Study of a few significant clustering methods

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ABSTRACT

Data analysis is an important tool in contemporary scientific research, including that conducted in the biology sciences, computer sciences, and social sciences. In order to accurately analyze the enormous number of data produced by contemporary applications, clustering algorithms have become a potent alternative meta-learning technique. However, because of the complex nature of the information, each clustering algorithm has sole advantages and disadvantages. This paper presents some significant clustering methods, their technique, performance along with advantages and disadvantages.

Keywords—Partition based clustering, particle swarm intelligence, ant colony optimization, fuzzy-c-means, bee colony optimization.

I. INTRODUCTION

Late advancements in information technology and innovations in data processing have brought numerous applications in different business areas. Every organization uses a large amount of raw data for different applications. Therefore, the importance of information management has increased. Discovery of knowledge from the huge amount of data used by these organizations is a big challenge. Knowledge discovery is one of the notable parts of data mining. The objective of data mining is the extraction of patterns and knowledge from large data sets, not the extraction of data itself [1]. Different data mining tasks include classification, summarization, association rule learning, regression, clustering, and anomaly detection.

Clustering is one of the significant research areas in data mining. Clustering is the process of collecting a set of entities so that objects in a similar group are progressively comparative to one another than to those in a different group [2, 3]. Clustering techniques can be used in many different fields including machine learning, image processing, data compression, pattern recognition, information retrieval, bioinformatics, etc [3]. There are nine categories that the conventional clustering algorithms fall under. These are based on hierarchy, partition, fuzzy theory, distributions, density, graph theory, grid, fractal theory, and models. But there are two major classes: (i) hierarchical clustering [1, 2, 4] and (ii) partitional clustering [1, 2, 4]. Hierarchical clustering aims at building a hierarchy of data objects/groups. Hierarchical clustering is again of two types: agglomerative or divisive [4]. The agglomerative approach begins with each item framing different groups, and progressively combines the objects/groups near each other until all the groups are converged into one. The divisive approach begins with all the items in the same group and progressively splits the group into sub-groups until each item is in one group. On the other hand, the partitional clustering techniques mostly based on a distance measure. Given n number of objects and k number of clusters, the partitioning technique starts with creating initial partitioning and then in several iterations tries to improve the partitions by moving the objects in between them. Some of the problems with hierarchical clustering include: once the cluster formation has done it cannot be modified, thus reallocation of objects is not possible; it cannot detect erroneous data, and because of its hierarchical nature, difficulty in handling larger datasets [4]. The partitional clustering overcomes all these problems, but with a limitation that it is not suitable for non-convex data [5].

The modern clustering techniques are basically based on kernels, swarm intelligence, quantum theory, spectral graph theory, affinity propagation, etc [5]. Swarm intelligence-based methods of modern clustering are the most widely employed. . Swarm intelligent algorithms are basically optimization algorithms that have been successfully applied for clustering technique. The fundamental goal of these clustering algorithms is to mimic the biological population's natural process of change. The primary benefit of these algorithms is that they avoid being easily drawn into local optimality while obtaining global optimality. This report is a study of certain significant clustering approaches that are used traditionally along with some modern algorithms along with their benefits and limitations. Here we have studied clustering approaches based on hierarchy, k-means, k-medoids, fuzzy-c-means and density under traditional techniques and approaches based on particle swarm optimization, ant colony optimization, bee colony optimization, whale optimization, kernel, and graph theory under modern techniques.

Following is how the remainder of the paper is structured: Sections II and III offer various traditional and modern clustering strategies, respectively, and Section IV concludes up the work with a strategy for further research.

II. TRADITIONAL CLUSTERING TECHNIQUES

A. Hierarchy based Clustering

The essential idea behind this kind of clustering procedure is to organize information by creating hierarchical connections between them [6]. It is presumable that every point of data originally represents a different cluster. Then the two clusters that lie nearest to one another are merged to form a single cluster. As an alternative, turn it around. The BIRCH [7], CURE [8], and ROCK [9] are the algorithms that use this kind of clustering. By building the feature tree (CF tree) of clustering, BIRCH realizes the clustering result. If a new data point is received, the CF tree will grow dynamically. CURE, which is appropriate for extensive clustering, uses a sampling method based on randomization to group each model separately before integrating the outcomes. For handling enumeration-type data, ROCK is an enhancement of CURE that takes into account the influence of the data surrounding the cluster on the similarity of the data. Hierarchy-based clustering has the advantage of being able to handle data of any size and shape, but it also has a high time complexity.

B. K-Means Clustering

K-Means clustering is used in the fields of data science and machine learning to address clustering problems which is an unsupervised learning algorithm and falls under partition based technique. Here, the unlabeled dataset is divided into K distinct clusters. The technique is centroid-based, so every cluster is assigned a centroid to it. Reducing the overall distances of the data points and their related cluster is the main objective of this technique [10].

The k-means clustering technique primarily accomplishes the following tasks.

1) Start by initializing K points, as initial cluster centroids, at random.
2) Create cluster by assigning the data elements to the closest centroid using a distance metric.
3) Update the cluster centroid by averaging the data points of the individual clusters.
4) Repeat steps 3 and 4 as necessary to determine the best centroids and ensure that the data objects are being allotted to the right clusters without changing their placement.

When, n is the number of data elements, k is the number of clusters and t is the number of iterations the time complexity of the algorithms is $O(nkt)$. Hence, it is a faster clustering technique. But the main drawbacks of k-means clustering include its susceptibility to initial centroids, applicability for only convex data, and tendency to fall in local optimum regions.

C. K-Medoids Clustering

The K-Medoids [11] clustering technique divides a set of data points into K clusters utilizing a distance measure. In this case, K-medoids function like K-means clustering and medoid indicates the centroid of a cluster. The key benefit of this approach is its resistance to anomaly for spherical data. More significantly, its convergence is quicker and with fewer steps. Although it might not be effective for non-spherical data, it can be a useful tool for research across domains.

The basic steps for K-medoids clustering is as follows:

1) Pick K medoids at random.
2) To create the initial cluster, assign data objects to the nearby medoids using a distance metric.
3) Add up the distances between each cluster and its corresponding medoid.
4) Replace the medoids with a different data member within the cluster randomly.
5) To obtain an updated clustering result, assign each data point to the nearest medoids.
6) Add up the distances between each cluster and its corresponding medoid.
7) Update the medoids if the summation of distances with newly created medoids is less than with the old medoids.
8) Repeat steps 4 to 7 until sum of the distances of old and new medoids are not same.

Empty cluster construction, K-means problem solving, and sensitivity to noise are some of its advantages. Additionally, it chooses the cluster member with the greatest degree of centering. Its drawbacks include the need for accuracy and complexity.

D. Fuzzy-c-means Clustering

Hard or crisp clustering refers to the clustering methods we've covered up to this point in which just one cluster is assigned to each object. This restriction is eased when using soft clustering or fuzzy clustering, and an object can have some degree of membership in all of the clusters. This is especially helpful when the boundaries between the clusters are unclear and poorly defined. Additionally, the memberships might let us identify more complex connections between a certain object and the exposed clusters. The fuzzy c-means

clustering (FCM) approach is the most popular soft clustering technique [12]. FCM seeks to minimize the cost function while trying to locate a partition (fuzzy clusters) for a set of data elements.

Each data point's membership score is determined by the FCM clustering algorithm based on the Euclidean distance between it and the cluster center. The membership ratings are higher for the nearby data points. The membership score and cluster centers are updated after every iteration as follows:

$$a_{ij} = 1/\sum_{k=1}^{c} (dis_{ij}/dis_{ik})^{(2/m-1)}, \quad (1)$$

$$b_j = \frac{\sum_{i=1}^{n} a_{ij}{}^m x_i}{\sum_{i=1}^{n} a_{ij}{}^m}, \quad (2)$$

In this equation, a_{ij} is the membership score, i is data point index, j is cluster center index, b_j is the j^{th} cluster center, *dis* is the Euclidean distance, c is the number of clusters, m is the fuzziness parameter and n is the number of data points.

The steps that the FCM clustering algorithm takes to complete its work are as follows:

1) Create n random centers to initiate n clusters.
2) Utilize (1) to determine the membership score for every data point.
3) Up until membership levels exceed a threshold value, repeat steps 4 through 6 as necessary.
4) Find the cluster centers using (2).
5) Calculate the centroid's Euclidean distance from each data point.
6) Utilize (1) to update the membership score for every data point.
7) Print the centroids of the clusters.

Due to the need to calculate each data point's membership in each cluster, the technique is comparatively slower and depends on how the weight matrix is initialized.

E. **Density based Clustering**

These clustering technique's central principle is that any data that are found in a region of dense information space are assumed to be members of the same cluster [13]. Common ones include DBSCAN [14], OPTICS [15], and Mean-shift [16]. Directly derived from the core idea of this group of clustering algorithms is the DBSCAN method. The OPTICS technique is an enhancement over DBSCAN process and it fixes the flaw that DBSCAN had in that it was sensitive to the neighborhood radius and the required adequate quantity of points. In mean-shift process, the current data point's mean offset is first determined, followed by the calculation of the next data point's mean using the current offset value and recent data points, and finally, the process repeated until certain termination measures are met. Benefits include high-efficiency clustering that works with arbitrary-shaped data; and the drawbacks include resulting in low-quality clustering results when the density of the data space is uneven, large memory requirements when the data size is large, and a clustering outcome that is very parameter-sensitive.

III. MODERN CLUSTERING TECHNIQUES

A. **Particle Swarm Optimization (PSO) based Clustering**

The concept of particle swarm optimization [17] is founded on the collective bird-like seeking behavior of swarms. It is a meta-heuristic populace search technique. By altering their position and velocity, the particles fly towards the location of food. Each location of the particle is a potential solution (pbest), and the particle that acquires the best location is the overall solution. Up until the ideal solution (gbest) is discovered, the particles travel. For every iteration of the algorithm, the velocity and locations are restructured according on the objective function defined. The following equations can be used to update the velocity and position:

$$V_i^{k+1} = \omega V_i^k + c1 * r1 * \left(P_i^k - X_i^k\right) + c2 * r2 * \left(G_i^k - X_i^k\right) \quad (3)$$

$$X_i^{k+1} = X_i^k + V_i^{k+1} \quad (4)$$

Where, V_i , P_i , X_i , G_i , respectively, stand for velocity, pbest, current location, and gbest. The steps in PSO based clustering are as follows:

1) Make the cluster centers (Particle) initialized at random.
2) For a maximum number of iterations, repeat steps 3 through 7.
3) Repeat steps 4 through 7 for every particle.
4) Repeat steps 5-7 for each data vector.

5) Determine the distance between centroid and its associated data vectors, then, allocate the data vector to the cluster with the shortest distance.
6) Update pbest and gbest and compute the fitness value.
7) Utilizing position formula (4) and velocity (3), update cluster centers.

Better precision, compact clusters, and repeatability are benefits of PSO-based clustering. The limitation is that for huge datasets it requires higher execution time. Again, PSO falls in the local optimum and is dependent on initial cluster centers.

B. Ant Colony Optimization based Clustering

The ant's movement to different locations is the basis for ant colony optimization. The direction and distance of the pheromone have an impact on this movement [18]. (5) is used to determine whether an ant will migrate from source *s* to destination *d* at time *t*. and after some time *t'* the intensity of the pheromone is computed using (6).

$$P_{sd}^{k}(t) = \frac{[\tau_{sd}(t)]^{\alpha}[\eta_{sd}]^{\beta}}{\sum_{k\in \text{allowed}(k)}[\tau_{sk}(t)]^{\alpha}[\eta_{sk}]^{\beta}} \quad \text{if } d \in \text{allowed}(k) \tag{5}$$

$$\tau_{sd}(t+t') = (1-\rho)\tau_{sd}(t) + \Delta\tau_{sd} \tag{6}$$

Here, τ_{sd} represents the pheromone's intensity along the path, η_{sd} = 1/ distance$_{sd}$, and α and β indicate the pheromone's impact. The rate of evaporation is ρ, and the total amount of pheromones released by all ants is $\Delta\tau_{sd}$. Although ant colony optimization (ACO) performs well in the area of discrete problem solving, it unavoidably has some drawbacks. It has good stability, however when working with a lot of data, it has some issues with convergence speed and solution accuracy. ACO has drawbacks including a sluggish convergence rate, weak similarity, high computational complexity, and a tendency to settle in local optima.

C. Bee Colony Optimization based Clustering

The traditional Bee Colony Optimization (BCO) [19] clustering technique operates alternating stages, called the forward and the backward pass. The objective of the forward pass is to survey the search area and gather some useful information. By assessing an objective function, the fitness of these practicable solutions is calculated. In the initial step of the backward pass, each bee chooses whether to stick with its own answer or to adopt one from another. The bee transforms into a recruiter if it chooses to keep going. Other bees in the hive searching for a recruiter are recruited by it, and they all move to where it has been located. If not, the bee chooses a recruiter and follows it in finding a solution. Once the backward pass is finished, all bees have a partial solution. The optimal partial solution is chosen as the local best. If the fitness of the most recent local best solution is greater than the fitness of the most recent global best solution found up until the previous iteration, the global best upgrades to the most recent local best. The algorithm must meet a termination requirement in order to stop operation.

The following steps are performed in the algorithm:

1) Initialize all the bees and their clusters.
2) Repeat steps 3 to 6 until termination.
3) Perform forward pass to collect feasible solutions.
4) Perform backward pass and do the following:
   - Compute the stickiness probability of bee.
   - If the probability of stickiness is less, chose another bee to follow.
5) Assign the remaining data objects after all stages complete.
6) Update the global best.
7) Return global best.

The likelihood that a bee will adhere to a solution is determined by the following equation [11].

$$P_b(k+1,t) = e^{-O_b(k,t)/(k\times t)}, \tag{7}$$

$$O_b(k,t) = \frac{SICD_b(k,t) - SICD_{min}(k,t)}{SICD_{max}(k,t) - SICD_{min}(k,t)}, \tag{8}$$

Where, *b* is the bee, *k* is stage, and *t* is iterations. $O_b(k,t)$ is the normalized *SICD*, $SICD_{max}$, and $SICD_{min}$ are the largest and smallest *SICD* value. The BCO clustering is renowned for its adaptability, dependability, and

capacity to investigate regional solutions. However, it has numerous drawbacks, including a stumpy convergence rate, uneven exploitation and exploration, and delayed sequential processing.

D. Whale Optimization Algorithm based Clustering

The Humpback Whale Optimization Algorithm is based on how humpback whales hunt. Around 12 metres below the surface, whales dive and blow bubbles all around the object. Afterward, ascend in the water to assault the target [20]. The term for this is "bubble-net attacking". The bubble-net attack works like this: The whales constrict and surround the prey by referring to its current best location as the target subject's position, while the other whales adjust their places in response.

The steps in Whale optimization-based clustering algorithm are as follows:

1) Make the cluster centers (Particle) initialized at random.
2) Repeat the steps 3 to 8 until termination.
3) Repeat steps 4 to 6 for each particle.
4) Repeat steps 5 and 6 for each data vector.
5) Calculate the distance between centroid and its associated data vectors, then allocate the data vector to the cluster with the shortest distance.
6) Determine the fitness value and make updates to the best search agent X*.
7) Repeat step 8 for every agent X.
8) Using either a spiral move or a shrink, update the location of agent X.

Different areas have favored the whale optimization algorithm (WOA), an advanced optimization method with a straightforward layout. WOA does have certain drawbacks, including a sluggish convergence rate, poor precision, and a tendency to quickly converge to local optimal values.

E. Kernel based Clustering

The fundamental tenet of this class of clustering techniques is that nonlinear mapping is used to transfer information from the space of inputs into a high dimension space of features for the cluster study. Kernel K-means [21], kernel SOM [22], and kernel FCM [23] are common clustering techniques. Kernel K-means, kernel SOM, and kernel FCM are algorithms that use the kernel method and transform the original information into an extremely large feature space. Benefits include: easier clustering in extremely large feature space, suitability for information of any shape, ability to investigate noise and distinguish overlying clusters, and lack of need for prior knowledge of data topology. The clustering outcome is very dependent on the kernel type and its factors, the computational time is considerably high, and the method is not appropriate for handling big amounts of data.

F. Graph Theory based Clustering

The fundamental concept behind these clustering methods is to turn the clustering task into a graph partitioning task by regarding every element as a vertex and the level of similarity over items as a weighted edge. The aim is to discover a strategy for graph partitioning that maximizes the total weight of connections among edges within a group while minimizing the weight of connections between distinct groups. Recursive spectral and multi-way spectral are the two categories into which the standard algorithms for this type of clustering can be broadly subdivided, and the classic algorithms for these two classes are, respectively, SM [50] and NJW [51]. The fundamental principle of SM, which is typically applied to image segmentation, is to reduce the Normalized Cut using a heuristic technique based on the eigenvector. In the feature space created by the eigenvectors corresponding to the k greatest eigenvalues of the Laplacian matrix, NJW also performs the clustering analysis. These algorithms are appropriate for the arbitrary-shaped, high-dimensional data set, which converged to the global optimal. The time complexity is relatively large, the clustering outcome is sensitive to the scaling parameter.

IV. CONCLUSION

The goal of this study is to present a summary of the algorithms used in various clustering techniques, along with each algorithm's benefits and drawbacks. The various clustering techniques that have been studied include density-based, hierarchy based, and partition based under traditional techniques. Additionally, we have provided PSO-based, ACO-based, BCO-based, Whale optimization-based, and kernel-based strategies under modern clustering algorithms. Different clustering algorithms produce noticeably different findings on the same data, which is the major difficulty with clustering analysis. Furthermore, no algorithm is currently available that provides all needed results. Due to this, a significant amount of research is being done.

For application domains like medicine and healthcare, the future work will concentrate on building clustering algorithms based on BCO, Fuzzy-c-means, k-means, and k-medoids. The field of anomaly detection may also be further tested.

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