

A Deterministic Seeding Approach for k-means Clustering

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ABSTRACT

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In this work, a simple and efficient approach is proposed to initialize the k-means clustering algorithm. The complexity of this method is $O(nk)$, where n is the number of data and k the number of clusters. Performance evaluation was done by applying this approach on various benchmark datasets and comparing with the related deterministic KKZ seed algorithm. Experimental results have demonstrated that this approach produces more consistent clustering results in term of average silhouette index.

Keywords: clustering, k-means, initialization, KKZ, silhouette.

I. INTRODUCTION

Cluster analysis is the most widely used technique in Data Mining. Clustering consists of grouping a given dataset into a predefined number of disjoint sets, called clusters, so that the elements in the same cluster are more comparable to each other and more different from the elements in the other cluster. This optimization problem is known to be NP-hard, even when the clustering process deals with only two clusters [1]. Therefore, many heuristics have been proposed, in order to find near optimal clustering solution in reasonable computational time. The most prominent clustering method k-means is a greedy algorithm which has two stages: Initialization, in which we set the seed set of centroids, and an iterative stage, called Lloyd's algorithm [6]. Additionally, Lloyd's algorithm has two steps: The assignment step, in which each object is assigned to its closest centroid, and the centroid's update step. The time required for the assignment step is $O(nkd)$,

while the centroid's update step and the computation of the error function is $O(nd)$. The main advantage of k-means is its fast convergence to a local minimum. A major drawback of k-means is its sensitivity to the initial clustering centers (namely, seed). To achieve a better initialization, many techniques have been proposed. In this study, yet another k-means initialization technique is proposed.

In the next section, some related works are briefly discussed. Then the proposed method and its computational complexity are described in Section 3. Section 4 consists to apply this approach to some standard data sets and reports its performance. Finally, conclusion of the paper is summarized in Section 5.

II. RELATED WORK

Several initialization methods have been proposed in the literatures. Among them, Katsavounidis et al. [4]

utilize the sorted pairwise distances for initialization which has been termed as the KKZ algorithm. This algorithm chooses the vector with maximal norm as the first seed, then For $j = 2, \dots, k$, each centroid m_j is set in the following way: For any remaining data x_i , its distance d_i to the existing centroids is computed. d_i is calculated as the distance between x_i to its closest existing centroid. Then, the point with the largest d_i is selected as m_j . The computational complexity of KKZ is $O(nk)$.

Another initialization method that is based on simple probabilistic seeding procedures. In particular, the k-means++ method, proposed by Arthur and Vassilvitskii in [3], consists of randomly selecting only the first centroid from the dataset. The greedy k-means++ method probabilistically selects k centers in each round and then greedily selects the center that most reduces the SSE. It chooses the first center randomly and the i -th ($i \in \{2, 3, \dots, k\}$) center is chosen to be $x' \in X$ with a probability of

$$md(x')^2 / \sum_{j=1}^n md(x_j)^2 \tag{1}$$

where $md(x)$ denotes the minimum-distance from a point x to the previously selected centers. The drawback of this approach is referred to its sequential nature, as well as to the fact that it requires k scans of the entire dataset, therefore it has a complexity of $O(nkd)$.

III. PROPOSED APPROACH

Pseudo-code:

INPUT: a dataset X whose cardinality is n and an integer k

OUTPUT: k seeds c_i

$c = \text{mean}(X)$

for $i=1$ to k **do**

$j = \text{ArgMax}(d(X_h, c))$

$1 \leq h \leq n$

$c = c + X_j$

$\text{output}(c)$

end;

Complexity:

Clearly, the complexity of this method is $O(nk)$.

IV. EXPERIMENTAL RESULTS

Algorithm validation is conducted using different data sets from the UCI Machine Learning Repository [2]. We evaluated its performance by applying on several benchmark datasets and compare with KKZ_k-means. In preprocessing step, the data were normalized.

Silhouette index [5] which measures the cohesion based on the distance between all the points in the same cluster and the separation based on the nearest neighbor distance, was used in these experiments in order to evaluate clustering accuracy.

The proposed approach was compared with a related deterministic clustering method: KKZ_k-means (k-means initialized by KKZ).

Experimental results are reported in table 1 and figure 1.

Table 1. Experimental results of KKZ_k-means and proposed approach on different datasets in term of average Silhouette value.

Data set	k	KKZ_k-means	Proposed
Iris	3	0.7542	0.8152
Ruspini	4	0.9086	0.9097
Aggregation	7	0.6536	0.7410
Compound	6	0.6484	0.7464
Pathbased	3	0.7316	0.7253
Spiral	3	0.5206	0.4953
D31	31	0.5881	0.7629
R15	15	0.5966	0.7475

Jain	2	0.6719	0.9078
Flame	2	0.5347	0.8760
s1	15	0.7333	0.7262
s2	15	0.6024	0.7375
s3	15	0.6117	0.6253
s4	15	0.6330	0.6303
t4.8k	8	0.5841	0.6789
dim2	9	0.7816	0.7896
dim3	9	0.3966	0.6190
dim4	9	0.5849	0.8716
dim5	9	0.4490	0.7565
dim6	9	0.6308	0.7346
dim7	9	0.5652	0.8858
dim8	9	0.4604	0.6553
dim9	9	0.3778	0.4865
dim10	9	0.3738	0.6424
dim11	9	0.5092	0.4209
dim12	9	0.4329	0.6813
dim13	9	0.6241	0.6637
dim14	9	0.6909	0.4973
dim15	9	0.5527	0.3829
a1	20	0.5542	0.7048
a2	35	0.5970	0.6811
a3	50	0.5752	0.6917

V. CONCLUSION

In this study, a deterministic initialization method for the k-means algorithm was suggested. Its time complexity is $O(nk)$ and experimental results have demonstrated that the proposed approach produces quickly consistent clustering results in term of average silhouette index. Future work will consist to consider a possible improvement of this method by avoiding dataset outliers, in order to obtain more accurate clustering results.

VI. REFERENCES

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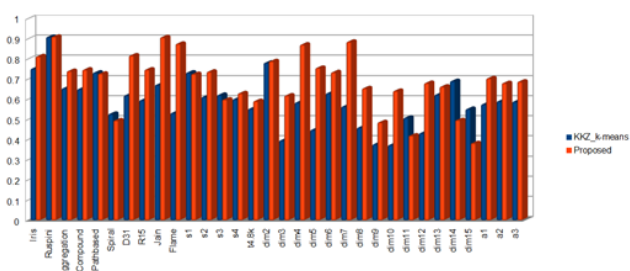


Fig 1: Chart of *kkz_kmeans* and proposed approach on different datasets in term of average Silhouette value

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