.613	0.475	0.285
Average, KL	0.821	0.621	0.530	0.966	0.866	0.941
Average, CH	0.968	0.876	0.937	0.968	0.875	0.937
Average, Sil	0.968	0.876	0.937	0.968	0.875	0.937
Average, Gap	0.582	0.476	0.285	0.582	0.469	0.285
Centroid, KL	0.736	0.546	0.483	0.739	0.552	0.485
Centroid, CH	0.960	0.844	0.921	0.936	0.854	0.926
Centroid, Sil	0.960	0.844	0.921	0.963	0.854	0.926
Centroid, Gap	0.128	0.354	0.144	0.305	0.386	0.242
Ward.D2, KL	0.940	0.776	0.878	0.959	0.844	0.919
Ward.D2, CH	0.945	0.768	0.885	0.959	0.844	0.919
Ward.D2, Sil	0.940	0.776	0.878	0.959	0.844	0.919
Ward.D2, Gap	0.527	0.428	0.285	0.607	0.467	0.285
Median, KL	0.317	0.394	0.250	0.248	0.355	0.214
Median, CH	0.860	0.610	0.648	0.835	0.551	0.676
Median, Sil	0.860	0.610	0.648	0.853	0.551	0.676
Median, Gap	0.317	0.394	0.250	0.248	0.355	0.214

Table 11. Number of clusters for data points (Model 4) using clustering methods with internal indices and two types of distance measures (Euclidean and Manhattan)

	Euclidean Distance				**Manhattan Distance**			
	KL	CH	Sil	Gap	KL	CH	Sil	Gap
Single	6	8	8	2	3	2	2	4
Complete	4	10	8	2	4	10	8	2
Average	4	10	10	2	4	10	11	2
Centroid	4	12	8	2	4	8	8	3
Ward.D2	10	10	10	2	10	10	10	2
Median	4	11	6	4	9	7	7	9

Table 12. The rate of agreement between the true clusters and the partitions that we have computed for (Model 4) using external similarity indices under Euclidean distance and Manhattan distance

	Euclidean Distance			**Manhattan Distance**		
Clustering Methods	Rand	F-M	Purity	Rand	F-M	Purity
Single, KL	0.673	0.482	0.400	0.674	0.471	0.347
Single, CH	0.860	0.644	0.631	0.508	0.412	0.231
Single, Sil	0.860	0.644	0.631	0.508	0.412	0.231
Single, Gap	0.255	0.344	0.200	0.681	0.489	0.431
Complete, KL	0.795	0.573	0.431	0.795	0.573	0.431
Complete, CH	0.974	0.874	0.917	0.965	0.834	0.894
Complete, Sil	0.949	0.803	0.829	0.939	0.775	0.814
Complete, Gap	0.581	0.440	0.231	0.601	0.448	0.231
Average, KL	0.795	0.573	0.431	0.795	0.573	0.431
Average, CH	0.989	0.948	0.972	0.989	0.946	0.972
Average, Sil	0.989	0.948	0.972	0.989	0.946	0.972
Average, Gap	0.581	0.440	0.231	0.581	0.440	0.231
Centroid, KL	0.795	0.573	0.431	0.795	0.573	0.431
Centroid, CH	0.989	0.944	0.972	0.949	0.802	0.814
Centroid, Sil	0.941	0.790	0.823	0.949	0.802	0.814
Centroid, Gap	0.255	0.344	0.200	0.634	0.464	0.315
Ward.D2, KL	0.989	0.948	0.972	0.988	0.941	0.968
Ward.D2, CH	0.989	0.948	0.972	0.988	0.941	0.968
Ward.D2, Sil	0.989	0.948	0.972	0.988	0.941	0.968
Ward.D2, Gap	0.581	0.440	0.231	0.581	0.440	0.231
Median, KL	0.746	0.507	0.400	0.912	0.683	0.711
Median, CH	0.955	0.798	0.848	0.913	0.696	0.711
Median, Sil	0.812	0.565	0.600	0.913	0.696	0.711
Median, Gap	0.746	0.507	0.400	0.912	0.683	0.711

5. CONCLUSION AND FUTURE WORKS

5.1 Conclusion

Different models and different distance measures have been used in this paper to evaluate the performance of some clustering methods (single linkage, complete linkage, average inkage, centroid, ward.2D, median) under different validity indices (KL, CH, Sil, Gap), different simulated data with different sample sizes using R software 3.1. Also, some external indices (Rand, F-M, Purity) are used to get the rate of agreement between the true clusters of the data points and the partitions that we have computed using clustering methods. For the results we noticed the following:

- All models show that the clustering method, average linkage, with CH index match the true clusters about more that 90% with different distance measure and different sample sizes.
- Single linkage clustering results with all internal indices (KL, CH, Sil, Gap) and different distance measure doesn't match the true clusters.
- Under different distance measure (Euclidean and Manhattan) and different models the results of the clustering methods, average linkage and ward.D2, with CH index match the true clusters.
- Median clustering method with Euclidean distance match the true clusters with three indices (KL, CH, Gap), for Model 1.
- The complete linkage clustering method with different distance measure (Euclidean and Manhattan) match the true clustering with CH index, for Model 2. As a result, we recommend to use the average linkage clustering method with CH index for clustering data points, and we can use them for comparing with the new clustering technique.

5.2 Future works

In this study, we only evaluate the performance of some clustering methods with some indices under linear data only, but it will be also interesting to explore how these clustering methods and indices works under circular data. Also, in the future we look forward to construct a novel clustering method and evaluate the performance of the proposed clustering method with the average linkage method with CH index.

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