Semi-Supervised Algorithms for Approximately Optimal and Accurate Clustering

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Abstract

We study k-means clustering in a semi-supervised setting. Given an oracle that returns whether two given points belong to the same cluster in a fixed optimal clustering, we investigate the following question: how many oracle queries are sufficient to efficiently recover a clustering that, with probability at least $(1-\delta)$, simultaneously has a cost of at most $(1+\epsilon)$ times the optimal cost and an accuracy of at least $(1-\epsilon)$?

We show how to achieve such a clustering on n points with $O((k^2 \log n) \cdot m(Q, \epsilon^4, \delta/(k \log n)))$ oracle queries, when the k clusters can be learned with an ϵ' error and a failure probability δ' using $m(Q, \epsilon', \delta')$ labeled samples, where Q is the set of candidate cluster centers. We show that $m(Q, \epsilon', \delta')$ is small both for k-means instances in Euclidean space and for those in finite metric spaces. We further show that, for the Euclidean k-means instances, we can avoid the dependency on n in the query complexity at the expense of an increased dependency on k: specifically, we give a slightly more involved algorithm that uses $O(k^4/(\epsilon^2\delta) + (k^9/\epsilon^4)\log(1/\delta) + k \cdot m(Q, \epsilon^4/k, \delta))$ oracle queries.

Finally, we show that the number of queries required for $(1-\epsilon)$-accuracy in Euclidean k-means must linearly depend on the dimension of the underlying Euclidean space, whereas, for finite metric space k-means, this number must at least be logarithmic in the number of candidate centers. This shows that our query complexities capture the right dependencies on the respective parameters.

1 Introduction

Clustering is a fundamental problem that arises in many learning tasks. Given a set P of data points, the goal is to output a k-partition $C_1 \dot\cup \ldots \dot\cup C_k$ of P according to some optimization criteria. In unsupervised clustering, the data points are unlabeled. The classic k-means problem and other well-studied clustering problems such as k-median fall into this category.

In a general k-means clustering problem, the input comprises a finite set of n points P that is to be clustered, a set of candidate centers Q, and a distance metric d giving the distances between each pair of points in $P \cup Q$. The goal is to find k cluster centers $c_1, \ldots, c_k \in Q$ that minimizes the cost, which is the sum of squared distances between each point in P and its closest cluster center. In this case, the clustering $\mathcal{C}$ is defined by setting $C_i = \{x \in P : c_i \text{ is the closest center to } x\}$ for all $i = 1, \ldots, k$ and breaking ties arbitrarily. Two widely studied special cases are the k-means problem in Euclidean space (where $P \subset \mathbb{R}^r, Q = \mathbb{R}^r$, and d is the Euclidean distance function) and the k-means problem in finite metric spaces (where $(P \cup Q, \mathrm{d})$ forms a finite metric space).

Despite its popularity and success in many settings, there are two known drawbacks of the unsupervised k-means problem:

1. Finding the centers that satisfy the clustering goal is computationally hard. For example, even the special case of 2-means problem in Euclidean space is NP-hard [9].

2. There could be multiple possible sets of centers that minimize the cost. However, in practical instances, not all such sets are equally meaningful, and we would like our algorithm to find one that corresponds to the concerns of the application.

Since k-means is NP-hard, it is natural to seek approximation algorithms. For the general k-means problem in Euclidean space, notable approximation results include the local search by Kanungo et al. [15]

with an approximation guarantee of $(9+\epsilon)$ and the recent LP-based 6.357-approximation algorithm by Ahmadian et al. [1]. On the negative side, Lee et al. [16] ruled out arbitrarily good approximation algorithms for the k-means problem on general instances. For several special cases, however, there exist PTASes. For example, in the case when k is constant, Har-Peled and Mazumdar [12] and Feldman et al. [10] showed how to get a PTAS using weak coresets, and in the case when the dimension d is constant, Cohen-Addad et al. [7] and Friggstad et al. [11] gave PTASes based on a basic local search algorithm. In addition, Awasthi et al. [4] presented a PTAS for k-means, assuming that the input is "clusterable" (satisfies a certain stability criterion).

Even if we leave aside the computational issues with unsupervised k-means, we still have the problem that there can be multiple different clusterings that minimize the cost. To see this, consider the 2-means problem on the set of vertices of an equilateral triangle. In this case, we have three different clusterings that give the same minimum cost, but only one of the clusterings might be meaningful. One way to avoid this issue is to have strong assumptions on the input. For example, Balcan et al. [5] considered the problem in a restricted setting where any c-approximation to the problem also classifies at least a $(1-\epsilon)$ fraction of the points correctly.

Ashtiani et al. [3] recently proposed a different approach for addressing the aforementioned drawbacks. They introduced a semi-supervised, active clustering framework where the algorithm is allowed to make queries of the form *same-cluster(x, y)* to a domain expert, and the expert replies whether the points x and y belong to the same cluster in some fixed optimal clustering. Under the additional assumptions that the clusters are contained inside k balls in $\mathbb{R}^r$ that are sufficiently far away from each other, they presented an algorithm that makes $O(k^2 \log k + k(\log n + \log(1/\delta)))$ same-cluster queries, runs in $O(kn \log n + k^2 \log(1/\delta))$ time, and recovers the clusters with probability at least $(1-\delta)$. Their algorithm finds approximate cluster centers, orders all points by their distances to the cluster centers, and performs binary searches to determine the radii of the balls. Although it recovers the exact clusters, this approach works only when the clusters are contained inside well-separated balls. When the clusters are determined by a general Voronoi partitioning, and thus distances to the cluster boundaries can differ in different directions, this approach fails.

A natural question arising from the work of Ashtiani et al. [3] is whether such strong assumptions on the input structure are necessary. Ailon et al. [2] addressed this concern and considered the problem without any assumptions on the structure of the underlying true clusters. Their main result is a polynomial-time $(1+\epsilon)$-approximation scheme for k-means in the same semi-supervised framework as in Ashtiani et al. [3]. However, in contrast to Ashtiani et al. [3], their work gives no assurance on the accuracy of the recovered clustering compared to the true clustering. To achieve their goal, the authors utilized importance sampling to uniformly sample points from small clusters that significantly contribute to the cost. Their algorithm makes $O(k^9/\epsilon^4)$ same-cluster queries, runs in $O(nr(k^9/\epsilon^4))$ time, and succeeds with a constant probability.

In this work, we investigate the k-means problem in the same semi-supervised setting as Ailon et al. [2], but, in addition to approximating the cost, we seek a solution that is also accurate with respect to the true clustering. We assume that the underlying true clustering minimizes the cost, and that there are no points on cluster boundaries (i.e., the margin between each pair of clusters can be arbitrarily small but not zero). This last assumption is what differentiates our setup from that of Ailon et al. [2]. It is reasonable to assume that no point lies on the boundary of two clusters, as otherwise, to achieve constant accuracy, we would have to query at least a constant fraction of the boundary points. Without querying each boundary point, we have no way of determining to which cluster it belongs.

Observe that if we label all the points correctly with respect to the true clustering, the resulting clustering automatically achieves optimal cost. However, such perfect accuracy is difficult to achieve as there may be points that are arbitrarily close to each other but belong to different clusters. Using only a reasonable number of samples, the best we can hope for is to recover an approximately accurate solution. PAC (Probably Approximately Correct) learning helps us achieve this goal and provides a trade-off between the desired accuracy and the required number of samples.

Suppose that we have a solution where only a small fraction of the input points is incorrectly classified. In this case, one would hope that the cost is also close to the optimal cost. Unfortunately, the extra cost incurred by the incorrectly classified points can be very high depending on their positions, true labels, and the labels assigned to them. Our main concern in this paper is controlling this additional cost.

We show that if we start with a constant-factor approximation for the cost, we can refine the clustering with PAC learning. This yields a simple polynomial-time algorithm that, given a k-means instance and $(\epsilon, \delta) \in (0,1)^2$ as parameters, with probability at least $(1-\delta)$ outputs a clustering that has a cost of at most $(1+\epsilon)$ times the optimal cost and that classifies at least a $(1-\epsilon)$ fraction of the points

correctly with respect to the underlying true clustering. To do so, the algorithm makes $O((k^2 \log n) \cdot m(Q, \epsilon^4, \delta/(k \log n)))$ same-cluster queries, where $m(Q, \epsilon', \delta')$ is the number of labeled samples needed by the PAC learning algorithm to learn k clusters in a k-means instance (P, Q, d) with an ϵ' error and a failure probability δ' (recall that Q is the set of candidate centers for a k-means instance). We further show that our algorithm can be easily adapted to k-median and other similar problems that use the ℓ'th power of distances in place of squared distances for some $\ell > 0$. We formally present this result as Theorem 11 in Section 3. An informal statement for the case of k-means is given below in Theorem 1.

Theorem 1 (An informal version of Theorem 11)**.** *There exists a semi-supervised learning algorithm that, given a k-means instance, oracle access to same-cluster queries that are consistent with some fixed optimal clustering, and parameters $(\epsilon, \delta) \in (0, 1)^2$, outputs a clustering that, with probability at least $(1 - \delta)$, correctly labels (up to a permutation of the labels) at least a $(1 - \epsilon)$ fraction of the points and, simultaneously, has a cost of at most $(1 + \epsilon)$ times the optimal cost. In doing so, the algorithm makes $O((k^2 \log n) \cdot m(Q, \epsilon^4, \delta/(k \log n)))$ same-cluster queries.*

Our algorithm is general and applicable to any family of k-means, k-median, or similar distance based clustering instances that can be efficiently learned with PAC learning. As shown in Appendix A, these include Euclidean and general finite metric space clustering instances. In contrast, both Ashtiani et al. [3] and Ailon et al. [2], considered only the Euclidean k-means problem. To the best of our knowledge, ours is the first such result applicable to finite metric space k-means and both Euclidean and finite metric space k-median problems.

Ideally, we want $m(Q, \epsilon, \delta)$ to be small. Additionally, the analysis of our algorithm relies on two natural properties of learning algorithms. Firstly, we require PAC learning to always correctly label all the sampled points. Secondly, we also require it to not 'invent' new labels and only output labels that it has seen on the samples. We show that such learning algorithms with small $m(Q, \epsilon, \delta)$ exist both for k-means instances in Euclidean space and for those in finite metric spaces with no points on the boundaries of the optimal clusters. For r-dimensional Euclidean k-means, $m(Q = \mathbb{R}^r, \epsilon, \delta)$ has a linear dependency on r. For the case of finite metric spaces, $m(Q, \epsilon, \delta)$ has a logarithmic dependency on $|Q|$, which is the size of the set of candidate centers. In fact, these learning algorithms are applicable not only to k-means instances but also to instances of any similar distance-based clustering problems whose costs are defined in terms of the ℓ'th power $(\ell > 0)$ of distances as opposed to squared distances.

Our semi-supervised learning algorithm is inspired by the work of Feldman et al. [10] on weak coresets. They construct the weak coresets by first obtaining an intermediate clustering with a constant-factor approximation algorithm and refining each intermediate cluster using random samples. In order to get good guarantees on the cost, they partition each cluster into an inner ball that contain the majority of the points, and an outer region with the remaining points. We proceed similarly to this construction; however, we further partition the outer region into $O(\log n)$ concentric rings and use PAC learning to label the points in the inner ball and in each of the outer rings. For Euclidean k-means instances, the number of same-cluster queries needed by the algorithm has a logarithmic dependency on the number n of points that is similar (up to a $\mathrm{poly}(\log \log n)$ factor) to that of the algorithm by Ashtiani et al. [3]. The advantage of our algorithm is that it works for a much broader range of k-means instances whereas the applicability of the algorithm of Ashtiani et al. [3] is restricted to those instances whose clusters are contained in well-separated balls in Euclidean space.

This algorithm is effective in many natural scenarios where the number of clusters k is larger than $\log n$. However, as the size of the k-means instance (i.e., the number of points) becomes large, the $\log n$ factor becomes undesirable. In Euclidean k-means, the number of samples needed by the learning algorithm for error ϵ and failure probability δ does not depend on n. The $\log n$ dependency in the final query complexity is exclusively due to repeating the PAC learning step on $\Omega(k \log n)$ different partitions of P. To overcome this problem, we present a second algorithm, which is applicable only to Euclidean k-means instances, inspired by the work of Ailon et al. [2]. This time, we start with a $(1+\epsilon)$-approximation for the cost and refine it using PAC learning. Unlike our first algorithm, we only run the PAC learning once on the whole input, and thus we completely eliminate the dependency on n. The disadvantages of this algorithm compared to our first algorithm are the slightly more involved nature of the algorithm and its increased dependency on k in its query complexity. Theorem 2 below formally states this result. The proof follows from the analysis our algorithm in Section 4.

Theorem 2. *There exists a polynomial-time algorithm that, given a k-means instance in r-dimensional Euclidean space, oracle access to same-cluster queries that are consistent with some fixed optimal clustering, and parameters $(\epsilon, \delta) \in (0, 1)^2$, outputs a clustering that, with probability at least $(1 - \delta)$, correctly labels (up to a permutation of the labels) at least a $(1 - \epsilon)$ fraction of the points and, simultaneously, has*

a cost of at most $(1+\epsilon)$ *times the optimal cost. The algorithm makes* $O(k^4/(\epsilon^2\delta) + (k^9/\epsilon^4)\log(1/\delta) + k \cdot m(Q, \epsilon^4/k, \delta))$ *same-cluster queries.*

For the Euclidean setting, query complexities of both our algorithms have a linear dependency on the dimension of the Euclidean space. The algorithm of Ashtiani et al. [3] does not have such a dependency due to their strong assumption on the cluster structure, whereas the one by Ailon et al. [2] does not have it as it only approximates the cost. We show that, in our scenario, such a dependency is necessary to achieve the accuracy guarantee of our algorithms. For the finite metric space k-means, the query complexity of our general algorithm has an $O(\text{poly}(\log|P|, \log|Q|))$ dependency. The dependency on $|P|$ comes from the repeated application of the learning algorithm on $\Omega(k \log|P|)$ different partitions, and whether we can avoid this is an open problem. However, we show that an $\Omega(\log|Q|)$ query complexity is necessary for the accuracy. Formally, we prove the following theorem in Section 5.

Theorem 3. *Let* K *be a family of* k*-means instances. Let* $\mathcal{A}$ *be an algorithm that, given a* k*-means instance in* K*, oracle access to same-cluster queries for some fixed optimal clustering, and parameters* $(\epsilon, \delta) \in (0,1)^2$*, outputs a clustering that, with probability at least* $(1-\delta)$*, correctly labels (up to a permutation of the cluster labels) at least a* $(1-\epsilon)$ *fraction of the points. Then, the following statements hold:*

1. *If* K *is the family of* k*-means instances in* r*-dimensional Euclidean space that have no points on the boundaries of optimal clusters,* $\mathcal{A}$ *must make* $\Omega(r)$ *same-cluster queries.*
2. *If* K *is the family of finite metric space* k*-means instances that have no points on the boundaries of optimal clusters,* $\mathcal{A}$ *must make* $\Omega(\log|Q|)$ *same-cluster queries.*

The outline of this extended abstract is as follows. In Section 2 we introduce the notation, formulate the problem and present the learning theorems that we use in the subsequent sections. In Section 3 we present our first algorithm, which is simple and applicable to general k-means instances that admit efficient learning algorithms, but has a dependency of $\log n$ in its query complexity. In Section 4 we discuss how to remove the $\log n$ dependency in the query complexity for the special case of Euclidean k-means instances and present our second algorithm. In Section 5, we prove our query lower bound claims of Theorem 3. In Appendix A, we introduce the basic concepts and tools of PAC learning and explain how to design learning algorithms for Euclidean and finite metric space k-means instances.

2 Preliminaries

In this section, we introduce the basic notation and two common families of k-means instances, and formally define the k-means problem that we address in this work. We also introduce the notion of *learnability* for families of k-means instances and state two learning theorems, which we prove later in Appendix A.

2.1 k-Means Problem in a Semi-supervised Setting

Let P and Q be two sets of points where $|P| = n$, and let $\mathrm{d} : (P \cup Q) \times (P \cup Q) \to \mathbb{R}_+$ be a distance metric. We denote a k-means instance by the triple (P, Q, d). Two common families of k-means instances we consider in this work are:

1. k-means instances in Euclidean space, where $P \subset \mathbb{R}^r$, $Q = \mathbb{R}^r$, and $\mathrm{d}(x_1, x_2) = \|x_1 - x_2\|$ is the Euclidean distance between x_1 and x_2, and
2. k-means instances in finite metric spaces, where $(P \cup Q, \mathrm{d})$ forms a finite metric space.

Let $[k] := \{1, \ldots, k\}$. We identify a k-clustering $\mathcal{C}$ of (P, Q, d) by a labeling function $f_{\mathcal{C}} : P \to [k]$, and a set of k centers, $c_1, \ldots, c_k \in Q$, associated with each label, $1, \ldots, k$. For each label $i \in [k]$ of a clustering $\mathcal{C}$, let $C_i := \{p \in P : f_{\mathcal{C}}(p) = i\}$ be the set of points whose label is i. For convenience, we may use the labeling function $f_{\mathcal{C}}$ or the set of clusters $\{C_1, \ldots, C_k\}$ interchangeably to denote a clustering $\mathcal{C}$.

For a subset $C \subseteq P$ and a point $q \in Q$, define $\mathrm{cost}(C, q) := \sum_{p \in C} \mathrm{d}^2(p, q)$. For each i, define center $c_i := \mathrm{argmin}_{q \in Q} \mathrm{cost}(C_i, q)$, i.e., each center is a point in Q that minimizes the sum of squared distances between itself and each of the points assigned to it. For a k-clustering $\mathcal{C}$, we define its *k-means cost* as $\mathrm{cost}(\mathcal{C}) := \sum_{i \in [k]} \mathrm{cost}(C_i, c_i)$. Let $\mathcal{C}^*$ be the set of all k-clusterings of (P, Q, d). Then, the

optimal k-means cost of (P, Q, d) is defined as $OPT := \min_{\mathcal{C} \in \mathcal{C}^*} \mathrm{cost}(\mathcal{C})$. We say that a k-clustering $\mathcal{C}$ α-approximates the k-means cost if $\mathrm{cost}(\mathcal{C}) \leq \alpha OPT$.

Let $\mathcal{O}$ be a fixed k-clustering of (P, Q, d) that achieves the optimal k-means cost, and let $\mathcal{C}$ be any k-clustering of P. Let $f_{\mathcal{O}}$ and $f_{\mathcal{C}}$ be the labeling functions that correspond to $\mathcal{O}$ and $\mathcal{C}$ respectively. We assume that we have oracle access to the labeling function $f_{\mathcal{O}}$ of the optimal target clustering up to a permutation of the labels. We can simulate a single query to such an oracle with $O(k)$ queries to a same-cluster oracle as explained in Algorithm 1. A same-cluster oracle is an oracle that answers *same-cluster*(p_1, p_2) queries with 'yes' or 'no' based on whether p_1 and p_2 belong to the same cluster in the fixed optimal clustering $\mathcal{O}$.

The error of a clustering $\mathcal{C}$ with respect to the clustering $\mathcal{O}$ for a k-means instance (P, Q, d) is now defined as $\mathrm{error}(\mathcal{C}, \mathcal{O}) := |\{p \in P : f_{\mathcal{O}}(p) \neq f_{\mathcal{C}}(p)\}|$. In other words, $\mathrm{error}(\mathcal{C}, \mathcal{O})$ is the number of points wrongly labeled by the clustering $\mathcal{C}$ with respect to the optimal clustering $\mathcal{O}$. We note that the error is only up to a permutation of the cluster labels because we only have access to a simulated (up to a permutation of the cluster labels) version of $f_{\mathcal{O}}$ instead of the true $f_{\mathcal{O}}$. We say that a k-clustering $\mathcal{C}$ is $(1-\alpha)$-accurate with respect to $\mathcal{O}$ if $\mathrm{error}(\mathcal{C}, \mathcal{O}) \leq \alpha n$.

Input : A point $x \in X$, oracle access to *same-cluster*(x_1, x_2).
Output: A label $i \in [k]$.
Global : A list of points $S = [\ ]$.

```
for 1 ≤ i ≤ length(S) do
    if same-cluster(x, S[i]) then
        Return i
Append x to S.
Return length(S).
```

Algorithm 1: Simulating a labeling oracle with the same-cluster oracle.

Given (P, Q, d), parameters k and $(\epsilon, \delta) \in (0,1)^2$, and oracle access to $f_{\mathcal{O}}$, our goal is to output a k-clustering $\hat{\mathcal{O}}$ of (P, Q, d) that, with probability at least $(1-\delta)$, satisfies $\mathrm{error}(\hat{\mathcal{O}}, \mathcal{O}) \leq \epsilon n$ and $\mathrm{cost}(\hat{\mathcal{O}}) \leq (1+\epsilon) OPT$.

2.2 PAC Learning for k-Means

Let K be a family of k-means instances, and let $m(Q, \epsilon, \delta)$ be a positive integer-valued function. We say such a family K is *learnable* with *sample complexity* m if there exists a learning algorithm $\mathcal{A}_L$ such that the following holds: Let $\epsilon \in (0,1)$ be an error parameter and let $\delta \in (0,1)$ be a probability parameter. Let (P, Q, d) be a k-means instance in class K. Let $\mathcal{O}$ be a fixed optimal k-means clustering and let $f_{\mathcal{O}}$ be the associated labeling function. Let T be a fixed subset of P, and let S be a multiset of at least $m(Q, \epsilon, \delta)$ independently and uniformly distributed samples from T. The algorithm $\mathcal{A}_L$, given input (P, Q, d) and $(s, f_{\mathcal{O}}(s))$ for all $s \in S$, outputs a function $h : P \to [k]$. Moreover, with probability at least $(1-\delta)$ over the choice of S, the output h agrees with $f_{\mathcal{O}}$ on at least a $(1-\epsilon)$ fraction of the points in T (i.e., $|\{p \in T : h(p) = f_{\mathcal{O}}(p)\}| \geq (1-\epsilon)|T|$).

We say that such a learning algorithm $\mathcal{A}_L$ has the *zero sample error* property if the output h of $\mathcal{A}_L$ assigns the correct label to all the sampled points (i.e., $h(s) = f_{\mathcal{O}}(s)$ for all $s \in S$). Furthermore, we say that such a learning algorithm $\mathcal{A}_L$ is *non-inventive* if it does not 'invent' labels that it has not seen. This means that the output h of $\mathcal{A}_L$ does not assign labels that were not present in the input (sample, label) pairs (i.e., if $h(x) = c$ for some $x \in P$, then for some sample point $s \in S$, $f_{\mathcal{O}}(s) = c$).

In Section 3, we present a simple algorithm for $(1+\epsilon)$-approximate and $(1-\epsilon)$-accurate k-means clustering for a family K of k-means instances, assuming that K is learnable with a zero sample error, non-inventive learning algorithm. In the analysis, zero sample error and non-inventive properties play a key role in the crucial step of bounding the cost of incorrectly labeled points in terms of that of correctly labeled nearby points.

We now present two learning theorems for the Euclidean setting and the finite metric space setting. Assuming no point lies on cluster boundaries, the theorem states that the labeling function $f_{\mathcal{O}}$ of the optimal clustering is learnable with a zero sample error, non-inventive learning algorithm. We say that a k-means instance (P, Q, d) has *no boundary points* if in any optimal clustering $\mathcal{O}$ with optimal clusters $O_1, \ldots, O_k$ and respective centers $o_1, \ldots, o_k$, the closest center to any given point $p \in P$ is unique (i.e., if $p \in O_i$, $\mathrm{d}(p, o_i) < \mathrm{d}(p, o_j)$ for all $j \neq i$).

Theorem 4 (Learning k-Means in Euclidean Space). *Let* $\mathrm{d}(p_1, p_2) = \|p_1 - p_2\|$ *be the Euclidean distance function. Let* $K = \{(P, \mathbb{R}^r, \mathrm{d}) : P \subset \mathbb{R}, |P| < \infty, (P, \mathbb{R}^r, \mathrm{d})$ *has no boundary points*$\}$ *be the family of* k*-means instances that are in* r*-dimensional Euclidean space and that have no boundary points. The family* K *is learnable with sample-complexity*[1] $m(\mathbb{R}^r, \epsilon, \delta) = \tilde{O}((k^2 r \log(k^2 r)(\log(k^3 r/\epsilon)) + \log(1/\delta))/\epsilon)$.

Theorem 5 (Learning k-Means in Finite Metric Spaces). *Let* $K = \{(P, Q, \mathrm{d}) : (P \cup Q, \mathrm{d})$ *is a finite metric space, and* (P, Q, d) *has no boundary points*$\}$ *be the family of finite metric space* k*-means instances that have no boundary points. The family* K *is learnable with sample-complexity*[2] $m(Q, \epsilon, \delta) = \tilde{O}((k^2(\log k)(\log |Q|)(\log k + \log 1/\epsilon) + \log(1/\delta))/\epsilon)$.

We prove Theorem 4 and Theorem 5 in Appendix A, where we also introduce the necessary PAC learning concepts and tools.

3 A Simple Algorithm for $(1+\epsilon)$ Cost and $(1-\epsilon)$ Accuracy

Let K be a family of k-means instances that is learnable with sample complexity m using a zero sample error, non-inventive learning algorithm $\mathcal{A}_L$. Let $\mathcal{A}_\alpha$ be a constant-factor approximation algorithm, and let $\mathcal{A}_1$ be a polynomial-time algorithm for the 1-means problem (i.e., given $(P, Q, \mathrm{d}) \in K$, $\mathcal{A}_1$ finds $\operatorname{argmin}_{q \in Q} \mathrm{cost}(P, q)$ in polynomial time). We present a simple semi-supervised learning algorithm that, given a k-means instance (P, Q, d) of class K and oracle access to the labeling function $f_{\mathcal{O}}$ of a fixed optimal clustering $\mathcal{O}$ of (P, Q, d), outputs a clustering $\hat{\mathcal{O}}$ that, with probability at least $(1-\delta)$, satisfies $\mathrm{cost}(\hat{\mathcal{O}}) \leq (1+\epsilon)OPT$ and $\mathrm{error}(\hat{\mathcal{O}}, \mathcal{O}) \leq \epsilon|P|$. Our algorithm uses $\mathcal{A}_\alpha$, $\mathcal{A}_1$, and $\mathcal{A}_L$ as subroutines and makes $O((k \log |P|) \cdot m(Q, \epsilon^4, \delta/(k \log |P|)))$ oracle queries. We show that our algorithm can be easily modified for $(1+\epsilon)$-approximate and $(1-\epsilon)$-accurate k-median and other similar distance-based clustering problems. Towards the end of this section, we discuss several applications of this result, namely, for Euclidean and finite metric space k-means and k-median problems.

Let us start by applying the learning algorithm $\mathcal{A}_L$ to learn all the cluster labels. If we get perfect accuracy, the cost will be optimal. A natural question to ask in this case is: what happens to the cost if the learning output has ϵ error? In general, even a single misclassified point can incur an arbitrarily large additional cost. To better understand this, consider the following: Let $O_i, O_j \subseteq P$ be two distinct optimal clusters in the target clustering, and let o_i, o_j be their respective cluster centers. Let $p \in O_i$ be a point that is incorrectly classified and assigned label $j \neq i$ by $\mathcal{A}_L$. Also assume that the number of misclassified points is small enough so that the centers of the clusters output by the learning algorithm are close to those of the optimal clustering. Thus, in the optimal clustering, p incurs a cost of $\mathrm{d}^2(p, o_i)$, whereas according to the learning outcome, p incurs a cost that is close to $\mathrm{d}^2(p, o_j)$. In the worst case, $\mathrm{d}(p, o_j)$ can be arbitrarily larger than $\mathrm{d}(p, o_i)$.

Now suppose that, within distance r from p, there exists some point $q \in O_j$. In this case, we can bound the cost incurred due to the erroneous label of p using the true cost of p in the target clustering. To be more specific, using the triangle inequality, we get the following bound for any metric space: $\mathrm{d}(p, o_j) \leq \mathrm{d}(p, q) + \mathrm{d}(q, o_j) \leq r + \mathrm{d}(q, o_j)$. Furthermore, due to the optimality, $\mathrm{d}(q, o_j) \leq \mathrm{d}(q, o_i) \leq \mathrm{d}(q, p) + \mathrm{d}(p, o_i) \leq r + \mathrm{d}(p, o_i)$. Hence, it follows that $\mathrm{d}(p, o_j) \leq 2r + \mathrm{d}(p, o_i)$. To utilize this observation in an algorithmic setting, we need to make sure that, for every point that is misclassified into cluster j, there exists a correctly classified nearby point q that belongs to the optimal cluster O_j. Luckily, this is ensured by the combination of zero sample error and non-inventive properties of $\mathcal{A}_L$. If a point is misclassified into cluster j, the non-inventive property says that $\mathcal{A}_L$ must have seen a sample point q from cluster j. The zero sample error property ensures that q is labeled correctly by $\mathcal{A}_L$. To make sure that such correctly labeled points are sufficiently close to their incorrectly labeled counterparts, we run $\mathcal{A}_L$ separately on certain suitably bounded partitions of P.

The formal description of our algorithm is given in Algorithm 2. The outline is as follows: First, we run $\mathcal{A}_\alpha$ on (P, Q, d) and obtain an intermediate clustering $\mathcal{C} = \{C_1, \ldots, C_k\}$. For each C_i, we run $\mathcal{A}_1$ to find a suitable center c_i. Next, we partition each intermediate cluster C_i into an inner ball and $O(\log |P|)$ outer rings centered around c_i. We run the learning algorithm $\mathcal{A}_L$ separately on each of these partitions. We choose the inner and outer radii of the rings so that, in each partition, the points that are incorrectly classified by the learning algorithm only incur a small additional cost compared to that of the correctly classified points. The final output is a clustering $\hat{\mathcal{O}}$ that is consistent with the learning outputs on each of the partitions. For each cluster $\hat{O}_i$, we associate the output of running $\mathcal{A}_1$ on $(\hat{O}_i, Q, \mathrm{d})$ as its center.

[1] $\tilde{O}$ hides $\mathrm{poly}(\log\log k, \log\log r)$ factors.
[2] $\tilde{O}$ hides $\mathrm{poly}(\log\log k, \log\log |Q|)$ factors.

Note that, due to the accuracy requirements, the cluster center to which a point is assigned in the output may not be the cluster center closest to that point in the output. It remains an interesting problem to find an accurate clustering in which every point is always assigned to its nearest cluster center.

Input : k-Means instance (P, Q, d), oracle access to $f_{\mathcal{O}}$, constant-factor approximation algorithm $\mathcal{A}_\alpha$, 1-means algorithm $\mathcal{A}_1$, zero sample-error, non-inventive learning algorithm $\mathcal{A}_L$ with sample complexity m, accuracy parameter $0 < \epsilon < 1$, and failure probability $0 < \delta < 1$.

Output: A clustering $\hat{\mathcal{O}} = \{\hat{O}_1, \ldots, \hat{O}_k\}$ defined by a labeling $f_{\hat{\mathcal{O}}} : P \to [k]$. The respective cluster centers are $\hat{o}_i = \operatorname{argmin}_{q \in Q} \operatorname{cost}(\hat{O}_i, q)$. For each $i \in [k]$, run $\mathcal{A}_1$ on $(\hat{O}_i, Q, \mathrm{d})$ to find $\hat{o}_i$.

Let $n = |P|$, and let $\gamma = \epsilon^2/(288\alpha)$.
Run $\mathcal{A}_\alpha$ and obtain an α-approximate k-means clustering $\mathcal{C} = \{C_1, \ldots, C_k\}$. For each $i \in [k]$, run $\mathcal{A}_1$ on (C_i, Q, d) and find centers $c_i = \operatorname{argmin}_{q \in Q} \operatorname{cost}(C_i, q)$.
for $C_i \in \mathcal{C}$ **do**
    Let $r_i = \sqrt{\operatorname{cost}(C_i, c_i)/(\gamma |C_i|)}$.
    Let $C_{i,0}$ be all points in C_i that are at most r_i away from c_i.
    Let $C_{i,j}$ be the points in C_i that are between $2^{j-1} r_i$ and $2^j r_i$ away from c_i for $j = 1, \ldots, (\log n)/2$.
    Let $m' = m(Q, \gamma^2, \delta/(k \log n))$.
    for *each non-empty* $C_{i,j}$ **do**
        Sample m' points $x_1, \ldots, x_{m'} \in C_{i,j}$ independently and uniformly at random.
        Query the oracle on $x_1, \ldots, x_{m'}$ and let $S_{i,j} = \{(x_i, f_{\mathcal{O}}(x_i)) : i = 1, \ldots, m'\}$.
        Run $\mathcal{A}_L$ on input (P, Q, d) and $S_{i,j}$, and obtain a labeling $h_{i,j} : C_{i,j} \to [k]$.
Output the clustering $\hat{\mathcal{O}}$ defined by the following labeling function:
for *each* i, j, $x \in C_{i,j}$ **do**
    Set $f_{\hat{\mathcal{O}}}(x) = h_{i,j}(x)$.

Algorithm 2: A simple algorithm for $(1+\epsilon)$-approximate $(1-\epsilon)$-accurate k-means clustering.

We now analyze Algorithm 2 and show that, with probability at least $(1-\delta)$, it outputs a $(1+\epsilon)$-approximate and $(1-\epsilon)$-accurate k-means clustering.

Let $n = |P|$ be the total number of points in the k-means instance. Assume that $0 < \gamma < 1/2$. For all i, j, p, let $H_{i,j,p} = \{x \in C_{i,j} : h_{i,j}(x) = p\}$ be the set of points that are in $C_{i,j}$ and labeled p by the output $h_{i,j}$ of the learning algorithm $\mathcal{A}_L$. Call a point $x \in P$ *bad* if $x \in H_{i,j,p}$ but $f_{\mathcal{O}}(x) \neq p$; otherwise, call it *good*. Denote the set of bad points by B and let the complement B^c of B be the set of good points. For each i, let $o_i = \operatorname{argmin}_{q \in Q} \operatorname{cost}(O_i, q)$ denote the center of cluster i in $\mathcal{O}$. For any point $x \in P$, let $o(x)$ denote the center of the optimal cluster for x under the clustering $\mathcal{O}$. Thus, $o(x) = o_p \Leftrightarrow f_{\mathcal{O}}(x) = p$.

Notice that, for all i, all the points in C_i belong to one of the $C_{i,j}$'s. In other words, no point in C_i is more than $2^{(\log n)/2} r_i$ away from c_i, where $r_i = \sqrt{\operatorname{cost}(C_i, c_i)/(\gamma |C_i|)}$. To see this, suppose $x \in C_i$ is a point that is more than $2^{(\log n)/2} r_i$ away from c_i. Then, $\mathrm{d}^2(x, c_i) \geq 2^{\log n} \cdot \operatorname{cost}(C_i, c_i)/(\gamma |C_i|) > \operatorname{cost}(C_i, c_i)$ which is a contradiction.

Lemma 6. *With probability at least* $(1-\delta)$*, all non-empty* $C_{i,j}$*'s satisfy* $|C_{ij} \cap B| \leq \gamma^2 |C_{ij}|$.

Proof. Recall that we run $\mathcal{A}_L$ with $m_K(P, Q, \mathrm{d}, \gamma^2, \delta/(k \log n))$ samples. Thus, by definition, $\mathcal{A}_L$, each run of $\mathcal{A}_L$ succeeds with probability at least $(1 - \delta/(k \log n))$. Since we only run $\mathcal{A}_L$ at most $k \log n$ times, the claim follows from the union bound. □

We continue the rest of the analysis conditioned on $|C_{i,j} \cap B| \leq \gamma^2 |C_{i,j}|$ for all $C_{i,j}$. In proving the subsequent results, we use the following observations.

Observation 7. *No two points in* $C_{i,j}$ *are more than distance* $R = 2 \cdot 2^j r_i$ *apart. Note that, according to the definition of* $C_{i,j}$ *in the algorithm,* R *is the outer diameter of the ring that bounds* $C_{i,j}$*.*

Observation 8. *For* $j \geq 1$*, the inner radius of the ring that bounds* $C_{i,j}$ *is* $2^{j-1} r_i$*. Therefore, we have the following lower bound for the cost of* $C_{i,j}$*:* $\operatorname{cost}(C_{i,j}, c_i) \geq |C_{i,j}| (2^{j-1} r_i)^2$.

Lemma 9. *For all* i, j *and* p*, if* $x \in H_{i,j,p} \cap B$ *then* $\mathrm{d}(x, o_p) \leq 4 \cdot 2^j r_i + \mathrm{d}(x, o(x))$.

Proof. If $x \in H_{i,j,p} \cap B$, then x is in some optimal cluster denoted by O_q for some $q \neq p$. Note that if $h_{i,j}$ (i.e., the output of the algorithm $\mathcal{A}_L$) gives label p to some point x, then the non-inventive property of $\mathcal{A}_L$ ensures that it has seen at least one point $y \in C_{i,j}$ that is in O_p, and the zero sample-error property ensures that y is labeled correctly by $h_{i,j}$. Thus, $o_p = o(y)$ and $o_q = o(x)$. Hence, y is a *good* point with label p, and consequently, we have

$$\begin{aligned}\mathrm{d}(x, o_p) &\leq \mathrm{d}(x, y) + \mathrm{d}(y, o_p) \leq \mathrm{d}(x, y) + \mathrm{d}(y, o_q) \leq 2\,\mathrm{d}(x, y) + \mathrm{d}(x, o(x)) \\ &\leq 4 \cdot 2^j r_i + \mathrm{d}(x, o(x)),\end{aligned}$$

where the last inequality follows from Observation 7. □

Lemma 10 (Squared Triangle Inequality)**.** *For any $a, b \geq 0$ and $0 < \epsilon < 1$, we have*

$$(a+b)^2 \leq (1+\epsilon)a^2 + \left(1 + \frac{1}{\epsilon}\right) b^2 \leq (1+\epsilon)a^2 + \left(\frac{2}{\epsilon}\right) b^2 \,.$$

Proof. The first inequality follows from the AM-GM inequality because $2ab \leq \epsilon a^2 + b^2/\epsilon$. The second inequality holds because $\epsilon < 1$ implies $1 < 1/\epsilon$. □

Now, let us analyze the cost of the labeling output by Algorithm 2:

$$\mathrm{cost}(P, \hat{\mathcal{O}}) = \sum_{p \in [k]} \mathrm{cost}(\hat{\mathcal{O}}_p, \hat{o}_p) \leq \sum_{p \in [k]} \mathrm{cost}(\hat{\mathcal{O}}_p, o_p) = \sum_{i,j,p} \mathrm{cost}(H_{i,j,p}, o_p).$$

Splitting the cost contributions of good and bad points, we get

$$\begin{aligned}\mathrm{cost}(P, \hat{\mathcal{O}}) &\leq \sum_{x \in B^c} \mathrm{d}^2(x, o(x)) + \sum_{i,j,p} \mathrm{cost}(H_{i,j,p} \cap B, o_p) \\ &= \sum_{x \in B^c} \mathrm{d}^2(x, o(x)) + \sum_{i,j,p} \sum_{x \in H_{i,j,p} \cap B} \mathrm{d}^2(x, o_p).\end{aligned}$$

Applying Lemma 9 together with Lemma 10, for any $\epsilon \in (0, 1)$, we have

$$\begin{aligned}\mathrm{cost}(P, \hat{\mathcal{O}}) &\leq \sum_{x \in B^c} \mathrm{d}^2(x, o(x)) + \sum_{i,j,p} \sum_{x \in H_{i,j,p} \cap B} \left(\left(1 + \frac{\epsilon}{3}\right) \mathrm{d}^2(x, o(x)) + \frac{2 \cdot 3}{\epsilon} (4 \cdot 2^j r_i)^2 \right) \\ &\leq \left(1 + \frac{\epsilon}{3}\right) \sum_{x \in P} \mathrm{d}^2(x, o(x)) + \sum_{i,j,p} \sum_{x \in H_{i,j,p} \cap B} \frac{96}{\epsilon} (2^j r_i)^2 \\ &= \left(1 + \frac{\epsilon}{3}\right) OPT + \sum_{i,j} \sum_{x \in C_{i,j} \cap B} \frac{96}{\epsilon} (2^j r_i)^2.\end{aligned}$$

From Lemma 6, we have $|C_{i,j} \cap B| \leq \gamma^2 |C_{i,j}|$, and it follows that

$$\begin{aligned}\mathrm{cost}(P, \hat{\mathcal{O}}) &\leq \left(1 + \frac{\epsilon}{3}\right) OPT + \sum_{i,j} \gamma^2 |C_{i,j}| \frac{96}{\epsilon} (2^j r_i)^2 \\ &= \left(1 + \frac{\epsilon}{3}\right) OPT + \sum_{i} \gamma^2 |C_{i,0}| \frac{96}{\epsilon} r_i^2 + \sum_{i,j:j \geq 1} \gamma^2 |C_{i,j}| \frac{96}{\epsilon} (2^j r_i)^2. \qquad (1)\end{aligned}$$

Consider the last two terms of Equation 1 individually. For the first summation, we have

$$\sum_i \gamma^2 |C_{i,0}| \frac{96}{\epsilon} r_i^2 = \sum_i \gamma^2 |C_{i,0}| \frac{96}{\epsilon} \frac{\mathrm{cost}(C_i, c_i)}{\gamma |C_i|} \leq \sum_i \frac{96\gamma}{\epsilon} \mathrm{cost}(C_i, c_i) \leq \frac{96\gamma\alpha}{\epsilon} OPT.$$

In the last inequality, we used the fact that $\mathcal{C}$ gives an α-approximation for the optimal cost. For the second summation of Equation 1, Observation 8 gives

$$\begin{aligned}\sum_{i,j:j \geq 1} \gamma^2 |C_{ij}| \frac{96}{\epsilon} (2^j r_i)^2 &= \sum_{i,j:j \geq 1} \frac{4 \cdot 96\gamma^2}{\epsilon} |C_{ij}| (2^{j-1} r_i)^2 \leq \sum_{i,j:j \geq 1} \frac{384\gamma^2}{\epsilon} \mathrm{cost}(C_{ij}, c_i) \\ &\leq \sum_i \frac{384\gamma^2}{\epsilon} \mathrm{cost}(C_i, c_i) \leq \frac{384\gamma^2\alpha}{\epsilon} OPT.\end{aligned}$$

Here, we have again used the approximation guarantee of $\mathcal{C}$ in the final inequality.

Choosing $\gamma = \epsilon^2/(288\alpha)$ makes sure that both $96\gamma\alpha/\epsilon \leq \epsilon/3$ and $384\gamma^2\alpha/\epsilon \leq \epsilon/3$, and consequently, we get a final cost of at most $(1+\epsilon)OPT$. Recall that we established this bound conditioned on $|C_{i,j} \cap B| \leq \gamma^2 |C_{i,j}|$ for all i, j. In Lemma 6, we saw that all the $O(k \log n)$ runs of the learning algorithm $\mathcal{A}_L$ succeed with probability at least $(1-\delta)$. Hence, the condition $|C_{i,j} \cap B| \leq \gamma^2 |C_{i,j}|$ is true for all i, j with the same probability. Summing the inequality over all i, j yields $|B| \leq \gamma^2 |P| \leq \epsilon |P|$. Consequently, the output of Algorithm 2, with probability at least $(1-\delta)$ over the choice of samples in step 10, outputs a $(1+\epsilon)$-approximate and $(1-\epsilon)$-accurate k-means clustering.

In Algorithm 2, instead of an exact algorithm $\mathcal{A}_1$ for the 1-means problem, we can also use a PTAS. Using a PTAS to approximate 1-means up to a $(1+\epsilon)$ factor will only cost an additional $(1+\epsilon)$ factor in our cost analysis. As a result, we get the same approximation and accuracy guarantees if we replace ϵ with $\epsilon/3$.

Algorithm 2 makes $O((k \log n) \cdot m(Q, \epsilon^4, \delta/(k \log n)))$ queries to the oracle $f_{\mathcal{O}}$ in total. Recall that simulating an oracle query to $f_{\mathcal{O}}$ takes $O(k)$ same-cluster queries. Therefore, the total number of same-cluster queries is $O((k^2 \log n) \cdot m(Q, \epsilon^4, \delta/(k \log n)))$.

Our definition of a learning algorithm in Section 2.2 has nothing to do with whether the input is a k-means instance or a k-median instance. In fact, it applies to any similar clustering scenario where the cost is defined in terms of the ℓ'th power ($\ell > 0$) of distances instead of squared distances. The analysis of Algorithm 2 can be adapted to any fixed ℓ where we have a suitable triangle inequality analogous to Lemma 10. For example, when $\ell \leq 1$, we can simply use the trivial inequality $(a+b)^\ell \leq a^\ell + b^\ell$. Thus, for such clustering problems, Algorithm 2, with a slight modification on choice of radii in Step 4 and a little adjustment to the parameter γ, will give the same guarantees. Hence, we have the following theorem which is the formal version of Theorem 1. The proof follows from the analysis of Algorithm 2.

Theorem 11. *Let K be a family of k-means (k-median) instances. Suppose that K is learnable with sample complexity $m(Q, \epsilon, \delta)$ using a zero sample error, non-inventive learning algorithm $\mathcal{A}_L$. Let $\mathcal{A}_\alpha$ be a constant-factor approximation algorithm, and let $\mathcal{A}_1$ be a PTAS for the 1-means (1-median) problem. There exists a polynomial-time algorithm that, given an instance $(P, Q, \mathrm{d}) \in K$, oracle access to same-cluster queries for some fixed optimal clustering $\mathcal{O}$, and parameters $(\epsilon, \delta) \in (0,1)^2$, outputs a clustering that, with probability at least $(1-\delta)$, is $(1-\epsilon)$-accurate with respect to $\mathcal{O}$, and simultaneously has a cost of at most $(1+\epsilon)OPT$. The algorithm uses $\mathcal{A}_L$, $\mathcal{A}_\alpha$, and $\mathcal{A}_1$ as subroutines. The number of same-cluster queries made by the algorithm is*

1. $O((k^2 \log |P|) \cdot m(Q, \epsilon^4, \delta/(k \log |P|)))$ *for the k-means setting and*
2. $O((k^2 \log |P|) \cdot m(Q, \epsilon^2, \delta/(k \log |P|)))$ *for the k-median setting.*

For k-means and k-median instances in Euclidean space and those in finite metric spaces, there exist several constant-factor approximation algorithms (for example, Ahmadian et al. [1] and Kanungo et al. [15]). Solving the 1-means problem in Euclidean space is straightforward: The solution to $\operatorname{argmin}_{q \in \mathbb{R}^r} \operatorname{cost}(P, q)$ is simply $q = (\sum_{p \in P} p)/|P|$. For the k-median problem in Euclidean space, the problem of 1-median does not have an exact algorithm but several PTASes exist (for example, Cohen et al. [6]). In a finite metric space, to solve $\operatorname{argmin}_{q \in Q} \operatorname{cost}(P, q)$, we can simply try all possible $q \in Q$ in polynomial time, and this holds for the k-median setting as well. Thus, for Euclidean and finite metric space k-means and k-median instances that have no boundary points, Theorem 11, together with Theorem 4 and Theorem 5, gives efficient algorithms for $(1+\epsilon)$-approximate, $(1-\epsilon)$-accurate semi-supervised clustering.

4 Removing the Dependency on Problem Size in the Query Complexity for Euclidean k-Means

For the family of Euclidean k-means instances, the query complexity of Algorithm 2 suffers from a $\tilde{O}(\log n)$ dependency (where n is the number of points in the input k-means instance, and $\tilde{O}$ hides $\operatorname{poly}(\log \log n)$ factors) due to the repeated use of the learning algorithm $\mathcal{A}_L$. Specifically, we run $\mathcal{A}_L$ with a failure probability of $\delta/(k \log n)$, $O(\log n)$ times per cluster. Note that the sample complexity of $\mathcal{A}_L$ itself, in the case of Euclidean k-means instances, does not have this dependency.

In this section, we show that we can avoid this dependency on n using a slightly more involved algorithm at the cost of increasing the query complexity by an extra $\operatorname{poly}(k)$ factor. Nevertheless, this

algorithm has superior performance when the size of the input instance (i.e., the number of points) is very large (when $\log n = \Omega(k^{10})$ for example).

Recall that, for a set $C \subset \mathbb{R}^r$, $\text{cost}(C, y)$ is minimized when y is the centroid of C, denoted by $\mu(C) = (\sum_{x \in C} x)/|C|$. Define the fractional size of an optimal cluster O_i as the fraction of points that belong to O_i, i.e., the ratio $|O_i|/n$. Suppose we only want to get a good approximation for the cost, and that we know that all the clusters in the target solution have sufficiently large fractional sizes. In this case, naive uniform sampling will likely pick a large number of samples from each of the clusters. This observation, together with Lemma 12, allows us to approximate the centroid and the cost of each cluster to any given accuracy.

Lemma 12 (Lemma 1 and Lemma 2 of Inaba et al. [13]). *Let $(\epsilon, \delta) \in (0, 1)^2$, let $m \geq 1/(\epsilon\delta)$ be a positive integer, and let $S = \{p_1, \ldots, p_m\}$ be a multiset of m i.i.d. samples from the uniform distribution over some finite set $C \subset \mathbb{R}^r$. With probability at least $(1 - \delta)$, $\text{d}^2(\mu(S), \mu(C)) \leq \epsilon \cdot \text{cost}(C, \mu(C))/|C|$ and $\text{cost}(C, \mu(S)) \leq (1 + \epsilon)\,\text{cost}(C, \mu(C))$.*

However, the above approach fails when some clusters in the optimal target solution contribute significantly to the cost, but have small fractional sizes (that is because uniform sampling is not guaranteed to pick sufficient numbers of samples from the small clusters). Ailon et al. [2] circumvented this issue with an algorithm that iteratively approximates the centers of the clusters using a distance-based probability distribution (D^2-sampling). We will refer to their algorithm as $\mathcal{A}^*$.

Note that when it comes to accuracy, we can totally disregard clusters with small fractional sizes; we only have to correctly label a sufficiently large fraction of the points in large clusters. With this intuition, we present the outline of our algorithm.

Let $(P, \mathbb{R}^r, \text{d})$ be a k-means instance in Euclidean space that has no boundary points. For simplicity, we refer to the instance $(P, \mathbb{R}^r, \text{d})$ by just P where possible, as for Euclidean k-means, the other two parameters are fixed. We start with a naive uniform sampling step that gives a good approximation for the centers of large clusters. Starting with these centers, we run a slightly modified version of algorithm $\mathcal{A}^*$ to approximate the centers of the remaining small clusters. Thus, at this point, we have a clustering with a good cost and we know which clusters are large. We now run the learning algorithm $\mathcal{A}_L$ on input P and obtain a labeling of the points. For each point, we assign its final label based on

1. the label assigned to it by the learning algorithm $\mathcal{A}_L$, and
2. its proximity to large cluster centers.

In particular, if the output of $\mathcal{A}_L$ decides that a point p should be in some large cluster i, and if p is sufficiently close to the approximate center for cluster i, we label it according to the learning output; otherwise, we label it according to its nearest approximate center. We show that this approach retains a cost that is close to the cost of the clustering output by $\mathcal{A}^*$. The accuracy guarantee comes from the facts that a large fraction of the points are sufficiently close to the centers of large clusters, and that $\mathcal{A}_L$ labels most of them correctly with a good probability.

We now review the key properties of algorithm $\mathcal{A}^*$ (the algorithm of Ailon et al. [2]). Let $0 < \epsilon < 1$. Call a k-means instance P is (k, ϵ)-irreducible if no $(k-1)$-means clustering gives an $(1+\epsilon)$-approximation for the k-means problem, i.e., if OPT^k denotes the optimal k-means cost of P, then P is (k, ϵ)-irreducible if $OPT^{k-1} > (1 + \epsilon)OPT^k$. Suppose that P is (k, ϵ)-irreducible. Let $\mathcal{O} = \{O_1, \ldots, O_k\}$ be the target optimal clustering, and let $o_1, \ldots, o_k$ be the respective centers. Let $C_i = \{c_1, \ldots, c_i\}$ denote a set of i centers and let $Z(i)$ denote the following statement: There exists a set of i distinct indices $j_1, \ldots, j_i$ such that, for all $r \in [i]$, $\text{cost}(O_{j_r}, c_r) \leq (1 + \epsilon/16)\,\text{cost}(O_{j_r}, o_{j_r})$. To put it differently, $Z(i)$ says that C_i is a set of good candidate centers for i-many distinct clusters in the target optimal solution. Assuming P is (k, ϵ)-irreducible, the algorithm $\mathcal{A}^*$ yields a method to incrementally construct sets $C_1, \ldots, C_k$ (i.e., $C_{i+1} = C_i \cup \{c_{i+1}\}$) such that, conditioned on $Z(i)$ being true, $Z(i+1)$ is true with probability at least $(1 - 1/k)$. Now suppose that P is $(k, \epsilon/(4k))$-irreducible. Then $\mathcal{A}^*$ gives a $(1 + \epsilon/(4 \cdot 16k))$-approximation for k-means with probability at least $(1 - 1/k)^k \geq 1/4$. Otherwise, $\mathcal{A}^*$ gives a $(1 + \epsilon/(4 \cdot 16k))$-approximation for the i-means problem for some $i < k$, where i is the largest integer such that P is $(i, \epsilon/4k)$-irreducible. In the latter case, it will give a $(1 + \epsilon/(4 \cdot 16k))(1 + \epsilon/(4k))^{k-i}$-approximation with probability at least $1/4$. In either case, the output of $\mathcal{A}^*$ is a $(1 + \epsilon)$-approximation.

In our algorithm, we first find the centers of large clusters using uniform sampling, and then run $\mathcal{A}^*$ find the remaining centers. This allows us to know which clusters are large, which is a crucial information needed for the final labeling. Suppose that in the target optimal solution we have $k_0 \leq k$ clusters whose fractional sizes are at least ϵ/k. Note that k_0 is at least 1 due to the Pigeonhole Principle, since at

least one cluster should have a fractional size of at least $1/k > \epsilon/k$. By Lemma 12, using uniform sampling, we can approximate the centroid of each of these large clusters with a good accuracy. Hence, we can have a set C_{k_0} of k_0 centers such that $Z(k_0)$ is true with probability $(1-\delta)$. Afterwards, we use $\mathcal{A}^*$ to incrementally construct $C_{k_0+1}, \ldots, C_k$. Conditioned on $Z(k_0)$ being true, the output C_k will be a $(1+\epsilon)$-approximation with probability $(1-1/k)^{k-k_0} \geq (1-1/k)^k \geq 1/4$ for $k \geq 2$. However, by independently running this incremental construction $O(\log(1/\delta))$ times and choosing the set of centers with the minimum total cost, we can boost this probability to $(1-\delta)$. This observation gives the following generalization of Theorem 10 of Ailon et al. [2].

Theorem 13. *Consider a Euclidean k-means instance $(P, \mathbb{R}^r, \mathrm{d})$. Let $O_1, \ldots, O_k$ be a fixed optimal clustering with respective centers $o_1, \ldots, o_k$. Let $k_0 \leq k$ and let $C_{k_0} = \{c_1, \ldots, c_{k_0}\}$ be a set of points such that, with probability at least p_0, $\mathrm{cost}(O_i, c_i) \leq (1 + \epsilon/(64k))\,\mathrm{cost}(O_i, o_i)$ for all $i \in [k_0]$. There exists an algorithm $\mathcal{A}_{cost}$ that, given P, C_{k_0}, and parameters $(\epsilon, \delta) \in (0,1)^2$ as input, outputs a set of centers $C_k = C_{k_0} \cup \{c_{k_0+1}, \ldots, c_k\}$ such that $\sum_{i\in[k]} \mathrm{cost}(O_i, c_i) \leq (1+\epsilon)\sum_{i\in[k]} \mathrm{cost}(O_i, o_i)$ with probability at least $p_0(1-\delta)$. Moreover, $\mathcal{A}_{cost}$ uses $O((k^9/\epsilon^4)\log(1/\delta))$ same-cluster queries and runs in time $O(nr(k^9/\epsilon^4)\log(1/\delta))$.*

Theorem 13 implies a method to get a good approximation for the cost that also reveals which clusters are large. Specifically, we first perform uniform sampling over the whole set P and approximate the centers of the large clusters. If we get a sufficient number of samples, the approximate centers will satisfy the precondition of Theorem 13 with a good probability. Thus, using algorithm $\mathcal{A}_{cost}$ from Theorem 13, we get the desired approximation for the cost. What remains now is to use PAC learning and to appropriately label the points according to the learning outcome.

We present the pseudo-code of our algorithm in Algorithm 3, where we use the algorithm $\mathcal{A}_{cost}$ from Theorem 13 and the learning algorithm $\mathcal{A}_L$ guaranteed by Theorem 4. In Algorithm 3, $Q_1(k,\epsilon,\delta) = 256k^3/(\epsilon^2\delta)$ is the number of samples needed to ensure that we pick a sufficient number of samples from each of the clusters with fractional sizes of at least ϵ/k, $Q_2(k,\epsilon,\delta)$ is the sample complexity of the algorithm $\mathcal{A}_{cost}$, and $Q_3(k,r,\epsilon,\delta) = m(\mathbb{R}^r,\epsilon,\delta)$ is the sample complexity of the learning algorithm $\mathcal{A}_L$ for an error ϵ and a failure probability δ. Note that Algorithm 3 only outputs a labeling; the corresponding centers are the centroids of the clusters defined by the labeling. As with Algorithm 2, the center that a point is assigned to in the final output may not be the closest center to that point.

Input : Point set $P \subset \mathbb{R}^r$, oracle access to $f_{\mathcal{O}}$, parameter k, accuracy parameter ϵ, failure probability δ, and algorithms $\mathcal{A}_{cost}$ and $\mathcal{A}_L$.
Output: A clustering $\hat{\mathcal{O}}$ defined by the labeling $f_{\hat{\mathcal{O}}} : P \to [k]$. The cluster centers are the centroids of the clusters defined by $f_{\hat{\mathcal{O}}}$.

1 Draw $Q_1(k,\epsilon,\delta)$ samples from P independently and uniformly at random, and query $f_{\mathcal{O}}$ to get their true cluster labels in $\mathcal{O}$. Denote the set of sampled points by S, and for all $i \in [k]$, denote the set of sampled points that belong to class i by S_i.
2 Let k' be the number of distinct cluster labels with more than $(\epsilon/(2k))Q_1(k,\epsilon,\delta)$ samples. Let $C_{k'} := \{\mu(S_i) : |S_i| > (\epsilon/(2k))Q_1(k,\epsilon,\delta)\}$. Without loss of generality, assume that the class labels for centers in $C_{k'}$ are $1, \ldots, k'$.
3 Run the algorithm $\mathcal{A}_{cost}$, starting from $C_{k'}$ as the partial set of centers. This takes $Q_2(k,\epsilon,\delta)$ more queries. Let $C_k = \{c_1, \ldots, c_k\}$ be the output, and let OPT^* be the cost of the clustering obtained by assigning each point to its nearest c_i.
4 Use the PAC learning algorithm $\mathcal{A}_L$ on $Q_3(k, r, \epsilon^4/k, \delta)$ uniform i.i.d. samples from P to learn a classifier for the k classes that is $\left(1-\epsilon^4/k\right)$-accurate with probability at least $(1-\delta)$. Let $H_1, \ldots, H_k$ be the sets of points that are labeled $1, \ldots, k$ respectively by the classifier.
5 Output the clustering $\hat{\mathcal{O}}$ defined by the following labeling function: for each $i \in [k']$ and $p \in H_i$ such that $\mathrm{d}^2(p, c_i) \leq kOPT^*/(n\epsilon^3)$, set $f_{\hat{\mathcal{O}}}(p) = i$. For any other point p, set $f_{\hat{\mathcal{O}}}(p) = i$ if the nearest cluster center to p in C_k is c_i.

Algorithm 3: Algorithm whose query complexity is independent of n

4.1 Analysis of Algorithm 3

Assume $0 < \epsilon < 1/4$. For an optimal cluster O_i with center o_i, denote by $\overline{\Delta}(O_i) := \mathrm{cost}(O_i, o_i)/|O_i|$ the average squared distance from the points in O_i to their center o_i. Let $c_1, \ldots, c_{k'}$ be the points in $C_{k'}$ where c_i is the approximate centroid for the cluster with label i found in Step 2 of Algorithm 3.

First, we show that Step 2 of Algorithm 3 approximates all the large cluster centers accurately enough so that the precondition for applying Theorem 13 is satisfied (recall that the precondition is to have a set of $k' < k$ approximate centers for k' distinct optimal clusters in the target solution). Lemma 14 ensures this, and also makes sure that the clusters that are too small are not picked as large clusters. This last fact is useful in the proof of Lemma 15.

Lemma 14. *With probability at least $1-\delta$, the following statements are true:*

1. *For all $i \in [k']$, $\mathrm{d}^2(o_i, c_i) \leq (\epsilon/(64k))\,\overline{\Delta}(O_i)$.*
2. *For all $i \in [k']$, $\mathrm{cost}(O_i, c_i) \leq (1+\epsilon/(64k))\,\mathrm{cost}(O_i, o_i)$.*
3. *Let $L = \{i \in [k] : |O_i| \geq (\epsilon/k)n\}$ be the set of the labels of the optimal clusters with a fractional size of at least ϵ/k. Then, $L \subseteq [k']$.*
4. *Let $T = \{i \in [k] : |O_i| \leq (\epsilon^2/k)n\}$ be the set of the labels of the optimal clusters with fractional size of at most ϵ^2/k. Then $T \cap [k'] = \emptyset$.*

Proof. Notice that for each $i \in [k']$, we have at least $(\epsilon/(2k))Q_1(k,\epsilon,\delta) = 128k^2/(\epsilon\delta)$ samples in Step 2. Thus, using Lemma 12 on each cluster with error parameter $\epsilon/(64k)$ and failure probability $\delta/(2k)$, and applying the union bound, the first two statements hold with probability at least $(1-\delta/2)$.

As for the final two statements, note the following. Let $q = Q_1(k,\epsilon,\delta)$, and let the random variables $X_{i,j} : j = 1,\ldots,q$ be such that $X_{i,j} = 1$ if the j-th sample is from O_i. Otherwise, $X_{i,j} = 0$. Let $X_i = \sum_{j\in[q]} X_{i,j}$ be total number of samples picked from O_i and $p_i = \Pr[X_{i,j} = 1]$. Since we pick identical samples, this probability does not depend on j.

If $i \in L$, then $p_i \geq \epsilon/k$ and $\mathbb{E}[X_i] = q \cdot p_i \geq q \cdot \epsilon/k$. Applying a standard Chernoff bound, we get

$$\Pr\left[X_i < \frac{1}{2}\cdot\frac{\epsilon}{k}q\right] \leq \Pr\left[X_i < \frac{1}{2}\,\mathbb{E}[X_i]\right] \leq \exp\left(-\frac{q\cdot\epsilon}{2^2\cdot 3\cdot k}\right) \leq \exp\left(-\frac{32k^2}{3\epsilon\delta}\right) \leq \frac{\delta}{2k}.$$

For $i \in T$, observe that $p_i \leq \epsilon^2/k$ and $\mathbb{E}[X_i] = q\cdot p_i \leq q\cdot\epsilon^2/k$. Since $\epsilon < 1/4$, we further have that $\epsilon/(2k) > 2\epsilon^2/k$. Applying another standard Chernoff bound, we now get

$$\begin{aligned}\Pr\left[X_i > \frac{1}{2}\cdot\frac{\epsilon}{k}q\right] &\leq \Pr\left[X_i > 2\cdot\frac{\epsilon^2}{k}q\right] \leq \Pr\left[X_i > 2\,\mathbb{E}[X_i]\right] \\ &\leq \exp\left(-\frac{q\cdot\epsilon^2}{2^2\cdot 3\cdot k}\right) \leq \exp\left(-\frac{32k^2}{3\delta}\right) \leq \frac{\delta}{2k}.\end{aligned}$$

Applying the union bound, we get that the final two statements are also true with probability at least $(1-\delta/2)$. Thus, all four statements are true with probability at least $(1-\delta)$. □

Recall that OPT^* is the cost of the clustering defined by the centers C_k after Step 3 of Algorithm 3. Lemma 14, together with Theorem 13, implies that, with probability at least $(1-2\delta)$,

$$OPT^* \leq \sum_{i\in[k]} \mathrm{cost}(O_i, c_i) \leq (1+\epsilon)\sum_{i\in[k]} \mathrm{cost}(O_i, o_i) \leq (1+\epsilon)OPT.$$

Also note that the PAC learning of Step 4 has at most ϵ^4/k error with probability at least $(1-\delta)$.

The following lemma thus provides the final ingredient of our proof. Conditioned on Steps 1, 2, 3, and 4 of Algorithm 3 being successful, Lemma 15 shows that the clustering defined in Step 5 achieves the desired accuracy of the algorithm with only a marginal increase in the cost.

Lemma 15. *Consider an outcome of Algorithm 3 where all four statements of Lemma 14 are true. Additionally, suppose that $\sum_{i\in[k]} \mathrm{cost}(O_i, c_i) \leq (1+\epsilon)OPT$, and that the PAC learning of Step 4 of Algorithm 3 has at most ϵ^4/k error. Then, the output clustering $\hat{\mathcal{O}}$ is $(1-6\epsilon)$-accurate with respect to the target optimal clustering $\mathcal{O}$ and $(1+3\epsilon)$-approximates the k-means cost.*

Proof. It is easy to see that the points that are incorrectly labeled by $f_{\hat{\mathcal{O}}}$ are fully contained inside the union of the following three disjoint sets:

1. Points that belong to the target optimal clusters whose fractional sizes are at most ϵ/k.

2. Points that are incorrectly labeled by the clustering algorithm in Step 4 but are not in the set defined above.

3. Points that do not satisfy the distance criterion in Step 5 but are correctly classified and are assigned a label from $\{1, \ldots, k'\}$ by the PAC learning output in Step 4.

At most a $k(\epsilon/k) = \epsilon$ fraction of the points are in the first set. By the accuracy of the PAC learning step, the second set has at most ϵ^4/k fraction of the points. As for the third set, we consider the following: By the fourth statement of Lemma 14, for $i = 1, \ldots, k'$, O_i has a fractional size of at least ϵ^2/k; therefore, $\text{cost}(O_i, o_i)/(n(\epsilon^2/k)) \geq \overline{\Delta}(O_i)$. Recall that H_i is the set of points that are assigned label i in the PAC learning step. Let $i \in \{1, \ldots, k'\}$, and let $p \in H_i$ be a point that is correctly labeled in the PAC learning output and that satisfies $\mathrm{d}^2(p, c_i) > kOPT^*/(n\epsilon^3)$. For such a point p, we can lower bound the distance to its approximate center at follows:

$$\mathrm{d}^2(p, c_i) > \frac{kOPT^*}{n\epsilon^3} \geq \frac{kOPT}{n\epsilon^3} \geq \frac{k\,\text{cost}(O_i, o_i)}{n\epsilon^3} \geq \frac{\overline{\Delta}(O_i)}{\epsilon}.$$

Also, since $2\,\mathrm{d}^2(p, o_i) + 2\,\mathrm{d}^2(o_i, c_i) \geq \mathrm{d}^2(p, c_i)$, and $\mathrm{d}^2(o_i, c_i) \leq (\epsilon/(64k))\,\overline{\Delta}(O_i)$ by Lemma 14 (1), we get

$$\mathrm{d}^2(p, o_i) > \frac{1}{2}\left(\frac{\overline{\Delta}(O_i)}{\epsilon} - 2\,\mathrm{d}^2(o_i, c_i)\right) > \frac{1}{2}\left(\frac{\overline{\Delta}(O_i)}{\epsilon} - 2\frac{\epsilon\,\overline{\Delta}(O_i)}{64k}\right) > \frac{\overline{\Delta}(O_i)}{4\epsilon}.$$

Hence, there can be at most $4\epsilon|O_i|$ such points. Summing over all O_i, we conclude that at most 4ϵ fraction of the points are in the final set. Hence, the resulting clustering is at least $(1 - 6\epsilon)$ accurate.

It remains to show that the cost increase in Step 5 is small. Let $\text{cost}' = \sum_{i\in[k]} \text{cost}(O_i, c_i)$ be the cost of assigning each optimal cluster O_i to its approximate center c_i. We know $cost'$ is close to the optimal cost by Theorem 13. We now show that the label assignment in Step 5 does not increase this cost by too much. Observe that for the points that are not labeled according to the PAC learning output, the contribution to cost$'$ can only decrease by assigning it to the nearest c_i. For the points that are labeled according to the PAC output, if the learning algorithm has assigned them the correct labels, then there is no change in their contribution to cost$'$.

Thus, it is sufficient to bound the cost of those points that are incorrectly labeled by the PAC learning and are labeled according to the learning output in the final assignment. There can be at most $(\epsilon^4/k)n$ such points due to the learning accuracy, and assigning such a point p to c_i can incur at most an extra $\mathrm{d}^2(p, c_i)$ cost. However, due to the distance constraint of Step 5 of Algorithm 3, $\mathrm{d}^2(p, c_i) \leq kOPT^*/(n\epsilon^3)$. Therefore, the total cost increase by these points is at most

$$\frac{\epsilon^4 n}{k}\frac{kOPT^*}{n\epsilon^3} \leq \epsilon OPT^* \leq \epsilon(1+\epsilon)OPT \leq 2\epsilon OPT.$$

Consequently, the cost of the output clustering of the algorithm is at most $(1 + 3\epsilon)OPT$. □

Combining Lemma 14, Theorem 13, and Lemma 15, we have the proof of Theorem 2. We need each of the Steps 1, 3, and 4 to succeed with probability at least $(1-\delta/3)$ so that we get a final failure probability of δ, which can be easily achieved by replacing the probability parameter δ of Algorithm 3 with $\delta/3$. Furthermore, according to the statement of Lemma 15, we also need to replace the accuracy parameter ϵ by $\epsilon/6$. As for the claim on the query complexity, we recall that we only need $O(k)$ same-cluster queries per single $f_{\mathcal{O}}$ query, and Algorithm 3 makes a total number of $Q_1(k, \epsilon, \delta) + Q_2(k, \epsilon, \delta) + Q_3(k, r, \epsilon^4/k, \delta)$ queries to $f_{\mathcal{O}}$. We remark that the sample complexity $m(P, \mathbb{R}^r, \mathrm{d}, \epsilon, \delta)$ for learning Euclidean k-means instances is independent of P.

5 Lower Bounds for $(1 - \epsilon)$-Accurate k-Means

The results we presented in Section 3 and Section 4 uses PAC learning to achieve $(1 - \epsilon)$-accuracy. Considering the class of Euclidean k-means instances, the query complexities of both our results have a linear dependency on the dimension of the Euclidean space. This is in contrast to the query complexities of the algorithms in Ashtiani et al. [3], which had strong assumptions on the input, and Ailon et al. [2], which was only aiming to approximate the optimal cost. In this section, we argue that the linear dependency on dimension is necessary for accuracy for Euclidean k-means instances. This result, as shown in the latter half of this section, also implies that the dependency on $\log|Q|$ is necessary for the k-means instances in finite metric spaces, where Q is the set of candidate centers.

Let $r > 0$ be an integer, and $e_1, \ldots, e_r$ be the standard basis in $\mathbb{R}^r$. Consider the 2-means instance $(P, \mathbb{R}^r, \mathrm{d})$ in r-dimensional Euclidean space, where $P = \{-e_1, e_1, \ldots, -e_r, e_r\}$. There are $2r$ points in P. In Lemma 16, we show that any optimal solution for this instance contains exactly one of $\pm e_i$ in each optimal cluster for all $i = 1, \ldots, r$. Hence, there are 2^r different optimal solutions. This means that, without querying at least one of $\pm e_i$, it is information-theoretically impossible to know which cluster e_i and $-e_i$ each belong to, and thus to achieve constant classification error, the query complexity must be linear in r. This proves the first claim of Theorem 3.

Lemma 16. *Consider the k-means instances $(P, \mathbb{R}^r, \mathrm{d})$ defined as above. Let $\mathcal{O} = \{O_1, O_2\}$ be any fixed optimal clustering on $(P, \mathbb{R}^r, \mathrm{d})$. For each $i \in [r]$, either $e_i \in O_1$ and $-e_i \in O_2$ or $e_i \in O_2$ and $-e_i \in O_1$.*

Proof. Consider a bi-partition $A \dot\cup B = \{\pm e_1, \ldots, \pm e_r\}$. We first observe the following: Let $i \in [r]$ be such that $-e_i \in A$ and $e_i \in B$. Define $A' := A \setminus \{-e_i\} \cup \{e_i\}$ and $B' := B \setminus \{e_i\} \cup \{-e_i\}$. Then the cost of the solution (A, B) is the same as the cost of (A', B'). This is because e_i and $-e_i$ are at the same distance to all points in $P \setminus \{\pm e_i\}$.

Therefore, without loss of generality, we only need to consider bi-partitions where the set A can be described as $A = \{e_{r_0+1}, \ldots, e_{r_0+r_1}\} \cup \{\pm e_{r_0+r_1+1}, \ldots, \pm e_{r_0+r_1+r_2}\}$, for some r_0, r_1 and r_2 where $r_0 + r_1 + r_2 = r$. Consequently, we have that $B = \{\pm e_1, \ldots, \pm e_{r_0}\} \cup \{-e_{r_0+1}, \ldots, -e_{r_0+r_1}\}$. To put differently, A contains only the positive points on axes $r_0 + 1, \ldots, r_0 + r_1$ whereas B contains only the negative points on the same axes. For axes $r_0 + r_1 + 1, \ldots, r_0 + r_1 + r_2$, A contains both positive and negative points on those axes. Similarly, for axes $1, \ldots, r_0$, B contains both points on those axes. The center of A is

$$\Big(\underbrace{0, \ldots, 0}_{r_0}, \underbrace{\frac{1}{r_1 + 2r_2}, \ldots, \frac{1}{r_1 + 2r_2}}_{r_1}, \underbrace{0, \ldots, 0}_{r_2}\Big),$$

and the center of B is

$$\Big(\underbrace{0, \ldots, 0}_{r_0}, \underbrace{-\frac{1}{r_1 + 2r_0}, \ldots, -\frac{1}{r_1 + 2r_0}}_{r_1}, \underbrace{0, \ldots, 0}_{r_2}\Big).$$

The cost of set A is

$$\begin{aligned}
& r_1 \cdot \left(\left(1 - \frac{1}{r_1 + 2r_2}\right)^2 + (r_1 - 1)\frac{1}{(r_1 + 2r_2)^2}\right) + 2r_2 \cdot \left(1 + r_1 \frac{1}{(r_1 + 2r_2)^2}\right) \\
&= \frac{1}{(r_1 + 2r_2)^2}\left(r_1(r_1 + 2r_2 - 1)^2 + r_1(r_1 - 1) + 2r_2(r_1 + 2r_2)^2 + 2r_1 r_2\right) \\
&= \frac{1}{(r_1 + 2r_2)^2}\left(r_1(r_1 + 2r_2)^2 - 2r_1(r_1 + 2r_2) + r_1 + r_1(r_1 - 1) + 2r_2(r_1 + 2r_2)^2 + 2r_1 r_2\right) \\
&= \frac{1}{(r_1 + 2r_2)^2}\left((r_1 + 2r_2)^3 - r_1(r_1 + 2r_2)\right) \\
&= (r_1 + 2r_2) - \frac{r_1}{r_1 + 2r_2}.
\end{aligned}$$

Similarly, the cost of set B is

$$\begin{aligned}
& r_1 \cdot \left(\left(1 - \frac{1}{r_1 + 2r_0}\right)^2 + (r_1 - 1)\frac{1}{(r_1 + 2r_0)^2}\right) + 2r_0 \cdot \left(1 + r_1 \frac{1}{(r_1 + 2r_0)^2}\right) \\
&= (r_1 + 2r_0) - \frac{r_1}{r_1 + 2r_0}.
\end{aligned}$$

The total cost of this clustering is therefore

$$2r - \left(\frac{r_1}{r_1 + 2r_2} + \frac{r_1}{r_1 + 2r_0}\right).$$

It remains to show that the maximum of

$$\left(\frac{r_1}{r_1 + 2r_2} + \frac{r_1}{r_1 + 2r_0}\right) = \left(\frac{r_1}{r_1 + 2r_2} + \frac{r_1}{2r - 2r_2 - r_1}\right)$$

is achieved by setting $r_1 = r$ and $r_0 = r_2 = 0$. For a fixed r_1, the last expression gives a convex function in variable r_2, and therefore either $r_2 = 0$ or $r_2 = r - r_1$ maximizes the expression. In either case, we have that the maximum of this expression for a fixed r_1 is

$$1 + \frac{r_1}{2r - r_1} = \frac{2r}{2r - r_1},$$

which in turn achieves maximum when $r_1 = r$. □

Now consider the hard example for Euclidean setting with $r = (\log n/2)$. Thus, we have $\log n$ points in P. Start with an empty set Q, and for each subset P' of P, add $\mu(P') = (\sum p \in P' p)/|P'|$ to Q. This forms a finite metric space k-means instance (P, Q, d) that has no boundary points. From the claim on dimension dependency for the Euclidean setting discussed above, it follows that $\Omega(r) = \Omega(\log n) = \Omega(\log |Q|)$ samples are necessary to achieve $(1 - \epsilon)$-accuracy. This proves the second claim of Theorem 3.

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A PAC Learning

In this section, we introduce some fundamental concepts and tools from PAC learning theory, and prove Theorem 4 and Theorem 5. We start by introducing some necessary notations.

Let $\mathcal{X}$ be an arbitrary domain set, $\mathcal{Y}$ be a label set, and $\mathcal{H} \subseteq \{h : \mathcal{X} \to \mathcal{Y}\}$ be a hypothesis class. Let $\mathcal{D}$ be some arbitrary distribution over $\mathcal{X} \times \mathcal{Y}$. The error of a hypothesis $h \in \mathcal{H}$ with respect to $\mathcal{D}$ is defined as

$$L_{\mathcal{D}}(h) := \Pr_{(x,y)\sim\mathcal{D}}[h(x) \neq y] \,. \tag{2}$$

We say that $\mathcal{H}$ satisfies *the realizability assumption* if there exists some $h^* \in \mathcal{H}$ such that $L_{\mathcal{D}}(h^*) = 0$. A learning algorithm $\mathcal{A}$ for hypothesis class $\mathcal{H}$ receives as input a sequence $S := ((x_1, y_1), \ldots, (x_m, y_m))$ of m pairs of domain points and their labels, where each domain point is sampled independently from $\mathcal{D}$. The learning algorithm should output a predictor $\mathcal{A}(S) \in \mathcal{H}$. The goal of the algorithm is to minimize the generalization error $L_{\mathcal{D}}(\mathcal{A}(S))$ with respect to the unknown $\mathcal{D}$. We define the empirical error (risk) on S for a hypothesis h as

$$L_S(h) := \frac{|\{i \in [m] : h(x_i) \neq y_i\}|}{m} \,. \tag{3}$$

We call the algorithm $\mathcal{A}$ an *empirical risk minimization (ERM)* algorithm if

$$\mathcal{A}(S) \in \operatorname*{argmin}_{h\in\mathcal{H}} L_S(h) \,.$$

Let $\mathcal{H}$ be a hypothesis class for some discrete domain $\mathcal{X}$. If the realizability assumption holds for $\mathcal{H}$, and if $\mathcal{A}$ is an ERM algorithm for $\mathcal{H}$, then $L_S(\mathcal{A}(S)) = 0$.

Clearly, $\mathcal{A}(S)$ depends on S. Hence, the generalization error, $L_D(A(S))$, is a random variable whose randomness depends on S. We are interested in establishing an upper bound on the number of samples that $\mathcal{A}$ needs in order to guarantee that the generalization error is small with a good probability.

Definition 17 (Sample Complexity of a Learning Algorithm)**.** *Let $\mathcal{A}$ be a learning algorithm for a hypothesis class $\mathcal{H}$. We define the sample complexity of $\mathcal{A}$, $m_{\mathcal{A},\mathcal{H}}(\epsilon, \delta)$, as the minimum natural number such that, if S is sequence of $m \geq m_{\mathcal{A},\mathcal{H}}(\epsilon, \delta)$ i.i.d. samples from $\mathcal{D}$, with probability at least $1 - \delta$, $L_{\mathcal{D}}(\mathcal{A}(S)) \leq \epsilon$.*

We now introduce some terminology from learning theory. We first define the notions of *shattering* and *VC-dimension* for a *binary* hypothesis class $\mathcal{H} \subseteq \{h : \mathcal{X} \to \{1, 2\}\}$.

Definition 18 (Shattering)**.** *We say a binary hypothesis class $\mathcal{H}$ shatters a finite set*

$$C = \{c_1, \ldots, c_m\} \subseteq \mathcal{X},$$

if $\{(h(c_1), \ldots, h(c_m)) : h \in \mathcal{H}\} = \{1, 2\}^{|C|}$.

Definition 19 (Vapnik–Chervonenkis (VC) Dimension)**.** *The VC-dimension of a binary hypothesis class $\mathcal{H}$, denoted* $\mathrm{VCdim}(\mathcal{H})$*, is the maximum size of a set $C \subset \mathcal{X}$ that can be shattered by $\mathcal{H}$. If $\mathcal{H}$ shatters sets of arbitrarily large size, we say that $\mathcal{H}$ has infinite VC-dimension.*

By definition, to shatter a set C, a hypothesis class $\mathcal{H}$ must have at least $2^{|C|}$ distinct elements. Hence, we have the following lemma.

Lemma 20. *Let $\mathcal{H}$ be a finite hypothesis class. Then,* $\mathrm{VCdim}(\mathcal{H}) = O(\log |\mathcal{H}|)$.

For a k-ary hypothesis class $\mathcal{H} \subseteq \{h : \mathcal{X} \to [k]\}$, we define the analogous notions of *multiclass shattering* and *Natarajan dimension*. As we will see below, the notion of multiclass shattering is a generalization of the notion of shattering for the binary hypothesis classes. Consequently, the Natarajan dimension is a generalization of the VC-dimension.

Definition 21 (Multiclass Shattering)**.** *We say that a set $C \subseteq \mathcal{X}$ is shattered by a k-ary hypothesis class $\mathcal{H}$ if there exist two functions $f_0, f_1 : C \to [k]$ such that,*

- *For every $x \in C$, $f_0(x) \neq f_1(x)$.*
- *For every $B \subset C$, there exists a function $h \in \mathcal{H}$ such that,*

$$\forall x \in B, h(x) = f_0(x) \text{ and } \forall x \in C \backslash B, h(x) = f_1(x).$$

Definition 22 (Natarajan Dimension)**.** *The Natarajan dimension of a k-ary hypothesis class $\mathcal{H}$, denoted by* $\mathrm{Ndim}(\mathcal{H})$*, is the maximal size of a set $C \subseteq \mathcal{X}$ that can be shattered by $\mathcal{H}$.*

Suppose $k = 2$. If a binary hypothesis class $\mathcal{H}_{\text{bin}} : \mathcal{X} \to \{1, 2\}$ shatters a set $C \subseteq \mathcal{X}$ according to Definition 18, then for all subsets B of C, there exists a hypothesis $h \in \mathcal{H}_{\text{bin}}$ that maps all points in B to 1 and all points in $C \backslash B$ to 2. Thus, setting $f_0(x) = 1$ and $f_1(x) = 2$ to be constant functions, it follows that $\mathcal{H}_{\text{bin}}$ shatters C according to Definition 21 as well.

For the converse, suppose that $\mathcal{H}_{\text{bin}}$ is hypothesis class that shatters a set $C \subseteq \mathcal{X}$ according to Definition 21. Definition 21 essentially says that, any mapping $C \to \{1, 2\}^{|C|}$ must be achievable with one of the hypotheses in $\mathcal{H}_{\text{bin}}$ which is equivalent to Definition 18. To see this, notice that $f_0(x) \neq f_1(x)$, and that we only have two labels.

In the remainder of this appendix, we prove Theorem 4 and Theorem 5. We proceed with defining a new hypothesis class for binary classification which is associated with non-homogeneous halfspaces in $\mathbb{R}^r$. Formally, given a non-homogeneous hyperplane $\ell \subset \mathbb{R}^r$, let h_ℓ be the binary classifier that assigns labels ± 1 to points based on which side of the hyperplane the point lies on. We define the binary hypothesis class $\mathcal{H}_{\text{b}}^{\text{EUC}}$ as

$$\mathcal{H}_{\text{b}}^{\text{EUC}} = \{h_\ell : \ell \text{ is a (non-homogeneous) hyperplane in } \mathbb{R}^r\}.$$

Lemma 23 (Theorem 9.3 of Shalev-Shwartz and Ben-David [17])**.** *The VC-dimension of $\mathcal{H}_{\text{b}}^{\text{EUC}}$ is $r+1$.*

Let $(P, \mathbb{R}^r, \mathrm{d})$ be a k-means instance in Euclidean space. Let $\mathcal{O}$ be a fixed optimal clustering of P, and let $f_{\mathcal{O}}$ be the labeling function of $\mathcal{O}$. Assume that $(P, \mathbb{R}^r, \mathrm{d})$ has no boundary points (i.e., in an optimal clustering, for any given point $p \in P$, the closest optimal center is unique). Let $A, B \subset P$ two non-empty disjoint subsets of points of two different labels under $f_{\mathcal{O}}$. Due to the assumption of having no boundary points, there exists a hypothesis $h \in \mathcal{H}_{\text{b}}^{\text{EUC}}$ that perfectly separates points in A from those in B. That is to say, it assigns -1 to all points in A and $+1$ to all points in B. Such a hypothesis h can be learned in polynomial-time using standard SVM (Support Vector Machine) training algorithms like the one proposed by Joachims [14].

Let $S = \{(x_1, y_1), \ldots, (x_m, y_m)\}$ be a multiset of sample-label pairs from $P \times Q$. Fix a pair of distinct cluster labels $a, b \in [k']$ and let $S_{a,b}$ be the subset of the samples-label pairs in S whose labels are either a or b. Since each pair of original clusters can be separated with a hyperplane in $\mathbb{R}^r$, there exists a hypothesis $g_{a,b} \in \mathcal{H}_b^{\text{EUC}}$ that perfectly labels the samples in $S_{a,b}$; that is to say that for all $(x, y) \in S_{a,b}$, $g_{a,b}(x) = 1$ if $y = a$ and $g_{a,b}(x) = -1$ if $y = b$. Suppose for each pair $a, b \in [k]$, $a \neq b$, we find a hypothesis $g_{a,b}$. Then, for all samples $(x, a) \in S$, $\sum_{b \neq a} g_{a,b}(x) = k - 1$. Moreover, for any sample $(x, a) \in S$, and for any $a' \neq a$, $\sum_{b \neq a'} g_{a',b}(x) < k - 1$. This is because $g_{a',a}(x) = -1$. Consequently, the function g defined as

$$g(x) = \operatorname*{argmax}_{a \in [k]} \sum_{b \in [k], b \neq a} g_{a,b}(x)$$

returns the correct label y for all $(x, y) \in S$. Hence, the aforementioned procedure gives an ERM algorithm for the hypothesis class $\mathcal{H}^*$ which is formally defined follows: for $\bar{g} = (g_{a,b})_{[a,b\in[k],a\neq b]} \in \left(\mathcal{H}_{\mathrm{b}}^{\mathrm{EUC}}\right)^{k(k-1)}$, a $(k(k-1))$-tuple of binary hypotheses, let $h_{\bar{g}}(x) = \operatorname{argmax}_{a\in[k]} \sum_{b\in[k],b\neq a} g_{a,b}(x)$. Define

$$\mathcal{H}^* = \left\{ h_{\bar{g}} : \bar{g} \in \left(\mathcal{H}_{\mathrm{b}}^{\mathrm{EUC}}\right)^{k(k-1)} \right\}.$$

The pseudo-code of the algorithm is presented in Algorithm 7. This algorithm is an adaptation of the All-Pairs algorithm described in Chapter 17.1 of Shalev-Shwartz and Ben-David [17]. An observant reader may notice that learning two hypotheses, namely $g_{a,b}$ and $g_{b,a}$, per each distinct a, b is redundant as one can set $g_{a,b}(x) = -g_{b,a}(x)$. However, for the ease of presentation, we stick with the idea that $g_{a,b}$ and $g_{b,a}$ are picked independently from each other.

Input : A set of samples $S = (x_1, y_1), \ldots, (x_m, y_m)$ and an ERM algorithm $\mathcal{B}$ for learning $\mathcal{H}_{\mathrm{b}}^{\mathrm{EUC}}$.
Output: A hypothesis $g \in \mathcal{H}^*$.

for $a, b \in [k]$ *such that* $a \neq b$ **do**
  Let $S_{a,b} = [\,]$ be an empty list.
  for $t = 1, \ldots, m$ **do**
    If $y_t = a$ add $(x_t, 1)$ to $S_{a,b}$.
    If $y_t = b$ add $(x_t, -1)$ to $S_{a,b}$.
  Let $g_{a,b} = \mathcal{B}(S_{a,b})$.
Let $g(x) = \operatorname{argmax}_{a\in[k]} \left(\sum_{b\in[k],b\neq a} g_{a,b}(x) \right)$.

Algorithm 4: An ERM algorithm for k-category classification.

The corollary to the following lemma bounds the Natarajan dimension of $\mathcal{H}^*$.

Lemma 24 (Lemma 29.6 of Shalev-Shwartz and Ben-David [17])**.** *Consider a multiclass predictor derived in the following way. Train l binary classifiers from a binary hypothesis class $\mathcal{H}_{\mathrm{bin}}$ and let $v : \{-1, 1\}^l \to [k]$ be a mapping from the l predictor results to a class label. Let $\mathcal{H}_{\mathrm{bin}}^v$ be the class of multiclass predictors obtained in this manner. If $\mathrm{VCdim}(\mathcal{H}_{\mathrm{bin}}) = d$ then, $\mathrm{Ndim}(\mathcal{H}_{\mathrm{bin}}^v) \leq 3dl \log(ld)$.*

Corollary 25. *The Natarajan dimension of the hypothesis class $\mathcal{H}^*$ is $O(rk^2 \log(rk))$ where r is the dimension of the Euclidean space and k is the number of clusters in the k-means instance.*

The following lemma, combined with Corollary 25 yields that

$$m_{\mathrm{ERM},\mathcal{H}^*}(\epsilon, \delta) = O\left(\frac{k^2 r \log(k^2 r) \left(\log\left(\frac{k^3 r}{\epsilon} \right) \right) + \log\left(\frac{1}{\delta} \right)}{\epsilon} \right).$$

Lemma 26 (Theorem 3.7 of Daniely et al. [8])**.** *Let $\mathcal{H} \subseteq \{h : \mathcal{X} \to [k]\}$ be a hypothesis class, for which the realizability assumption holds with respect to some distribution $\mathcal{D}$, and let $d = \mathrm{Ndim}(\mathcal{H})$. Let*

$$m_{\mathrm{ERM},\mathcal{H}}(\epsilon, \delta) = \sup_{\mathcal{A}\in\mathrm{ERM}} m_{\mathcal{A},\mathcal{H}}(\epsilon, \delta),$$

where the supremum is taken over all ERM algorithms for $\mathcal{H}$. Then,

$$m_{\mathrm{ERM},\mathcal{H}}(\epsilon, \delta) = O\left(\frac{d\left(\log\left(\frac{kd}{\epsilon} \right) \right) + \log\left(\frac{1}{\delta} \right)}{\epsilon} \right).$$

Thus, if $m \geq m_{\mathrm{ERM},\mathcal{H}^*}(\epsilon, \delta)$ i.i.d. samples from Q and their respective labels were input to Algorithm 7, the output hypothesis h, with probability at least $(1 - \delta)$, will have at most an ϵ error.

To prove Theorem 4, what remains is to ensure that the learned hypothesis does not output class labels that the learning algorithm has not seen in the samples. For this, we propose a simple modification to Algorithm 7. That is, if a' is a class label that is not present in the samples, for all class labels a from which we have seen at least 1 sample, we set $g_{a,a'}(x) = 1$ and $g_{a',a}(x) = -1$ to be constant functions which may correspond to hyperplanes that are infinitely far away from the origin. Without loss of generality, assume that we have seen samples with labels $1, \ldots, k'$, and we have not seen samples with

labels $k'+1,\ldots,k$. Let $a \in k'$ be a label that that we have seen and let $a' \in [k]\backslash[k']$ be a label that we have not seen. Therefore we have

$$\sum_{b\neq a} g_{a,b}(x) = \sum_{b\in[k'],b\neq a} g_{a,b}(x) + \sum_{b\in[k]\backslash[k']} g_{a,b}(x) \geq -(k'-1) + (k-k') = k - 2k' + 1,$$

and

$$\sum_{b\neq a'} g_{a',b}(x) = \sum_{b\in[k']} g_{a',b}(x) + \sum_{b\in[k]\backslash[k'],b\neq a'} g_{a',b}(x) \leq -k' + (k-k'-1) = k - 2k' - 1.$$

Consequently, the output $g(x)$ of Algorithm 7 will never assign a label from $[k]\backslash[k']$ to any $x \in \mathbb{R}^d$.

To prove Theorem 5, all we need to do is to replace the binary hypothesis class $\mathcal{H}_{\mathrm{b}}^{\mathrm{EUC}}$ used in the preceding discussion with the binary hypothesis class $\mathcal{H}_{\mathrm{b}}^{\mathrm{FMS}}$ which we introduce next. We show that $\mathcal{H}_{\mathrm{b}}^{\mathrm{FMS}}$ satisfies the realizability assumption. We further show that there exists an ERM algorithm for $\mathcal{H}_{\mathrm{b}}^{\mathrm{FMS}}$ and the VC-dimension of $\mathcal{H}_{\mathrm{b}}^{\mathrm{FMS}}$ is small.

Let (P, Q, d) be k-means instance in a finite metric space where $|Q| < \infty$, and define the binary hypothesis class $\mathcal{H}_{\mathrm{b}}^{\mathrm{FMS}}$ as follows:

$$\mathcal{H}_{\mathrm{b}}^{\mathrm{FMS}} = \{h_{q_1,q_2} : (q_1, q_2) \in Q \times Q\},$$

where $h_{q_1,q_2} : P \to \{-1, +1\}$ is a binary labeling function define as

$$h_{q_1,q_2}(p) = \begin{cases} -1, & \text{if } \mathrm{d}(p,q_1) \geq \mathrm{d}(p,q_2) \\ +1, & \text{otherwise.} \end{cases}$$

Observe that this is a finite hypothesis class with at most $|Q|^2$ hypotheses. Furthermore, based on the assumption on no boundary points, for any two subsets P of two different labels, there exists an $h \in \mathcal{H}_{\mathrm{b}}^{\mathrm{FMS}}$ that perfectly separates them. Hence, pairwise binary classification of any two labels is realizable under $\mathcal{H}_{\mathrm{b}}$. To find such h in polynomial-time, we simply iterate over all possible hypotheses and pick the one that gives zero error. Lemma 20 yields that the VC-dimension of $\mathcal{H}_{\mathrm{b}}^{\mathrm{FMS}}$ is $O(\log |Q|)$.