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A Better k -means++ Algorithm via Local Search

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Abstract

In this paper, we develop a new variant of k -means++ seeding that in expectation achieves a constant approximation guarantee. We obtain this result by a simple combination of k -means++ sampling with a local search strategy. We evaluate our algorithm empirically and show that it also improves the quality of the solution in practice.

1. Introduction

As a central problem in unsupervised learning clustering received a lot of attention in the past decades. The goal of clustering is to partition a given set of objects into clusters with the idea that objects in the same cluster should be similar to each other while objects in different clusters should be less similar. One basic formulation of clustering is the k -clustering problem with sum-of-squared-error objective function. In this problem, the objects are represented as vectors in \mathbb{R}^d and we think of the squared Euclidean distance as a measure of dissimilarity. Formally, in this setting we want to find a set C of k centers that minimizes

$$\sum_{p \in P} \min_{c \in C} \|p - c\|^2.$$

The clusters are defined by assigning each point to their closest center. It is known that the optimal center of a given cluster is the average or mean of the cluster, which is why the problem is also often called k -means clustering.

k -means has been extensively studied in literature, and several heuristic have been proposed to solve the problem. Probably the most celebrated heuristic for k -means is the well-known Lloyd's algorithm (Lloyd, 2006). The algorithm is also often called the k -means algorithm. The algorithm usually performs very well in practice, but it does not provide a

theoretical approximation guarantee. → 이론 해결하는 논문

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center vs optimal center

계산 기준으로 생각. $T(n) = 2T\left(\frac{n}{2}\right) = 2 \cdot 3T\left(\frac{n}{2 \cdot 3}\right) = 2^k T\left(\frac{n}{2^k}\right)$

The k -means++ seeding algorithm (Arthur & Vassilvitskii, 2007) is a simple way to improve Lloyd's algorithm. The algorithm incrementally chooses a set of k centers by sampling the next center from a distribution where every point has probability proportional to its squared distance to the currently closest center. The solution computed by the seeding algorithm has expected cost of $O(\log k)$ times the cost of the optimum solution. In practice, it is then often used as a starting solution for Lloyd's algorithm (which never decreases the objective function).

k -means++ is easy to implement and is known to sometimes heavily outperform Lloyd's algorithm with random initialization in terms of the cost of the computed solution (Arthur & Vassilvitskii, 2007). However, from a theoretical point of view, the approximation guarantee of $O(\log k)$ is not fully satisfying as constant approximation algorithms exist (Ahmadian et al., 2017). Unfortunately, it is known that the analysis is tight (Arthur & Vassilvitskii, 2007) and there are also input sets such that k -means++ achieves an $o(\log k)$ -approximation with probability at most $\exp(-k^{1-o(1)})$ (Bruns & Rögl, 2011). At the same time, it is known that k -means++ provides a constant bi-criteria approximation with constant probability, if one allows to sample $O(k)$ centers (Aggarwal et al., 2009). More recently, a more precise tradeoff with respect to the number of centers and the expected cost has been given by (Wei, 2016).

1.1. Our Contribution

We show that a simple combination of k -means++ seeding with $O(k \log \log k)$ rounds of local search gives a constant approximation guarantee in expectation. Our strategy is as follows. We start similarly as k -means++: We iteratively sample centers from a distribution where every point has probability proportional to its cost in the current clustering. However, after we have sampled k centers we continue for another $O(k \log \log k)$ rounds. In order to maintain a set of k centers, we exchange the newly sampled center with the old center, such that the swap improves the cost by the largest amount. If there is no improving swap, we discard the sampled center. We prove that after $O(k \log \log k)$ iterations our solution is in expectation a constant factor larger than the optimal solution.

- old center → new center (swap 시 cost의 변화가 클 때)
- cost 변화가 많지 X → sampled center 삭제

We remark that the analysis of the local search algorithm by Kanungo et al. (Kanungo et al., 2004) already implies that after some (potentially very large) number of rounds the algorithm ends up with a constant approximation. Their algorithm improves the current solution by swapping one center with an input point. Kanungo et al. proved that this algorithm gives in polynomial time a constant approximation (Kanungo et al., 2004). Unfortunately the running time of this simple swapping strategy can be very high. The main contribution of the paper is to introduce a new improvement strategy that is provably very fast: after only $O(k \log \log k)$ rounds the resulting center has constant approximation guarantee in expectation.

We empirically evaluated our algorithm. The evaluation shows that we improve the quality of the solution significantly (8-35%) compared with the basic k -means++ seeding when both algorithms are not using Lloyd's algorithm for postprocessing. In the case that both algorithms perform 10 steps of Lloyd's algorithm after the seeding the relative improvement over k -means++ is in the range of 1 - 18%.

1.2. Other Related Work

Kanungo et al. analyzed and empirically evaluated their local search algorithm as well as a few other variants of k -means clustering (Kanungo et al., 2004). In their experiments the local search based algorithm was converging very slowly. They achieved the best performance using a combination of local search and Lloyd's algorithm (Lloyd, 2006). A combination of local search and Lloyd's algorithm with a coresets construction has been developed (Frahling & Sohler, 2008). In the setting of streaming algorithms, as part of the StreamKM++ algorithm a heuristic is given to quickly approximate the k -means++ seeding using coresets trees (Ackermann et al., 2012). A more recent approach to approximately sample from the k -means++ distribution uses the Metropolis-Hastings algorithm to approximately sample from the k -means++ distribution (Bachem et al., 2016). In order to make the seeding applicable in a parallel setting, the k -means|| algorithm (Bahmani et al., 2012) reduces the number of rounds by sampling centers independently with (probability proportional) to the squared distance. This allows to sample sets of centers in parallel.

In terms of (mostly) theoretical results, it is known that there are different constant approximation algorithms for the k -clustering problem with sum of squared errors (" k -means clustering") (Jain & Vazirani, 2001; Kanungo et al., 2004; Ahmadian et al., 2017). Currently, the best approximation ratio is 6.357 (Ahmadian et al., 2017). It is also known that it is NP-hard to obtain a solution with approximation factor less than 1.0013, i.e. there is no $(1 + \epsilon)$ -approximation algorithm for arbitrary small $\epsilon > 0$, if k and d can be large (Lee et al., 2017). For constant d , one can obtain $(1 + \epsilon)$ -

approximation algorithms using local search (Cohen-Addad, 2018; Cohen-Addad et al., 2016; Friggstad et al., 2016) (see also (Bandyapadhyay & Varadarajan, 2016)). However, the running time of these algorithm depends doubly exponential on the dimension. If k and ϵ are considered to be constant, there are many $(1 + \epsilon)$ approximation algorithms available that are based on reducing the input size or the number of candidate solutions (see, for example, (Har-Peled & Mazumdar, 2004; Feldman et al., 2007; Chen, 2009; Kumar et al., 2010)).

2. Preliminaries

Let $P = \{p_1, \dots, p_n\}$ be a point set in \mathbb{R}^d . For two points $p, q \in \mathbb{R}^d$ we use $\|p - q\|$ to denote their Euclidean distance. In the sum-of-squared-error problem (or k -means problem) we aim to find a set C of k centers in \mathbb{R}^d that minimizes the following objective function over all such sets C :

$$\text{cost}(P, C) = \sum_{i=1}^n \min_{c \in C} \|p_i - c\|^2.$$

For a point set P we define its mean or center of gravity to be

$$\mu(P) = \frac{1}{|P|} \sum_{p \in P} p.$$

We note that $\mu(P)$ is an optimal solution to the 1-means problem. Finally we refer to the set of optimal centers as C^* . We use P_1^*, \dots, P_k^* to be the partitioning into clusters induced by the optimal centers and we refer to the cost of the optimal solution as Opt_k .

The following lemma is folklore:

Lemma 1. Let $P \subseteq \mathbb{R}^d$ be a set of points and let $c \in \mathbb{R}^d$ be a center. Then we have $\text{cost}(P, \{c\}) = |P| \cdot \|c - \mu(P)\|^2 + \text{cost}(P, \mu(P))$.

We will also use the following lemma (rephrased from Corollary 21 in (Feldman et al., 2018)).

Lemma 2. Let $\epsilon > 0$. Let $p, q \in \mathbb{R}^d$ and let $C \subseteq \mathbb{R}^d$ be a set of k centers. Then $|\text{cost}(\{p\}, C) - \text{cost}(\{q\}, C)| \leq \epsilon \cdot \text{cost}(\{p\}, C) + (1 + \frac{1}{\epsilon}) \|p - q\|^2$.

3. An improved k -means++ algorithm

We analyze the following algorithm. Starting with an empty solution C we sample a point p at random from P where the probability to sample $p \in P$ is proportional to $\text{cost}(\{p\}, C)$ (in the first step we sample uniformly at random). Then if $|C| < k$, we add the sampled point to C . Otherwise we check whether there exists a point $c \in C$ such that $\text{cost}(P, C \setminus \{c\} \cup \{p\}) < \text{cost}(P, C)$. If this is the case, we replace c by the point in C that reduces the cost function by

$C \rightarrow P$ 변경

initial clustering \hat{C} . Furthermore:

$$\begin{aligned} E[X] &= 500\text{Opt}_k + \text{cost}(P, \hat{C}) \\ &= \sum_{i=0}^Z \binom{Z}{i} \frac{1}{1000} \frac{999}{1000}^{Z-i} \left(1 - \frac{1}{100k}\right)^i \\ &= \text{cost}(P, \hat{C}) \left(1 - \frac{1}{100000k}\right)^{100000k \log \log k} \\ &\leq \frac{\text{cost}(P, \hat{C})}{\log k} + 500\text{Opt}_k \end{aligned}$$

This implies that $E[\text{cost}(P, \hat{C})] \leq \frac{\text{cost}(P, \hat{C})}{\log k} + 500\text{Opt}_k$. But now:

$$\begin{aligned} E[\text{cost}(P, C)] &= \sum_{\hat{C}} E[\text{cost}(P, C) | \hat{C}] P(\hat{C}) \\ &= \sum_{\hat{C}} P(\hat{C}) \left(\frac{\text{cost}(P, \hat{C})}{\log k} + 500\text{Opt}_k \right) \\ &= \frac{E[\text{cost}(P, \hat{C})]}{\log k} + 500\text{Opt}_k \end{aligned}$$

Now the theorem follows from (Arthur & Vassilvitskii, 2007) where the authors prove that $E[\text{cost}(P, \hat{C})] \leq (8 \log k + 2)\text{Opt}_k$. So $E[\text{cost}(P, C)] \leq 509\text{Opt}_k$. \square

In the rest of section we show Lemma 3, the main idea behind the proof is to compare the current set of centers and the optimal set of centers and to show that if the cost of the current solution is high ($> 500\text{Opt}_k$) we are likely to sample a node that will improve the clustering. Our general proof strategy is inspired to the analysis of the single swap heuristic (Kanungo et al., 2002), although we modified them to make them work in our context.

4.1. Proof of Lemma 3

We assume that the optimal solution $C^* = \{c_1^*, \dots, c_k^*\}$ is unique (this can be enforced using proper tiebreakers) and use P_1^*, \dots, P_k^* to denote the corresponding optimal partition. We will also use $C = \{c_1, \dots, c_k\}$ to refer to our current clustering with corresponding partition P_1, \dots, P_k . When the indices are not relevant, we will drop the index and write, for example, $c \in C$.

We use some ideas from (Kanungo et al., 2002) that have been used to analyze the single swap heuristic. We say that an optimal center c^* is captured by a center $c \in C$, if c is the nearest center to c^* among all centers in C . Note that a center $c \in C$ may capture more than one optimal center and every optimal center is captured by exactly one center from

$C^* = \mathcal{M}(P)$ 는 C 와 매칭된다.

\hookrightarrow 가까운 하나와 1:1 매칭

but C^* 와 가장 가까운 C 는 하나이지만 C 가 매칭 X 일수도

C (ties are dealt with in an arbitrary way). Hence, some center in C may not capture any optimal center. Similarly to (Kanungo et al., 2002) we call these centers lonely. Let L be the index set of lonely centers and let H be the index set of centers capturing exactly one cluster. Wlog. we assume that for $h \in H$ we have that $c_h \in C$ captures $c_h^* \in C^*$, i.e. the indices of the clusters with a one-to-one correspondence are identical. \rightarrow 1:1 대응이 됨

We will use the above definition in the following way. If a center c captures exactly one cluster of the optimal solution, we think of it as a candidate center for this cluster. In this case, if c is far away from the center of this optimal cluster, we argue that with good probability we sample a point close to the center. In order to analyze the change of cost, we will argue that we can assign all points in the cluster of c that are not in the captured optimal cluster to a different center without increasing their contribution by too much. This will be called the reassignment cost and is formally defined in the definition below. We will show that with good probability we sample from a cluster such that the improvement for the points in the optimal cluster is significantly bigger than the reassignment cost.

\star If a center is lonely, we think of it as a center that can be moved to a different cluster. Again, we will argue that with high probability we can sample points from other clusters such that the reassignment cost is much smaller than the improvement for this cluster. \rightarrow 두가지의 영향이 다르네

Now we start to analyze the cost of reassignment of the points due to a center swap.

We would like to argue that reassigning the points currently assigned to a cluster center with index from H or L to other clusters is small. In the case of clusters with index $h \in H$, we will assign all points from P_h that are not in P_h^* to other centers. In the case of clusters with index $l \in L$ we will consider the cost of assigning all points in P_l to other clusters. We introduce the following definition to capture the cost of this reassignment.

Definition 1. Let $P \subseteq \mathbb{R}^d$ be a point set and $C \subseteq \mathbb{R}^d$ be a set of k cluster centers and let H be the subset of indices of cluster centers from $C = \{c_1, \dots, c_k\}$ that capture exactly one cluster center of an optimal solution $C^* = \{c_1^*, \dots, c_k^*\}$. Let $P_i, P_i^*, 1 \leq i \leq k$, be the corresponding clusters. Let $h \in H$ be an index with cluster P_h and wlog. let P_h^* be the cluster in the optimal solution captured by c_h . The reassignment cost of c_h is defined as $\rightarrow C_h$: 바뀌진 원래.

$\text{reassign}(P, C, c_h) = \text{cost}(P \setminus P_h^*, C \setminus \{c_h\}) - \text{cost}(P \setminus P_h^*, C)$ 아닌 거만 빼면 \rightarrow 면면 \uparrow

For $\ell \in L$ we define the reassignment cost of c_ℓ as

$\text{reassign}(P, C, c_\ell) = \text{cost}(P \setminus \{c_\ell\}) - \text{cost}(P, C) \rightarrow C$ 에 없던 거 빼면 \rightarrow 면면 \downarrow

We will now prove the following lemma on reassignment costs.

Lemma 4. For $r \in H \cup L$ we have

$$\text{reassign}(P, C, c_r) \leq \frac{21}{100} \text{cost}(P_r, C) + 24 \text{cost}(P_r, C^*).$$

Proof. We only present the case $r \in H$. The case $r \in L$ is almost identical (in fact, simpler). We observe that $\text{reassign}(P, C, c_r) = \text{cost}(P_r \setminus P_r^*, C \setminus \{r\}) - \text{cost}(P_r \setminus P_r^*, C)$ since vertices in clusters other than P_r will still be assigned to their current center. Our main idea is as follows. If $r \in H$, we assign every point in $P_r \cap P_i^*$, $i \neq r$, to the center that captured the center of P_i^* . While this assignment may not be optimal, its cost gives an upper bound on the cost of reassigning the points. In order to get an estimate for the cost of reassigning the points, we proceed as follows: We move every point in $P_r \cap P_i^*$, $i \neq r$, to the center of P_i^* . After this movement, the closest center of C to these points is the center that captured the center of P_i^* , which, for points not in P_r^* , cannot be r , since r is in H . We then use the fact that the squared moved distance of each point equals its contribution to the optimal solution to get an upper bound on the cost change using Lemma 2. After this, we move the points back to their original location while keeping their cluster assignments fixed. Again we can use the bound on the overall moved distance together with Lemma 2 to obtain a bound on the change of cost. Combining the two bounds we obtain an upper bound on the increase of cost that comes from reassigning the points. Details follow.

Let Q_r be the (multi)set of points obtained from $P_r \setminus P_r^*$ by moving each point in $P_i^* \cap P_r$, $i \neq r$, to c_i^* . We apply Lemma 2 with $\epsilon = 1/10$ to get an upper bound for the change of cost with respect to C that results from moving the points to Q_r . For $p \in P_r \setminus P_r^*$ let $q_p \in Q_r$ be the point of Q_r to which p has been moved. We have:

$$\begin{aligned} & \rightarrow |\text{cost}(\{p\}, C) - \text{cost}(\{q_p\}, C)| \\ & \leq \frac{1}{10} \text{cost}(\{p\}, C) + 11 \cdot \text{cost}(\{p\}, C^*). \end{aligned}$$

Summing up over all points in $P_r \setminus P_r^*$ yields

$$\begin{aligned} & |\text{cost}(P_r \setminus P_r^*, C) - \text{cost}(Q_r, C)| \\ & \leq \frac{1}{10} \text{cost}(P_r \setminus P_r^*, C) + 11 \cdot \text{cost}(P_r \setminus P_r^*, C^*). \end{aligned}$$

① center로 옮기기

Note that after this movement all points from $P_r \setminus P_r^*$ have been assigned to centers from $C \setminus \{r\}$. Now we analyze the cost of moving the points back to their original location while maintaining this assignment. Let $Q_{r,i}$ be the points in Q_r that are nearest to center $c_i \in C$ and let $P_{r,i}$ be the set of their original locations. For $p \in P_{r,i}$ that has been

moved to $q_p \in Q_{r,i}$ we have:

$$\begin{aligned} & |\text{cost}(\{q_p\}, \{c_i\}) - \text{cost}(\{p\}, \{c_i\})| \\ & \leq \frac{1}{10} \text{cost}(\{q_p\}, \{c_i\}) + 11 \cdot \text{cost}(\{p\}, \{c_i\}) \end{aligned}$$

Summing up over all points in Q_r and the corresponding points in Q_r yields

$$\begin{aligned} & |\text{cost}(Q_r, C) - \sum_{i=1}^k \text{cost}(P_{r,i}, \{c_i\})| \rightarrow \text{all } q_r \rightarrow p \text{ cost} \\ & \leq \frac{1}{10} \text{cost}(Q_r, C) + 11 \cdot \text{cost}(P_r \setminus P_r^*, C^*) \\ & \leq \frac{1}{10} \left(\frac{11}{10} \text{cost}(P_r \setminus P_r^*, C) + 11 \cdot \text{cost}(P_r \setminus P_r^*, C^*) \right) + 11 \cdot \text{cost}(P_r \setminus P_r^*, C^*) \\ & \leq \frac{11}{100} \text{cost}(P_r, C) + 13 \cdot \text{cost}(P_r, C^*). \end{aligned}$$

Hence,

$$\begin{aligned} \text{reassign}(P, C, c_r) &= |\text{cost}(P_r \setminus P_r^*, C) - \sum_i \text{cost}(P_{r,i}, \{c_i\})| \\ &\leq |\text{cost}(P_r \setminus P_r^*, C) - \text{cost}(Q_r, C)| + |\text{cost}(Q_r, C) - \sum_i \text{cost}(P_{r,i}, \{c_i\})| \\ &\leq \frac{21}{100} \text{cost}(P_r, C) + 24 \text{cost}(P_r, C^*). \end{aligned}$$

For the first equality note that $\sum_i \text{cost}(P_{r,i}, \{c_i\}) = \text{cost}(P_r \setminus P_r^*, C \setminus \{r\})$.

Now that we have a good bound on the reassignment cost we make a case distinction. Recall that we assume that for every $h \in H$ the optimal center captured by c_h is c_h^* , i.e. the indices are identical. We first consider the case that

$$\sum_{h \in H} \text{cost}(P_h^*, C) > \frac{1}{3} \text{cost}(P, C).$$

With the previous lemma at hand, we can focus on the centers $h \in H$ where replacing h by an arbitrary point close to the optimal cluster center of the optimal cluster captured by h improves the cost of the solution significantly. We call such clusters good and make this notion precise in the following definition.

Definition 2. A cluster index $h \in H$ is called good, if

$$\text{cost}(P_h^*, C) - \text{reassign}(P, C, c_h) - \frac{9 \text{cost}(P_h^*, \{c_h^*\})}{100k} > \frac{1}{100k} \cdot \text{cost}(P, C).$$

The above definition estimates the gain of replacing c_h by a point close to the center of P_h^* by considering a clustering

$$Q_{r,i} \rightarrow P_{r,i}$$

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that reassigns the points in (P_h) that do not belong to (P_h^*) and assigns all points in (P_h) to the new center. Now we want to show that we have a good probability to sample a good cluster. In particular, we first argue that the sum of cost of good clusters is large.

Lemma 5. If $3 \sum_{h \in H} \text{cost}(P_h^*, C) > \text{cost}(P, C) \geq 500 \text{Opt}_k$, then

$$\sum_{h \in H, h \text{ is good}} \text{cost}(P_h^*, C) \geq \frac{1}{25} \text{cost}(P, C).$$

Proof. We have $\sum_{h \in H} \text{cost}(P_h^*, C) \geq \frac{1}{3} \text{cost}(P, C)$ and by the definition of good and Lemma 4

$$\sum_{h \in H, h \text{ is not good}} \text{cost}(P_h^*, C) \leq \left\{ \sum_{h \in H} \text{reassign}(P, C, c_h) + 9 \text{Opt}_k + \frac{1}{100} \text{cost}(P, C) \right\} \leq \frac{22}{100} \text{cost}(P, C) + 33 \text{Opt}_k.$$

Using that $\text{cost}(P, C) \geq 500 \text{Opt}_k$ we obtain that

$$\sum_{h \in H, h \text{ is not good}} \text{cost}(P_h^*, C) \leq \frac{143}{500} \cdot \text{cost}(P, C).$$

So $\sum_{h \in H, h \text{ is good}} \text{cost}(P_h^*, C) \geq \frac{23}{500} \cdot \text{cost}(P, C)$. The lemma follows.

Now we show that whenever a cluster has high cost wrt. (C) it suffices to consider the points close to the optimal center to get an approximation of the cost of the cluster. We will then use this fact to argue that we sample with good probability a point close to the center. In the following lemma it will be helpful to think of (Q) as being a (good) cluster in the optimal solution and (C) being the centers of the current solution.

Lemma 6. Let $(Q) \subseteq \mathbb{R}^d$ be a point set and let $(C) \subseteq \mathbb{R}^d$ be a set of k centers and let $\alpha \geq 9$. If $\text{cost}(Q, C) \geq \alpha \cdot \text{cost}(Q, \{\mu(Q)\})$ then

$$\text{cost}(R, C) \geq \left(\frac{\alpha - 1}{8} \right) \cdot \text{cost}(Q, \{\mu(Q)\}),$$

where $(R) \subseteq (Q)$ is the subset of (Q) at squared distance at most $\frac{2}{|\alpha|} \cdot \text{cost}(Q, \{\mu(Q)\})$ from $\mu(Q)$.

Proof. We know that the closest center in (C) to $\mu(Q)$ has squared distance at least $\frac{\alpha - 1}{|\alpha|} \cdot \text{cost}(Q, \{\mu(Q)\})$ as otherwise $\text{cost}(Q, C) < \alpha \cdot \text{cost}(Q, \{\mu(Q)\})$ by Lemma 1. Hence, the squared distance of every point in (R) to (C) is at least

$$(\sqrt{\alpha - 1} - \sqrt{2})^2 \cdot \text{cost}(Q, \{\mu(Q)\}) / |\alpha| \geq (\alpha - 1) / 4 \cdot \text{cost}(Q, \{\mu(Q)\}) / |\alpha|.$$

where we use that $\alpha \geq 9$ and so $\sqrt{\alpha - 1} \geq 2\sqrt{2}$. Furthermore, by averaging we get $|R| \geq |Q|/2$, which together with the inequality above implies the result.

Now we can argue that sampling according to sum of squared distances will provide us with constant probability with a good center. Consider any index $h \in H$ with h being good. We will apply Lemma 6 with $Q = P_h^*$ and $\alpha = \text{cost}(Q, C) / \text{cost}(Q, \mu(Q))$. Note that by the definition of good, we have that $\alpha \geq 9$. Now let us define R_h^* to be the set (R) guaranteed by Lemma 6. We have $\text{cost}(R_h^*, C) \geq \frac{\alpha - 1}{8} \text{cost}(P_h^*, \{c_h^*\}) = \frac{\alpha - 1}{8\alpha} \text{cost}(P_h^*, C) \geq \frac{1}{9} \text{cost}(P_h^*, C)$ by our choice of α observe that c_h^* equals $\mu(P_h^*)$. Since the sum of squared distances of points in good clusters is at least $1/25 \text{cost}(P, C)$ by Lemma 5, we conclude that $\sum_{h \in H, h \text{ is good}} \text{cost}(R_h^*, C) \geq \frac{1}{9 \cdot 25} \text{cost}(P, C)$. Thus, the probability to sample a point from $\cup_{h \in H, h \text{ is good}} \text{cost}(R_h^*, C)$ is more than $1/1000$. By the definition of good, if we sample such a point $c \in R_h^*$ we can swap it with (c_h) to get a new clustering of cost at most $\text{cost}(P, C) - \text{cost}(P_h^*, C) + \text{reassign}(P, C, \{c_h\}) + \text{cost}(P_h^*, \{c\})$. By Lemma 1 we know that $\text{cost}(P_h^*, \{c\}) \leq 9 \text{cost}(P_h^*, \{c_h^*\})$. Hence, with probability at least $1/1000$ the new clustering has cost at most

$$\begin{aligned} & \text{cost}(P, C) - (\text{cost}(P_h^*, C) - \text{reassign}(P, H, c_h) - 9 \text{cost}(P_h^*, \{c_h^*\})) \\ & \leq (1 - \frac{1}{100k}) \cdot \text{cost}(P, C). \end{aligned}$$

This proves our lemma in the first case.

In the second case, we have $\sum_{h \in H} \text{cost}(P_h^*, C) < 1/3 \text{cost}(P, C)$. Now let $R = \{1, \dots, k\} \setminus H$, so we get $\sum_{r \in R} \text{cost}(P_r^*, C) \geq 2/3 \text{cost}(P, C)$. Observe that R equals the index set of optimal cluster centers that were captured by centers that capture more than one optimal center. This is because every optimal center is captured by one center and R does not include H . In this case, if the index of a center of our current solution is in $(R \setminus L)$ we cannot easily move the cluster center without having impact on other clusters. What we do instead is to use the centers in L as candidate centers for a swap. Similar to the case above we will argue that we can swap a center from L with a point that is close to an optimal center of a cluster (P_r^*) for some $r \in R$.

Recall that we have already bounded the cost of reassigning a center in L so we just need to argue that the probability of sampling a good center is high enough.

In particular, we focus on the centers $r \in R$ and swap an arbitrary center $\ell \in L$ with an arbitrary point close to one of the centers in R to improve the cost of the solution. Slightly overloading notation, we call such cluster centers good and make this notion precise in the following definition.

$$\text{Cost}(P, C) = |P| |C - \mu(P)|^2 + \text{cost}(P, \mu(P)) + \text{cost}(P, \mu(Q))$$

Definition 3. A cluster index $i \in \{1, \dots, k\}$ is called good, if there exists a center $\ell \in L$ such that

$$\text{cost}(P_i^*, C) - \text{reassign}(P, C, \ell) - 9\text{cost}(P_i^*, \{c_i^*\}) > \frac{1}{100k} \cdot \text{cost}(P, C).$$

The above definition estimates the cost of removing ℓ and inserting a new cluster center close to the center of P_i^* by considering a clustering that reassigns the points in P_i^* and assigns all points in P_i^* to the new center. In the following we will now argue that the sum of cost of good clusters is large, this will be useful to show that the probability of sampling such a cluster is high enough.

Lemma 7. If $3 \sum_{h \in H} \text{cost}(P_h^*, C) \leq \text{cost}(P, C)$ and $\text{cost}(P, C) \geq 500\text{Opt}_k$ we have

$$\left[\sum_{r \in R, r \text{ is good}} \text{cost}(P_r^*, C) \geq \frac{1}{20} \text{cost}(P, C). \right]$$

Proof. We have $\sum_{r \in R} \text{cost}(P_r^*, C) \geq 2/3 \text{cost}(P, C)$. Note that $|R| \leq 2|L|$. By the definition of good and Lemma 4

$$\begin{aligned} \sum_{r \in R, r \text{ is not good}} \text{cost}(P_r^*, C) &\leq 2|L| \min_{\ell \in L} \text{reassign}(P, C, \ell) + 9\text{Opt}_k \\ &\leq \frac{1}{100} \text{cost}(P, C) \\ &\leq 2 \sum_{\ell \in L} \text{reassign}(P, C, \ell) + 9\text{Opt}_k \\ &\leq \frac{1}{100} \text{cost}(P, C) \\ &\leq \frac{43}{100} \text{cost}(P, C) + 57\text{Opt}_k. \end{aligned}$$

Using that $\sum_{i \in \{1, \dots, k\}} \text{cost}(P_i^*, C) \geq 500\text{Opt}_k$ we obtain that

$$\sum_{r \in R, r \text{ is not good}} \text{cost}(P_r^*, C) \leq \frac{11}{20} \text{cost}(P, C)$$

Now the bound follows by combining the previous inequality with $\sum_{r \in R} \text{cost}(P_r^*, C) \geq 2/3 \text{cost}(P, C)$. \square

Note that also in this case we can now argue similarly as in the other case that sampling according to sum of squared distances will provide us with constant probability with a good center using Lemma 6. In fact, since the sum of squared distances of points in good centers is at least $1/20 \text{cost}(P, C)$ by Lemma 7, it follows together with Lemma 6 that we sample a point from a good cluster P_r^* that is within distance two times the average cost of the cluster with probability $\frac{1}{1000}$. By the definition of good, we know that such a point improves the cost of the current clustering by at least a factor of $(1 - \frac{1}{100k})$. Thus, Lemma 3 follows.

5. Experiments

In this experiment we study the performance of our algorithm in practice. In particular, we have two main goals:

- Study the reduction in the cost that we obtain by running our local search post-processing after k -means++
- Study the reduction in the cost that we obtain by running our local search post-processing after k -means++ and then we run the Lloyd's algorithm on the set of obtained centers

Algorithms. We compare four different algorithms:

- KM++: the classic k -means++ algorithm (Arthur & Vassilvitskii, 2007)
- LS++: our algorithm presented in Section 3
- LL-KM++: the classic k -means++ algorithm (Arthur & Vassilvitskii, 2007) followed by 10 steps of the Lloyd's algorithm (Lloyd, 2006)²
- LL-LS++: our algorithm presented in Section 3 followed by 10 steps of the Lloyd's algorithm (Lloyd, 2006)

Datasets. We consider the k -means clustering for $k = 25$ or 50 on 3 different datasets:

- RNA – 8 features from 488565 RNA input sequence pairs (Uzilov et al., 2006)
- KDD-BIO – 145751 samples with 74 features measuring the match between a protein and a native sequence (KDD)
- KDD-PHY – 100000 samples with 78 features representing a quantum physic task (KDD)

We run all our experiments 3 times and we report the average of the results.

Results. In Figure 1 we compare the performance of our algorithm with the classic k -means++ for $k = 50$ and $k = 25$. We note that our algorithm improves substantially the performance of the classic k -means++ algorithm with a cost reduction that spans from the 8% to 35%. We also note that the gain that we obtain with our algorithm is stable across different datasets.

²We stop the Lloyd's algorithm when the incremental improvement of an iteration was small. In particular, after 10 steps of Lloyd's the improvement that we observed was less 0.4% per iteration for all considered datasets and for all different choices on the number of centers.

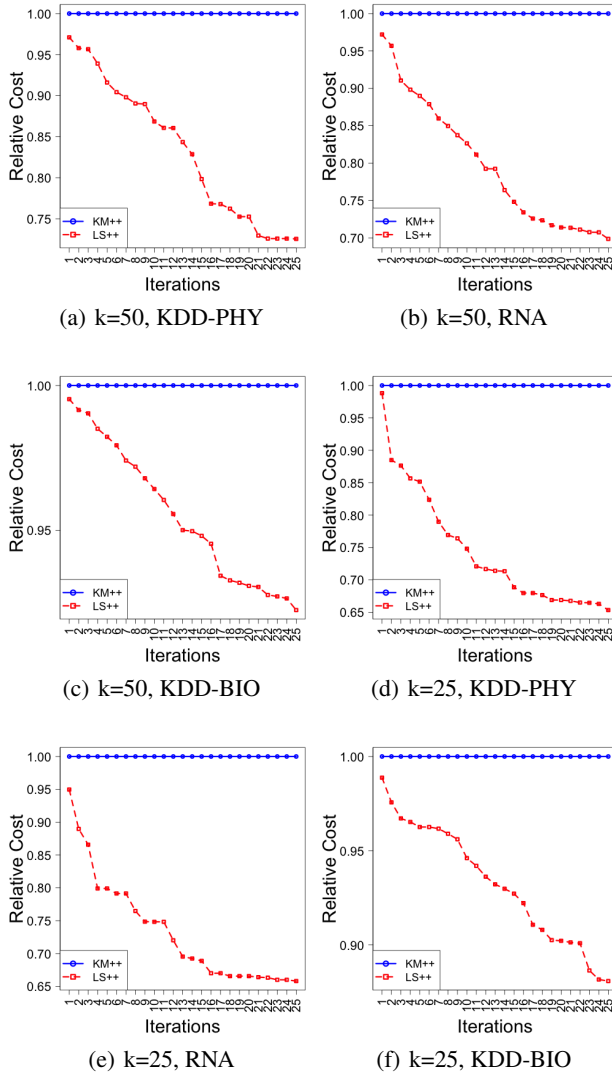


Figure 1. Comparison between the cost of KM++ and LS++. The x axes is the number of local search iterations that we run for our algorithm. The y axes show the relative cost of the algorithm compared with the cost of KM++.

In Figure 2 we compare the performance of LL-LS++ with LL-KM++ for $k = 50$ and $k = 25$. We can observe that the reduction of the cost after Lloyd's is significantly reduced and it is between 1% and 18%. We also note that the reduction is slightly less stable, especially for $k = 25$ and that in KDD-bio the gain is reduced substantially after running Lloyd's but the algorithm still outperform the baseline. Nevertheless we note that LL-LS++ almost always obtain better results than LL-KM++. Confirming the effectiveness of our seeding procedure.

Finally we observe that our algorithm is very efficient in practice. In fact, the time spent to run 25 iteration of our algorithm is smaller than the time spent in a single Lloyd's iteration.

6. Conclusions

We propose a simple variation of k -means++ algorithm based on local search and prove that the algorithm achieves a constant factor approximation. Furthermore we show experimentally the impact the effectiveness of our method.

It is an interesting open question to improve our analysis to reduce the number of local search steps needed in our analysis to obtain a constant factor approximation. In particular it would be nice to show that $O(k)$ steps are sufficient.

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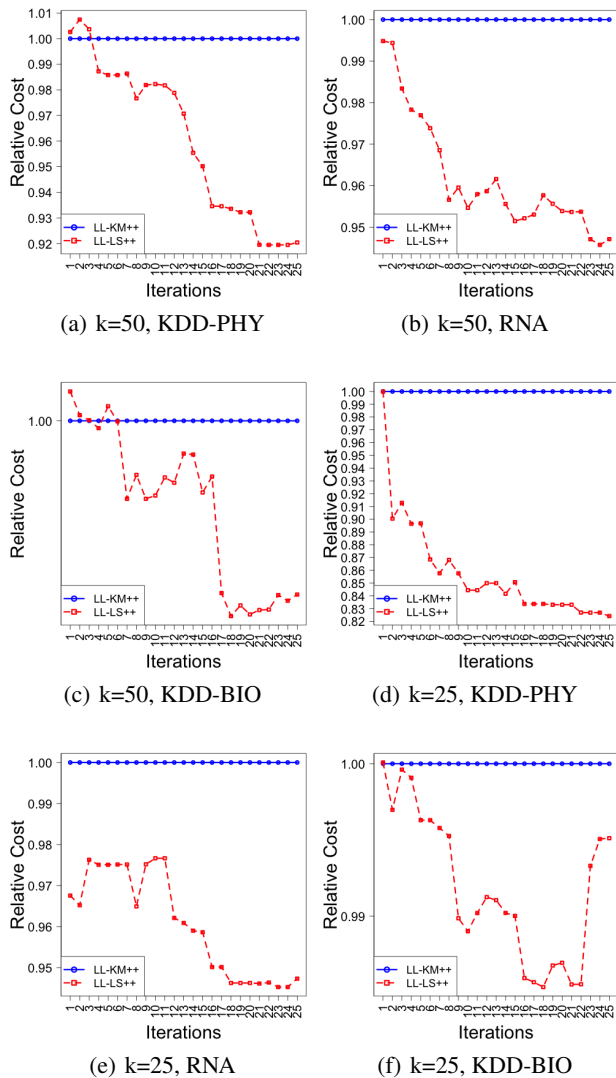


Figure 2. Comparison between the cost of LL-KM++ and LL-LS++. The x axes is the number of local search iterations that we run for our algorithm. The y axes show the relative cost of the algorithm compared with the cost of LL-KM++.

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