A Faster $k$-means++ Algorithm

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Abstract

$k$-means++ is an important algorithm for choosing initial cluster centers for the $k$-means clustering algorithm. In this work, we present a new algorithm that can solve the $k$-means++ problem with nearly optimal running time. Given $n$ data points in $\mathbb{R}^d$, the current state-of-the-art algorithm runs in $\tilde{O}(k)$ iterations, and each iteration takes $\tilde{O}(ndk)$ time. The overall running time is thus $\tilde{O}(ndk^2)$. We propose a new algorithm FASTKMEANS++ that only takes in $\tilde{O}(nd + nk^2)$ time, in total.

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1 Introduction

$k$-means clustering aims to cluster $n$ data points from $\mathbb{R}^d$ into $k$ clusters, such that the average distance between a data point and the center of the cluster it belongs to is minimized. $k$-means has many important real-world applications in signal processing [GG12, DMC15] and unsupervised machine learning [DH04, CN12].

A central problem in $k$-means is how to pick the initial locations of the $k$ clusters to avoid $k$-means from finding poor clusters. Much work focuses on finding a “good” initialization for the $k$-means algorithm. The well-known heuristic Lloyd algorithm [Llo82] performs well in practice while there is no theoretical guarantee for its approximation at initialization. There are already constant approximation algorithms with theoretical guarantee [JV01, KMN+04]. Unfortunately, $(1 + \epsilon)$-approximation algorithm for arbitrary small $\epsilon > 0$ does not exist if $k$ and $d$ can be large [LSW17]. In recent works [BV15, CA18, CAKM19, FRS19], one achieved $(1 + \epsilon)$ approximation algorithm. However, the running time of these algorithms depends on $d$ double exponentially. For fixed $k$ and $\epsilon$, one may reduce input size or number of potential solutions to achieve constant approximation [HPM04, HPK05, FMS07, Che09, KSS10].

$k$-means++ [AV06] is an algorithm that can find a center set that achieves $O(\log k)$ approximation for the optimal center set. $k$-means++ has thus been integrated into many standard machine learning libraries and is used as the default initialization method, replacing the traditional random initialization method. If allowed to sample $O(k)$ centers, [ADK09] shows that $k$-means++ achieves constant bi-criteria approximation with constant probability. The more accurate trade-off between the number of centers to be sampled and the expected cost can be found in [Wei16]. [ANFSW19] provides a 6.357 ratio approximation guarantee using primal-dual algorithm.

We note that applying a local search algorithm is one feasible way to achieve constant approximation for $k$-means clustering [KMN+04, FS08, CA18, FRS19]. However, these algorithms suffer from a potentially large number of iterations. A more efficient $k$-means++ algorithm via local search was proposed in [LS19] to achieve constant approximation. It is an iterative method that requires $\tilde{O}(k)$ iterations, and each iteration has to take $\tilde{O}(nk^2)$ time. The overall running time is thus $\tilde{O}(nk^2)$. This running time is fine for small and low-dimensional data, but it is increasingly insufficient for today’s explosion of dataset sizes ($n$), data dimensionality ($d$), and the number of clusters ($k$).

In this paper, we propose a faster version of the $k$-means++ algorithm, called FastKMeans++. We show that choosing initial cluster locations can be much faster for constant approximation. We observe that the major computation cost originates from distance calculation. To accelerate the algorithm, especially for high dimensional situations, we design a distance oracle using JL lemmas [JL84] to approximate distance. We can approximate the $k$-means++ algorithm in $\tilde{O}(nd + nk^2)$ time and maintain constant approximation. When $k = O(\sqrt{d})$, we obtain optimal running time. In experiments, we use the $k$-means++ algorithm [LS19] and FastKMeans++ algorithm to cluster the same synthetic point set respectively. We use $k$-means++ as a baseline to evaluate the performance of FastKMeans++. Our experimental results demonstrate that FastKMeans++ is faster than $k$-means++ in practice.

1.1 Our Results

We state an informal version of our results as follows.

**Theorem 1.1** (Informal Version of Theorem 5.1). Given point set $P \subset \mathbb{R}^d$ and $Z = \tilde{O}(k)$, the running time of Algorithm 3 is $\tilde{O}(n(d + k^2))$ which uses $O(n(d + k))$ space.
We use $C$ to denote the result of Algorithm 3. Let $C^\ast$ be the set of optimum centers. Then we have

$$\mathbb{E}[\text{cost}(P, C)] = O(\text{cost}(P, C^\ast)).$$

Our result shows that our algorithm using a distance oracle still achieves constant approximation in expectation and runs in nearly optimal running time.

2 Related Work

Clustering In [HPM04], they showed the existence of small coresets for the problems of computing $k$-means clustering for points in low dimensions. In [HPK05], when they got clusterings for many different values of $k$, they used a quality measure of clusterings that is independent of $k$ to determine a good choice of $k$, like the average silhouette coefficient. In [FMS07], they use a weak ($\epsilon, k$)-coreset to obtain a PTAS for the $k$-means clustering problem with running time $O(nkd + d \cdot \text{Poly}(k/\epsilon) + 2\tilde{O}(k/\epsilon))$. In [Che09], they use coresets whose size is with polynomial dependency on the dimension $d$ to maintain a $(1 + \epsilon)$-approximate $k$-means clustering of a stream of points in $\mathbb{R}^d$. In [KSS10], they provide simple randomized algorithms for the $k$-means that yield $(1 + \epsilon)$ approximations with probability $\geq 1/2$ and running times of $O(2^{k/\epsilon}O(1)\cdot d\cdot n)$. In [LS19], they provide a $O(1)$-approximation algorithm and runs in $O(nk^2)$ time. In [CALNF+20], they provide a log($k$)-approximation and runs in $(nd + dk^3)$ time. Our algorithm achieves $O(1)$-approximation and runs in $O(nd + nk^2)$. The approximation factor of [LS19] is the same as ours, but their running time is always slower than ours. Also when $d \approx n$, their algorithm [CALNF+20] takes $O(nk^3)$ while ours takes only $O(nk^2)$.

Sketching for Iterative Algorithm Sketching is an effective method to increase the speed of machine learning algorithms and optimization techniques. It involves compressing the large input matrix down to a much smaller sketching matrix that retains most of the key features of the original. As the algorithm now processes this smaller representation rather than the full high-dimensional input, its runtime can be substantially reduced. The core benefit is that the key information is preserved while removing redundant data that would otherwise slow computations. By working with this concise sketch version, large performance gains are possible without significantly impacting output quality.

In this work, we apply the sketching technique to an iterative algorithm. It is well-known that the sketching technique can be applied to many fundamental problems that are solved by the iterative type of algorithm. For example, linear programming [CLS19, JSWZ21, SY21, GS22], empirical risk minimization [LSZ19, QSZZ23], cutting plane method [JLSW20], computing John Ellipsoid [CCLY19, SYYZ22], low-rank approximation [SYYZ23a], tensor decomposition [DSY23], integral minimization problem [JLSZ23], federated learning [BSY23], linear regression problem [CW13, NN13, SYYZ23b, SYZ23b], matrix completion [GSYZ23], training over-parameterized neutral tangent kernel regression [BPSW21, SZZ21, Zha22, ALS+22], attention computation problem [SYZ23a, GSWY23, GSY23], and matrix sensing [DLS23].

Roadmap In Section 3, we introduce preliminary knowledge including notation and folklore lemmas. In Section 4, we present our data structure of DISTANCEORACLE. In Section 5, we present the main results for FASTKMEANS++ algorithm. In Section 6, we demonstrate the running time and space storage for the algorithm. We provide the pseudocode of our algorithms and use a
series of experiments to justify the advantages of our FastKMeans++ algorithm in Section 7. In Section 8, we draw our conclusion.

3 Preliminary

In Section 3.1, we first introduce several basic notations, such as the number of elements in a set, the distance between two nodes, and mathematical expectation. We introduce related definitions throughout the paper in Section 3.2, such as the sum of the distance between each node and its closest center and the mass center of multiple points. We present useful lemmas in Section 3.3, such as the method to calculate or estimate the sum of the distance between each node in a point set and a specific center or between a given node and each node in a center point set.

3.1 Notation

We use \([n]\) to denote set \(\{1, 2, \cdots, n\}\). Given finite set \(S\), we use \(|S|\) to denote the number of elements in set \(S\). We use \(\| \cdot \|_2\) to denote \(\ell_2\) norm in Euclidean space. We use \(| \cdot |\) to denote absolute value. Given random variable \(X\), we use \(E[X]\) to denote its expectation. For any function \(f\), we use \(O(f)\) to denote \(f \cdot \text{poly}(\log f)\).

3.2 Related Definitions

We define the cost given data set \(P\) and center set \(C\).

**Definition 3.1 (Cost).** Given set \(P \subset \mathbb{R}^d\) and set \(C \subset \mathbb{R}^d\), we define \(\text{cost}(P, C) := \sum_{i=1}^{n} \min_{c \in C} \|p_i - c\|^2_2\).

Also, we define the mean or center of gravity for a point set.

**Definition 3.2 (Mean).** Given data set \(P \subset \mathbb{R}^d\), we define the mean of this set \(\mu(P) := \frac{1}{|P|} \sum_{p \in P} p\).

3.3 Useful Lemmas

The following JL Lemma provides guidance for achieving distance oracle data structure.

**Lemma 3.3 (JL Lemma, [JL84]).** For any \(X \subset \mathbb{R}^d\) of size \(n\), there exists an embedding \(f : \mathbb{R}^d \rightarrow \mathbb{R}^m\) where \(m = O(\epsilon^{-2} \log n)\) such that

\[
(1 - \epsilon) \cdot \|x - y\|^2_2 \leq \|f(x) - f(y)\|^2_2 \leq (1 + \epsilon) \cdot \|x - y\|^2_2
\]

The following lemma is folklore which bridges the cost (Definition 3.1) and mean (Definition 3.2)

**Lemma 3.4.** Let \(P \subset \mathbb{R}^d\) be a point set. Let \(c \in \mathbb{R}^d\) be a center. Let \(\mu(P)\) be defined as \(\mu(P) := \frac{1}{|P|} \sum_{p \in P} p\) (Definition 3.2). Then we have

\[
\text{cost}(\{p\}, C) = |P| \cdot \|c - \mu(P)\|^2_2 + \text{cost}(P, \mu(P))
\]

We present a variation of Corollary 21 in [FSS20] which gives an upper bound on the cost difference.

**Lemma 3.5.** For arbitrary \(\epsilon > 0\), let \(p, q\) be two different points in \(\mathbb{R}^d\) and \(C \subset \mathbb{R}^d\) be the center set. Then

\[
|\text{cost}(\{p\}, C) - \text{cost}(\{q\}, C)| \leq \epsilon \cdot \text{cost}(\{p\}, C)
\]

\[
+ (1 + \frac{1}{\epsilon})\|p - q\|^2_2
\]
4 Data Structure

In Section 4.1, we present the data structure of DistanceOracle. In Section 4.2, we state the running time results for DistanceOracle.

4.1 Distance Oracle

In this section, we state the result for the Distance Oracle data structure. In Init procedure, we preprocess the original data set \( P \subset \mathbb{R}^d \) using JL transform and store the transformed sketches. When we need to compute distance, we only use these sketches so that we can get rid of factor \( d \).

We also use index set \( S \subset [n] \) to denote current centers. We maintain a balanced search tree array \( v \) of size \( n \) that records the closet center for each data point and supports Insert, Delete, and GetMin operations. Using tree array \( v \), we are able to compute the current cost (Definition 3.1) with Cost operation and also the cost after adding a center with Query operation.

Theorem 4.1 (Distance Oracle). There is a data structure that uses space

\[
O(n(d + k + \varepsilon^{-2} \log n \log(n/\delta)))
\]

with the following procedures:

- **Init** Given data \( P \subset \mathbb{R}^d \), center \( S \subset [n] \), precision parameter \( \varepsilon \in (0, 0.1) \) and failure probability \( \delta \in (0, 0.1) \), it takes \( O(n \log n) \) time to initialize.

- **Cost** It returns an approximate cost \( \tilde{d} \) using \( O(n) \) time such that

\[
(1 - \varepsilon) \cdot \text{cost}(P, S) \leq \tilde{d} \leq (1 + \varepsilon) \cdot \text{cost}(P, S)
\]

- **Insert** Given index \( j \in [n] \), it inserts distances between \( y_j \) and all sketches to \( v \) using \( O(n \log n) \) time.

- **Delete** Given index \( j \in [n] \), it deletes all distances between \( y_j \) and all sketches using \( O(n \log n) \) time.

- **Sample** It samples an index \( j \) using \( O(n) \) time.

- **Query** Given an index \( j \in [n] \), it returns a value \( \tilde{q} \) that satisfies

\[
(1 - \varepsilon) \cdot \text{cost}(P, \{x_j\}) \leq \tilde{q} \leq (1 + \varepsilon) \cdot \text{cost}(P, \{x_j\})
\]

using \( O(n \log n) \) time.

Proof. By Lemma 4.2, Lemma 4.3, Lemma 4.4, Lemma 4.5, Lemma 4.6 and Lemma 4.7, we obtain the running time for procedure Init, Cost, Insert, Delete, Sample and Query, respectively. In each of these lemmas, we calculate and prove the time complexity of each procedure.

In DistanceOracle, it stores \( n \) data points in \( \mathbb{R}^d \), \( n \) sketches in \( \mathbb{R}^m \) and maintain an \( n \)-array. Each entry of the \( n \)-array is a balanced search tree with \( O(k) \) nodes. Also, we have \( m = O(\varepsilon^{-2} \log(n/\delta)) \). The total space storage is

\[
O(nd) + O(nm) + O(nk) = O(n(d + k + \varepsilon^{-2} \log(n/\delta)))
\]
Algorithm 1 Distance Oracle

1: data structure \textbf{DistanceOracle} \Comment{Theorem 4.1}
2: members
3: \texttt{n, m, d, k} $\in \mathbb{N}_+$
4: \texttt{P} = \{x_1, \ldots, x_n\} \Comment{|P| = n, \text{P} \subset \mathbb{R}^d}
5: \texttt{Q} = \{y_1, \ldots, y_n\} \Comment{|Q| = n, \text{Q} \subset \mathbb{R}^m}
6: \texttt{S} $\subset$ \texttt{[\texttt{n}]}
7: \texttt{v} \Comment{This is a length-\texttt{n} array and each entry in the array is a balanced search tree where the root has the minimum value.}
8: \texttt{sum}
9: end members
10: procedure \texttt{Init}(\texttt{P} $\subset$ \texttt{R}^d, \texttt{S} $\subset$ \texttt{[n]}, \texttt{\epsilon} $\in$ (0, 0.1), \texttt{\delta} $\in$ (0, 0.1))
11: \texttt{P} $\leftarrow$ \texttt{P}
12: \texttt{m} $\leftarrow$ $O(\epsilon^{-2} \log(n/\delta))$
13: for \texttt{i} = 1 $\rightarrow$ \texttt{n} do
14: \texttt{y}_i $\leftarrow$ \texttt{Pi} \texttt{x}_i
15: end for
16: \texttt{S} $\leftarrow$ \texttt{S}
17: end procedure
18: procedure \texttt{Cost}()
19: \texttt{sum} $\leftarrow$ 0
20: for \texttt{i} = 1 $\rightarrow$ \texttt{n} do
21: \texttt{sum} $\leftarrow$ \texttt{sum} + \texttt{v}[\texttt{i}].\texttt{GetMin}()
22: end for
23: return \texttt{sum}
24: end procedure
25: procedure \texttt{Insert}(\texttt{j} $\in$ \texttt{[n]})
26: \texttt{S} $\leftarrow$ \texttt{S} $\cup$ \texttt{j}
27: for \texttt{i} = 1 $\rightarrow$ \texttt{n} do
28: \texttt{v}[\texttt{i}].\texttt{Insert}(\texttt{j}, \|\texttt{y}_i - \texttt{y}_j\|_2^2)
29: end for
30: \texttt{Cost}()
31: end procedure
32: procedure \texttt{Delete}(\texttt{j} $\in$ \texttt{[n]})
33: \texttt{S} $\leftarrow$ \texttt{S} \texttt{\setminus} \texttt{j}
34: for \texttt{i} = 1 $\rightarrow$ \texttt{n} do
35: \texttt{v}[\texttt{i}].\texttt{Delete}(\texttt{j})
36: end for
37: \texttt{Cost}()
38: end procedure
39: end data structure

4.2 Running Time of Distance Oracle

We start to prove the running time for \texttt{Init}.

**Lemma 4.2** (Running Time of \texttt{Init}). Given data \texttt{P} $\subset$ \texttt{R}^d, index set \texttt{S} $\subset$ \texttt{[n]}, precision parameter \texttt{\epsilon} $\in$ (0, 0.1) and failure probability \texttt{\delta} $\in$ (0, 0.1), procedure \texttt{Init} takes $O(\epsilon^{-2}nd \log(n/\delta))$ time to
Algorithm 2 Distance Oracle

1: data structure DistanceOracle \>
   \text{Theorem 4.1}
2: procedure Sample()
3: \text{sum} \leftarrow 0
4: \textbf{for} \ i = 1 \rightarrow n \ \textbf{do}
5: \quad u_i \leftarrow v[i].\text{GetMin}()
6: \quad \text{sum} \leftarrow \text{sum} + u_i
7: \textbf{end for}
8: \text{Sample an index j via probability equal to } \frac{u_j}{\text{sum}}
9: \text{return } j
10: \textbf{end procedure}
11: procedure Query(j)
12: \text{tmp} \leftarrow 0
13: \textbf{for} \ i = 1 \rightarrow n \ \textbf{do}
14: \quad u_i \leftarrow \min\{v[i].\text{GetMin}(), \|y_i - y_j\|_2^2\}
15: \quad \text{tmp} \leftarrow \text{tmp} + u_i
16: \textbf{end for}
17: \text{return } \text{tmp}
18: \textbf{end procedure}
19: \textbf{end data structure}

\textit{initialize}.

\textit{Proof.} The running time is dominated by the for-loop in Line 13 with \(n\) iterations. In each iterations, it samples a sketch matrix \(\Pi\) from \(\mathbb{R}^{m \times d}\) and obtains a sketch \(\Pi x\) (Line 14), which takes \(O(md)\) time. Thus, the total running time is

\[
 n \cdot O(md) = O(\epsilon^{-2}nd \log(n/\delta))
\]

which follows from \(m = O(\epsilon^{-2} \log(n/\delta))\)

Next, we turn to prove the running time for \textit{Cost}.

\textbf{Lemma 4.3 (Running Time of Cost).} Procedure \textit{Cost} returns the current cost using \(O(n)\) time.

\textit{Proof.} Procedure \textit{Cost} runs a for-loop in Line 20 with \(n\) iterations. In each iteration, it runs in \(O(1)\) time (Line 21). Thus the total running time is \(O(n)\).

We show the running time of \textit{Insert} in the following lemmas.

\textbf{Lemma 4.4 (Running Time of Insert).} Given index \(j \in [n]\), it inserts distances between \(y_j\) and all sketches to \(v\) using \(O(\epsilon^{-2}n \log(n/\delta))\) time.

\textit{Proof.} Procedure \textit{Insert} runs a for-loop (Line 27) with \(n\) iterations then calls procedure \textit{Cost}. In each iteration \(i\), it first calculate \(\|y_i - y_j\|_2^2\) which takes \(O(m)\) time and insert into balanced tree \(v[i]\) using \(O(\log n)\) time (Line 28). After the for-loop, it calls \textit{Cost} which takes \(O(n)\) time. Thus, the total running time is \(n \cdot O(m + \log n) + O(n) = O(\epsilon^{-2}n \log(n/\delta))\) which follows from \(m = O(\epsilon^{-2} \log(n/\delta))\)

We turn to prove the running time of \textit{Delete}.
Lemma 4.5 (Running Time of DELETE). Given index \( j \in [n] \), procedure DELETE deletes all distances between \( y_j \) and all sketches using \( O(n \log n) \) time.

Proof. Procedure DELETE runs a for-loop (Line 34) with \( n \) iterations then calls procedure Cost. In each iteration \( i \), it delete node \( j \) in balanced tree \( v[i] \) (Line 35) using \( O(\log n) \) time. After the for-loop, it calls \( \text{Cost} \) (Line 37) which takes \( O(n) \) time. Thus, the total running time is \( n \cdot O(\log n) + O(n) = O(\epsilon^{-2} \log n \log(n/\delta)) \) which follows from \( m = O(\epsilon^{-2} \log(n/\delta)) \).

We present the running time of Sample

Lemma 4.6 (Running Time of SAMPLE). Procedure SAMPLE samples an index \( j \) according to probability

\[
\frac{\text{cost}\{x_j, C\}}{\sum_{i=1}^{n} \text{cost}\{x_i, C\}}
\]

using \( O(n) \) time.

Proof. Procedure SAMPLE first runs a for-loop (Line 4) with \( n \) iterations then sample an element from \([n]\). In each iteration, Line 5 and Line 6 runs in \( O(1) \) time. The sampling step in Line 8 runs in \( O(n) \) time. Thus, the total running time is \( O(n) \).

We show the running time of QUERY procedure.

Lemma 4.7 (Running Time of QUERY). Given an index \( j \in [n] \), procedure QUERY returns the sum of distances between \( y_j \) and all sketches using \( O(\epsilon^{-2} n \log(n/\delta)) \) time.

Proof. Procedure QUERY runs a for-loop (Line 13) with \( n \) iterations. In each iteration \( i \), it calculates \( \|y_i - y_j\|_2^2 \) which takes \( O(m) \) time and GetMin procedure for balanced search tree (Line 14) runs in \( O(\log n) \) time. Thus, the total running time is \( n \cdot O(m + \log n) = O(\epsilon^{-2} n \log(n/\delta)) \).

5 Main Result

We state the main result for our algorithm including running time, space storage, and constant approximation guarantee.

Theorem 5.1 (Formal Version of Theorem 1.1). Given data set \( P \subset \mathbb{R}^d \), number of centers \( k \in \mathbb{N} \), precision parameter \( \epsilon \in (0, 0.1) \), failure probability \( \delta \in (0, 0.1) \) and set \( Z = O(k \log \log k) \), the running time of the FASTKMEANS++ algorithm is

\[
O(\epsilon^{-2} n(d + k^2 \log \log k) \log(n/\delta)).
\]

Let \( C \) be the output of our FASTKMEANS++ Algorithm 3. Let \( C^* \) be the set of optimal centers. Then, we have \( E[\text{cost}(P, C)] = O(\text{cost}(P, C^*)) \).

In addition this algorithm requires \( O(n(d + k + \epsilon^{-2} \log(n/\delta))) \) space.

Proof. It follows from Lemma 6.3 (Space part), Lemma 6.1 (Running time part), and Lemma A.10 (Correctness part).

6 Running Time and Space

Section 6.1 presents the running time for FASTKMEANS++ algorithm. Section 6.2 shows the running time for LOCALSEARCH++. Section 6.3 states the space storage for FASTKMEANS++.
6.1 Running Time of FastKMeans++

In this section, we present the running time of the FastKMeans++ algorithm.

**Lemma 6.1** (Running Time of FastKMeans++, Running time of Theorem 5.1). Given data set $P \subset \mathbb{R}^d$, number of cluster centers $k \in \mathbb{N}$, precision $\epsilon \in (0, 0.1)$, failure probability $\delta \in (0, 0.1)$ and $Z = O(k \log \log k)$, the running time of Algorithm 3 is

$$O(\epsilon^{-2}n(d + k^2 \log \log k) \log(n/\delta)).$$

**Proof.** The running time consists of three parts.

- By Theorem 4.1, Line 7 takes $O(\epsilon^{-2}nd \log(n/\delta))$ time and Line 10 takes $O(\epsilon^{-2}n \log(n/\delta))$ time.
- In Line 11, there is a for-loop with $O(k)$ iterations. In each iteration, Line 12 takes $O(n)$ time and Line 14 runs in $O(\epsilon^{-2}n \log(n/\delta))$ time.
- In Line 16, there is another for-loop with $Z$ iterations. In each iteration, it calls LocalSearch++ which takes $O(\epsilon^{-2}nk \log(n/\delta))$ time by Lemma 6.2.

Thus, the total running time for FastKMeans++ is

$$O(\epsilon^{-2}nd \log(n/\delta)) + O(\epsilon^{-2}n \log(n/\delta))$$

$$+ k \cdot (O(n) + O(\epsilon^{-2}n \log(n/\delta)))$$

$$+ Z \cdot O((\epsilon^{-2}nk \log(n/\delta))$$

$$= O(\epsilon^{-2}n(d + \log n) \log(n/\delta))$$

$$+ O(\epsilon^{-2}nk \log(n/\delta))$$

$$+ O(\epsilon^{-2}nk^2 \log(k) \log(n) \log(n/\delta))$$

$$= O(\epsilon^{-2}n(d + k^2 \log \log k) \log(n/\delta))$$

where the first step follows from $Z = O(k \log \log k)$, and the last step follows from summing all terms in the first step.

Thus, we complete the proof. \qed

6.2 Running Time of LocalSearch++

In this section, we prove the running time for LocalSearch++ (Algorithm 4).

**Lemma 6.2** (Running Time of LocalSearch++). Given data set $P \subset \mathbb{R}^d$ and center set $C \subset \mathbb{R}^d$, the running time of LocalSearch++ is $O(\epsilon^{-2}nk \log(n/\delta))$.

**Proof.** In Line 3, it calls Sample procedure which takes $O(n)$ time. Line 6 takes $O(n)$ time. Line 7 is a for-loop with $k$ iterations. In each iteration, it takes $O(n \log n)$ time to run Delete (Line 8), $O(\epsilon^{-2}n \log(n/\delta))$ to run Query procedure (Line 9) and $O(\epsilon^{-2}n \log(n/\delta))$ to run Insert (Line 14). The running time for one step iteration is $O(\epsilon^{-2}n \log(n/\delta))$. Line 16 and Line 17 runs in $O(\epsilon^{-2}n \log(n/\delta)$ time.

Thus, the total running time for LocalSearch++ is

$$O(n) + k \cdot O(\epsilon^{-2}n \log(n/\delta)) + O(\epsilon^{-2}n \log(n/\delta))$$

$$= O(\epsilon^{-2}nk \log(n/\delta))$$

Thus, we complete the proof. \qed
6.3 Space Storage

In this section, we prove the space storage of FastKMeans++ algorithm.

**Lemma 6.3** (Space Storage For Algorithm 3, Space part of Theorem 5.1). The space storage of Algorithm 3 is \( O(n(d + k + \epsilon^2 \log(n/\delta))) \).

**Proof.** The space storage in Algorithm 3 comes from DistanceOracle and center set \( C \subset [n] \) (Line 4).

We have the total space storage for FastKMeans++

\[
O(n(d + k + \epsilon^2 \log(n/\delta))) + O(n) = O(n(d + k + \epsilon^2 \log(n/\delta)))
\]

Thus, we complete the proof.

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**Figure 1:** The relationship between each parameter and the running time, where original algorithm denotes Algorithm in [LS19], and our algorithm denotes FastKMeans++ in Theorem 5.1. Let \( n \) be the number of points in the point set. Let \( d \) denote the dimension of each node. Let \( m \) denote the dimension of each node after we process them with a sketching matrix. Let \( k \) be the number of clusters and centers.

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**Figure 2:** The running time of \( k \)-means++ and FastKMeans++ algorithm on SCADI and MUPCI data set. \( m \) denotes the dimension of each node after we transformed all of them, and \( k \) denotes the number of clusters. There are two figures for each data set. The left one shows the relationship between the running time of two algorithms and \( m \), and the right one shows the relationship between the running time of two algorithms and \( k \).
Figure 3: The running time of \( k \)-means++ and \textsc{FastKMeans++} algorithm on Libras Movement and STDW data set. \( m \) denotes the dimension of each node after we transformed all of them, and \( k \) denotes the number of clusters. There are two figures for each data set. The left one shows the relationship between the running time of two algorithms and \( m \), and the right one shows the relationship between the running time of two algorithms and \( k \).

7 Experiments

\textbf{Purpose.} In this section, we use \( k \)-means++ algorithm in [LS19] and \textsc{FastKMeans++} algorithm in Theorem 5.1 to cluster the same synthetic point set respectively. We use \( k \)-means++ as a baseline to evaluate the performance of \textsc{FastKMeans++}. We designed a new data structure \textsc{DistanceOracle} in Theorem 4.1. In \textsc{DistanceOracle}, we use a balanced search tree to store the nodes of each cluster to make the searching process faster. In order to shorten the time of calculating the distance between two nodes, we also create a sketching matrix that decreases the number of dimensions of each node. We adjust the parameters of our \textsc{FastKMeans++} and original \( k \)-means++ algorithm spontaneously to observe the influence of each parameter on their running time. Our summary of the result is as follows:

- Our \textsc{FastKMeans++} algorithm is much faster than original \( k \)-means++ algorithm if \( m \) is small enough.
- The running time of \( k \)-means++ and \textsc{FastKMeans++} algorithm will increase linearly as \( n \) increases.
- The running time of original \( k \)-means++ algorithm will increase linearly as \( d \) increases, but \( d \) doesn’t affect the running time of our \textsc{FastKMeans++} algorithm very much.
- The running time of our \textsc{FastKMeans++} algorithm will increase linearly as \( m \) increases, but \( m \) is unrelated with the running time of original \( k \)-means++ algorithm.
- The running time of \( k \)-means++ and \textsc{FastKMeans++} algorithm will increase squarely as \( k \) increases.

\textbf{Setup.} We use a computer of which the CPU is AMD Ryzen 7 4800H, GPU is RTX 2060 laptop. The operating system is Windows 11 Pro and we use Python as the code language. Let \( \ell_2 \) denote distance weights. Let \( n \) denote the number of points in the point set. Let \( d \) denote the dimension of each node. Let \( m \) denote the dimension of each node after we process them with a sketching matrix. Let \( k \) denote the number of clusters and centers. Let \( Z = O(k \log \log k) \) denote the number of iterations.

\textbf{Synthetic Data Generation.} We generate \( n \) random nodes of \( x_1, \cdots, x_n \in \mathbb{R}^d \) and each node is generated as follows
Table 1: Let $n$ denote the number of nodes and $d$ denote the dimension of each node. Here MUPCI denotes Mturk User-Perceived Clusters over Images. Let STDW denote the Sales Transactions Dataset Weekly Data Set. Let LM denote the Libras Movement. $m$ denotes the dimension of each node after we transformed all of them, and $k$ denotes the number of clusters.

| Dataset Names | $n$ | $d$ | $m$ | $k$ |
|---------------|-----|-----|-----|-----|
| SCADI         | 70  | 206 | [60, 80, 100, 120, 140] | [5, 10, 15, 20, 25] |
| MUPCI         | 180 | 500 | [150, 200, 250, 300, 350] | [5, 10, 15, 20, 25] |
| LM            | 360 | 91  | [30, 40, 50, 60, 70] | [10, 15, 20, 25, 30] |
| STDW          | 811 | 53  | [30, 40, 50, 60, 70] | [10, 15, 20, 25, 30] |

- Pick each coordinate of node from $[-1, 1]$.
- Normalize each vector so that its $\ell_2$ norm is 1.

In the original $k$-means++ algorithm, for node $x_i$ and node $x_j$, we use $\|x_i - x_j\|_2^2$ to denote the distance between them. This takes $O(d)$ time. As per update, it will take $O(nkd)$ time since there are $k$ clusters containing $n$ points. For $Z = O(k \log \log k)$ iterations, it takes $O(nkd^2 \log \log k)$ time.

In our FastKMEANS++ algorithm, we compute $y_i = Sx_i$ for $\forall i \in [n]$. It takes $O(nd)$ time since there are $n$ nodes in total. So when we initialize our data structure, it will take $O(nmd)$ time. In per update, we use $\|y_i - y_j\|_2^2$ to denote the distance between them. This takes $O(m)$ time. So it will take $O(nkm)$ time since we need to iterate over all clusters and calculate the distance to all other clusters.

For $Z = O(k \log \log k)$ iterations, it will take $O(nkd^2 \log \log k)$ time during the update process. Therefore, it will take

$$O(nmd + nmk^2 \log \log k)$$

time in total.

**Parameter Setting.** In our experiments, we choose $n = 150$, $d = 150$, $m = 75$ and $k = 15$ as primary condition.

**Real Datasets.** In this part, we run $k$-means++ and our FastKMEANS++ algorithm on real data sets from UCI library [DG17] to observe if our algorithm is better than the original one in a real-world setting.

- SCADI Data Set [ZBD18, BZ19]: This dataset contains 206 attributes of 70 children with physical and motor disability based on ICF-CY.
- Mturk User-Perceived Clusters over Images Data set [CLg+16]: This dataset random sampled 180 images from the NUS-WIDE image database. Each image has 500 features consisting of a bag of words based on SIFT descriptions.
- Libras Movement Data set [DMR+09]: The dataset contains 15 classes of 24 instances each. In the video pre-processing, a time normalization is carried out selecting 45 frames from each video, according to a uniform distribution. In each frame, the centroid pixels of the segmented objects (the hand) are found, which compose the discrete version of the curve $F$ with 45 points. Each instance contains 90 features of this curve $F$. 

11
• Sales Transactions Dataset Weekly Data set [TSL14]: This data set contains 811 sales transactions weekly. Each record has one product code and data for 52 weeks.

**Results.** To evaluate the influence of \( n \), we vary the value of \( n \in [50, 250] \) while keeping other parameters the same. Fig. 1a indicates the running time of original \( k \)-means++ and our FASTKMEANS++ algorithm increases linearly while \( n \) increases. We note that our FASTKMEANS++ algorithm is faster than the original \( k \)-means++ algorithm while \( n \) changes. The ratio of the running time of the original \( k \)-means++ to that of FASTKMEANS++ also increases from 8.26 to 8.33 as \( n \) increases.

Then we estimate the influence of \( d \), we vary the value of \( d \in [50, 250] \) while making sure \( n = 15, m = 75, k = 15 \) during the whole testing process. We compare the performance of the original \( k \)-means++ algorithm and our FASTKMEANS++ algorithm in Fig. 1b. It shows the running time of the original \( k \)-means++ algorithm increases linearly while \( d \) increases. The ratio of the running time of the original \( k \)-means++ to that of FASTKMEANS++ also increases from 2.77 to 14.30 as \( d \) increases. The running time of our FASTKMEANS++ seems unrelated with \( d \) because in this case, \( d \) is too small compared with other parameters like \( n \) and \( m \). To show the influence of \( d \) on our FASTKMEANS++ algorithm more clearly, we will explain it with more figures in the appendix.

To evaluate the influence of \( m \in [25, 125] \), we vary the value of \( m \) while keeping other parameters the same. Fig. 1c shows the running time of the original \( k \)-means++ algorithm doesn’t change but that of our algorithm increases linearly while \( m \) increases. And our FASTKMEANS++ algorithm runs faster compared to the original algorithm if \( m \) is small enough. The ratio of the running time of the original \( k \)-means++ to that of FASTKMEANS++ decreases from 17.73 to 5.59 as \( m \) increases. We vary the value of \( k \in [5, 25] \) and run \( k \)-means++ and FASTKMEANS++. From Fig. 1d we can see that the running time of original \( k \)-means++ and our algorithm increases squarely while \( k \) increases. We note that our FASTKMEANS++ algorithm is faster than the original \( k \)-means++ algorithm while \( k \) changes. The ratio of the running time of the original \( k \)-means++ to that of FASTKMEANS++ also increases from 2.95 to 13.04 as \( k \) increases. This is consistent with our original thought.

**Results for real data set.** Fig. 2a, Fig. 2b, Fig. 3a and Fig. 3b show the relationship between the running time of \( k \)-means++ algorithm and FASTKMEANS++ and parameter \( m \) and \( k \) on SCADI, MUPCI, Libras Movement and STDW data sets respectively. They show that our FASTKMEANS++ is much faster than the original \( k \)-means++ algorithm on real data sets.

### 8 Conclusion

In this paper, we accelerate the \( k \)-means++ algorithm using a distance oracle. We carefully design the data structure to support initialize, query, cost, etc. operations. We remove the factor \( d \) of running time in each iteration of the local search. Finally, we run our FASTKMEANS++ algorithm and the original \( k \)-means++ algorithm. In addition, we also implement our algorithm and obtain the experimental results which support our theoretical result. In this paper, we primarily focus on designing data structures and algorithms. We believe that proving a certain lower bound for our problem is also an interesting future direction. Our proposed FASTKMEANS++ algorithm not only improves computational efficiency but also maintains the quality of the clustering solution. We believe that our contributions will significantly advance the current state of scalable machine learning methods, opening up new possibilities for handling large-scale datasets.
Impact Statement

In this paper, we present the algorithm, theoretical analysis, and experiment. To the best of our knowledge, we do not foresee any potential negative societal consequences of our work.

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Appendix

Roadmap. In Section A, we provide the pseudocode of our algorithms and proof of the correctness result. In Section B, we provide more experimental results.

A Correctness

In Section A.1, we defined two operations capture and reassign respectively. Then in Section A.2, we prove the upper bound for reassign operation. In Section A.3, we defined a good cluster whose index is in $H$. $H$ is the subset of center set $C = \{c_1, \cdots, c_k\}$ that capture (Definition A.1) exactly one cluster center from optimal center set $C^* = \{c^*_1, \cdots, c^*_k\}$. Then we calculate a lower bound for the proportion of good clusters under certain conditions. In Section A.4, we calculate a lower bound for the cost related to the mean center (Definition 3.2). In Section A.5, similar to Section A.3, we provide a definition of a good cluster for general cases. And we calculate a lower bound for the proportion of such good clusters under certain conditions. With lemmas and definitions in these sections, we prove that in each iteration of LOCALSEARCH++, we can reduce the cost by $(1 - \frac{1}{100})$ with constant probability in Section A.6. Then in Section A.7, we prove the correctness of FastKMeans++.

Algorithm 3 Fast $k$-means++

```plaintext
1: data structure FastKMeans++▷ Theorem 5.1
2: members
3: DistanceOracle do
4: $C \subset [n]$  
5: end members
6: procedure Seeding($P \subset \mathbb{R}^d, k \in \mathbb{N}_+, Z \in \mathbb{N}_+, \epsilon \in (0, 0.1), \delta \in (0, 0.1)$)
7: do.Init($P, \epsilon, \delta$)
8: Sample index $j$ from $[n]$ uniformly at random
9: $C \leftarrow \{j\}$
10: do.Insert($j$)
11: for $i = 2 \to k$ do
12: $j \leftarrow$ do.Sample()
13: $C \leftarrow C \cup \{j\}$
14: do.Insert($j$)
15: end for
16: for $i = 2 \to Z$ do
17: LOCALSEARCH++()
18: end for
19: return $C$
20: end procedure
21: end data structure
```

A.1 Capture and Assign

In this section, we introduce two operations capture and assign.
**Algorithm 4 LocalSearch++**

```
1: data structure FastKMeans++
2: procedure LocalSearch++ () ▷ Lemma 6.2
3:   j ← DO.SAMPLE()
4:   a ← j
5:   q ← a
6:   tmpb ← DO.COST()
7:   for b ∈ C do
8:       DO.DELETE(b)
9:       tmpa ← DO.QUERY(a)
10:      if tmpa < tmpb then
11:          q ← b
12:          tmpb ← tmpa
13:      end if
14:     DO.INsert(b)
15:   end for
16:   DO.DELETE(q)
17:   DO.INsert(a)
18:   C ← (C \ q) ∪ a
19: end procedure
20: end data structure
```

**Definition A.1 (Capture).** Let $C^* = \{c_1^*, \cdots, c_k^*\}$ be optimal centers and $C = \{c_1, \cdots, c_k\}$ is current cluster centers. An optimal center $c^*$ is captured by a center $c \in C$ if

$$c = \arg \min_{c \in C} \|c^* - c\|^2_2.$$ 

Then, we state the definition of reassign operation as follows.

**Definition A.2 (Reassign).** Let $P \subset \mathbb{R}^d$ be a data set. Let $C \subset \mathbb{R}^d$ be cluster centers set and $C^* = \{c_1^*, \cdots, c_k^*\}$ be the optimal cluster centers set. Let $P_i, P_i^*, 1 \leq i \leq k$ be the corresponding clusters. Let $H$ denote the subset of center set $C = \{c_1, \cdots, c_k\}$ that capture (Definition A.1) exactly one cluster center from $C^*$. Let $L$ be the subset of cluster centers $C = \{c_1, \cdots, c_k\}$ that doesn’t capture (Definition A.1) any optimal centers. We use $P_h$ to denote the cluster with index $h \in H$ and use $P_h^*$ to denote the cluster in $C^*$ captured by $c_h$. We use a similar notation for the index $\ell \in L$.

For $h \in H$, we define the reassignment cost of $c_h$ as

$$\text{reassign}(P, C, c_h) := \text{cost}(P \setminus P_h^*, C \setminus \{c_h\}) - \text{cost}(P \setminus P_h^*, C)$$

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

$$\text{reassign}(P, C, c_\ell) := \text{cost}(P \setminus \{c_\ell\}) - \text{cost}(P, C)$$

**A.2 Upper Bound for Reassign Operation**

In this section, we calculate an upper bound for reassign operation.
Lemma A.3. For \( r \in H \cup L \) we have

\[
\text{reassign}(P, C, c_r) \leq \frac{21}{100} \cos(P_r, C) + 24 \cos(P_r, C^*)
\]

Proof. If a center \( c \in C \) does not capture any optimal center, we call it a lonely center. If a center is lonely, we think of it as a center that can be moved to a different cluster. We use \( Q_r \) to denote points obtained from \( P_r \setminus P_r^* \) by moving each point in \( P_r^* \cap P_r, i \neq r \), to \( c_i^* \). By Lemma 3.5 with \( \epsilon = 1/10 \), we obtain an upper bound for the change of cost with respect to \( C \), which results from moving the points to \( Q_r \). For \( p \in P_r \setminus P_r^* \), we use \( q_p \in Q_r \) to denote the point of \( Q_r \) to which \( p \) has been moved. We have:

\[
\left| \cos(\{p\}, C) - \cos(\{q_p\}, C) \right| \leq \frac{1}{10} \cos(\{p\}, C) + 11 \cdot \cos(\{p\}, C^*)
\]

Taking all points in \( P_r \setminus P_r^* \) into consideration,

\[
\left| \cos(P_r \setminus P_r^*, C) - \cos(Q_r, C) \right| \leq \frac{1}{10} \cos(P_r \setminus P_r^*, C) + 11 \cdot \cos(P_r \setminus P_r^*, C^*) \tag{1}
\]

Note that all points from \( P_r \setminus P_r^* \) have been assigned to centers from \( C \setminus \{r\} \). We turn to analyze the cost of moving the points back to the original location while maintaining the assignment. We use \( Q_{r,i} \) to denote the points in \( Q_r \) nearest to center \( c_i \in C \) and \( P_{r,i} \) to represent the set of their original locations. For \( p \in P_{r,i} \) that was moved to \( q_p \in Q_{r,i} \), we have:

\[
\left| \cos(\{q_p\}, \{c_i\}) - \cos(\{p\}, \{c_i\}) \right| \leq \frac{1}{10} \cos(\{q_p\}, \{c_i\}) + 11 \cdot \cos(\{p\}, \{q_p\})
\]

Taking all points in \( P_r \) and the corresponding points in \( Q_r \) into consideration,

\[
\left| \cos(Q_r, C) - \sum_{i=1}^{k} \cos(P_{r,i}, \{c_i\}) \right| \leq \frac{1}{10} \cos(Q_r, C) + 11 \cdot \cos(P_r \setminus P_r^*, C^*) \leq \frac{11}{100} \cos(P_r, C) + 13 \cdot \cos(P_r, C^*).
\]

where the first step follows \( \sum_{i=1}^{k} \cos(P_{r,i}, c_i) = \cos(P_r \setminus P_r^*, C \setminus \{r\}) \), the second step follows from Eq. (1) and the last step follows from \( \cos(P_r \setminus P_r^*, C^*) \leq \cos(P_r, C^*) \).

Hence,

\[
\text{reassign}(P, C, c_r) = \left| \cos(P_r \setminus P_r^*, C) - \sum_{i=1}^{k} \cos(P_{r,i}, \{c_i\}) \right| \leq \frac{21}{100} \cos(P_r, C) + 24 \cos(P_r, C^*)
\]
\[
\leq |\text{cost}(P_r \setminus P^*_r, C) - \text{cost}(Q_r, C)| + |\text{cost}(Q_r, C) - \sum_i \text{cost}(P_{r,i}, c_i)|
\]
\[
\leq \frac{21}{100} \text{cost}(P_r, C) + 24 \text{cost}(P_r, C^*)
\]

where the first step follows from definition of reassign and \(\sum_{i=1}^k \text{cost}(P_{r,i}, c_i) = \text{cost}(P_r \setminus P^*_r, C \setminus \{r\})\), the second step follows from inserting \(\text{cost}(Q_r, C)\) and the last step follows from Eq. (1) and Eq. (2).

\[\square\]

### A.3 Good Cluster

In this section, we introduce the definition of "good" for an index in \(H\) (Definition A.2).

**Definition A.4.** We define a good cluster index \(h \in H\) to be the one satisfying

\[
\text{cost}(P^*_h, C) - \text{reassign}(P, C, c_h) - 9 \text{cost}(P^*_h, \{c^*_h\}) > \frac{1}{100k} \cdot \text{cost}(P, C)
\]

The following lemma shows a lower bound for the proportion of good clusters under condition \(3 \sum_{h \in H} \text{cost}(P^*_h, C) > \text{cost}(P, C)\).

**Lemma A.5.** Let \(c_0 > 300\) be a constant. If \(3 \sum_{h \in H} \text{cost}(P^*_h, C) > \text{cost}(P, C) \geq 500 \text{OPT}_k\), then

\[
\sum_{h \in H, h \text{ is good}} \text{cost}(P^*_h, C) \geq \left(\frac{1}{9} - \frac{33}{c_0}\right) \cdot \text{cost}(P, C)
\]

**Proof.** We already have \(\sum_{h \in H} \text{cost}(P^*_h, C) \geq \frac{1}{3} \text{cost}(P, C)\). By the definition of good (Definition A.4) and Lemma A.3

\[
\sum_{h \in H, h \text{ is not good}} \text{cost}(P^*_h, C) \leq \sum_{h \in H} \text{reassign}(P, C, c_h) + 9 \text{OPT}_k + \frac{1}{100} \text{cost}(P, C)
\]
\[
\leq \frac{22}{100} \text{cost}(P, C) + 33 \text{OPT}_k
\]

where the first step follows from Definition A.4 and the last step follows from Lemma A.3.

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

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

To the opposite, we have \(\sum_{h \in H, h \text{ is good}} \text{cost}(P^*_h, C) \geq \frac{23}{900} \cdot \text{cost}(P, C)\).

Thus, we complete the proof. \(\square\)

### A.4 Lower Bound for Cost

In this section, the following lemma provides a lower bound for the cost related to the mean center (Definition 3.2)
Lemma A.6. Given point set $Q \subset \mathbb{R}^d$, center set $C \subset \mathbb{R}^d$ of size $k$ and parameter $\alpha \geq 9$. Let $R \subset Q$ be the subset of $Q$ such that $\text{cost}(R, \{\mu(Q)\}) = \frac{2}{|Q|} \cdot \text{cost}(Q, \{\mu(Q)\})$ from $\mu(Q)$. If 
$\text{cost}(Q, C) \geq \alpha \cdot \text{cost}(Q, \{\mu(Q)\})$, we have 
$$\text{cost}(R, C) \geq \frac{(\alpha - 1)}{8} \cdot \text{cost}(Q, \{\mu(Q)\}),$$

\textbf{Proof.} Lemma 3.4 implies that the closest center in $C$ to $\mu(Q)$ has squared distance at least $\frac{\alpha - 1}{|Q|} \cdot \text{cost}(Q, \{\mu(Q)\})$. Hence, the squared distance of points in $R$ to $C$ is at least 
$$(\sqrt{\alpha - 1} - \sqrt{2})^2 \cdot \text{cost}(Q, \{\mu(Q)\})/|Q| \geq (\alpha - 1)/4 \cdot \text{cost}(Q, \{\mu(Q)\})/|Q|$$
where we use that $\alpha \geq 9$ so that $\sqrt{\alpha - 1} \geq 2\sqrt{2}$. By taking average, we get $|R| \geq |Q|/2$. With the inequality above we obtain the result. \qed

\section{A.5 Good Cluster for General Cluster}
In this section, we introduce definition of "good" for general cluster index.

\textbf{Definition A.7.} Let $L$ be the subset of cluster centers $C = \{c_1, \cdots, c_k\}$ that doesn’t capture (Definition A.1) any optimal centers. For a general cluster index $i \in \{1, \cdots, k\}$, we say it is good if there exists a center $\ell \in L$ such that 
$$\text{cost}(P_i^*, C) - \text{reassign}(P, C, \ell) - 9 \text{cost}(P_i^*, \{c_i^*\}) > \frac{1}{100k} \cdot \text{cost}(P, C)$$

We prove a lower bound similar to Lemma A.5 in the case $3\sum_{h \in H} \text{cost}(P_h^*, C) \leq \text{cost}(P, C)$.

\textbf{Lemma A.8.} Let $c_0 > 300$ denote a constant. 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 
$$\sum_{r \in R, r \text{ is good}} \text{cost}(P_r^*, C) \geq \left(\frac{71}{300} - \frac{57}{c_0}\right) \text{cost}(P, C).$$

\textbf{Proof.} We already 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 (Definition A.7) and Lemma A.3
$$\sum_{r \in R, r \text{ is not good}} \text{cost}(P_r^*, C) \leq 2|L| \min_{\ell \in L} \text{reassign}(P, C, \ell) + 9 \text{OPT}_k + \frac{1}{100} \text{cost}(P, C)$$
$$\leq 2 \sum_{\ell \in L} \text{reassign}(P, C, \ell) + 9 \text{OPT}_k + \frac{1}{100} \text{cost}(P, C)$$
$$\leq \frac{43}{100} \text{cost}(P, C) + 57 \text{OPT}_k,$$
where the first step follows from Definition A.7, the second step follows from $|L| \min_{\ell \in L} \text{reassign}(P, C, \ell) \leq \sum_{\ell \in L} \text{reassign}(P, C, \ell)$ and the last step follows from Lemma A.3.
Using $\sum_{i \in \{1, \cdots, k\}} \text{cost}(P_i^*, C) \geq 500 \text{OPT}_k$, we obtain that
$$\sum_{r \in R, r \text{ is not good}} \text{cost}(P_r^*, C) \leq \frac{11}{20} \text{cost}(P, C)$$

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

22
A.6 Cost Reduction

Now, we can prove Lemma A.9. It suffices to show that using `DISTANCEORACLE`, we can control the sampling error and give a constant lower bound for sampling probability.

**Lemma A.9.** Let $c_0 > 300$ denote a constant. Let $P$ be a point set in $\mathbb{R}^d$. Let $C$ center set satisfying $\text{cost}(P, C) > c_0 \text{OPT}_k$. Let $C' = \text{LOCALSEARCH++}(P, C)$. With probability $\frac{1}{1000}(1 - \delta)$, we have $\text{cost}(P, C') \leq (1 - \frac{1}{100k}) \text{cost}(P, C)$.

**Proof.** Let $R_h^*$ be the set $R$ defined in Lemma A.6. For the case $P \in H$ $\text{cost}(P^*, C) \geq \frac{1}{3} \text{cost}(P, C)$, we conclude that

$$\sum_{h \in H, h \text{ is good}} \text{cost}(R_h^*, C) \geq \frac{1}{9} \cdot \left( \frac{1}{9} - \frac{33}{c_0} \right) \text{cost}(P, C) \geq \frac{1 - \epsilon}{1 + \epsilon} \cdot \left( \frac{1}{9} - \frac{11}{3c_0} \right) \text{cost}(P, C) \geq \left( \frac{1}{162} - \frac{11}{6c_0} \right) \text{cost}(P, C)$$

where the first step follows from Lemma A.5 and Lemma A.6, the second step follows from Cost part of Theorem 4.1, and the last step follows from $\frac{1 - \epsilon}{1 + \epsilon} \leq \frac{1}{2}$ when $\epsilon \in (0, 0.1)$, with probability at least $1 - \delta$, $\delta \in (0, 0.1)$.

With probability $1 - \delta$, we obtain lower bound $\frac{1}{162} - \frac{11}{6c_0}$. Conditioned on this event happening, we have probability at least $\frac{1}{162} - \frac{11}{6c_0}$ to ensure the following analysis. The whole probability is $(\frac{1}{162} - \frac{11}{6c_0})(1 - \delta)$. Thus, we can sample a point from $\bigcup_{h \in H, h \text{ is good}} R_h^*$ with probability no less than $(\frac{1}{162} - \frac{11}{6c_0})(1 - \delta)$.

By Definition A.4, when we sample a point in $R_h^*$, we can replace it with $c_h$ to get an upper bound on the cost.

$$\text{cost}(P, C \setminus \{c_h\} \cup \{c\}) \leq \text{cost}(P, C) - \text{cost}(P_h^*, C) + \text{reassign}(P, C, \{c_h\}) + \text{cost}(P_h^*, \{c\})$$

which follows from Definition A.4.

By Lemma 3.4 we have $\text{cost}(P_h^*, \{c\}) \leq 9 \text{cost}(P_h^*, \{c_h\})$. Thus, with probability at least $(\frac{1}{162} - \frac{11}{6c_0})(1 - \delta)$, we have

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

For the case $\sum_{h \in H} \text{cost}(P_h^*, C) \leq \frac{1}{3} \text{cost}(P, C)$, Lemma A.8 gives a similar lower bound as Lemma A.5. Using a similar technique as above, we conclude the same result for this case.

Thus, we complete the proof. \square
A.7 Correctness of FastKMeans++

In this section, we show the correctness of our FastKMeans++ algorithm using Lemma A.9. We remark that as long as we prove Lemma A.9, then we can achieve the following result.

Lemma A.10 (Correctness of FastKMeans++, correctness part of Theorem 5.1). Given input data set $P \subset \mathbb{R}^d$, we set $Z = O(k \log \log k)$ and use $C$ to denote the outcome of Algorithm 3. Let $C^*$ be the set of optimum centers. Then we have $\mathbb{E}[\text{cost}(P, C)] = O(\text{cost}(P, C^*))$.

Proof. Let $c_1 > 10^4$ be a constant.

Let $\hat{C}$ be the output of the first for-loop in Algorithm 3. Let $C$ be the final output of Algorithm 3. By Lemma A.9, conditioned on the fact that the cost of the centers is bigger than 5000 OPT before the first call of LocalSearch++, we reduce the cost by a $(1 - \frac{1}{100k})$ multiplicative factor with probability $\frac{1}{1000}$.

We construct an auxiliary random process $X$ to model the evolution of our algorithm. It starts with initial value $\text{cost}(P, \hat{C})$. Then, it goes through $Z = 10^5k \log \log k$ iterations and reduces its value by a $(1 - \frac{1}{100k})$ multiplicative factor with probability $1/1000$ per iteration.

At the end of the process, it increases its value by adding quantity $5000 OPT_k$.

We note that the value of $X$ after $Z$ iterations stochastically dominates the cost of the clustering. Thus, we have

$$
\mathbb{E}[X] = 500\text{OPT}_k + \text{cost}(P, \hat{C}) \sum_{i=0}^{Z} \left(\frac{Z}{i}\right) \left(\frac{1}{1000}\right)^i \left(\frac{999}{1000}\right)^{Z-i} \left(1 - \frac{1}{100k}\right)^i
$$

$$
= \text{cost}(P, \hat{C})(1 - \frac{1}{100k})^{10^5k \log \log k} + 500\text{OPT}_k
$$

$$
\leq \frac{\text{cost}(P, \hat{C})}{\log k} + 500\text{OPT}_k
$$

where the first step follows from the expectation of binomial distribution, the second step follows from combining $(\frac{1}{1000})^i$ and $(1 - \frac{1}{100k})^i$ and the last step follows from $(1 - \frac{1}{n})^n \leq \frac{1}{e}$ when $n > 10^5$.

This implies that $\mathbb{E}[\text{cost}(P, C) | \hat{C}] \leq \frac{\text{cost}(P, \hat{C})}{\log k} + 5000\text{OPT}_k$. In the meanwhile,

$$
\mathbb{E}[\text{cost}(P, C)] = \sum_{\hat{C}} \mathbb{E}[\text{cost}(P, C) | \hat{C}] P(\hat{C})
$$

$$
= \sum_{\hat{C}} P(\hat{C}) \left(\frac{\text{cost}(P, \hat{C})}{\log k} + 500\text{OPT}_k\right)
$$

$$
= \mathbb{E}[\text{cost}(P, \hat{C})] \frac{\text{log k}}{\log k} + 500\text{OPT}_k
$$

(3)

where the first step follows from the definition of conditional expectation, the second step follows from Eq. (3) and the last step follows from $\sum_{\hat{C}} P(\hat{C}) = 1$.

Now the theorem follows from the following results in [AV06]

$$
\mathbb{E}[\text{cost}(P, \hat{C})] \leq (8 \log k + 2) \text{OPT}_k .
$$

Hence,

$$
\mathbb{E}[\text{cost}(P, C)] \leq 509\text{OPT}_k .
$$

$\square$
B More Experiments

Here we provide the links for the four real datasets.

- SCADI Data Set [ZBD18, BZ19] ¹
- Mturk User-Perceived Clusters over Images Data set [CLg+16]²
- Libras Movement Data set [DMR+09]³
- Sales Transactions Dataset Weekly Data set [TSL14]⁴

Let \( n \) be the number of points in the point set. Let \( d \) denote the dimension of each node. We use \( m \) to denote the dimension of each node after we process them with a sketching matrix. Let \( k \) be the number of clusters and centers. We provide more results of experiments to show the influence of \( n, d, m, \) and \( k \) in this part.

To evaluate if the influence of parameter \( n \) will be affected by other parameters, we set different values for other parameters and run the original \( k \)-means++ algorithm and our FastKMeans++ algorithm. Fig. 4 and Fig. 5 show that the running time of original \( k \)-means++ and FastKMeans++ increase linearly as \( n \) increases no matter what the value of other parameters is.

To evaluate if the influence of parameter \( d \) will be affected by other parameters, we set different values for other parameters and run the original \( k \)-means++ algorithm and our FastKMeans++ algorithm. To make the influence of \( d \) on our FastKMeans++ more clear, I set \( d \) large enough compared with \( n, m, \) and \( k \). Fig. 6 and Fig. 7 show that the running time of original \( k \)-means++ and FastKMeans++ increase linearly as \( d \) increases no matter what the value of other parameters is.

To evaluate if the influence of parameter \( m \) will be affected by other parameters, we set different values for other parameters and run the original \( k \)-means++ algorithm and our FastKMeans++ algorithm. Fig. 8 shows that \( m \) is irrelevant to the running time of the original \( k \)-means++ algorithm. Fig. 9 shows that the running time of FastKMeans++ increases linearly as \( m \) increases no matter what the value of other parameters is.

To evaluate if the influence of parameter \( k \) will be affected by other parameters, we set different values for other parameters and run the original \( k \)-means++ algorithm and our FastKMeans++ algorithm. Fig. 10 and Fig. 11 show that the running time of original \( k \)-means++ and FastKMeans++ increase squarely as \( k \) increases no matter what the value of other parameters is.

**When should we use FastKMeans++ algorithm?** The result above demonstrates that our FastKMeans++ algorithm much faster than original \( k \)-means++ algorithm. It also shows that if we set \( m \) smaller, the running time of our algorithms will decrease too. Our FastKMeans++ algorithm behaves better compared with original \( k \)-means++ algorithm especially when \( d \) is very large. Therefore, our FastKMeans++ algorithm can handle the \( k \)-means problem with high dimensional points.

¹https://archive.ics.uci.edu/ml/datasets/SCADI
²https://archive.ics.uci.edu/ml/datasets/Mturk+User-Perceived+Clusters+over+Images
³https://archive.ics.uci.edu/ml/datasets/Libras+Movement
⁴https://archive.ics.uci.edu/ml/datasets/Sales_Transactions_Dataset_Weekly
Figure 4: The relationship between running time of original \(k\)-means++ algorithm and parameter \(n\).

Figure 5: The relationship between running time of our FASTKMEANS++ algorithm and parameter \(n\).

Figure 6: The relationship between running time of original \(k\)-means++ algorithm and parameter \(d\).
Our Fast KMeans++ Algorithm

Figure 7: The relationship between running time of our FastKMeans++ algorithm and parameter $d$

Figure 8: The relationship between running time of original k-means++ algorithm and parameter $m$

Figure 9: The relationship between running time of our FastKMeans++ algorithm and parameter $m$
Figure 10: The relationship between running time of original \( k \)-means++ algorithm and parameter \( k \)

Figure 11: The relationship between running time of our FastKMeans++ algorithm and parameter \( k \)