How Fast is the k-means Method?*

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Abstract

We present polynomial upper and lower bounds on the number of iterations performed by the k-means method (a.k.a. Lloyd's method) for k-means clustering. Our upper bounds are polynomial in the number of points, number of clusters, and the spread of the point set. We also present a lower bound, showing that in the worst case the k-means heuristic needs to perform $\Omega(n)$ iterations, for n points on the real line and two centers. Surprisingly, the spread of the point set in this construction is *polynomial*. This is the first construction showing that the k-means heuristic requires more than a polylogarithmic number of iterations. Furthermore, we present two alternative algorithms, with guaranteed performance, which are simple variants of the k-means method.

1 Introduction

In a (geometric) *clustering* problem, we are given a finite set $X \subset \mathbb{R}^d$ of n points and an integer $k \geq 2$, and we seek a partition (clustering) $\mathcal{S} = (S_1, \ldots, S_k)$ of X into k disjoint nonempty subsets along with a set $C = \{c_1, \ldots, c_k\}$ of k corresponding *centers*, that minimizes a suitable cost function among all such k-clusterings of X. The cost function typically represents how tightly each cluster is packed and how separated different clusters are. A center c_i *serves* the points in its cluster S_i.

We consider the *k-means* clustering *cost function* $\phi(\mathcal{S}, C) = \sum_{i=1}^{k} \psi(S_i, c_i)$, in which $\psi(S, c) = \sum_{x \in S} \|x - c\|^2$, where $\|\cdot\|$ denotes the Euclidean norm. It can be easily observed that for any cluster S_i, the point c that minimizes the sum $\sum_{x \in S_i} \|x - c\|^2$, is the centroid of S_i, denoted by $c(S_i)$, and therefore in an optimal clustering, $c_i = c(S_i)$. Thus the above cost function can be written as $\phi(\mathcal{S}) = \sum_{i=1}^{k} \sum_{x \in S_i} \|x - c(S_i)\|^2$.

It can also be observed that in an optimal k-clustering, each point of S_i is closer to c_i, the center corresponding to S_i, than to any other center. Thus, an optimal k-clustering is imposed by a Voronoi diagram whose sites are the centroids of the clusters. Such partitions are related to centroidal Voronoi tessellations (see [4]).

A k-means clustering algorithm that is used widely because of its simplicity is the *k-means heuristic*, also called *Lloyd's method* [11]. This algorithm starts with an arbitrary k-clustering $\mathcal{S}_0$ of X with the initial k centers chosen to be the centroids of the clusters of $\mathcal{S}_0$. Then it repeatedly performs local improvements by applying the following "hill-climbing" step.

Definition 1.1 *Given a clustering $\mathcal{S} = (S_1, \ldots, S_k)$ of X, a* k-MEANS step *returns a clustering $\mathcal{S}' = (S'_1, \ldots, S'_k)$ by letting S'_i equal to the intersection of X with the cell of $c(S_i)$ in the Voronoi partitioning imposed by centers $c(S_1), \ldots, c(S_k)$. If a point of X has more than a single closest center, it is assigned to one of its incident Voronoi cells arbitrarily. The (new) center of S'_i will be $c(S'_i)$.*

In a clustering $\mathcal{S} = (S_1, \ldots, S_k)$ of X, a point $x \in X$ is misclassified *if there exists $1 \leq i \neq j \leq k$, such that $x \in S_i$ but $\|x - c(S_j)\| < \|x - c(S_i)\|$. Thus a* k-MEANS *step can be broken into two stages: (i) every misclassified point is assigned to its closest center (with ties broken arbitrarily), and (ii) all centers are moved to the centroids of their newly formed clusters.*

The k-means algorithm, to which we shall refer as "k-MEANSMTD" throughout this paper, performs the k-MEANS step repeatedly and stops when the assignment of the points to the centers does not change from that of the previous step. This happens when there remains no misclassified points and consequently in the last k-MEANS step $\mathcal{S}' = \mathcal{S}$. Clearly the clustering cost is reduced when each point is mapped to the closest center and also when each center moves to the centroid of the points it serves. Thus, the clustering cost is strictly reduced in each of the two stages of a k-MEANS step.

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This in particular implies that no clustering can be seen twice during the course of execution of k-MeansMtd. Since there are only finitely many k-clusterings, the algorithm terminates in finite time.

vThe algorithm k-MeansMtd and its variants are widely used in practice [5]. Convergence and consistency of k-MeansMtd in probabilistic settings is studied in [12] and [15]. It is known that the output of k-MeansMtd is not necessarily a global minimum, and it can be arbitrarily bad compared to the optimal clustering. Furthermore, the answer returned by the algorithm and the number of steps depend on the initial choice of the centers, i.e. the initial clustering [9]. These shortcomings of k-MeansMtd has led to development of efficient polynomial approximation schemes for the k-means clustering problem both in low [13, 6, 7, 10] and high dimensions [3]. Unfortunately, those algorithms have had little impact in practice, as they are complicated and probably impractical because of large constants. A more practical local search algorithm, which guarantees a constant factor approximation, is described by Kanungo *et al.* [9].

Up to this point, no meaningful theoretical bound was known for the number of steps k-MeansMtd can take to terminate in the worst case. Inaba *et al.* [8] observe that the number of distinct Voronoi partitions of a given n-point set $X \subset \mathbb{R}^d$ induced by k sites is at most $O(n^{kd})$ which gives a trivial similar upper bound on the number of steps of k-MeansMtd (by observing that the clustering cost monotonically decreases and thus no k-clustering can be seen twice). However, the fact that k in typical application can be in the hundreds together with the relatively fast convergence of k-MeansMtd observed in practice, make this bound somewhat meaningless. The difficulty of proving any super-linear lower bound further suggests the looseness of this bound.

Our contribution. It thus appears that the combinatorial behavior of k-MeansMtd is far from being well understood. Motivated by this, in this paper we provide a lower bound and several upper bounds on the number of iterations performed by k-MeansMtd and some of its close variants. To our knowledge, our lower bound is the first that is super-polylogarithmic. Our upper bounds are *polynomial* in the spread Δ of the input point set, k, and n (the *spread* of a point set is the ratio between its diameter and the distance between its closest pair). The bounds are meaningful (i.e., polynomial) for most inputs.

In Section 2, we present an $\Omega(n)$ lower bound on the number of iterations performed by k-MeansMtd. More precisely, we show that for an adversarially chosen initial two centers and a set of n points on the line, k-MeansMtd takes $\Omega(n)$ steps. Note, that this matches the straightforward upper bound on the number of Voronoi partitions in one dimension with two centers, which is $O(n)$.

In Section 3, we provide a polynomial upper bound for the one-dimensional case. In Section 4, we provide an upper bound for the case where the points lie on a grid. In Section 5, we investigate two alternative algorithms, and provide polynomial upper bounds on the number of iterations they perform. Those algorithms are minor modifications of k-MeansMtd algorithm, and we believe that their analysis provides an insight about the behavior of k-MeansMtd. In Section 6, we conclude by mentioning a few open problems and a discussion of our results.

2 Lower Bound Construction for Two Clusters in One Dimension

In this section, we describe a set of $2n$ points, along with an initial pair of centers, on which k-MeansMtd takes $\Omega(n)$ steps.

Fix $n \geq 2$. Our set X will consist of $2n$ numbers $y_1 < \cdots < y_n < x_n < \cdots < x_1$ with $y_i = -x_i$, for $i = 1, \ldots, n$.

At the ith iteration, we denote by l_i and r_i the current left and right centers, respectively, and by L_i and R_i the new sets of points assigned to l_i and r_i, respectively. Furthermore, for each $i \geq 0$, we denote by α_i the Voronoi boundary $\frac{1}{2}(l_i + r_i)$ between the centers l_i and r_i. Thus $L_i = \{x \in X \mid x < \alpha_i\}$ and $R_i = \{x \in X \mid x \geq \alpha_i\}$.

Let x_1 be an arbitrary positive real number and let $x_2 < x_1$ be a positive real number to be specified shortly. Initially, we let $l_1 = x_2$ and $r_1 = x_1$ and consequently $\alpha_1 = \frac{1}{2}(x_1 + x_2)$. Thus in the first iteration, $L_1 = \{y_1, \ldots, y_n, x_n, \ldots, x_2\}$ and $R_1 = \{x_1\}$. We will choose $x_2, \ldots, x_n$ such that at the end of the ith step we have $L_i = \{y_1, \ldots, y_n, x_n, \ldots, x_{i+1}\}$ and $R_i = \{x_i, \ldots, x_1\}$. Suppose for the inductive hypothesis that at the $(i-1)$th step we have $L_{i-1} = \{y_1, \ldots, y_n, x_n, \ldots, x_{i+1}, x_i\}$ and $R_{i-1} = \{x_{i-1}, \ldots, x_1\}$.

Thus we can compute l_i and r_i as

$$l_i = \frac{y_1 + \cdots + y_n + x_n + \cdots + x_i}{2n - i + 1}$$

and

$$r_i = \frac{x_{i-1} + \cdots + x_1}{i - 1}.$$

Since $y_1 + \cdots + y_n + x_n + \cdots + x_i = -(x_{i-1} + \cdots + x_1)$,

we get for α_i:

$$\begin{aligned}\alpha_i &= \frac{1}{2}(l_i + r_i)\\ &= \frac{1}{2}\left(\frac{x_{i-1}+\cdots+x_1}{i-1} - \frac{x_{i-1}+\cdots+x_1}{2n-i+1}\right)\\ &= \frac{n-i+1}{(i-1)(2n-i+1)}(x_{i-1}+\cdots+x_1)\\ &= \frac{n-i+1}{(i-1)(2n-i+1)}\cdot s_{i-1},\end{aligned}$$

where $s_{i-1} = \sum_{j=1}^{i-1} x_j$.

To guarantee that only x_i deserts L_{i-1} to R_i, in the ith iteration, we need that $x_{i+1} < \alpha_i < x_i$. Thus, it is natural to set $x_i = \tau_i \alpha_i$, where $\tau_i > 1$, for $i = 1, \ldots, n$. Picking the coefficients $\tau_1, \ldots, \tau_n$ is essentially the only part of this construction that is under our control. We set

$$\tau_i = 1 + \frac{1}{n-i+1} = \frac{n-i+2}{n-i+1},$$

for $i = 1, \ldots, n$. Since $\tau_i > 1$, $x_i = \tau_i \alpha_i > \alpha_i$, for $i = 1, \ldots, n$. Next, we verify that $x_{i+1} < \alpha_i$. By definition,

$$\begin{aligned}x_{i+1} &= \tau_{i+1}\alpha_{i+1} = \tau_{i+1}\cdot\frac{n-i}{i(2n-i)}\cdot s_i\\ &= \tau_{i+1}\cdot\frac{n-i}{i(2n-i)}\cdot(x_i + s_{i-1})\\ &= \tau_{i+1}\cdot\frac{n-i}{i(2n-i)}\left(\tau_i + \frac{(i-1)(2n-i+1)}{n-i+1}\right)\alpha_i\\ &= \frac{n-i+1}{i(2n-i)}\left(\frac{n-i+2}{n-i+1} + \frac{(i-1)(2n-i+1)}{n-i+1}\right)\alpha_i.\end{aligned}$$

It can be verified through elementary simplifications that the coefficient of α_i above is always less than 1 implying that $x_{i+1} < \alpha_i < x_i$, for $i = 1, \ldots, n-1$.

We can compute a recursive formula for x_{i+1} in terms of x_i, as follows

$$\begin{aligned}x_{i+1} &= \tau_{i+1}\alpha_{i+1} = \frac{n-i+1}{n-i}\cdot\frac{n-i}{i(2n-i)}\cdot s_i\\ &= \frac{n-i+1}{i(2n-i)}\cdot(x_i + s_{i-1})\\ &= \frac{n-i+1}{i(2n-i)}\left(x_i + \frac{(i-1)(2n-i+1)}{n-i+1}\cdot\alpha_i\right)\\ &= \frac{n-i+1}{i(2n-i)}\left(x_i + \frac{(i-1)(2n-i+1)}{n-i+1}\cdot\left(1+\frac{1}{n-i+1}\right)^{-1}x_i\right)\\ &= \frac{n-i+1}{i(2n-i)}\left(1 + \frac{(i-1)(2n-i+1)}{n-i+2}\right)\cdot x_i,\end{aligned}$$

for $i = 1, \ldots, n-1$. Thus letting

$$\beta_i = \frac{n-i+1}{i(2n-i)}\left(1 + \frac{(i-1)(2n-i+1)}{n-i+2}\right)$$

we get that

$$x_{i+1} = \beta_i x_i, \tag{2.1}$$

for $i = 1, \ldots, n-1$.

Theorem 2.1 *For each $n \geq 2$, there exists a set of $2n$ points on a line with two initial center positions for which k-MeansMtd takes exactly n steps to terminate.*

2.1 The Spread of the Point Set. It is interesting to examine the spread of the above construction. As we show below, somewhat surprisingly, the spread of this construction is polynomial, hinting (at least intuitively) that "bad" inputs for k-MeansMtd are, arguably, not that contrived.

By Eq. (2.1), we have $x_{i+1} = \beta_i x_i$. Notice that by the given construction $\beta_i < 1$ for all $i = 1, \ldots, n-1$ since $x_{i+1} < x_i$. In the sequel we will show that x_n is only polynomially smaller than x_1, namely $x_n = \Omega(x_1/n^4)$. We then derive a bound on the distance between any consecutive pair x_i and x_{i+1}. These two assertions combined, imply that the point set has a spread bounded by $O(n^5)$. The following lemma follows from elementary algebraic simplifications.

Lemma 2.1 *For each $1 \leq i \leq n/2$, $\beta_i \geq (1-1/i)^2$, and for each $n/2 < i < n-1$, $\beta_i \geq (1-1/(n-i+1))^2$. Furthermore, for $i \geq 2$, we have $\beta_i \leq 1 - 1/2i$.*

Corollary 2.1 *For any $n > 0$ we have $x_n = \Omega(x_1/n^4)$.*

Proof. $x_n = \beta_1 \cdot \prod_{i=2}^{n-1} \beta_i \cdot x_1$

$$\begin{aligned}&\geq \beta_1 x_1 \cdot \prod_{i=2}^{\lfloor n/2\rfloor}\left(1-\frac{1}{i}\right)^2 \cdot \prod_{i=\lfloor n/2\rfloor+1}^{n-1}\left(1-\frac{1}{n-i+1}\right)^2\\ &= \beta_1 x_1 \cdot \left(1-\frac{1}{2}\right)^2 \cdots \left(1-\frac{1}{\lfloor n/2\rfloor}\right)^2 \cdot\left(1-\frac{1}{\lfloor n/2\rfloor}\right)^2 \cdots \left(1-\frac{1}{2}\right)^2\\ &= \beta_1 x_1 \cdot \left(\prod_{i=2}^{\lfloor n/2\rfloor}\frac{(i-1)^2}{i^2}\right)^2 = \beta_1 x_1 \cdot \left(\frac{1}{\lfloor n/2\rfloor}\right)^4\end{aligned}$$

The claim follows as $\beta_1 = n/(2n-1) = \Theta(1)$.

Lemma 2.2 *For each $i = 1, \ldots, n-1$, $x_i - x_{i+1} \geq x_i/3i$.*

Proof. Since $x_{i+1} = \beta_i x_i$, we have $x_i - x_{i+1} = x_i(1-\beta_i)$. For $i = 1$, we have $\beta_1 = n/(2n-1) \leq 2/3$, when $n \geq 2$.

Thus, we have $x_1 - x_2 \geq x_1/3$. For $i = 2, \ldots, n-1$, using Lemma 2.1 we get $1-\beta_i \geq 1/2i$. Thus, $x_i - x_{i+1} = x_i(1-\beta_i) \geq x_i \cdot 1/(2i) > x_i/3i$, as claimed.

Theorem 2.2 *The spread of the point set constructed in Theorem 2.1 is $O(n^5)$.*

Proof. By Lemma 2.2, for each $i = 1, \ldots, n-1$, $x_i - x_{i+1} \geq x_i/3i$. Since $x_i > x_n$ and by Corollary 2.1, $x_n = \Omega(x_1/n^4)$, it follows that $x_i - x_{i+1} = \Omega(x_1/n^5)$. This lower bound for the distance between two consecutive points is also true for y_i's due to the symmetric construction of the point set around 0. On the other hand, since $x_n = \Omega(x_1/n^4)$, $x_n - y_n = 2x_n = \Omega(x_1/n^4)$. Thus every pair of points are at distance at least $\Omega(x_1/n^5)$. Since the diameter of the point set is $2x_1$, we get a bound of $O(n^5)$ for the spread of the point set.

3 An Upper Bound for One Dimension

In this section, we prove an upper bound on the number of steps of k-MeansMtd in one dimensional Euclidean space. As we shall see, the bound does not involve k but is instead related to the spread Δ of the point set X. Without loss of generality we can assume that the closest pair of points in X are at distance 1 and thus the diameter of the set X is Δ. Before proving the upper bound, we mention a straightforward technical lemma from [9].

Lemma 3.1 ([9]) *Let S be a set of points in $\mathbb{R}^d$ with centroid $c = c(S)$ and let z be an arbitrary point in $\mathbb{R}^d$. Then $\psi(S,z) - \psi(S,c) = |S| \cdot \|c - z\|^2$.*

The above lemma quantifies the contribution of a center c_i to the cost improvement in a k-Means step as a function of the distance it moves. More formally, if in a k-Means step a k-clustering $\mathcal{S} = (S_1, \ldots, S_k)$ is changed to the other k-clustering $\mathcal{S}' = (S'_1, \ldots, S'_k)$, then

$$\phi(\mathcal{S}) - \phi(\mathcal{S}') \geq \sum_{i=1}^{k} |S'_i| \cdot \|c(S'_i) - c(S_i)\|^2 .$$

Note that in the above analysis we only consider the improvement resulting from the second stage of the k-Means step in which the centers are moved to the centroids of their clusters. There is an additional gain from reassigning the points in the first stage of a k-Means step that we currently ignore.

In all our upper bound arguments we use the fact that since the initial set of centers is chosen from inside the convex hull of the input point set X (the initial centers are the centroid of the initial arbitrary clustering and even if this was not the case, all centers would move inside the convex hull of X after one step), the initial clustering cost is no more than $n\Delta^2$. This simply follows from the fact that each of the n points in X is at distance no more than Δ from its assigned center.

Theorem 3.1 *The number of steps of k-MeansMtd on a set $X \subset \mathbb{R}$ of n points with spread Δ is at most $O(n\Delta^2)$.*

Proof. Consider a k-Means step that changes a k-clustering $\mathcal{S}$ into another k-clustering $\mathcal{S}'$. The crucial observation is that in this step, there exists a cluster that is only extended or shrunk from its right end. To see this consider the leftmost cluster S_1. Either S_1 is modified in this step, in which case this modification can only happen in form of extension or shrinking at its right end, or it remains the same. In the latter case, the same argument can be made about S_2, and so on.

Thus assume that S_1 is extended from right by receiving a set T or points from the cluster directly to its right, namely S_2 (S_2 cannot lose all its points to S_1 as it has at least one point to the right of c_2 and this point is closer to c_2 than to c_1 and cannot go to S_1). Notice that $c(T)$ is to the right of the leftmost point in T and at distance at least $(|T|-1)/2$ from this leftmost point (because every pair of points are at distance one or more in T and $c(T)$ gets closest to its leftmost point when every pair of consecutive points in T are placed at the minimum distance of 1 from each other). Similarly, the centroid of S_1 is to the left of the rightmost point of S_1 and at distance at least $(|S_1|-1)/2$ from it. Thus, $\|c(S_1) - c(T)\| \geq (|T|-1)/2 + (|S_1|-1)/2 + 1 = (|T| + |S_1|)/2$, where the extra 1 is added because the distance between the leftmost point in T and the rightmost point in S_1 is at least 1. The centroid of S'_1 will therefore be at distance

$$\frac{|T|}{|S_1| + |T|} \|c(S_1) - c(T)\| \geq \frac{|T|}{|S_1| + |T|} \cdot \frac{|T| + |S_1|}{2} = \frac{|T|}{2} \geq \frac{1}{2}$$

from $c(S_1)$ and to its right. Consequently, by Lemma 3.1, the improvement in clustering cost is at least $1/4$.

Similar analysis implies a similar improvement in the clustering cost for the case where we remove points from S_1. Since the initial clustering cost is at most $n\Delta^2$, the number of steps is no more than $n\Delta^2/(1/4) = 4n\Delta^2$.

Remark 1. The choice of $n\Delta^2$ as an upper-bound for the initial clustering cost in proving Theorem 3.1 as well as all other upper bounds proved later in this paper

can be slightly improved, tightening these upper bounds accordingly.

Since the initial centers are centroids of their clusters in the initial clustering, at the beginning of the first step, we have a clustering $\mathcal{S} = (S_1, \ldots, S_k)$ of the input point set X with centers $c_1, \ldots, c_k$, respectively, where for each $i = 1, \ldots, k$, $c_i = c(S_i)$. Let $\hat{c} = c(X)$ be the centroid of the entire input point set. By Lemma 3.1, we can write

$$\psi(S_i, c_i) = \psi(S_i, \hat{c}) - |S_i| \cdot \|\hat{c} - c_i\|^2 ,$$

for $1 \leq i \leq k$. Summing this equation, for $i = 1, \ldots, k$, we get

$$\begin{aligned} \phi(\mathcal{S}) &= \sum_{x \in X} \|x - \hat{c}\|^2 - \sum_{i=1}^{k} |S_i| \,.\, \|\hat{c} - c_i\|^2 \\ &< \sum_{x \in X} \|\hat{c} - x\|^2 = \frac{1}{n} \sum_{x,y \in X} \|x - y\|^2 . \end{aligned}$$

Thus, we get the more accurate upper bound of $1/n \sum_{x,y \in X} \|x - y\|^2$ that can replace the trivial bound of $n\Delta^2$. Note that depending on the input, this improved upper bound can be smaller than $n\Delta^2$ by a factor of $O(n)$. Nevertheless, in all our upper bound results we employ the weaker bound for the purpose of readability, while all those bounds can be made more precise by applying the above-mentioned improvement.

Remark 2. A slight technical detail in the implementation of k-MeansMtd algorithm, involves the event of a center losing all the points it serves. Candidate strategies used in practice to handle this problem include: placing the lonely center somewhere else arbitrarily or randomly, leaving it where it is to perhaps acquire some points in future steps, or completely removing it. For the sake of convenience in our analysis and in agreement with [11], we adopt the last strategy, namely, whenever a center is left serving no points, we remove that center permanently and continue with the remaining centers.

4 Upper Bound for Points on a d-Dimensional Grid

In this section, we prove an upper bound on the number of steps of k-MeansMtd when the input points belong to the integer grid $\{1, \ldots, M\}^d$. This is the case in many practical applications where every data point has a large number of fields with each field having values in a small discrete range. For example, this includes clustering of pictures, where every pixel forms a single coordinate (or three coordinates, corresponding to the RGB values) and the value of every coordinate is restricted to be an integer in the range 0–255.

The main observation is that the centroids of any two subsets of $\{1, \ldots, M\}^d$ are either equal or are suitably far away. Since each step of k-MeansMtd moves at least one center or else stops, this observation guarantees a certain amount of improvement to the clustering cost in each step.

Lemma 4.1 *Let S_1 and S_2 be two nonempty subsets of $\{1, \ldots, M\}^d$ with $|S_1| + |S_2| \leq n$. Then, either $c(S_1) = c(S_2)$ or $\|c(S_1) - c(S_2)\| \geq 1/n^2$.*

Proof. If $c(S_1) \neq c(S_2)$ then they differ in at least one coordinate. Let u_1 and u_2 be the values of $c(S_1)$ and $c(S_2)$ in one such coordinate, respectively. By definition, $u_1 = s_1/|S_1|$ and $u_2 = s_2/|S_2|$ where s_1 and s_2 are integers in the range $\{1, \ldots, nM\}$. In other words $|u_1 - u_2|$ is the difference of two distinct fractions, both with denominators less than n. It follows that $|u_1 - u_2| \geq 1/n^2$ and consequently $\|c(S_1) - c(S_2)\| \geq |u_1 - u_2| \geq 1/n^2$.

Theorem 4.1 *The number of steps of k-MeansMtd when executed on a point set X taken from the grid $\{1, \ldots, M\}^d$ is at most dn^5M^2.*

Proof. Note, that $U = n \cdot (\sqrt{d}M)^2 = ndM^2$ is an upper bound of for the clustering cost of any k-clustering of a point set in $\{1, \ldots, M\}^d$ and that at each step at least one center moves by at least $1/n^2$. Therefore, by Lemma 3.1, at every step the cost function decreases by at least $1/n^4$ and the overall number of steps can be no more than $U/(1/n^4) = dn^5M^2$.

5 Arbitrary Point Sets and Alternative Algorithms

Unfortunately proving any meaningful bounds for the general case of k-MeansMtd, namely with points in $\mathbb{R}^d$ with $d > 1$ and no further restrictions, remains elusive. However, in this section, we present two close relatives of k-MeansMtd for each of which we can bound the number of steps by a polynomial in the number of points, number of centers, and the spread of the point set. The first algorithm differs from k-MeansMtd in that it moves a misclassified point to its correct cluster, as soon as the misclassified point is discovered (rather than first finding all misclassified points and then reassigning them to their closest centers as is the case in k-MeansMtd). The second algorithm is basically the same as k-MeansMtd using a natural generalization of misclassified points. Our experimental results, reported in the full-version of this paper, further support the kinship of these two algorithms with k-MeansMtd.

As was the case with our previous upper bounds, our main approach in bounding the number of steps in both these algorithms is through showing substantial improvements in the clustering cost at each step.

5.1 The SinglePnt Algorithm. We introduce an alternative to the k-Means step which we shall call a SinglePnt step.

Definition 5.1 *In a* SinglePnt step *on a k-clustering $\mathcal{S} = (S_1, \ldots, S_k)$, a misclassified point x is chosen, such that $x \in S_i$ and $\|x - c(S_j)\| < \|x - c(S_i)\|$, for some $1 \leq i \neq j \leq k$, and a new clustering $\mathcal{S}' = (S'_1, \ldots, S'_k)$ is formed by removing x from S_i and adding it to S_j. Formally, for each $1 \leq l \leq k$,*

$$S'_l = \begin{cases} S_l & l \neq i, j, \\ S_l \setminus \{x\} & l = i, \\ S_l \cup \{x\} & l = j. \end{cases}$$

The centers are updated to the centroids of the clusters, and therefore only the centers of S_i and S_j change. Note that updating the centers takes constant time.

In a SinglePnt step, if the misclassified point is far away from at least one of $c(S_i)$ and $c(S_j)$, then the improvement in clustering cost made in the SinglePnt step cannot be too small.

Lemma 5.1 *Let S and T be two point sets of sizes n and m, respectively, and let $s = c(S)$ and $t = c(T)$. Suppose that x is a point in T with distances d_S and d_T from s and t, respectively, and such that $d_S < d_T$. Let $S' = S \cup \{x\}$ and $T' = T \setminus \{x\}$ and let $s' = c(S')$ and $t' = c(T')$. Then $\psi(S, s) + \psi(T, t) - \psi(S', s') - \psi(T', t') \geq (d_S + d_T)^2/(2(n + m))$.*

Proof. Indeed, $c(S') = \frac{n}{n+1} c(S) + \frac{1}{n+1} x$. Thus

$$\begin{aligned} \|s - s'\| &= \|c(S) - c(S')\| = \left\| \frac{1}{n+1} c(S) - \frac{1}{n+1} x \right\| \\ &= \frac{1}{n+1} \|c(S) - x\| = \frac{d_S}{n+1}. \end{aligned}$$

Similarly, $\|t - t'\| = d_T/(m-1)$. By Lemma 3.1 we obtain

$$\psi(S', s) - \psi(S', s') = (n+1) \left(\frac{d_S}{n+1} \right)^2 = \frac{d_S^2}{n+1},$$

and similarly $\psi(T', t) - \psi(T', t') = d_T^2/(m-1)$.

Since $d_S < d_T$, we have that $\psi(S, s) + \psi(T, t) \geq \psi(S', s) + \psi(T', t)$, and

$$\begin{aligned} \psi(S, s) &+ \psi(T, t) - \psi(S', s') - \psi(T', t') \\ &\geq \psi(S', s) + \psi(T', t) - \psi(S', s') - \psi(T', t') \\ &\geq \frac{d_S^2}{n+1} + \frac{d_T^2}{m-1} \geq \frac{d_S^2}{n+m} + \frac{d_T^2}{n+m} \\ &= \frac{d_S^2 + d_T^2}{n+m} \geq \frac{(d_S + d_T)^2}{2(n+m)}. \end{aligned}$$

Our modified version of k-MeansMtd, to which we shall refer as "SinglePnt", replaces k-Means steps with SinglePnt steps. Starting from an arbitrary clustering of the input point set, SinglePnt repeatedly performs SinglePnt steps until no misclassified points remain. Notice that unlike the k-Means step, the SinglePnt step does not maintain the property that the clustering achieved at the end of the step is imposed by some Voronoi diagram. However, this property must hold when the algorithm stops, or otherwise some misclassified points would exist and further steps would be possible.

Theorem 5.1 *On any input $X \subset \mathbb{R}^d$, SinglePnt makes at most $O(kn^2\Delta^2)$ steps before termination.*

Proof. Once again, we assume that no two points in X are less than unit distance apart. Call a SinglePnt step *weak*, if the misclassified point it considers is at distance less than $1/8$ from both *involved centers*, i.e., its current center and the center closest to it. We call a SinglePnt step *strong* if it is not weak. Since in a strong SinglePnt step, the sum of distances of the misclassified point to the involved centers is at least $1/8$, and the two involved clusters have at most n points combined, it follows by Lemma 5.1 that in such a step the clustering cost improves by at least $(1/8)^2/(2n) = 1/(128n)$. In the sequel we shall show that the algorithm cannot take more than k *consecutive* weak steps, and thus at least one out of every $k+1$ consecutive steps must be strong and thus result an improvement of $1/(128n)$ to the clustering cost; hence the upper bound of $O(kn^2\Delta^2)$.

Consider the beginning of a of SinglePnt step. Let $c_1, \ldots, c_k$ denote the current centers, and let $S_1, \ldots, S_k$ denote the corresponding clusters; namely, S_i is the set of points served by c_i, for $i = 1, \ldots, k$. Consider the balls $B_1, \ldots, B_k$ of radius $1/8$ centered at $c_1, \ldots, c_k$, respectively. Observe that since every pair of points in X are at distance at least 1 from each other, each ball B_i can contain at most one point of X. Moreover, the intersection of any subset of the balls $B_1, \ldots, B_k$ can contain at most one point of X. For a point $x \in X$, let $\mathcal{B}(x)$ denote the set of balls among $B_1, \ldots, B_k$ that contain the point x. We refer to $\mathcal{B}(x)$ as the *batch* of x.

By the above observation, the balls (and the corresponding centers) are classified according to the point of X they contain (if they contain such a point at all). Let $\mathcal{B}_X$ be the set of batches of balls that are induced by X and contain more than one ball. Formally, $\mathcal{B}_X = \{\mathcal{B}(x) : x \in X, |\mathcal{B}(x)| > 1\}$. The set of balls $\bigcup \mathcal{B}_X$ is the set of *active* balls.

A misclassified point x can participate in a weak SinglePnt step only if it belongs to more than one ball; i.e., when $|\mathcal{B}(x)| > 1$. Observe that, if we perform a weak step, and one of the centers moves such that the corresponding ball B_i no longer contains any point of X in its interior, then for B_i to contain a point again, the algorithm must perform a strong step. To see this, observe that (weakly) losing a point x may cause a center move a distance of at most 1/8. Therefore, once a center c_i loses a point x, and thus moves away from x, it does not move far enough for the ball B_i to contain a different point of X.

Hence, in every weak iteration a point x changes the cluster it belongs to in $\mathcal{B}(x)$. This might result in a shrinking of the active set of balls. On the other hand, while only weak SinglePnt steps are being taken, any cluster S_j can change only by winning or losing the point x_i that stabs the corresponding ball B_j. It follows that once a set S_j loses the point x, then it can never get it back since that would correspond to an increase in the clustering cost. Therefore the total number of possible consecutive weak SinglePnt steps is bounded by $\sum_{x \in X, |\mathcal{B}(x)|>1} |\mathcal{B}(x)| \leq k$.

5.2 The Lazy-k-Means algorithm. Our second variant to k-MeansMtd, which we name "Lazy-k-Means", results from a natural generalization of misclassified points (Definition 1.1). Intuitively, the difference between the Lazy-k-Means and k-MeansMtd is that Lazy-k-Means at each step only reassigns those misclassified points to their closest centers that are *substantially* misclassified, namely the points that benefit from reclassification by at least a constant factor.

Definition 5.2 *Given a clustering $\mathcal{S} = (S_1, \ldots, S_k)$ of a point set X, if for a point $x \in S_i$ there exists a $j \neq i$, such that $\|x - c(S_i)\| > (1+\varepsilon)\|x - c(S_j)\|$, then x is said to be* $(1+\varepsilon)$-misclassified *for center pair $(c(S_i), c(S_j))$. The centers $c(S_i)$ and $c(S_j)$ are referred to as* switch centers *for x. We also say that $c(S_i)$ is the* losing center *and $c(S_j)$ is the* winning center *for x.*

Thus Lazy-k-Means with parameter ε starts with an arbitrary k-clustering. In each step, it (i) reassigns every $(1+\varepsilon)$-misclassified point to its closest center and (ii) moves every center to the centroid of its new cluster. Indeed, k-MeansMtd is simply Lazy-k-Means with parameter $\varepsilon = 0$. Naturally, the algorithm stops when no $(1+\varepsilon)$-misclassified points are left.

In the sequel we bound the maximum number of steps taken by Lazy-k-Means. We shall use the following fact from elementary Euclidean geometry.

Fact 5.1 *Given two points c and c' with $\|c - c'\| = \ell$, the locus of the points x with $\|x - c'\| > (1+\varepsilon)\|x - c\|$ is an open ball of radius $R = \ell(1+\varepsilon)/(\varepsilon(2+\varepsilon))$ called the ε-Apollonius ball for c with respect to c'. This ball is centered on the line containing the segment cc' at distance $R + \ell\varepsilon/(2(2+\varepsilon))$ from the bisector of cc', and on the same side of the bisector as c.*

Lemma 5.2 *For any three points x, c, and c' in $\mathbb{R}^d$ with $\|x - c\| \leq \|x - c'\|$ we have $\|x - c'\|^2 - \|x - c\|^2 = 2h\|c - c'\|$, where h is the distance from x to the bisector of c and c'.*

Proof. Let y be the intersection point of the segment cc' with the $(d-1)$-dimensional hyperplane parallel to the bisector of c and c' and containing x. By Pythagorean equality we have $\|x - c\|^2 = \|x - y\|^2 + \|y - c\|^2$ and $\|x - c'\|^2 = \|x - y\|^2 + \|y - c'\|^2$. Subtracting the first equality from the second, we obtain

$$\begin{aligned} \|x - c'\|^2 &- \|x - c\|^2 \\ &= \|y - c'\|^2 - \|y - c\|^2 \\ &= (\|y - c'\| + \|y - c\|)(\|y - c'\| - \|y - c\|) \\ &= 2h\|c - c'\|, \end{aligned}$$

since $\|y - c'\| - \|y - c\| = 2h$.

Theorem 5.2 *For $\varepsilon > 0$, the number of steps of* Lazy-k-Means *is $O(n\Delta^2\varepsilon^{-3})$.*

Proof. We will show that every two consecutive steps of Lazy-k-Means make an improvement of at least

$$\lambda^* = \frac{\varepsilon^3(2+\varepsilon)}{256(1+\varepsilon)^2} \geq \frac{\varepsilon^3}{512} = \Omega(\varepsilon^3).$$

Let $\ell_0 = \varepsilon(2+\varepsilon)/(16(1+\varepsilon))$. Notice that $\ell_0 < 1/8$ for $0 < \varepsilon \leq 1$. We call a misclassified point x *strongly* misclassified, if its switch centers c and c' are at distance at least ℓ_0 from each other, and *weakly* misclassified otherwise.

If at the beginning of a Lazy-k-Means step there exists a strongly misclassified point x for a center pair (c, c'), then since every point in the ε-Apollonius ball for c' with respect to c is at distance at least $\ell_0\varepsilon/(2(2+\varepsilon))$ from the bisector of cc', by Lemma 5.2 the reclassification improvement in clustering cost resulting from assigning x to c' is

$$\|x - c\|^2 - \|x - c'\|^2 = \frac{\ell_0^2\varepsilon}{2+\varepsilon} \geq \frac{\varepsilon^3(2+\varepsilon)}{256(1+\varepsilon)^2} = \lambda^*.$$

Thus we assume that all misclassified points are weakly misclassified. Let x be one such point for center pair (c, c'). By our assumption $\|c - c'\| < \ell_0$. Observe that in such a case, the radius of the ε-Apollonius ball for c' with respect to c is $\ell(1+\varepsilon)/(\varepsilon(2+\varepsilon)) < 1/16$. In particular, since there exists a ball of radius $1/16$ containing both x and c', the ball of radius $1/8$ centered at c', which we denote by $B(c', 1/8)$, includes x. Also since $\|c - c'\| < 1/8$ as verified above, we get $c \in B(c', 1/8)$ as well. In other words, both switch centers c and c' are at distance less than $1/4$ from x. Now, since every pair of points in X are at distance 1 or more, any center can be a switch center for at most one weakly misclassified point. This in particular implies that in the considered Lazy-k-Means step, no cluster is modified by more than a single point.

When the misclassified points are assigned to their closest centers, the centers that do not lose or win any points stay at their previous locations. A center c' that wins a point x moves closer to x since x is the only point it wins while losing no other points. Similarly, a center c that loses a point x moves away from x since x is the only point it loses without winning any other points. A losing center c moves away from its lost point x by a distance of at most $\|c - x\| < 1/4$ since its previous number of served points was at least 2 (otherwise, we would have $c = x$ and thus x could not be misclassified). Therefore, when c moves to the centroid of its cluster (now missing x), $\|x - c\| < 1/2$ and consequently $\|c - y\| > 1/2$ for any $x \neq y \in X$. As a result, c can not be a switch center for any weakly misclassified point in the subsequent Lazy-k-Means step.

On the other hand, the winning center c' to whose cluster x is added, moves closer to x and since no center other than c and c' in $B(x, 1/4)$ moves (as there is no point other than x they can win or lose), x will not be misclassified in the next Lazy-k-Means step.

It follows from the above discussion that the next Lazy-k-Means step cannot have any weakly misclassified points and thus either the algorithm stops or some strongly misclassified point will exist, resulting an improvement of at least λ^*. Thus the total number of steps taken by Lazy-k-Means with parameter ε is at most $2n\Delta^2/\lambda^* = O(n\Delta^2\varepsilon^{-3})$.

6 Conclusions

We presented several results on the number of iterations performed by the k-MeansMtd clustering algorithm. To our knowledge, our results are the first to provide combinatorial bounds on the performance of k-MeansMtd. We also suggested related variants of k-MeansMtd algorithm, and proved upper bounds for their performance. We implemented those algorithms and compared their performance in practice [16]. We conjecture that the upper bounds we proved for SinglePnt hold also for k-MeansMtd. Maybe the most surprising part in those bounds for the number of iterations performed is the lack of dependence on the dimension of the data.

We consider this paper to be a first step in understanding the k-means method. It is our belief that both our lower and upper bounds are loose, and one might need to use other techniques to improve them. In particular, we mention some open problems:

1. There is still a large gap between our lower and upper bounds. In particular, a super-linear lower bound would be interesting even in high-dimensional space.

2. Our current upper bounds include the spread as a parameter. It would be interesting to prove (or disprove) that this is indeed necessary.

3. We have introduced alternative, easy to analyze algorithms, that are rather close to k-MeansMtd in their description. We have performed a series of experiments to compare these alternative algorithms with k-MeansMtd [16] and the results of these experiments on several artificial and real-world point-sets are reported in the full-version of this paper. These results suggest that these alternative algorithms perform quite closely to k-MeansMtd both in the number of steps they take and the quality of the clustering they produce. It would be interesting to show provable connections between these algorithms and compare the bounds on the number of steps they require to terminate.

6.1 Dependency on the spread. A shortcoming of our results, is the dependency on the spread of the point set in the bounds presented. However:

1. This can be resolved by doing a preprocessing stage, snapping together points close to each other, and breaking the input into several parts to be further clustered separately. This is essentially what fast provable approximation algorithms for TSP, k-means, and k-median do [1, 7]. This results in point sets with polynomial spread, which can be used instead of the original input to compute a good clustering. This is outside the scope of our analysis, but it can be used in practice to speedup k-MeansMtd algorithm.

2. In high dimensions, it seems that in many natural cases the spread tends to shrink and be quite small.

As such, we expect our bounds to be meaningful in such cases.

To see an indication of this shrinkage in the spread, imagine picking n points randomly from a unit hypercube in $\mathbb{R}^d$ with volume one. It is easy to see that the minimum distance between any pair of points is going to be at least $L = 1/n^{3/d}$, with high probability, since if we center around each such point a hypercube of side length L, it would have volume $1/n^3$ of the unit hypercube. As such, the probability of a second point falling inside this region is polynomially small.

However, L tends to 1 as d increases. Thus, for $d = \Theta(\log n)$ the spread of such random point set is $\Theta(\sqrt{d}/(L/2)) = \Theta(\sqrt{\log n})$. (An alternative way to demonstrate this is by picking points randomly from the unit hypersphere. By using a concentration of mass argument [14] on a hypersphere, we get a point-set with spread $O(1)$ with high probability.)

6.2 Dependency on the initial solution. The initial starting solution fed into k-MeansMtd is critical in the time it takes to converge, and in the quality of the final clustering generated. Of course, one can use a (rough) approximation algorithm [7] to come up with a better starting solution. While this approach might be useful in practice, it again falls outside the scope of our analysis.

In particular, it would be nice to improve our lower bound, so that it holds, with reasonable probability, for randomly chosen initial solution.

6.3 Similar results. Recently, independently of our results, Sanjoy Dasgupta [2] announced results which are similar to a *subset* of our results. In particular, he mentions the one-dimensional lower bound, and a better upper bound for $k < 5$ but only in one dimension. This work of Sanjoy Dasgupta and Howard Karloff seems to be using similar arguments to ours (personal communication) although to our knowledge it has not been written or published yet.

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