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# The global k-means lustering algorithm

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**Intelligent Autonomous Systems**

We present the global k-means algorithm which is an incremental approach to clustering that dynamically adds one cluster center at a time through a deterministic global search procedure consisting of  $N$  (with  $N$  being the size of the data set) exe
utions of the k-means algorithm from suitable initial positions. We also propose modifications of the method to reduce the computational load without significantly affecting solution quality. The proposed clustering methods are tested on well-known data sets and they ompare favorably to the k-means algorithm with random restarts.

Keywords: Clustering; K-means algorithm; Global optimization; k-d trees, Data mining.



Submitted to Pattern Recognition

# **Contents**



## Intelligent Autonomous Systems

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#### 1 **Introduction**

A fundamental problem that frequently arises in a great variety of fields such as pattern recognition, image processing, machine learning and statistics is the clustering problem [1]. In its basic form the clustering problem is defined as the problem of finding groups of data points in a given data set. Each of these groups is called a cluster and can be defined as a region in which the density of objects is locally higher than in other regions.

The simplest form of clustering is partitional clustering which aims at partitioning a given data set into disjoint subsets (clusters) so that specific clustering criteria are optimized. The most widely used criterion is the clustering error criterion which for each point computes its squared distance from the corresponding cluster center and then takes the sum of these distances for all points in the data set. A popular clustering method that minimizes the clustering error is the k-means algorithm. However, the k-means algorithm is a local search procedure and it is well-known that it suffers from the serious drawback that its performance heavily depends on the initial starting conditions [2]. To treat this problem several other techniques have been developed that are based on sto
hasti global optimization methods (eg. simulated annealing, geneti algorithms). However, it must be noted that these te
hniques have not gained wide acceptance and in many practical applications the clustering method that is used is the k-means algorithm with multiple restarts  $[1]$ .

In this work we propose the global k-means clustering algorithm, which constitutes a deterministic effective global clustering algorithm for the minimization of the clustering error that employs the k-means algorithm as a local search procedure. The algorithm proceeds in an incremental way: to solve a clustering problem with  $M$  clusters, all intermediate problems with  $1, 2, \ldots, M-1$  clusters are sequentially solved. The basic idea underlying the proposed method is that an optimal solution for a clustering problem with  $M$  clusters can be obtained using a series of local searches (using the k-means algorithm). At each local search the  $M-1$  cluster centers are always initially pla
ed at their optimal positions orresponding to the lustering problem with  $M-1$  clusters. The remaining M-th cluster center is initially placed at several positions within the data space. Since for  $M = 1$  the optimal solution is known, we can iteratively apply the above procedure to find optimal solutions for all k-clustering problems  $k = 1, \ldots, M$ . In addition to effectiveness, the method is deterministic and does not depend on any initial conditions or empirically adjustable parameters. These are significant advantages over all clustering approa
hes mentioned above.

In the following section starts with a formal definition of the clustering error and a brief des
ription of the k-means algorithm and then des
ribes the proposed global k-means algorithm. Section 3 describes modifications of the basic method that require less computation at the expense of being slightly less effective. Section 4 provides experimental results and comparisons with the k-means algorithm with multiple restarts. Finally Section 5 provides conclusions and des
ribes dire
tions for future resear
h.

## 2 The global k-means algorithm

Suppose we are given a data set  $X = \{x_1, \ldots, x_N\}$ ,  $x_n \in R^+$ . The *M*-clustering problem aims at partitioning this data set into M disjoint subsets (clusters)  $C_1, \ldots, C_M$ , such that a clustering riterion is optimized. The most widely used lustering riterion is the sum of the squared Euclidean distances between each data point  $x_i$  and the centroid  $m_k$  (cluster center) of the subset  $C_k$  which contains  $x_i$ . This criterion is called clustering error and depends on the cluster

centers  $m_1, \ldots, m_M$ :

$$
E(m_1, \ldots, m_M) = \sum_{i=1}^{N} \sum_{k=1}^{M} I(x_i \in C_k) |x_i - m_k|^2
$$
 (1)

where  $I(X) = 1$  if X is true and 0 otherwise.

The k-means algorithm finds locally optimal solutions with respect to the clustering error. It is a fast iterative algorithm that has been used in many clustering applications. It is a point-based lustering method that starts with the luster enters initially pla
ed at arbitrary positions and pro
eeds by moving at ea
h step the luster enters in order to minimize the lustering error. The main disadvantage of the method lies in its sensitivity to initial positions of the luster enters. Therefore, in order to obtain near optimal solutions using the k-means algorithm several runs must be scheduled differing in the initial positions of the cluster centers.

In this paper, the global k-means clustering algorithm is proposed, which constitutes a deterministi global optimization method that does not depend on any initial parameter values and employs the k-means algorithm as a local search procedure. Instead of randomly selecting initial values for all cluster centers as is the case with most global clustering algorithms, the proposed te
hnique pro
eeds in an in
remental way attempting to optimally add one new luster enter at ea
h stage.

More specifically, to solve a clustering problem with  $M$  clusters the method proceeds as follows. We start with one cluster  $(k = 1)$  and find its optimal position which corresponds to the centroid of the data set X. In order to solve the problem with two clusters  $(k = 2)$  we perform <sup>N</sup> exe
utions of the k-means algorithm from the following initial positions of the luster enters: the first cluster center is always placed at the optimal position for the problem with  $k = 1$ , while the second center at execution n is placed at the position of the data point  $x_n$   $(n = 1, \ldots, N)$ . The best solution obtained after the  $N$  executions of the k-means algorithm is considered as the solution for the clustering problem with  $\kappa = z$ . In general, let  $(m_1(\kappa), \ldots, m_k(\kappa))$  denote the final solution for k-clustering problem. Once we have found the solution for the  $(k - 1)$ clustering problem, we try to find the solution of the k-clustering problem as follows: we perform N runs of the k-means algorithm with  $k$  clusters where each run  $n$  starts from the initial state  $(m_1(\kappa-1), \ldots, m_{(k-1)}(\kappa-1), x_n)$ . The best solution obtained from the N runs is considered as the solution  $(m_1(k), \ldots, m_k(k))$  of the k-clustering problem. By proceeding in the above fashion we finally obtain a solution with  $M$  clusters having also found solutions for all k-clustering problems with  $k < M$ .

The latter characteristic can be advantageous in many applications where the aim is also to discover the 'correct' number of clusters. To achieve this, one has to solve the k-clustering problem for various numbers of clusters and then employ appropriate criteria for selecting the most suitable value of  $k$  [3]. In this case the proposed method directly provides clustering solutions for all intermediate values of  $k$ , thus requiring no additional computational effort.

In what concerns computational complexity, the method requires  $N$  executions of the kmeans algorithm for each value of  $k$  ( $k = 1, \ldots, M$ ). Depending on the available resources and the values of N and M, the algorithm may be an attractive approach, since, as experimental results indicate, the performance of the method is excellent. Moreover, as we will show later there are several modifications that can be applied in order to reduce the computational load.

The rationale behind the proposed method is based on the following assumption: an optimal clustering solution with  $k$  clusters can be obtained through local search (using k-means) starting from an initial state with

- the k is the contract position at the optimized positions for the (i) I contracted problem and the
- the remaining k-th enter pla
ed at an appropriate position to be dis
overed.

This assumption seems very natural: we expect that the solution of the k-clustering problem to be reachable (through local search) from the solution of  $(k-1)$ -clustering problem, once the additional enter is pla
ed at an appropriate position within the data set. It is also reasonable to restrict the set of possible initial positions of the k-th center to the set X of available data points. It must be noted that this is a rather omputational heavy assumption and several other options (examining fewer initial positions) may also be onsidered. The above assumptions are also verified experimentally, since in all experiments (and for all values of  $k$ ) the solution obtained by the proposed method was at least as good as that obtained using numerous random restarts of the k-means algorithm. In this spirit, we an autiously state that the proposed method is experimentally optimal (although it is difficult to prove theoretically).

## 3 Speeding-up execution

Based on the general idea of the global k-means algorithm, several heuristics can be devised to reduce the computational load without significantly affecting the quality of the solution. In the following subsections two modifications are proposed, each one referring to a different aspect of the method.

### 3.1 The fast global k-means algorithm

The fast global k-means algorithm constitutes a straightforward method to accelerate the global k-means algorithm. The difference lies in the way a solution for the k-clustering problem is obtained, given the solution of the  $(k-1)$ -clustering problem. For each of the N initial states  $(m_1(\kappa-1), \ldots, m_{(k-1)}(\kappa-1), x_n)$  we do not execute the k-means algorithm until convergence to obtain the final clustering error  $E_n$ . Instead we compute an upper bound  $E_n \leq E - b_n$ on the resulting error  $E_n$  for all possible allocation positions  $x_n$ , where E is the error in the  $(k-1)$ -clustering problem. We then initialize the position of the new cluster center at the point  $x_i$  that minimizes  $E_n$ , or equivalently that maximizes  $b_n$ , and execute the k-means algorithm to obtain the solution with  $k$  clusters. Formally we have

$$
b_n = \sum_{j=1}^{N} \max(d_{k-1}^j - |x_n - x_j|^2, 0), \tag{2}
$$

$$
i = \arg\max_{n} b_n \tag{3}
$$

where  $d'_{k}$  $k-1$  is the square distance set the signal distance of  $\mathcal{L}$  and the k  $\mathcal{L}$  and  $\mathcal{L}$  and  $\mathcal{L}$  and  $\mathcal{L}$ centers obtained so far (ie., center of the cluster where  $x_i$  belongs). The quantity  $b_n$  measures the guaranteed reduction in the error measure obtained by inserting a new cluster center at position  $x_n$ .

Suppose the solution of the  $(\kappa - 1)$ -clustering problem is  $(m_1(\kappa - 1), \ldots, m_{(k-1)}(\kappa - 1))$  and a new cluster center is added at location  $x_n$ . Then the new center will allocate all points  $x_i$  whose squared distance from  $x_n$  is smaller than the distance  $d_k^{\gamma}$  $\kappa-1$  in the set of t Therefore, for each such data point  $x_j$  the clustering error will decrease by  $d_{k-1}^i - |x_n - x_j|^2$ . The summation over all such data points  $x_i$  provides the quantity  $b_n$  for a specific insertion location  $x_n$ . Since the k-means algorithm is guaranteed to decrease the clustering error at each step,  $E - b_n$  upper bounds the error measure that will be obtained if we run the algorithm until convergence after inserting the new center at  $x_n$  (this is the error measure used in the global k-means algorithm).

Experimental results (see next section) suggest that using the data point that minimizes this bound leads to results almost as good as those provided by the global k-means algorithm.



Moreover, the cluster insertion procedure can be efficiently implemented by storing in a matrix all pairwise squared distan
es between points when the algorithm starts, and using this matrix for directly computing the upper bounds above. A similar 'trick' has been used in the related problems of greedy mixture density estimation using the EM algorithm  $[4]$  and principal curve fitting  $[5]$ .

Finally, we may still apply this method as well as the global k-means algorithm when we do not consider every data point  $x_n$   $(n = 1, ..., N)$  as possible insertion position for the new center, but use only a smaller set of appropriately selected insertion positions. A fast and sensible choice for selecting such a set of positions based on k-d trees is discussed next.

#### 3.2 Initialization with  $k$ -d trees

A k-d tree  $[6, 7]$  is a multi-dimensional generalization of the standard one-dimensional binary search tree, that facilitates storage and search over  $k$ -dimensional data sets. A  $k$ -d tree defines a recursive partitioning of the data space into disjoint subspaces. Each node of the tree defines a subspa
e of the original data spa
e and, onsequently, a subset ontaining the data points residing in this subspace. Each nonterminal node has two successors, each of them associated with one of the two subspaces obtained from the partitioning of the parent space using a cutting hyperplane. The k-d tree structure was originally used for speeding up distance-based search operations like nearest neighbors queries, range queries, et
.

In our case we use a variation of the original  $k$ -d tree proposed in [7]. There, the cutting hyperplane is defined as the plane that is perpendicular to the direction of the principal component of the data points orresponding to ea
h node, therefore the algorithm an be regarded as a method for nested (re
ursive) prin
ipal omponent analysis of the data set. The re
ursion usually terminates if a terminal node (called bucket) is created containing less than a prespecified number of points b (called bucket size) or if a prespecified number of buckets have been reated. It turns out that, even if the algorithm is not used for nearest neighbor queries, merely the onstru
tion of the tree provides a very good preliminary lustering of the data set. The idea is to use the bu
ket enters (whi
h are fewer than the data points) as possible insertion lo
ations for the algorithms presented previously.

In Figure 1 average performan
e results are shown on 10 data sets ea
h one onsisting of 300 data points drawn from the same mixture of 15 Gaussian omponents. The omponents of the Gaussian mixture are well separated and exhibit limited eccentricity.

We compare the results of three methods to the clustering problem with  $k = 15$  centers: (i) The dashed line depicts the results when using the fast global k-means algorithm with all data points onstituting potential insertion lo
ations. The average lustering error over the 10 data sets is 15.7 with standard deviation 1.2. (ii) The solid line depicts results when the standard k-means algorithm is used: one run for each data set was conducted. At each run the 15 cluster enters were initially positioned to the entroids of the bu
kets obtained from the appli
ation of the k-d tree algorithm until 15 bu
kets were reated. The average lustering error over the 10 data sets is 24:4 with standard deviation 9:8. (iii) The solid line (with error bars) shows the results when using the fast global k-means algorithm with the potential insertion locations constrained by the centroids of the buckets of a  $k$ -d tree. On the horizontal axis we vary the number of buckets for the k-d tree of the last method.

We also computed the 'theoretical' clustering error for each data set, ie., the error computed by using the true cluster centers. The average error value over the 10 data sets was 14.9 with standard deviation 1.3. These results were too close to the results of the standard fast global k-means to include them in the figure.

We can conclude from this experiment that (a) the fast global k-means approach gives rise to performan
e signi
antly better than when starting with all enters at the same time initialized using the  $k$ -d tree method, and (b) restricting the insertion locations for the fast global k-means to those given by the  $k$ -d tree (instead of using all data points) does not significantly degrade performance if we consider a sufficiently large number of buckets in the k-d tree (in general larger than the number lusters).

Obviously, it is also possible to employ the above presented  $k$ -d tree approach with the global k-means algorithm.

#### 4 **Experimental results**

We have tested the proposed clustering algorithms on several well-known data sets, namely the iris data set [8], the synthetic data set  $[9]$  and the image segmentation data set [8]. In all data sets we conducted experiments for the clustering problems obtained by considering only feature vectors and ignoring class labels. The iris data set contains 150 four-dimensional data points. the syntheti data set 250 two-dimensional data points and the for the image segmentation data set we onsider 210 six-dimensional data points obtained through PCA on the original 18-dimensional data points. The quality of the obtained solutions was evaluated in terms of the values of the final clustering error.

For each data set we conducted the following experiments:

- one run of the global k-means algorithm for <sup>M</sup> = 15.
- one run of the fast global k-means algorithm for  $\mathbf{15}$ .
- the complete algorithm for the statistic statistic control in the complete algorithm was algorithm was algorit executed N times (where  $N$  is the number of data points) starting from random initial positions for the <sup>k</sup> enters and we omputed the minimum and average lustering error as well as its standard deviation.

For each of the three data sets the experimental results are displayed in Figures 2, 3 and 4 respectively. Each figure plot displays the clustering error value as a function of the number of clusters. It is clear that the global k-means algorithm is very effective providing in all cases solutions of equal or better quality with respect to the k-means algorithm. In what concerns the fast version of the algorithm, it is very encouraging that, although executing significantly







faster, it provides solutions of ex
ellent quality, omparable to those obtained by the original method. Therefore, it constitutes a very efficient algorithm, both in terms of solution quality and computational complexity and can run even faster if k-d trees are employed as explained in the previous se
tion.

Matlab implementations of the fast global k-means and the k-d tree building algorithms an be downloaded from http://www.science.uva.nl/research/ias.

#### 5 **Discussion and conclusions**

We have presented the global k-means clustering algorithm, which constitutes a deterministic clustering method providing excellent results in terms of the clustering error criterion. The method is independent of any starting onditions and ompares favorably to the k-means algorithm with multiple random restarts. The deterministic nature of the method is particularly important in cases where the clustering method is used either to specify initial parameter values for other methods (for example RBF training) or onstitutes <sup>a</sup> module in <sup>a</sup> more omplex system. In such a case we can be almost certain that the employment of the global k-means (or any of the fast variants) will always provide sensible clustering solutions. Therefore, one can evaluate the complex system and adjust critical system parameters without having to worry for dependen
e of system performan
e on the lustering method employed.

Another advantage of the proposed technique is that in order to solve the  $M$ -clustering problem, all intermediate k-clustering problems are also solved for  $k = 1, \ldots, M$ . This may prove useful in many applications where we seek for the actual number of clusters and the k-clustering problem is solved for several values of  $k$ . We have also developed the fast global k-means algorithm, which significantly reduces the required computational effort, while at the same time providing solutions of almost the same quality.

We have also proposed two modification of the method that reduce the computational load without significantly affecting solution quality. These methods can be employed to find solutions to lustering problems with thousands of high-dimensional points and one of our primary aims is to test the te
hniques on large s
ale data mining problems.

Another direction of future work is related with the use of parallel processing for accelerating the proposed methods since, for every  $k$ , the N executions of the k-means algorithm are independent and can be performed in parallel. Another research direction concerns the application of the proposed method to other types of clustering (for example fuzzy clustering), as well as to topographi methods like SOM. Moreover, an important issue that deserves further study is related with the possible development of theoreti
al foundations for the assumptions behind the method. Finally, it is also possible to employ the global k-means algorithm as a method for providing effective initial parameter values for RBF networks and data modeling problems using Gaussian mixture models and compare the effectiveness of the obtained solutions with other training techniques for Gaussian mixture models [10, 11].

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