A new algorithm for choosing initial cluster centers for k-means

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Abstract—The k-means algorithm is widely used in many applications due to its simplicity and fast speed. However, its result is very sensitive to the initialization step: choosing initial cluster centers. Different initialization algorithms may lead to different clustering results and may also affect the convergence of the method. In this paper, we propose a new algorithm for improving the initialization of the cluster centers by reducing dimensions followed by moving cluster centers towards high density regions. Our algorithm is compared with three other initialization algorithms for k-means. And the effectiveness of our approach is shown by a series of carefully designed experiments.

Keywords—K-means, cluster analysis

I. INTRODUCTION

Because of the importance of clustering algorithm in data mining and pattern recognition, many different clustering algorithms have been developed. With the fast development of technologies, such as data storage, camera acquisition, and medical equipment data acquisition, the increasingly inflation of the data, puts forwards the requirements for data clustering with high speed. Although the k-means algorithm has been proposed a long time ago [1], it is still the most widely used clustering method for its simplicity and fast speed which makes it a suitable method for clustering large amounts of data [2].

However, the clustering result of k-means is severely affected by the choice of initial cluster centers, especially in the case of a large number of clusters. The traditional k-means method chooses initial cluster centers arbitrarily, which may affect its accuracy in the clustering [3], [4].

K-means++ [3] is an improved version of k-means. The first center is chosen from the data set randomly, the other centers are chosen with a probability: the further a point is from the selected centers the larger the probability for the point to be chosen as a new center. The improvement not only speeds up the convergence of the clustering process but yields a better clustering result than k-means [3]. However, k-means++ may choose outliers or data points located at low density area as cluster centers, which may lead to sub-optimal solutions.

To overcome the disadvantages of the randomness in selecting initial cluster centers, another method for choosing cluster centers has been proposed by Murat Erisoglu, et al. [4]. This method first chooses two main dimensions that best represent the distribution of the dataset, and then computes Euclidean distances between each data point and the centroid of the data in the subspace defined by the two selected dimensions. The first cluster center is the data point with the longest distance from the centroid in the subspace. The i-th cluster center is the data point with the maximum combined distance from the previous (i-1) cluster centers. The algorithm has been shown to be effective in improving the k-means method when applied to some real data sets [4]. However, in our study of the algorithm, it is found that when it is applied to some synthetic data sets containing noise, the algorithm sometimes chooses noise data point far away from the centroid as the cluster center. Moreover, when the algorithm is launched multiple times on the same data set, it produces the same result.

To overcome the drawbacks of the available methods, we propose a new algorithm for initializing the cluster centers for k-means algorithm. After reducing the number of the dimensions of data sets, the candidate cluster centers are chosen similarly as k-means++, the final cluster centers are chosen by moving the candidate centers towards high density area.

The rest of the paper is organized as follows. The proposed algorithm for choosing initial cluster centers is introduced in Section 2. The experimental results are presented in Section 3. Conclusions are drawn in Section 4.

II. PROPOSED ALGORITHM

In this section, the proposed algorithm for choosing initial cluster centers is described. It consists of three parts.

A. Reducing the number of dimensions

First, in order to speed up the process of choosing the initial cluster centers, a two dimensional subspace is selected from the feature space, in other words, two main variables which are most representative for the original data are selected for initializing the cluster centers, which is similar to the method used by Murat Erisoglu, et al. [4]. The first variable is the one which has the maximum absolute value of the coefficient of variation, where the coefficient of variation is determined by

\[ CV_j = \frac{s(x_j)}{\bar{x}_j} \quad j = 1, 2, ..., p \]  \hspace{1cm} (1)

where \(s(x_j)\) is the standard deviation, \(\bar{x}_j\) is the mean of the \(j\)-th attribute variable, and \(p\) is the number of features. Then, we make use of the correlation coefficient of the variables to select the second main variable. The correlation coefficient is defined as
The proposed algorithm utilizes a method similar to Mean Shift to move the candidate cluster centers to high density area, avoiding the issue of choosing cluster centers at low density area. Fig. 1 shows the shifting process. The four circles with a dot in the middle indicate the initial candidate centers, the four circles with asterisks in the middle represent the final cluster centers, and the other circles show the process of center shifting.

B. Experiments on several data sets

The performance of our proposed method is compared with k-means, k-means++ and a method proposed by Murat Erisoglu, et al. [[4]] on three synthetic data sets. Each data set is generated by Gaussian distribution function. FM Index [错误!未找到引用源。] is used to evaluate the clustering results of the four methods. By running each algorithm 100 times on the identical data set, the maximum and average of FM indices are recorded in Table I through Table III.

The first group of data sets is produced by changing the total number of data points while fixing the number of dimensions to 5 and the number of clusters to 8. The clustering results on this data set are showed in Table I. Our method produces the highest maximum FM indices when the number of data points is 5000 and 20000. The average FM indices from our method are the highest in the four algorithms applied on four data sets.

The second group of data sets is generated by varying the number of clusters and fixing the number of data points to 10000 in 5-dimension space. Table II shows the FM indices of the clustering results. The average FM indices of all the methods are decreasing with the increasing of the number of clusters. The maximum and the average FM indices produced by our method are higher than these of the other three algorithms when the number of the clusters reaches 10 and then 20. And it is noticed that the increase of the speed of our method is lower than these of the other three algorithms when the number of the clusters reaches 10 and then 20. And it is noticed that the increase of the speed of our method is lower than these of the other three algorithms when the number of the clusters reaches 10 and then 20. And it is noticed that the increase of the speed of our method is lower than these of the other three algorithms when the number of the clusters reaches 10 and then 20.

The third group of data sets is generated by varying the number of dimensions while fixing the total number of data points to 10000 and the number of clusters to 10. Table III shows the results for the data sets. Due to the increased distances between the centroids of different clusters included in four synthetic data sets in high-dimensional space, the maximum and average FM indices are increasing as the number of dimensions increasing. Our method has the best performance indicated by the average FM Indices on four data sets. Considered together, our method has a stable performance on a large part of tested data sets.

A. Comparison of the methods

The random initial cluster centers in k-means method sometimes leads to bad clustering result. Similarly, the first cluster center of k-means++ is selected arbitrarily, so it can be an outlier or a data point located at low density area, which is also possible for other cluster centers.

$$CC_j = \frac{\sum_{i=1}^{n}(x_i - \bar{x}_j)(\bar{x}_j - \bar{x}_j)}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x}_j)^2} \sqrt{\sum_{j=1}^{m}(\bar{x}_j - \bar{x}_j)^2}}$$

(2)
IV. CONCLUSION

Because of the fast speed and wide applications of k-means, several algorithms are proposed in recent years to optimize the initialization of cluster centers in k-means. Most of the current methods may select initial cluster centers in low density region which may result in bad clustering results. So we propose a new method for choosing cluster centers using a combination of dimension reduction, selecting cluster centers with a probability, and followed by shifting the cluster centers towards high density area.

By reducing the number of dimensions to 2, we speed the process of the initialization. By shifting the candidate centers to high density area, the final clustering results can be improved. Experiments show the effectiveness of our method compared with three other methods. There are still problems with our proposed method: the speed of our method is not as good as k-means. So our future work will be concentrating on how to make the method more efficient.

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VI. REFERENCES


