

Novel Approach of K-Mean Algorithm

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-----ABSTRACT -----

Emergence of modern techniques for scientific data collection has resulted in large scale accumulation of data pertaining to diverse fields. Conventional database querying methods are inadequate to extract useful information from huge data banks. Cluster analysis is one of the major data analysis methods and the k-means clustering algorithm is widely used for many practical applications. But the original k-means algorithm is computationally expensive and the quality of the resulting clusters heavily depends on the selection of initial centroids. Several methods have been proposed in the literature for improving the performance of the k-means clustering algorithm. This paper proposes a method for making the algorithm more effective and efficient; so as to get better clustering with reduced complexity.

KEY WORDS: Data Analysis, Clustering, k-means Algorithm, Enhanced k-means Algorithm.

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I. INTRODUCTION

Advances in scientific data collection methods have resulted in the large scale accumulation of promising data pertaining to diverse fields of science and technology. Owing to the development of novel techniques for generating and collecting data, the rate of growth of scientific databases has become tremendous. Hence it is practically impossible to extract useful information from them by using conventional database analysis techniques. Effective mining methods are absolutely essential to unearth implicit information from huge databases. Cluster analysis [3] is one of the major data analysis methods which is widely used for many practical applications in emerging areas like Bioinformatics [1, 2]. Clustering is the process of partitioning a given set of objects into disjoint clusters. This is done in such a way that objects in the same cluster are similar while objects belonging to different clusters differ considerably, with respect to their attributes. The k-means algorithm [3, 4, 5, 6, 7] is effective in producing clusters for many practical applications. But the computational complexity of the original k-means algorithm is very high, especially for large data sets. Moreover, this algorithm results in different types of clusters depending on the random choice of initial centroids. Several attempts were made by researchers for improving the performance of the k-means clustering algorithm for improving the accuracy and efficiency of the k-means algorithm.

II. BASIC K-MEANS CLUSTERING ALGORITHM

The K-Means clustering algorithm is a partition-based cluster analysis method [10]. According to the algorithm we firstly select k objects as initial cluster centers, then calculate the distance between each object and each cluster center and assign it to the nearest cluster, update the averages of all clusters, repeat this process until the criterion function converged. Square error criterion for clustering

mi is the center of i-class, ni is the number of samples of i-class. Algorithm process is shown in Fig K-means clustering algorithm is simply described as follows:

Input: N objects to be cluster (xj, $Xz \dots xn$), the number of clusters k;

Output: k clusters and the sum of dissimilarity between each object and its nearest cluster center is the smallest; 1) Arbitrarily select k objects as initial cluster centers (m], m2 ... mk);

2) Calculate the distance between each object Xi and each cluster center, then assign each object to the nearest cluster, formula for calculating distance as:

d(x''m,) = Id(xil-mjl)', i=l...N; j=l...k; /=1 d(Xi, mJ) is the distance between data i and cluster j;

3) Calculate the mean of objects in each cluster as the new cluster centers, 1 "" m = -Ix, $i=1, 2 \dots k$; Nds the number of samples of, NFI" current cluster i;

4) Repeat 2) 3) until the criterion function E converged, return (m), m2 . . . mk). Algorithm terminates.

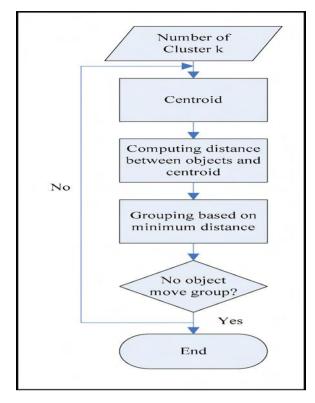


Fig 2.1 K mean algorithm process

III. RELATED WORK

Several attempts were made by researchers to improve the effectiveness and efficiency of the k-means algorithm [8]. A variant of the k-means algorithm is the k-modes [9]. Method which replaces the means of clusters with modes. Like the k-means method, the k-modes algorithm also produces locally optimal solutions which are dependent on the selection of the initial modes. The k-prototypes algorithm [9] integrates the k-means and k-modes processes for clustering the data. In this method, the dissimilarity measure is defined by taking into account both numeric and categorical attributes. The original k-means algorithm consists of two phases: one for determining the initial centroids and the other for assigning data points to the nearest clusters and then recalculating the cluster means. The second phase is carried out repetitively until the clusters get stabilized, i.e., data points stop crossing over cluster boundaries. Fang Yuan et al. [8] proposed a systematic method for finding the initial centroids. The centroids obtained by this method are consistent with the distribution of data. Hence it produced clusters with better accuracy, compared to the original k-means algorithm. However, Yuan's method does not suggest any improvement to the time complexity of the k-means algorithm. Fahim A M et al. proposed an efficient method for assigning data-points to clusters. The original k-means algorithm is computationally very expensive because each iteration computes the distances between data points and all the centroids. Fahim's approach makes use of two distance functions for this purpose- one similar to the k-means algorithm and another one based on a heuristics to reduce the number of distance calculations. But this method presumes that the initial centroids are determined randomly, as in the case of the original k-means algorithm. Hence there is no guarantee for the accuracy of the final clusters.

IV. PROPOSED ALGORITHM

In the novel clustering method discussed in this paper, both the phases of the original k-means algorithm are modified to improve the accuracy and efficiency. Input: $D = \{d1, d2,...,dn\} // \text{ set of } n \text{ data items}$

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A set of k clusters.
Steps:
Phase 1: Determine the initial centroids of the clusters

Input:

 $D = \{d1, d2,..., dn\}$ // set of *n* data items *k* // Number of desired clusters Output: A set of *k* initial centroids . Steps:

1. Set m = 1;

2. Compute the distance between each data point and all other data- points in the set D;

3. Find the closest pair of data points from the set D and form a data-point set Am $(1 \le m \le k)$ which contains these two data-points, Delete these two data points from the set D;

4. Find the data point in D that is closest to the data point set Am, Add it to Am and delete it from D;

5. Repeat step 4 until the number of data points in Am reaches 0.75*(n/k);

6. If m < k, then m = m+1, find another pair of data points from D between which the distance is the

shortest, form another data-point set Am and delete them from D, Go to step 4;

7. for each data-point set Am (1<=m<=k) find the arithmetic mean of the vectors of data points in Am, These means will be the initial centroids.

Phase 2: Assign each data point to the appropriate clusters

Input:

D = {d1, d2,.....,dh} // set of *n* data-points.
C = {c1, c2,.....,ck} // set of *k* centroids
Output:
A set of *k* clusters
Steps:
1. Compute the distance of each data-point *di* (1<=i<=n) to all the centroids *cj* (1<=j<=k) as *d(di, cj)*;
2. For each data-point *di*, find the closest centroid *cj* and assign *di* to cluster *j*.
3. Set ClusterId[i]=j; // j:Id of the closest cluster
4. Set Nearest_Dist[i]= *d(di, cj)*;
5. For each cluster *j* (1<=j<=k), recalculate the centroids;
6. Repeat
7. For each data-point *di*, 7.1 Compute its distance from the centroid of the present nearest cluster;
7.2 If this distance is less than or equal to the present nearest distance, the data-point stays in the

cluster; Else

7.2.1 For every centroid c_i (1<=j<=k) Compute the distance $d(d_i, c_i)$;

Endfor;

7.2.2 Assign the data-point *di* to the cluster with

the nearest centroid cj

7.2.3 Set ClusterId[i]=j;

7.2.4 Set Nearest_Dist[i]= d(di, cj);

Endfor;

8. For each cluster j (1<=j<=k), recalculate the centroids; Until the convergence criteria is met.

In the first phase, the initial centroids are determined systematically so as to produce clusters with better accuracy [8]. The second phase makes use of a variant of the clustering method discussed in . It starts by forming the initial clusters based on the relative distance of each data-point from the initial centroids. These clusters are subsequently fine-tuned by using a heuristic approach, thereby improving the efficiency. In this phase initially, compute the distances between each data point and all other data points in the set of data points. Then find out the closest pair of data points and form a set A1 consisting of these two data points, and delete them from the data point set D. Then determine the data point which is closest to the set A1, add it to A1 and delete it from D. Repeat this procedure until the number of elements in the set A1 reaches a threshold. At that point go back to the second step and form another data-point set A2. Repeat this till 'k' such sets of data points are obtained. Finally the initial centroids are obtained by averaging all the vectors in each data-point set. The Euclidean distance is used for determining the closeness of each data point to the cluster centroids. The distance between one vector X = (x1, x2, ..., xn) and another vector Y = (y1, y2, ..., yn) is obtained as d(X, Y) =Square root of $\{(x1-y1)2 + (x2 - y2)2 + ..., + (xn - yn)2\}$ The distance between a data point X and a data-point set D is defined as $d(X, D) = \min(d(X, Y), where Y \in D)$. The initial centroids of the clusters are given as input to the second phase, for assigning data-points to appropriate clusters.

The first step in Phase 2 is to determine the distance between each data-point and the initial centroids of all the clusters. The data-points are then assigned to the clusters having the closest centroids. This results in an initial grouping of the data-points. For each data-point, the cluster to which it is assigned (ClusterId) and its distance from the centroid of the nearest cluster (Nearest_Dist) are noted. Inclusion of data-points in various clusters may lead to a change in the values of the cluster centroids. For each cluster, the centroids are recalculated by taking the mean of the values of its data-points. Up to this step, the procedure is almost similar to the original k-means algorithm except that the initial centroids are computed systematically. The next stage is an iterative process which makes use of a heuristic method to improve the efficiency. During the iteration, the data-points may get redistributed to different clusters. The method involves keeping track of the distance between each data-point and the centroid of its present nearest cluster. At the beginning of the iteration, the distance of each data-point from the new centroid of its present nearest cluster is determined. If this distance is less than or equal to the previous nearest distance, that is an indication that the data point stays in that cluster itself and there is no need to compute its distance from other centroids. This result in the saving of time required to compute the distances to k-1 cluster centroids. On the other hand, if the new centroid of the present nearest cluster is more distant from the data-point than its previous centroid, there is a chance for the data-point getting included in another nearer cluster. In that case, it is required to determine the distance of the data-point from all the cluster centroids. Identify the new nearest cluster and record the new value of the nearest distance. The loop is repeated until no more data-points cross cluster boundaries, which indicates the convergence criterion. The heuristic method described above results in significant reduction in the number of computations and thus improves the efficiency.

V. CONCLUSION

The k-means algorithm is widely used for clustering large sets of data. But the standard algorithm do not always guarantee good results as the accuracy of the final clusters depend on the selection of initial centroids. Moreover, the computational complexity of the standard algorithm is objectionably high owing to the need to reassign the data points a number of times, during every iteration of the loop. This paper presents an enhanced k-means algorithm which combines a systematic method for finding initial centroids and an efficient way for assigning data points to clusters. This method ensures the entire process of clustering in O(n2) time without sacrificing the accuracy of clusters. The previous improvements of the k-means algorithm compromise on either accuracy or efficiency. A limitation of the proposed algorithm is that the value of k, the number of desired clusters, is still required to be given as an input, regardless of the distribution of the data points. Evolving some statistical methods to compute the value of k, depending on the data distribution, is suggested for future research. A method for refining the computation of initial centroids is worth investigating.

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