P-k-means: k-means using Partition based Cluster Initialization Method

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A B S T R A C T

The k-Means algorithm is extensively used in a number of data clustering applications. In basic k-means, initial cluster centroids are selected on random basis. As a result, every run of k-means leads to the formation of different clusters. Hence, accuracy and performance of k-means is susceptible to the selection of initial cluster centroids. Therefore, careful initialization of cluster centroids plays a major role on accuracy and performance of the k-means algorithm. In view of this, a new k-means using Partition based Cluster Initialization method called as 'P-k-means' is proposed in this paper. The experiment is carried out on six different datasets. The empirical results are compared using various external and internal clustering validation measures. The comparative results show that P-k-means is better than basic k-means.

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1. Introduction

Data mining is commonly used in numerous applications (Arora & Gupta, 2017; Han, Kamber & Pei, 2012). Clustering is one of the essential functions of data mining which is based on unsupervised learning (or learning by observations). It groups the data objects based on the distance or similarity. The objects which are similar or close to each other are grouped in the same cluster whereas the objects which are dissimilar or far off are grouped in another cluster (Han, Kamber & Pei, 2012; Jain & Dubes, 1988). The distance or similarity is defined based on the behavior or characteristics of the data objects by the various clustering methods (Gupta & Chandra, 2019; Jain, Murty, & Flynn, 1999).

A number of clustering methods have been proposed by many researchers so far. Out of these methods, basic k-means is considered as oldest and commonly used clustering algorithm to identify spherical-shaped clusters. Basic k-means is described as follows (*Algorithm 1*):

Algorithm 1: Basic k-means

1. *Decide k (no. of clusters)*
2. *Randomly initialize cluster centroids* $C = \{c_1, c_2, \dots, c_k\}$
3. *Repeat*
    a. *For each data point* (x_i) *in data set (D)*
        i. *Compute distance* dis(x_i, C) *between* x_i *and all cluster centroids*
        ii. *Assign* d_i *to the nearest cluster*
    b. *Re-compute cluster centroids as the mean of all cluster members.*
4. *Until cluster membership stabilizes.*

As per Step 2 of basic k-means, the randomized selection of initial cluster centroids leads to a different set of clusters in every run of the algorithm.

Related work done by some leading researchers in the area of cluster centroid initialization for k-means is presented in *section 2* of this paper. The new approach called as P-k-means for initialization of cluster centroid is proposed and described in *section 3*. In *section 4*, the empirical results are presented. The results are compared based on the several metrices such as accuracy, performance, Within-cluster Sum of Squared Error (WSSE), Between-cluster Sum of Squared Error (BSSE), Purity, Precision, Recall and F-Measure. Finally in *section 5*, the conclusion is drawn. The results show that P-k-means outperforms the basic k-means in terms of the aforesaid metrics.

2. Related Work

The accuracy, performance and reliability of basic k-means is majorly depends on the selection of initial cluster centroids. Therefore, if the initial clusters centroids are chosen which are closer to the actual cluster centroids then accuracy, performance and reliability of the k-means will be better. In view of this, many researchers have modified the basic k-means and proposed a number of different methods to initialize the cluster centroids (Gan, Ma, & Wu, 2007; Motwani, Arora, & Gupta, 2019; Jain, 2010; Xu, & Tian, 2015).

The initial attempt for cluster initialization was made by Forgy (Forgy, 1965) based on the random selection. The Forgy's method was slightly modified by several researchers (McQueen, 1967; Kaufman & Rousseeuw, 1990; Katsavounidis, Kuo & Zhang, 1994; Bradley & Fayyad, 1998). New methods based on data distribution, estimation of density, deterministic divisive method, maximin initialization and hierarchical method was proposed in (Pei, Fan & Xie, 1999; Khan & Ahmad, 2004; Su & Dy, 2004; Hathaway, Bezdek & Huband, 2006; Arai & Barakbah, 2007) respectively. Arthur and Vassilvitskii (2007) proposed k-means algorithm based on improved cluster initialization method called as k-means++. A number of attempts have been made by several other researchers (Wu, Jiang & Huang, 2007; Kang & Cho, 2009; Maitra, 2009; Xu, Xu & Zhang, 2009; Dang, Xuan, Rong & Liu, 2010; Naldi, Campello, Hruschka & Carvalho, 2011; Reddy, Mishra & Jana, 2011; Bai, Liang, Dang & Cao, 2012; Chen, 2012; Aldahdooh & Ashour, 2013; Goyal & Kumar, 2014; Duwairi & Abu-Rahmeh, 2015; Poomagal, Saranya & Karthik, 2016; Dhanabal & Chandramathi, 2017; Golasowski, Martinovič & Slaninová, 2017; Kumar & Reddy, 2017; Ismkhan, 2018; Nguyen, Duc & Duong, 2018; Sandhya & Sekar, 2018; Yu, Chu, Wang, Chan & Chang, 2018; Kurada & Kanadam, 2019).

3. Proposed Method

In order to improve the accuracy, performance and objective function of k-means, a novel scheme for initializing cluster centroids has been devised. In this method, the range of each dimension (or attribute), dim_i, of the data set is logically divided in k equi-sized partitions, where k refers to the # of clusters. The collection of k equi-sized partitions of all dimensions is modeled as $k \times d$ Matrix where d is the # of dimensions. From this Matrix, k distinct sets, where each set consists of one randomly selected partition from each dimension, are selected as k centroids for the k-means algorithm. From each selected partition, a randomized value is selected in the set. The motivation behind this method is that the clusters may spread horizontally, vertically, diagonally or in arc shaped. Therefore, to guess the centroids randomly from these cells will be more near to the actual centroids which results in the higher accuracy and performance of the k-means. The proposed method, k-means using Participation Based Cluster Initialization Method called as P-k-means, is presented as *Algorithm 2*.

Algorithm 2: P-k-means: k-means using Partition Based Cluster Initialization Method

1. *Decide k (no. of clusters)*
2. *Initialize cluster centroids* $C = \{c_1, c_2, \ldots, c_k\}$ *as*
   a. *Divide the range of data of each dimension,* dim_i *into k equi-ranged partitions.*
   b. *Repeat*
   c. *Randomly choose one partition from each dimension* (dim_i)*, which was not selected earlier.*
   d. *Find the randomized value of each partition selected for centroid.*
   e. *Until all centroids are chosen.*
3. *Repeat*
   a. *For each data point* (x_i) *in data set (D)*
      i. *Compute distance* $dis(x_i, C)$ *between* x_i *and all cluster centroids*
      ii. *Assign* x_i *to the nearest cluster*
   b. *Re-compute cluster centroids as the mean of all cluster members.*
4. *Until cluster membership stabilizes.*

4. Experiment Design and Results

The k-Means based on the both proposed and the traditional methods have been implemented in MATLAB. Both the methods have been executed on 6 data sets taken from UCI and Hartigan. The results computed and compared based on the average of 200 runs of each of the methods on each of the data sets used.

4.1. Dataset used

Both the methods have been evaluated on six different datasets Pen Digit, Iris, Image Segmentation, Spambase, Wine and Animal Milk. First five datasets are taken from UCI. The sixth data set Animal Milk is taken from Hartigan. The characteristics of these datasets are presented in Table 1.

Table 1 - Datasets Used

Dataset	No. of Instances	No. of Attributes	No. of Clusters
Pen Digit	7494	16	10
IRIS	150	4	3
Image Segmentation	2100	19	7
Spambase	4601	57	2
Wine	178	13	3
Animal Milk	16	4	5

4.2. Metric

The k-Mean algorithm has been tested using both the methods. The average of 200 runs of each of the methods on each of the above mentioned six datasets has been taken. The implementation is the standard one with no special optimizations.

4.3. Clustering Evaluation and Validation Measures

Clustering evaluation and validation measures are reliable and independent measures used to evaluate, assess the validity of goodness of the clustering (Halkidi, Batistakis & Vazirgiannis, 2001). These are also used for the comparison of experiments and results of the clustering algorithms. The measures are broadly classified into three categories external, internal and relative (Theodoridis & Koutroubas, 2003).

4.3.1. External Measures

External measures are based on supervised learning in which clustering is compared against the prior or expert-specified knowledge (i.e. ground truth or manual classification). These measures do not employ criteria intrinsic to the dataset (Halkidi, Batistakis & Vazirgiannis, 2001; Rendón, Abundez, Arizmendi & Quiroz, 2011). A number of external measures are commonly used. In this paper, the empirical results are compared based on Purity, Precision, Recall and F-measure external measures.

4.3.2. Internal Measures

Internal measures evaluate the goodness of clustering. These are mostly based on two criteria intra-cluster compactness (or cohesion) and inter-cluster separation (Halkidi, Batistakis & Vazirgiannis, 2001). There is a trade-off in maximizing intra-cluster cohesion and inter-cluster separation. These measures employ criteria derived from the dataset itself. A number of internal measures are commonly used. The sum of squared error (SSE) is the widely used internal measure for clustering validation and also used in this paper.

4.3.3. Relative Measures

These are used to evaluate the results of clustering based on the different parameter settings for the same algorithm.

4.4. Results and Discussion

The comparative empirical evaluation of basic k-Means and P-k-means are presented in *Table 2* through *Table 8*. The results of both the methods are evaluated and compared based on (i) Iterations taken to converge, (ii) Accuracy of Cluster Assignment, (iii) Within-cluster SSE, (iv) Between-cluster SSE, (v) Purity / Precision of Clustering, (vi) Recall of Clustering and (vii) F-Measure of Clustering. As the purity and precision gives the same result hence the results of both purity and precision is presented in the same table.

The comparative performance based on average # of iterations taken to converge by both the methods is presented in *Tables 2*. In *Table 3*, the accuracy of the both the methods based on cluster assignments compared with ground truth are presented. *Table 4* and *Table 5* present the Within-cluster Sum of Squared Error (WSSE) and Between-cluster Sum of Squared Error (BSSE) of both the methods respectively. In *Table 6* through *Table 8*, the Purity / Precision, Recall and F-Measure of the clustering compared based on the ground truth of both the methods are presented respectively.

Table 2 shows that performance of P-k-means is better than basic k-means for all datasets except Animal Milk. The accuracy of P-k-means is better as compared to the basic k-means for all datasets as shown in *Table 3*. *Table 4* and *Table 5*, shows that WSSE and BSSE of P-k-means are also better than that of basic k-means. The Purity / Precision Measure of P-k-means in four data sets are better than that of basic k-means (*Table 6*). The Recall and F-Measure of P-k-means are also better than that of basic k-means for all datasets except Wine dataset as shown in *Table 7* and *Table 8*.

Table 2 - Iterations taken to Converge

Dataset	Basic K-means	P-k-means
Pen Digit	28.65	27.69
IRIS	9.22	8.62
Image Segmentation	13.89	13.79
Spambase	7.13	6.87
Wine	11.87	10.68
Animal Milk	38.42	38.90

Table 3 - Accuracy of the Cluster Assignment

Dataset	Basic K-means	P-k-means
Pen Digit	75.89%	76.09%
IRIS	88.81%	88.83%
Image Segmentation	97.09%	97.19%
Spambase	98.92%	98.92%
Wine	71.70%	72.57%
Animal Milk	96.96%	97.49%

Table 4 - Within-cluster SSE (WSSE)

Dataset	Basic K-means	P-k-means
Pen Digit	3510918.33	3502339.52
IRIS	27.14	26.83
Image Segmentation	4274503.45	4380699.66
Spambase	620211350.51	620211350.51
Wine	841436.80	867154.49
Animal Milk	7.67	7.28

Table 5 - Between-cluster SSE (BSSE)

Dataset	Basic K-means	P-k-means
Pen Digit	109851.99	109844.49
IRIS	13.05	13.08
Image Segmentation	2273924.87	2317511.20
Spambase	7088425076.79	7088425076.79
Wine	296495.06	305144.18
Animal Milk	682.73	692.07

Table 6 - Purity / Precision of Clusters

Dataset	Basic K-means	P-k-means
Pen Digit	0.7718	0.7651
IRIS	0.8972	0.9020
Image Segmentation	0.8042	0.8028
Spambase	0.6671	0.6875
Wine	0.7406	0.7433
Animal Milk	0.9582	0.9643

Table 7 - Recall of Clusters

Dataset	Basic K-means	P-k-means
Pen Digit	0.7167	0.7202
IRIS	0.8807	0.8869
Image Segmentation	0.2162	0.2175
Spambase	0.5073	0.5265
Wine	0.6561	0.6474
Animal Milk	0.9160	0.9280

Table 8 - F-Measure of Clusters

Dataset	Basic K-means	P-k-means
Pen Digit	0.7079	0.7102
IRIS	0.8789	0.8852
Image Segmentation	0.1151	0.1163
Spambase	0.3945	0.4379
Wine	0.6703	0.6632
Animal Milk	0.9125	0.9246

5. Summary and Conclusion

The basic k-Means is widely used because it is easy to implement and no complexity is involved in initializing the cluster centroids randomly. But, the accuracy and performance of k-means algorithm is sometimes extremely affected due to the initial cluster centroids. The proposed P-k-means is also easy to implement as it is also based on random selection. In P-k-means, k centroids are randomly selected which are having high probability to be closer to the actual cluster centroids. The empirical results presented in *Table 2* through *Table 8* show that P-k-means is better than basic k-means in terms of Accuracy, Performance, WSSE, BSSE, Purity / Precision, Recall and F-Measure. The results clearly shows that there is about 10% less number of iterations are required to converge the P-k-means and about 5% accuracy is increased in P-k-means as compared to basic k-means. In view of the above, the P-k-means outperformed the basic k-means algorithm.

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