Revisiting Agglomerative Clustering

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Abstract

In data clustering, emphasis is often placed in finding groups of points. An equally important subject concerns the avoidance of false positives. As it could be expected, these two goals oppose one another, in the sense that emphasis on finding clusters tends to imply in higher probability of obtaining false positives. The present work addresses this problem considering some traditional agglomerative methods, namely single, average, median, complete, centroid and Ward’s applied to unimodal and bimodal datasets following uniform, gaussian, exponential and power-law distributions. More importantly, we adopt a generic model of clusters involving a higher density core surrounded by a transition zone, followed by a sparser set of outliers. Combined with preliminary specification of the size of the expected clusters, this model paved the way to the implementation of an objective means for identifying the clusters from dendrograms. In addition, the adopted model also allowed the relevance of the detected clusters to be estimated in terms of the height of the subtrees corresponding to the identified clusters. More specifically, the lower this height, the more compact and relevant the clusters tend to be. Several interesting results have been obtained, including the tendency of several of the considered methods to detect two clusters in unimodal data. The single-linkage method has been found to provide the best resilience to this tendency. In addition, several methods tended to detect clusters that do not correspond directly to the cores, therefore characterized by lower relevance. The possibility of identifying the type of distribution of points from the adopted measurements was also investigated.

1 Introduction

The organization of entities into categories represents an exceedingly important activity underlying much of the human experience, including science and
technology. Typically, the objects in the same category share several of their properties, while presenting features that are distinct to those of entities in other categories. By abstracting entities into categories, several interesting advantages can be obtained. First, we have a more compact representation, as it is no longer necessary to have a specific identifier for each entity. Being compact, categories can be easily and effectively communicated between individuals. The identification of categories also provides an indication of which of the involved features are more relevant. An additional benefit of defining categories is that they can provide insights about their interrelationship, especially in the case of subcategorization, implying a hierarchical structure.

The task of categorization, also called classification, can take place according to the two following main paradigms: (i) supervised classification, in which prototypes and samples of pre-defined categories are available and used for comparison with the entities to be classified; and (ii) unsupervised classification, or clustering, characterized by the absence of any previous knowledge about the number of properties of the categories, which have to be otherwise abstracted [1, 2]. Needless to say, the latter type of classification is more challenging, being also particularly important as it presupposes any supervised scheme.

Clustering is not an easy endeavour, as it depends on several factors such as the choice of the features to be considered as well as on the type of classification method to be adopted. Indeed, especially when the entities belonging to different categories are not markedly distinct, different choices of features and/or clustering methods can lead to substantially diverging results. These challenges have motivated the development of several clustering approaches, of which hierarchical methods have received special attention. Hierarchical clustering can proceed by successively dividing or agglomerating the original entities into groups and subgroups according to some criteria. As such, hierarchical methods provide valuable information about the interrelationship between categories.

Hierarchical clustering methods may construct the hierarchy in two opposite directions, bottom-up (agglomerative) and top-down (divisive). Despite similar in concept, they may eventually come up with different solutions [3, 4]. Divisive algorithms are more robust in the early stages compared to its counterpart and agglomerative clustering techniques, in turn, are more understandable and by far the most popular [6].

The choice of the agglomerating criterion defines the respective hierarchical clustering method. These criteria are typically based on distances between clusters, such as the single-linkage approach, which considers the smallest distance between the points in two clusters. However, it is also possible to consider the minimization of dispersion of the points inside each cluster as a criterion, which gives rise to methods such as Ward’s agglomerative clustering [7]. In the present work, we consider the following methods: single-linkage, complete-linkage, median, average, and Ward’s.

The coexistence of many methods for the same finality often motivates efforts aimed at identifying their respective relative performance concerning specific size and types of data, choice of features, number of categories, etc. Therefore,
it is not surprising that agglomerative hierarchical clustering methods have been studied comparatively (e.g. \cite{8, 9}). Very often, these methods are investigated concerning their potential to separate existing clusters.

While the identification of existing clusters is undoubtedly an important performance factor to be taken into account, other aspects should be considered. Of particular relevance concerns the resilience to false-positive identification of clusters. This is often critical because data devoid of clusters should not lead to any significant cluster, which could have important implications in several clustering applications.

The comparative evaluation of the performance of the adopted agglomerative hierarchical methods regarding their robustness to false-positive constitutes the main objective of the present work. In order to do so, we consider several types of clusterless point distributions – more specifically uniform, linear, exponential, normal, and power-law – as input to the adopted agglomerative hierarchical methods. A relevance parameter is also proposed, capable of quantifying the prominence of the detected clusters, which is used to investigate the robustness of the adopted methods when applied to the above indicated clusterless datasets. More specifically, it would be expected that these methods never, or rarely, detect two or more clusters.

This article is organized as follows. In Section 2 some basics concepts and the cluster identification methodology are presented. The experiments are shown and discussed in Section 4. In Section 5 we present the final considerations.

2 Methodology

2.1 Linkage methods

Given a dataset containing \( N \) elements, where the \( i \)-th element is represented by a feature vector \( \vec{x}_i \), the initial step of agglomerative clustering is to link the points together to form candidate clusters according to a given metric. This is known as the linkage step.

Let the distance between any two clusters \( w \) and \( v \) be represented as \( D(w, v) \). Many distinct metrics can be used for defining \( D \), but here we only consider Euclidean distances. Initially, each cluster contains a single object, that is, the number of clusters is given by the number of objects. At each iteration, pairs of clusters that were not previously joined are inspected, and the pair of clusters having the minimum value in \( D \) is joined to form a new cluster \( u \). Let \( s \) and \( t \) be the pair of clusters that were joined, and define \( x[i] \) to represent an object \( i \) in cluster \( x \). After the clusters are joined, the distances \( D(u, v) \) between the new cluster \( u \) and all other clusters need to be calculated. Many methods have been defined to calculate the new distances, and they have a large impact on the resulting hierarchy. Common approaches are described below.

Single-linkage (SIN) \cite{10, 11, 12}: the distance between clusters \( u \) and \( v \) is
given by the smallest distance between every pair of objects \((u[i], v[j])\), that is,

\[
D(u, v) = \min_{ij} \{D(u[i], v[j])\} \tag{1}
\]

Complete-linkage (COM) \[13\]: calculated as the largest distance between every pair of objects between clusters \(u[i]\) and \(v[j]\],

\[
D(u, v) = \max_{ij} \{D(u[i], v[j])\} \tag{2}
\]

Average-linkage (AVG) \[14\]: also called Unweighted Pair Group Method with Arithmetic Mean (UPGMA) \[4\], defines the new distance as the average distance between objects in \(u\) and \(v\), that is,

\[
D(u, v) = \frac{\sum_{ij} D(u[i], v[j])}{|u||v|}, \tag{3}
\]

where \(|x|\) represents the number of objects in cluster \(x\).

Centroid-linkage (CEN) \[14\]: also called Unweighted Pair Group Method with Centroid (UPGMC) \[4\], uses the Euclidean distance between the clusters centroids,

\[
D(u, v) = ||C_u - C_v||, \tag{4}
\]

where \(C_x\) indicates the centroid of cluster \(x\).

Median-linkage (MED) \[15\]: also called Weighted Pair Group Method with Centroid (WPGMC) \[4\], uses Equation 4 to calculate the distances, but the centroid of cluster \(u\) is calculated as

\[
C_u = \frac{C_s + C_t}{2}, \tag{5}
\]

Ward-linkage (WAR) \[7\]: joins clusters leading to the minimum increase in within-cluster variance. This can be done by setting the distances as

\[
D(u, v) = \sqrt{|v| + |s| \frac{D(v, s)^2}{T} + |v| + |t| \frac{D(v, t)^2}{T} - \frac{|v|}{T} D(s, t)^2}, \tag{6}
\]

where \(T = |v| + |s| + |t|\).

The single-linkage method can be implemented using a minimum spanning tree \[16\]. The complete, average, weighted and ward methods are commonly implemented using the nearest-neighbor chain algorithm \[17\]. An efficient implementation for the centroid and median methods can be found in \[17\].

Figure 1 shows the dendrograms obtained by the considered methods when applied to a uniform distribution of points inside a circle.
2.2 Anatomy of a Cluster

One of the challenges in cluster detection is that the selection, parameter setting or even the development of effective methodologies rely critically on the properties of the typically expected clusters (e.g. [6]). Hierarchical approaches are no exception to this, especially given that the existing alternatives typically rely on distinct agglomeration schemes (e.g. minimal/maximal distance, dispersion, etc.).

Though a consensus, general definition of a cluster remains elusive, several real-world data yield respective point distributions in feature spaces that exhibit a a gradient of point density. For instance, Figure 2 depicts nine examples of real-data obtained from [18] mapped into a feature space that are characterized by this type of point distribution.

Figures 3 and 4 illustrate the model of cluster considered in the current work. It is characterized by a high density core (red), followed by a medium density transition region (black), and then a peripheral low density region (blue). Though the model shown in Figures 3 and 4 have circular symmetry, this is not a necessary condition for our approach. The regions shown in this figure were identified by the methodology to be described in Section 2.

Interestingly, these three regions tend to be well-preserved even when more than one cluster is present, as illustrated in Figure 5.
Figure 2: Scatterplots of pairs of features derived from problems of different nature (indicated in the respective titles) that present cluster structure compatible with that assumed in the present work, with the density of points increasing towards the respective core, and the presence of a peripheral region and outliers.

Moreover, several important types of statistical point distribution, such as those adopted in this work (uniform, Gaussian, power and exponential) are all characterized by presenting the 3 proposed types of regions when including one or more clusters.

The adoption of a reference model as that shown in Figure 3 allows several benefits.

First, it allows the prediction of the behavior of clustering approaches, which need to be capable of treating the varying density of points in an effective way. In addition, the availability of such models allow parameters of a chosen method to be set more properly, in a semi-supervised fashion. For instance, the number of points in the 3 regions — core, transition and periphery — provides, as we shall see in this work, an important subsidy not only for identifying clusters, but also to assigning relevance levels to the obtained results.

Second, the peripheral, relatively isolated points, can be understood as cor-
responding to outliers, or it is also possible to conceive methods that focus on the detection of the core and then, as post-processing, tries to rescue the peripheral points in case they are wanted. However, it seems reasonable that the consideration of very low-density regions simultaneously during cluster detection represents an additional, potentially substantial challenge to the considered algorithms.

Third, the identification of properties of the three parts of clusters provides a subsidy for trying to infer the type of point distributions characterizing the clusters by using pattern recognition resources.

The higher density of the core provides more statistical relevance, being
potentially less affected by noise and distortions. Even more importantly, in multimoideal datasets, the cores of the existing clusters are almost invariably more separated one another than would be the case if the other two regions were also taken into account. This is in contrast to several existing methodologies, which treat all density regions in a unified manner.

Consequently, our approach focuses on the identification of the core region in the dendrograms obtained by the considered agglomerative methodologies.

The varying density characterizing the adopted model has another important implication, namely that it would be interesting that the adopted clustering be capable of aggregating points into the core in a progressive and relatively
smooth manner, to avoid instabilities as the cluster merge along the obtained dendrograms.

Once the cores have been detected, hopefully with enhanced quality, it is always possible to perform some post-processing oriented to recovering the points in the transition and/or periphery regions or each detected group.

2.3 Cluster identification

After the application of a linkage methodology to a dataset, the results are usually visualized using a dendrogram, such as those shown in Figure 1. Next, a methodology for selecting a suitable cut of the dendrogram is applied, so as to define the clusters. For instance, a common strategy is to calculate the inconsistency of each merge performed during the linkage process, that is, each dendrogram bifurcation, and to find merges such that all the descendants have an inconsistency lower than a given threshold. Such a criterion usually disregard important prior knowledge one may have about the data, such as an estimation of the size of the clusters or the number of outliers expected in the data. An important situation is when the number of elements for each class is known, or can be estimated. In this case, one should search for clusters having specific sizes. Furthermore, the size of the clusters can also be predicted in cases where a prototype of the clusters is available or can be developed.

Figure 5 illustrates a possible prototype in a 2D feature space, involving two circular clusters of normally distributed data. The distribution of the data is shown in Figure 5(a). Two main clusters can be identified at a more macroscopic scale. Actually, these clusters might not coincide with the partition found if some of the aforementioned criteria were used. This partitioning implies a specific number of points for identifying the clusters, as shown in Figure 5(b). If the desired clusters are to be searched at a much smaller scale, such as the cluster shown in Figure 5(c), they will likely be ignored. Since the expected size of the clusters might be a piece of important information for defining their partitions, it is a crucial parameter of our methodology.

As discussed in Section 2.2 an estimation of the number of outliers in the data is also relevant for cluster identification. Outliers in the data that do not belong to specific clusters should not be assigned to any cluster. Despite being an evident requirement, many cluster identification methods, most notably partitional methods, do not follow this principle. Therefore, we also consider the expected number of outliers as a parameter of the method.

The methodology works as follows. Given the desired cluster size s and a number of clusters k, the dendrogram is first obtained and then analysed in a bottom-up approach. Clusters are merged until k clusters having at least s elements are identified for the first time. Since the last cluster merge might generate a cluster having size much larger than s, it is checked if the last merge should be undone. Let u represent the cluster formed after the most recent merge, and let q and t indicate the two clusters that were joined to defined u. Representing as su, sq and st the respective sizes of clusters u, q and t, we calculate sm = max{sq, st}. Then, if (su − s) < (s − sm) the last cluster merge
is kept. Otherwise, the final clusters will include the largest cluster between \( q \) and \( t \), and will not include \( u \). If \( k \) clusters cannot be identified by the method, the first merge where \( k - 1 \) clusters are identified is used. The same happens if \( k - 1 \) clusters cannot be identified, and so on.

This method is illustrated in Figure 3. The points in Figure 3(a) yielded, by using the single-linkage method, the dendrogram in Figure 3(b). If the red points in Figure 3(a) are to be detected as the resulting cluster, the respective number of points is determined and used for selecting the corresponding subtree in the dendrogram by using the here proposed methodology, marked in red in Figure 3(b). A similar situation is shown in Figures 3(c) and 3(d) for a bimodal distribution.

In addition to the identified clusters, outliers are also detected and pruned from the dendrogram using a top-down approach. Starting from the top, it is verified if one of the two clusters joined in the current merge has a size smaller than \( c \). If that is the case, the small cluster is considered an outlier. The
same criterium is applied to the next merges until a merge having both clusters larger than $c$ is identified. The detected outliers are represented as blue points in Figures 3(a) and 3(c) and as a blue line in the dendrograms shown in Figures 3(b) and 3(d).

Some hierarchical clustering methods, such as Ward’s, try to minimize the variance of the points inside a cluster while maximizing the inter-cluster distance. This approach might be appropriate when the distribution of the points representing the objects in the feature space is bimodal at the selected scale. On the other hand, if the distribution of the data is unimodal, the minimization of the variance and maximization of the inter-cluster distance might lead to the detection of false clusters. Furthermore, outliers are not taken into account by such methods. For instance, the Ward method applied to the points shown in Figure 4(a) will generate the dendrogram shown in Figure 4(b), where no outlier points were detected.

It is important to identify cases when a linkage methodology, and respective strategy for cluster identification, lead to the detection of false clusters. Thus, a criteria for quantifying the quality of the obtained partition, henceforth called relevance, needs to be defined. Figures 4(c) and 4(d) show the result of the application of the Ward-linkage method to a bimodal distribution of points. The core of the green cluster was not detected correctly. Comparing Figures 3 and 4 it is clear that the cores identified by the single-linkage method in both the unimodal and bimodal distributions are more compact and central than those identified by the Ward method. As a result, the cores identified by the single-linkage method were found to be more relevant than those detected by the Ward method.

The above considerations suggest that the relevance of a cluster identified by the methodology can be measured in terms of the height of the red line indicated in the respective dendrograms. Whenever a single cluster is identified, its relevance is given by the dendrogram height where the last merge occurred. If more than one cluster is detected, the relevance is calculated as the average of the heights of the last merges from each cluster.
3 Inferring the Types of Clusters

The proposed approach for identifying the clusters in dendrograms and assigning respective relevance intrinsically provides subsidies that can be further considered for identifying the type of point distribution type of the respective dataset. Such information could be valuable not only for a better understanding of the analyzed data, but also be used for tuning and enhancing the cluster detection methodology. Interestingly, the identification of the type of point distributions represents itself as a pattern recognition approach applied to pattern recognition.

Here, we illustrate the above possibility with respect to identifying the type of point distribution in unimodal datasets. The first step while trying to identify the type of distribution in a set of points is to define a reasonable and effective set of respective features. Natural candidates are the position of the outliers height, the cluster height, as well as the size of the outliers set and the size of the detected cluster set.

Another potentially useful set of features is related to the number of points that are incorporated into the dendrogram as the respective height variable changes. Figure 8(b) depicts an example of the variation of the number of points incorporated into the dendrogram (y-axis) in terms of the heights (x-axis). One possibility is to consider the whole curve of the number of points × height. But since the number of elements in these curves can vary among different datasets, it is necessary to implement an interpolation of the curve, allowing respective resampling with a constant number of elements.

Figure 8 illustrates the whole feature vector \( \mathbf{f} \) that can be defined while
incorporating the whole set of elements in the number of incorporated points curve.

$\mathbf{f} = [\text{outliers, outliers, cluster, cluster, link, size, height, size avg., height avg., heights}]$

**Figure 8:** Set of features used for the cluster identification including the dendrogram link heights.

Another possibility is to fit the curve expressing the number of incorporated points by a polynomial. We have found that a cubic polynomial, $y = ax^3 + bx^2 + cx + d$, where $x$ is the dendrogram height, tends to provide good fitting for the obtained number of incorporated elements curves. Figure 9 shows the alternative feature vector that can be therefore obtained.

$\mathbf{f} = [\text{outliers, outliers, cluster, cluster, a, b, c, d, size, height, size avg., height avg.}]$

**Figure 9:** Set of features used for the cluster identification, including the curve fit.

Once feature vectors have been obtained for a representative set of point distributions of diverse types, it is possible to apply principal component analysis
(PCA, e.g. [26]) to investigate possible formation of clusters respective to the considered types of point distributions.

4 Experiments and discussion

Eight synthetic data distributions were considered, including unimodal and bimodal configurations derived from random distributions. The four unimodal distributions were the uniform, Gaussian, power-law and exponential. For each distribution, $D$ independent and identically distributed random variables were used, which defined the dimension of the generated dataset. The bimodal data corresponding to a given zero-centered unimodal distribution was generated using the following approach. Two sets of points $S_1$ and $S_2$ were drawn from the unimodal distribution and the respective standard deviations $\sigma_1$ and $\sigma_2$ of the generated points were calculated. Then, the average $\sigma = (\sigma_1 + \sigma_2)/2$ of the standard deviations was calculated, and used for defining a distance $d$ given by

$$d = \alpha\sigma/2$$

Next, the coordinates of the points in set $S_1$ were all translated by $d$, while the coordinates of points in $S_2$ were translated by $-d$. A value of $\alpha = 4$ was used for all distributions. Thus, $\alpha = 2d/\sigma$ is the same for all bimodal distributions. The procedure for generating a power-law bimodal distribution was slightly different. Before translation, the coordinates of the points in set $S_2$ were multiplied by $-1$, so that the tails of the distributions of the two sets of points were placed on opposing directions. Please refer to Table 1 for more details about the adopted parameters of the distributions and to Figure 10 for contour-level plots of the distributions.

| Index | $N_{clusters}$ | Distribution | Param. |
|-------|----------------|--------------|--------|
| A     | 1              | uniform      | r: 1.0 |
| C     | 1              | power        | exp: 2 |
| D     | 1              | gaussian     | cov: (1.0 0.0) |
| E     | 1              | exponential  | –      |
| F     | 2              | uniform      | r: 1.0 |
| G     | 2              | power        | exp: 2 |
| H     | 2              | gaussian     | cov: (1.0 0.0) |
| I     | 2              | exponential  | –      |

For each considered distribution, $M = 400$ datasets containing $N = 500$ points were generated. The dimension of the datasets was changed in the experiments, going from $D = 2$ up to $D = 10$. Thus, for a given number of dimensions $D$, each linkage method was evaluated on 3200 datasets. After generating the dendrograms and applying the methodology described in Section 2,
using $K = 2$, $S = 0.3N$ as cluster size and $P = 0.02N$ for removing outliers, the number of detected clusters and the respective relevance of the clusters found were calculated to define the performance vectors described in Section 2. The results are shown in Figures 12 and 13 for, respectively, unimodal and bimodal data.

In all experiments, the hypothesis is that there are two clusters in the data. However, in the case of unimodal data, the linkage methods should yield a dendrogram that when analyzed should not lead to the detection of two clusters. Thus, an ideal method should detect a single cluster with relevance equal to 1 for all the 400 considered unimodal datasets. This ideal situation is represented as a black vector in Figure 7.

The results show that the number of detected clusters varies among the distributions and the linkage methods. For the uniform unimodal distribution, most methods detected 2 clusters in almost all datasets, with the notable exception of the single-linkage method that detected the correct number of clusters in 76% of the cases. For the gaussian and power-law distributions, the number of detected clusters fluctuates for all linkage methods with the exception of the single-linkage, that detected the correct number of clusters in all cases. The average, centroid, and single linkage methods detected the correct number of clusters in almost all realizations of the exponential distribution.

The reason for the variation in performance among the distributions is the difference between the cores of these distributions. While the uniform distribution does not have a well-defined core, the other three distributions contain high-density cores that are easier for the methods to detect. This corroborates the importance of considering the cores during cluster detection. It is interesting to note that the Ward method resulted in the worst performance in all cases, leading to the detection of false clusters in 82% of all datasets.

When bimodal data is considered, in almost all situations the methods detected the correct number of clusters, being different only regarding the relevance of the clusters found. The single-linkage method resulted in the lowest relevance for the uniform distribution, that is, it indicates that the two clusters found are not particularly relevant even though it is known that the data have two clusters. This could be interpreted as the single-linkage method not performing well for bimodal data, but we argue that this is not the case for the data used in the experiments. In order to understand why a small relevance should be desired in such situations, Figure 6 shows an example of bimodal data generated from the uniform distribution and adopted for evaluating the methods. It is clear that the clusters are very close to one another. Actually, the distances among some points inside the clusters are larger than the distance between the clusters. Thus, depending on the criteria used for defining the clusters, these two clusters could be taken as a single cluster since there is no evident separation between their points. For instance, consider a situation where a clustering algorithm is applied for categorizing apples as ripe and unripe based on color. In this situation, it would be easy to categorize the limiting cases, but a nearly continuous variation would be observed between the two limits. Thus, the intermediate colors would not imply the clustering of the data.
A summary of the results obtained for each type of dataset is presented in Figure 14. The ordinate axis for each plot indicates the average value of \( l \) obtained for a linkage method applied to 400 datasets having the indicated dimension and distribution. As in the previous results, \( k = 2 \) is used when applying the cluster partition methodology. Figure 14 shows that the value of \( l \) for the Ward method is very different between the unimodal and bimodal distributions. In the unimodal case, the Ward method tends to detect two clusters with high relevance, as indicated by the results in Figure 14. Therefore, it results in the worst performance among all methods. In the case of bimodal data, it tends to detect two clusters with high relevance, leading to small values of \( l \). Also, the performance of the method was very similar for all bimodal distributions, which indicates that the considered distributions did not significantly influence the clusterization. The single-linkage method resulted in the smallest values of \( l \) for 2D, 4D and 5D data, which is the desired behavior since in the case of unimodal data \( l \) should be small. Interestingly, for 10 dimensions the centroid method performed slightly better than the single linkage. Figure 14 also indicates that the complete and median methods tend to have similar performance. The same is observed for the average and centroid methods.
To complement our experiments, we also performed an evaluation of the proposed methodology for identifying types of point distributions, described in Section 4.

We adopted the same number of realizations, 400, of point distributions described in Table 1. The two alternative feature vectors, i.e. incorporating all points in the curves of incorporated points as well as the respective fitting by cubic polynomials. Figure 12 depicts the results of PCA of the so-obtained feature vectors with respect to point distributions in 2-D (a), 4-D (b), 5-D (c) and 10-D (d). In (a) and (d), the link heights were utilized for the PCA while in (b) and (c) the polynomial fit coefficients were used instead.

Observe that the total variance explanation, shown along the respective principal axes, tends to decrease with the dimension, achieving nearly 100% for 2D. As can be readily appreciated from the obtained results, several well-separated clusters have been obtained in all considered situations. As could be expected, the two uniform types of points distributions always appeared further away from the other clusters. This is a consequence of the fact that
Figure 13: Vectorial visualization of the method proposed evaluated using bi-modal distributions.

uniform distribution of points has no definite core, with all points keeping similar
distances one another. For 2D, except for the two uniform distributions, which
completely merged one another while remaining away from the other clusters,
the other point distributions tended to occupy respective areas, but with little
separation between the groups. The results obtained for the other 3 dimensions
all exhibit well-separated clusters, with a significant separation being observed
for 10D.

These results corroborate the potential of the suggested methodology for
identifying the types of point distributions in the analyzed data, which could
be achieved by applying supervised pattern recognition on the obtained feature
spaces. The identification of the types of clusters has potential not only for
better understanding the data under analysis, but also for providing subsidies for
enhancing the clustering methodology. For instance, parameters of the proposed
clustering identification method can be fine-tuned adaptively while considering
the observed types of clusters.
5 Conclusion

In spite of continuing research efforts since the 70’s, clustering identification remains a challenging issue. In particular, specific implementations need to balance a trade-off between false positives and false negatives, as well as being able to cope with outliers, varying types of point distributions and feature space dimensionality, among other issues.

Hierarchical clustering methods represent a particularly interesting and effective approach because the number of groups can be chosen, normally by analyzing the respectively obtained dendrograms. Also, they also tend to perform well respectively to real-world data [27]. The agglomerative type of hierarchical clustering has been frequently adopted in theoretical and applied clustering research.

Agglomerative clustering methods differ from one another by the type of group linkage criteria, which can be based on distance, dispersion, etc. Six types are commonly found in the respective literature: single, complete, average, centroid, median, and Ward. Because these methods can perform differently regarding, for instance, false positives, it becomes important to consider
comparative approaches. One related difficulty commonly found concerns the
definition of a stable and meaningful measurement of the relevance of the clus-
ters. Ultimately, despite several efforts, there is still a need for more objective
comparative approaches.

The difficulties in comparing clustering methods are, at least partially, re-
lated to the definition of what are the properties of the expected clusters. Ac-
tually, this point is also fundamental in devising clustering methods. In the
present work, we developed a model-based approach to the important issues
not only of identifying clusters from dendrograms obtained from agglomerative
methods, but also assigning respective relevance figures of merit.

More specifically, we assumed a model involving three main components:
core, periphery, and transition. As such, the adopted model intrinsically takes
into account gradients of point densities, which are commonly found in real-
world datasets. In addition, we assume that some information is known or
hypothesized about the size of the expected clusters. The adopted model al-

tows the identification of the clusters to be performed in a bottom-up manner,
starting from the leaves of the dendrogram and moving upward the height until
clusters having the desired sizes are found. Another procedure can be applied to
identify the outliers, proceeding top-down the dendrogram and removing groups
having a size smaller than a given parameter.

Thanks to the combination of the bottom-up and top-down adopted ap-
proaches, the core and outliers components of the model can be properly identified, so that the remaining points are understood as composing the transition region. The latter group provides a stable and intuitive indication about the relevance of the obtained cluster, in the sense that it indicates how far the core is to the outliers. Consequently, we defined the relevance of the cluster as the average height of the dendrogram subtrees associated to the detected clusters.

A number of interesting results have been obtained and discussed. Among them, we have that several methods tend to find two clusters in unimodal data, with the noticeable exception of the single-linkage method. At the same time, several methods tended to yield clusters that do not correspond closely to the cores, also including points from the transition or even outlier zones. These situations were duly characterized by lower relevance values. All methods except for the single-linkage were mostly unable to detect outliers, an often desired task.

The reported developments pave the way to some interesting future investigations. For instance, it would be interesting to extend the proposed approach to datasets with larger number of clusters and to other types of point distributions. Another interesting perspective would be to compare divisive hierarchical methods.

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