Provably faster randomized and quantum algorithms for k-means clustering via uniform sampling

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Abstract

The k-means algorithm (Lloyd's algorithm) is a widely used method for clustering unlabeled data. A key bottleneck of the k-means algorithm is that each iteration requires time linear in the number of data points, which can be expensive in big data applications. This was improved in recent works proposing quantum and quantum-inspired classical algorithms to approximate the k-means algorithm locally, in time depending only logarithmically on the number of data points (along with data dependent parameters) [q-means: A quantum algorithm for unsupervised machine learning; Kerenidis, Landman, Luongo, and Prakash, NeurIPS 2019; Do you know what q-means?, Doriguello, Luongo, Tang]. In this work, we describe a simple randomized mini-batch k-means algorithm and a quantum algorithm inspired by the classical algorithm. We prove worse-case guarantees that significantly improve upon the bounds for previous algorithms. Our improvements are due to a careful use of $uniform\ sampling$, which preserves certain symmetries of the k-means problem that are not preserved in previous algorithms that use data norm-based sampling.

1 Introduction

The k-means clustering objective aims to partition a set of data points $\mathbf{v}_1, \dots, \mathbf{v}_n \in \mathbb{R}^d$ into k disjoint sets (also called clusters) such that points within a cluster are close to each other and points in different clusters are far from one another. Specifically, we are are tasked with finding k cluster centers $\mathbf{c}_1, \dots, \mathbf{c}_k \in \mathbb{R}^d$ such that the cost function

$$\mathcal{L}(\mathbf{c}_1, \dots, \mathbf{c}_k) \coloneqq \frac{1}{n} \sum_{i \in [n]} \min_{j \in [k]} \|\mathbf{v}_i - \mathbf{c}_j\|^2, \tag{1.1}$$

is minimized. Assigning each point \mathbf{v}_i to the nearest cluster center gives a partition of the data.

Perhaps the most influential algorithm for k-means clustering is the k-means algorithm (also called Lloyd's algorithm) [Llo82]. The k-means algorithm is a greedy heuristic algorithm¹ that takes as input k initial centers (e.g., from k-means++ [AV07]) and iteratively performs two locally optimal steps: (i) the data points are partitioned based on the promixity to the current centroids, and (ii) new centroids are chosen to optimize the cost function with respect to this partitioning.

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¹ Finding the optimal partition of k clusters, given the set of n data points is NP-hard [Das08].

We describe *a single iteration* of this algorithm in Algorithm 1. Typically this procedure is then repeated (using the output of the previous iteration for the initial centers of the next iteration) for some fixed number of iterations or until a given convergence criteria has been satisfied; e.g., until the centroids or cost do not vary much from iteration to iteration [Mac67, Llo82].

Algorithm 1 (Standard k-means (one iteration)).

Input: Data points $\mathbf{v}_1,\dots,\mathbf{v}_n\in\mathbb{R}^d$, initial centers $\mathbf{c}_1^0,\dots,\mathbf{c}_k^0\in\mathbb{R}^d$

1: **for** $j \in [k]$ **do**

2:
$$C_j^0 = \left\{ i \in [n] : j = \operatorname{argmin}_{j' \in [k]} \| \mathbf{v}_i - \mathbf{c}_{j'}^0 \| \right\}$$

3:
$$\mathbf{c}_j = \frac{1}{|C_j^0|} \sum_{i \in C_j^0} \mathbf{v}_i$$

Output: Updated centers $\mathbf{c}_1, \dots, \mathbf{c}_k \in \mathbb{R}^d$

1.1 Prior work

Each iteration of the k-means algorithm requires O(ndk) time. While significant work using classical methods has focused on improving this per-iteration cost, over recent years quantum and quantum-inspired algorithms have been proposed to reduce the per-iteration cost of k-means [KLLP19, DLT25]. These algorithms perform an approximate k-means step with runtime depending just poly-logarithmically on the number of data points n. When the number of data points n is large, such methods offer potential speedups. We provide an overview of the theoretical guarantees provided by these existing works in Sections 1.1.1 and 1.1.2 respectively. Finally, in Section 1.1.3, we discuss classical mini-batch algorithms that aim to reduce the per-iteration cost of the k-means algorithm.

1.1.1 q-means: A quantum algorithm for unsupervised machine learning [KLLP19]

q-means is a quantum algorithm which aims to mimic the k-means algorithm over one step. The algorithm assumes superposition query-access to the dataset containing n data points via quantum-random-access-memory (QRAM) in time logarithmic in the size of the dataset, where each data point is encoded into the amplitude-encoding quantum state using the KP-tree data structure [KP17]. Given the initial centroids $\mathbf{c}_1^0,\ldots,\mathbf{c}_k^0$, the q-means algorithm produces centroids $\widehat{\mathbf{c}}_1,\ldots,\widehat{\mathbf{c}}_k$ that are close to the classical k-means algorithm (see [KLLP19, §1.3]) in the sense that the approximate centers satisfy

$$\forall j \in [k]: \quad \left\| \hat{\mathbf{c}}_j - \frac{1}{|\check{C}_j^0|} \sum_{i \in \check{C}_j^0} \mathbf{v}_i \right\| \le \varepsilon, \tag{1.2}$$

where $(\check{C}_1^0, \dots, \check{C}_k^0)$ is some partition of [n] for which

$$\forall j \in [k], \ i \in \check{C}_{j}^{0}: \quad \|\mathbf{v}_{i} - \mathbf{c}_{j}^{0}\|^{2} \leq \min_{j' \in [k]} \|\mathbf{v}_{i} - \mathbf{c}_{j'}^{0}\|^{2} + \varepsilon. \tag{1.3}$$

That is, the approximate centers are nearly the mean of the right partition of the dataset. The parameter ε measures the nearness to the k-means algorithm; if $\varepsilon = 0$, then $\widehat{\mathbf{c}}_1, \dots, \widehat{\mathbf{c}}_k$ must match the centroids produced by the k-means algorithm.²

²Note that the units on ε are inconsistent between (1.2) and (1.3). This is implicitly mitigated by the assumption that $\|\mathbf{v}_i\| \ge 1$ for each $i \in [n]$.

Under the assumptions that $\min_{i \in [n]} \|\mathbf{v}_i\| \ge 1$ and that the initial cluster sizes are roughly balanced $(|C_j^0| = \Theta(n/k))$, [KLLP19, Theorem 5.1] asserts that the *q*-means algorithm runs in

$$\tilde{O}\left(\frac{kd}{\varepsilon^2}\eta\kappa\left(\mu + \frac{k\eta}{\varepsilon}\right) + \frac{k^2\eta^{3/2}\kappa\mu}{\varepsilon^2}\right) \text{ time per-iteration,}$$
 (1.4)

where $\tilde{O}(\cdot)$ hides poly-logarithmic dependencies, $\eta \coloneqq \max_i \|\mathbf{v}_i\|^2$, κ is the condition number of data matrix $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_n]^\mathsf{T}$, and $\mu \le \|\mathbf{V}\|_\mathsf{F}$ is a data-dependent quantity which arises from the use of black-box quantum linear algebra subroutines within the q-means algorithm. The main primitives used in the q-means algorithm include quantum distance estimation, minimum distance finding, and quantum linear algebra subroutines to approximate a matrix-vector product.

1.1.2 Do you know what q-means? [DLT25]

The authors in [DLT25] introduce an "improved" version of the q-means algorithm which avoids the need to use quantum linear algebra subroutines required by [KLLP19], while still maintaining a polylogarithmic dependence in n. As such, the dependence on most parameters is improved. Additionally, they introduce a "quantum-inspired" classical algorithm that maintains the poly-logarithmic dependence in n, although with a quadratically worse bound in data-dependent parameters. Additionally, they strengthen the approximation guarantee over [KLLP19] by producing clustering centers $\hat{\mathbf{c}}_1, \ldots, \hat{\mathbf{c}}_k$ satisfying

$$\forall j \in [k]: \quad \|\widehat{\mathbf{c}}_j - \mathbf{c}_j\| \le \varepsilon, \tag{1.5}$$

where $\mathbf{c}_1, \dots, \mathbf{c}_k$ are the centroids output by the k-means algorithm. This guarantee corresponds to that of [KLLP19] with ε in (1.3) set to zero.

The quantum algorithm of [DLT25] assumes query-access to the data-set via QRAM which is able to prepare row-norm weighted superpositions over *binary encoding* of the data points. Then, under the same assumptions $\min_{i \in [n]} \|\mathbf{v}_i\| \ge 1$ and $|C_j^0| = \Theta(n/k)$, [DLT25, Theorem 11] asserts that the quantum algorithm runs in

$$\tilde{O}\left(\frac{k^2 d\sqrt{\tilde{\eta}}}{\varepsilon}(\sqrt{k} + \sqrt{d})\right) \text{ time per-iteration,}^3$$
(1.6)

where $\bar{\eta} = n^{-1} \sum_{i \in [n]} \|\mathbf{v}_i\|^2 = n^{-1} \|\mathbf{V}\|_{\mathsf{F}}^2 \le \eta$.

The quantum-inspired classical algorithm of [DLT25] mimics the quantum algorithm by assuming access to the sample-and-query (SQ) access model to draw a subset of the data, where data points are drawn proportional to the squared row-norms $\|\mathbf{v}_i\|^2$ [DLT25]. Under the same balanced clusters assumption, [DLT25, Theorem 10] asserts that the dequantized algorithm uses

$$O\left(\frac{k^2 \log(k)\bar{\eta}}{\varepsilon^2}\right)$$
 samples per-iteration. (1.7)

The KP-tree data-structure [KP17] enables SQ access by sampling an index $i \in [n]$ proportional to the squared row-norms in $\tilde{O}(1)$ time, and reading a data point in $\tilde{O}(d)$ time respectively. Thus the total runtime cost of the algorithm is $\tilde{O}(\# \text{samples} \times kd)$ time per iteration.

We emphasize that both the quantum and quantum-inspired algorithm of [DLT25] make use of importance sampling: data points \mathbf{v}_i , for which $\|\mathbf{v}_i\|$ is large, are deemed to be more important in estimating the centroids.

³To the best of our knowledge, only the query complexity (and not time-complexity) of the mean estimation procedure used by [DLT25] was analyzed. Hence, the bound they state is more analogous to a bound on the QRAM query complexity (assuming $\tilde{O}(d)$ time/query) than a true runtime guarantee.

1.1.3 Other mini-batch algorithms

Unsurprisingly, over the past several decades the classical computing community has also developed algorithms to avoid the O(ndk) work per iteration of the k-means algorithm. An important class of these algorithms are based on a technique called *mini-batching*, whereby updates at a given iteration are computed using a small fraction of the total dataset, typically chosen uniformly at random [BB94, SMD22, TM17, Scu10, NF16].⁴ Such algorithms are widely used in practice, appearing in popular machine learning libraries such as scikit-learn [PVG+11].

A number of works aim to provide insight into such algorithms by providing theoretical bounds on the the batch-size and iteration count required for the algorithm to converge (to e.g., a local minimum) [TM17, Sch23]. Often, these mini-batch algorithms make use of additional algorithmic tools such as damping, which helps to reduce variability due to randomness in the algorithms. Unlike the past work described in Section 1.1, such methods do not aim to mimic the behavior of the *k*-means algorithm over one step. In Appendix C, we show that one-step guarantees, similar to those proved by the past work in Section 1.1, can be used to derive near-monotonicity bounds for damped mini-batch algorithms.

1.2 Outline and contributions

Our first main contribution is an analysis of a simple mini-batch algorithm based on *uniform sampling* (Algorithm 2). The algorithm, about whose novelty we make no claims, is extremely simple: it selects a subset of b data points uniformly at random, and then performs one step of the k-means algorithm on this subset. Our main result is that, if the initial clusters are of roughly equal size, i.e., $|C_j^0| = \Theta(n/k)$ then the output $\widehat{\mathbf{c}}_1, \dots, \widehat{\mathbf{c}}_k$ of Algorithm 2 satisfy, for all $j \in [k]$, $\|\mathbf{c}_j - \widehat{\mathbf{c}}_j\| \le \varepsilon$, if the algorithm uses

$$O\left(\frac{k^2}{\varepsilon^2}\phi + \log(k)\right)$$
 samples per-iteration, (1.8)

where the parameter

$$\phi \coloneqq \frac{1}{n} \sum_{j \in [k]} \sum_{i \in C_i^0} \|\mathbf{v}_i - \mathbf{c}_j\|^2$$
(1.9)

measures of the quality of the partition induced by the initial cluster center.

That our bounds depend on ϕ is a notable improvement over past work (recall [KLLP19] incurs dependency on the quantity $\eta = \max_i \|\mathbf{v}_i\|^2$, while [DLT25] depends on $\bar{\eta} = n^{-1} \sum_i \|\mathbf{v}_i\|^2 = \mathcal{L}(\mathbf{0},...,\mathbf{0})$). Indeed, it always holds that

$$\phi \le \bar{\eta} \le \eta,\tag{1.10}$$

and in many cases we expect $\phi \ll \bar{\eta}$. As we discuss in Section 1.3, a key limitation of the previous works is the unavoidable dependency on η and $\bar{\eta}$, which arises from failing to respect the k-means objective problem symmetry.

Our second main contribution is a quantum algorithm (Algorithm 3) which can be viewed as a quantum analog of Algorithm 2. Assuming superposition quantum access to the data using QRAM, and leveraging quantum mean estimation [CHJ22], we showcase a quadratic improvement in the ε dependence compared to our classical algorithm. Specifically, under the same balanced clusters assumption, we obtain the same guarantee using

$$\tilde{O}\left(\frac{k^{5/2}\sqrt{d}}{\varepsilon}\sqrt{\phi}\right)$$
 QRAM queries per-iteration. (1.11)

⁴The dequantized algorithm of [DLT25] can be viewed as a mini-batch algorithm with non-uniform sampling.

As with Algorithm 2, our guarantees improve on the quantum algorithms from past work [KLLP19, DLT25], most notably with regards to the dependence on ϕ rather than $\bar{\eta}$ or η . In addition, since we only use uniform superposition over the data, we do not require access to a KP-tree data structure. We note that the precise access model for the quantum algorithms in [KLLP19], [DLT25], and our work are all slightly different, so direct comparisons of costs are not reasonable.

Finally, in the appendix, we provide some additional results that may be of independent interest. In particular, in Appendix C we analyze a generalization of Algorithm 2 which uses damping and is closely related to the implementation of mini-batch k-means in scikit-learn. Our main result is to show that, under certain assumptions, the cost (1.1) of the cluster centers produced is nearly monotonic (i.e., does not increase by more than a multiplicity factor $(1 + \gamma)$, for some small parameter γ).

1.3 k-means problem invariance

The k-means clustering objective is invariant to rigid-body transforms of the data (e.g., shifting the data points by some constant vector or rotating the data). The k-means algorithm (Algorithm 1) respects this problem symmetry; if run on transformed data (with initial cluster centers transformed accordingly), then the outputs on the transformed problem will be the transformed version of the outputs of the algorithms run on the original data. Uniform sampling (and hence Algorithm 2) also respect this symmetry (and our bounds for the algorithm reflect this).

On the other hand, algorithms which depend on the relative sizes of the row-norms can behave drastically different depending on how the data is transformed (see Fig. 1). This invariance is reflected in the analyses of past algorithms, which depend on quantities like η and $\bar{\eta}$ [KLLP19, DLT25]. In realistic scenarios, both η and $\bar{\eta}$ can be large, and it is easy to see that a dependence on an aspect-ratio is inherent to algorithms which uses some type of magnitude based importance sampling.

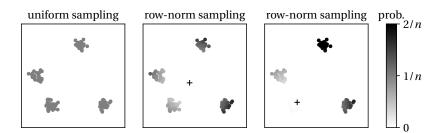


Figure 1: Visualization of the probability of sampling a given data point when using uniform sampling or row-norm sampling. For row-norm sampling, we show two versions of the data-set, corresponding to a shift (origin is indicated with a plus). Row-norm sampling is sensitive to rigid-body transforms of the data (which do not change the clustering objective (1.1)) and is unlikely to sample points in clusters near the origin when the smoothed aspect ratio $\bar{\eta}$ is large.

Example 1.1. Consider a dataset $\mathbf{v}_1, \dots, \mathbf{v}_n \in \mathbb{R}^1$ where $\mathbf{v}_1, \dots, \mathbf{v}_{n/2} = -1$ and $\mathbf{v}_{n/2+1}, \dots, \mathbf{v}_n = \alpha \ge 1$. This is a perfectly clusterable dataset when k = 2 (i.e., there are centers for which the cost (1.1) is zero). Suppose we initialize with clusters $\mathbf{c}_1^0 = 0$ and $\mathbf{c}_2^0 = \alpha$.

• The k-means algorithm (Algorithm 1) produces the correct cluster centers $\mathbf{c}_1 = -1$ and $\mathbf{c}_2 = \alpha$.

- The mini-batch k-means algorithm (Algorithm 2) which samples points uniformly produces the correct cluster centers if and only if B contains at least one entry from $\{1, ..., n/2\}$ and at least one entry from $\{n/2+1, ..., n\}$. This happens with probability $1-\delta$ if we use $b=1+\log_2(1/\delta)=\Theta(\log(1/\delta))$ samples.
- Suppose instead we observe points proportional to their squared row-norms (this is what is done in [DLT25]). When $\alpha \gg 1$, we are unlikely to see any points in the cluster at -1, in which case we cannot hope to produce an accurate update. Specifically,

$$\Pr\left(\text{observe at least one point from cluster at } -1\right) = 1 - \left(1 - \frac{1}{(1 + \alpha^2)}\right)^b$$
,

so that we need at least $b = \Omega(\alpha^2 \log(1/\delta))$ samples to observe a point from the cluster at -1 with probability $1 - \delta$.

Since $\eta = \max_i \|\mathbf{v}_i\|^2 = \alpha^2$ and $\bar{\eta} = \frac{1}{n} \sum_{i \in [n]} \|\mathbf{v}_i\|^2 = (1 + \alpha^2)/2$, this example demonstrates that a dependence on such quantities is inherent to this sampling scheme.

Example 1.1 highlights a fundamental weakness of distance-based sampling. Intuitively, in order to produce cluster centers similar to those produced by the k-means algorithm, we must observe a reasonable number of points from each of the C_j^0 . However, even if the clusters are all of similar size (i.e., $|C_j^0| = \Theta(n/k)$) if all the points in C_j^0 are near the origin, then we may require a larger number of total samples in order to ensure that we sample enough points in C_j^0 . On the other hand, uniform sampling allows to observe a constant fraction samples from each cluster, resulting in a more reliable update.

1.4 Notation and conventions

We write $[k] := \{1, 2, ..., k\}$, and use $\tilde{O}(\cdot)$ is used to hide poly-logarithmic terms in all parameters, including n, $\mathcal{L}(\mathbf{c}_1^0, ..., \mathbf{c}_k^0)$, η , etc. We use $\|\mathbf{x}\|$ to indicate the Euclidean norm of a vector \mathbf{x} , $\|\mathbf{X}\|_{\mathsf{F}}$ to indicate the Frobenius norm of a matrix \mathbf{x} , and |C| the cardinality of a set C.

All of our theoretical guarantees are local per-iteration guarantees, which relate the performance of approximate algorithms to the true k-means algorithm. Throughout, we will write

$$\mathbf{c}_{j} = \frac{1}{|C_{j}^{0}|} \sum_{i \in C_{j}^{0}} \mathbf{v}_{i}, \qquad C_{j}^{0} = \left\{ i \in [n] : j = \underset{j' \in [k]}{\operatorname{argmin}} \|\mathbf{v}_{i} - \mathbf{c}_{j'}^{0}\| \right\}$$
(1.12)

as in the k-means algorithm. 5 Most of the bounds depend on the parameters

$$k_C := \frac{n}{\min_{j \in [k]} |C_j^0|}, \qquad \phi := \frac{1}{n} \sum_{j \in [k]} \sum_{i \in C_j^0} \|\mathbf{v}_i - \mathbf{c}_j\|^2,$$
 (1.13)

which respectively control the relative size of the clusters induced by the initial cluster centers and the quality of these clusters. Previous works assume balanced cluster sizes $k_C = \Theta(k)$ [KLLP19, DLT25].

When describing quantum algorithms, U^{\dagger} will denote the conjugate transpose of a unitary U, and $|0\rangle$ will be some easy to prepare state, whose size can be determined from context.

 $^{^{5}}$ In the case that a data point has multiple nearest initial cluster centers, we assume the tie is broken based on some fixed rule.

2 Mini-batch algorithm

We now present Algorithm 2, which is a mini-batch version of Algorithm 1. The algorithm is simple; in each iteration, a random subset of data points b is drawn from the full dataset uniformly at random (with replacement) and the k-means algorithm is applied to this subset.

Algorithm 2 (Mini-batch *k*-means (one iteration)).

Input: Data $\mathbf{v}_1, ..., \mathbf{v}_n \in \mathbb{R}^d$, initial centers $\mathbf{c}_1^0, ..., \mathbf{c}_k^0 \in \mathbb{R}^d$

1: Sample *b* indices $B = \{s_1, ..., s_b\} \in [n]^b$, each independently such that $\Pr(s_\ell = i) = 1/n$.

2: **for** $j \in [k]$ **do**

3:
$$\widehat{C}_{j}^{0} = \left\{ i \in B : j = \operatorname{argmin}_{j' \in [k]} \| \mathbf{v}_{i} - \mathbf{c}_{j'}^{0} \| \right\}$$

4:
$$\widehat{\mathbf{c}}_j = \frac{1}{|\widehat{C}_j^0|} \sum_{i \in \widehat{C}_j^0} \mathbf{v}_i$$

Output: Updated centers $\hat{\mathbf{c}}_1, \dots, \hat{\mathbf{c}}_k \in \mathbb{R}^d$

Strictly speaking, B and \widehat{C}^0_j are multisets (rather than sets), since they may have repeated entries. We expect an algorithm which draws the entries of B without replacement may perform slightly better. However, the algorithm presented is easier to analyze due to the independence of the indices in B.

2.1 Main results

Our main result for Algorithm 2 is the following.

Theorem 2.1. Suppose

$$b \ge k_C \cdot \max \left\{ \frac{40\phi}{\varepsilon^2}, 8\log(20k) \right\},$$

where k_C and ϕ are defined in (1.13). Then, with probability at least 9/10, the output ($\hat{\mathbf{c}}_1, \dots, \hat{\mathbf{c}}_k$) of Algorithm 2 satisfies

$$\frac{1}{n} \sum_{j \in [k]} |C_j^0| \|\mathbf{c}_j - \widehat{\mathbf{c}}_j\|^2 \le \varepsilon^2.$$

As noted in the introduction, past work [KLLP19, DLT25] prove that their algorithms mimic, in a certain sense, the k-means algorithm. While Theorem 2.1 can be converted into a guarantee similar to past work.

Corollary 2.2. Suppose

$$b \ge k_C \cdot \max \left\{ \frac{40k_C \phi}{\varepsilon^2}, 8\log(20k) \right\},$$

where k_C and ϕ are defined in (1.13). Then, with probability at least 9/10, the output $(\hat{\mathbf{c}}_1, ..., \hat{\mathbf{c}}_k)$ of Algorithm 2 satisfies

$$\forall j \in [k]: \|\mathbf{c}_j - \widehat{\mathbf{c}}_j\| \le \varepsilon.$$

In particular, if $|C_j^0| = \Theta(n/k)$ (i.e., $k_C = \Theta(k)$) and $b = O(k^2 \varepsilon^{-2} \phi + \log(k))$, then for all $j \in [k]$, $\|\mathbf{c}_j - \widehat{\mathbf{c}}_j\| \le \varepsilon$, as mentioned in (1.8).

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Remark 2.3. While we state our bounds for constant failure probability $\leq 1/10$, the result can be efficiently improved to an arbitrary failure probability δ by repeating each iteration $O(\log(1/\delta))$ times and using a high-dimensional variant of the "median-trick"; see Theorem A.6.

2.2 Proofs

In this section we provide our analysis of Algorithm 2. Throughout, it will be useful to consider the quantities

$$\phi_j := \frac{1}{n} \sum_{i \in C_j^0} \|\mathbf{v}_i - \mathbf{c}_j\|^2, \qquad j \in [k].$$

$$(2.1)$$

Note that, by definition (see (1.9)), $\phi = \phi_1 + \cdots + \phi_k$.

Proof of Theorem 2.1. Let $\mathbf{V}^T = [\mathbf{v}_1, \dots, \mathbf{v}_n] \in \mathbb{R}^{d \times n}$ and, for each $j \in [k]$, define the characteristic vector

$$\mathbf{x}_j = \frac{1}{|C_j^0|} \sum_{i \in C_j^0} \mathbf{e}_i,\tag{2.2}$$

where $\mathbf{e}_i \in \mathbb{R}^n$ is the i-th standard basis vector. Then $(\mathbf{x}_j)_i = 1/|C_j^0|$ if $i \in C_j^0$ and 0 otherwise, and $\mathbf{1}^\mathsf{T}\mathbf{x}_j = 1$, where $\mathbf{1}$ is the all-ones vector. As with past work [KLLP19, DLT25], we will make use of the fact that $\mathbf{c}_j = \mathbf{V}^\mathsf{T}\mathbf{x}_j$.

Fix $j \in [k]$. Observe the j-th center output by Algorithm 2 can be written as

$$\widehat{\mathbf{c}}_{j} = \frac{1}{n|\widehat{C}_{j}^{0}|} \sum_{i \in \widehat{C}_{i}^{0}} \frac{1}{n^{-1}} \mathbf{v}_{i} = \mathbf{c}_{j} + \widehat{\lambda}_{j} \widehat{\mathbf{y}}_{j}, \tag{2.3}$$

where

$$\widehat{\lambda}_{j} = \frac{b|C_{j}^{0}|}{n|\widehat{C}_{j}^{0}|}, \qquad \widehat{\mathbf{y}}_{j} = \frac{1}{b|C_{j}^{0}|} \sum_{i \in \widehat{C}_{i}^{0}} \frac{1}{n^{-1}} (\mathbf{v}_{i} - \mathbf{c}_{j}).^{6}$$
(2.4)

Next, note that ℓ_2 -distance between the cluster centers produced by k-means and Algorithm 2 can be decomposed as

$$\|\mathbf{c}_{j} - \widehat{\mathbf{c}}_{j}\| = \|\widehat{\lambda}_{j}\widehat{\mathbf{y}}_{j}\| = |\widehat{\lambda}_{j}|\|\widehat{\mathbf{y}}_{j}\|. \tag{2.5}$$

We will now show that $|\hat{\lambda}_j| \le 2$ with a high probability, and that $\|\hat{\mathbf{y}}_j\|$ is small (relative to the per-cluster cost) in expectation. Subsequently employing the linearity of expectation, Markov's inequality, and a union bound gives us the desired bound.

Bound for $|\widehat{\lambda}_j|$: Since $|\widehat{C}_j^0|$ is a binomial random variable (with b draws and success probability $|C_j^0|/n$), then $|\widehat{\lambda}_j| = O(1)$ with good probability. In particular, a standard application of a multiplicative Chernoff bound (see e.g., Imported Theorem A.5) gives

$$\Pr\left(\widehat{\lambda}_j > 2\right) = \Pr\left(|\widehat{C}_j^0| < \frac{b|C_j^0|}{2n}\right) \le \exp\left(-\frac{b|C_j^0|}{8n}\right) \le \exp\left(-\frac{b}{8k_C}\right) \le \frac{1}{20k},\tag{2.6}$$

where the last inequality is due to our choice of $b \ge 8k_C \log(20k)$. Hence, applying a union bound, we have

$$\Pr\left(\forall j \in [k] : \widehat{\lambda}_j \le 2\right) \ge 1 - \frac{1}{20}. \tag{2.7}$$

⁶This implies that if $|\hat{C}_{j}^{0}| = 0$, then the algorithm should update $\hat{\mathbf{c}}_{j} = \mathbf{c}_{j}$, which would require performing a full k-means step. However, this case is avoided with high probability by (2.7).

Bound for $\|\hat{y}_i\|$: Observe, again using the definition of x_i , that \hat{y}_i can be written as

$$\widehat{\mathbf{y}}_j = \frac{1}{b|C_j^0|} \sum_{i \in \widehat{C}_i^0} \frac{1}{n^{-1}} (\mathbf{v}_i - \mathbf{c}_j)$$
(2.8)

$$= \frac{1}{b|C_i^0|} \sum_{i \in [b]} \frac{1}{n^{-1}} (\mathbf{v}_{s_i} - \mathbf{c}_j) \mathbb{1}[s_i \in C_j^0]$$
 (2.9)

$$= \frac{1}{b} \sum_{i \in [b]} \frac{1}{n^{-1}} (\mathbf{v}_{s_i} - \mathbf{c}_j) (\mathbf{x}_j)_{s_i}. \tag{2.10}$$

A standard direct computation (see Lemma A.3) reveals that

$$\mathbb{E}[\|\widehat{\mathbf{y}}_j\|^2] = \frac{1}{b} \left(\left(\sum_{i \in [n]} \frac{1}{n^{-1}} \|\mathbf{v}_i - \mathbf{c}_j\|^2 |(\mathbf{x}_j)_i|^2 \right) = \frac{1}{b} \left(\left(\frac{1}{|C_j^0|^2} \sum_{i \in C_i^0} \frac{1}{n^{-1}} \|\mathbf{v}_i - \mathbf{c}_j\|^2 \right).$$
(2.11)

Therefore,

$$\mathbb{E}\left[|C_{j}^{0}|\|\widehat{\mathbf{y}}_{j}\|^{2}\right] = \frac{n}{b|C_{j}^{0}|} \sum_{i \in C_{i}^{0}} \|\mathbf{v}_{i} - \mathbf{c}_{j}\|^{2} = \frac{n^{2}\phi_{j}}{b|C_{j}^{0}|},$$
(2.12)

where the last equality is by our definition (2.1) of ϕ_j . We now use linearity of expectation, the definition $k_C = n/\min_{j \in [k]} |C_i^0|$, and that $\phi = \phi_1 + \cdots + \phi_k$ to obtain a bound

$$\mathbb{E}\left[\frac{1}{n}\sum_{j\in[k]}|C_{j}^{0}|\|\widehat{\mathbf{y}}_{j}\|^{2}\right] = \sum_{j\in[k]}\frac{n\phi_{j}}{b|C_{j}^{0}|} \le \frac{k_{C}\phi}{b}.$$
(2.13)

Applying Markov's inequality (see Imported Theorem A.4) we find

$$\Pr\left(\frac{1}{n}\sum_{i\in[k]}|C_j^0|\|\widehat{\mathbf{y}}_j\|^2 > \frac{\varepsilon^2}{2}\right) \le \frac{2k_C\phi}{\varepsilon^2b} \le \frac{1}{20},\tag{2.14}$$

where the last inequality is due to our choice of $b \ge 40k_C\phi/\varepsilon^2$.

The result then follows from a union bound with compliment of the event that $|\hat{\lambda}_j| < 2$ for all $j \in [k]$.

2.2.1 Proof of ε -approximate k-means property

Corollary 2.2 follows from basic algebraic properties.

Proof of Corollary 2.2. We have that

$$\max_{j \in [k]} \|\mathbf{c}_{j} - \widehat{\mathbf{c}}_{j}\|^{2} = \max_{j \in [k]} \frac{n}{|C_{j}^{0}|} \frac{1}{n} |C_{j}^{0}| \|\mathbf{c}_{j} - \widehat{\mathbf{c}}_{j}\|^{2} \le k_{C} \frac{1}{n} \max_{j \in [k]} |C_{j}^{0}| \|\mathbf{c}_{j} - \widehat{\mathbf{c}}_{j}\|^{2} \le k_{C} \frac{1}{n} \sum_{j \in [k]} |C_{j}^{0}| \|\mathbf{c}_{j} - \widehat{\mathbf{c}}_{j}\|^{2}.$$
 (2.15)

The result then follows by Theorem 2.1, relabeling ε as appropriate.

3 Quantum algorithm

Changing the computational access model to the data from the classical random-access-memory (RAM) to the quantum superposition access model via QRAM allows for performing coherent operations on the quantum states, often resulting in quadratic reduction in the QRAM queries compared to the classical queries [Gro96, BHMT02]. In this section, simplifying the results by [KLLP19, DLT25], we propose an improved quantum algorithm for k- means clustering which returns a ε accurate approximation to the exact d-dimensional centroids per-iteration using using $\tilde{O}(\sqrt{d}/\varepsilon)$ queries (as opposed to $\tilde{O}(1/\varepsilon^2)$ queries required by classical algorithms).

3.1 Computational model

A key assumption of our quantum algorithm is that the input data can accessed in a coherent superposition using a quantum computer.

Assumption 3.1 (Quantum query access). We assume input data $\mathbf{x}_1, \dots, \mathbf{x}_q \in \mathbb{R}^d$ is available through a quantum data structure (which we call QRAM) that provides access to the unitary U implementing the map $|i\rangle|0\rangle \mapsto |i\rangle|\mathbf{x}_i\rangle$. A "query to the QRAM" refers to the use of this map (or its inverse).

This is similar to the RAM access model assumed for the classical algorithm, $i \mapsto \mathbf{x}_i$ (and as with the classical algorithm, we only read entire columns of the data-matrix at once). The main difference is that the unitary which implements $|i\rangle|0\rangle \mapsto |i\rangle|\mathbf{x}_i\rangle$ also allows us to act simultaneously on states in superposition

$$\sum_{i} \alpha_{i} |i\rangle |0\rangle \mapsto \sum_{i} \alpha_{i} |i\rangle |\mathbf{x}_{i}\rangle$$
(3.1)

for arbitrary $\alpha_i \in \mathbb{C}$ such that $\sum_i |\alpha_i|^2 = 1$.

Analogously to our analysis of the classical algorithm in Section 2, we measure the "cost" of our quantum algorithm in terms of the number of queries to the QRAM.⁷

There are a number of ways to encode a real-number x into the quantum state $|x\rangle$ [NC10]. The precise encoding is not important for us, so long as we can perform certain basic operations, which are used within our algorithm and subroutines such as quantum mean estimation [CHJ22].

Assumption 3.2 (Exact quantum arithmetic). We assume real-numbers x can be represented in a quantum state $|x\rangle$ and that we can perform basic arithmetic/comparison operations on such quantum states exactly; e.g., $|x\rangle|0\rangle \mapsto |x\rangle|\sqrt{x}\rangle$, $|x,y\rangle|0\rangle \mapsto |x,y\rangle|x+y\rangle$, $|x,y\rangle|0\rangle \mapsto |x,y\rangle|1$ [|x|], etc.

This is similar to the assumption we make in the analysis of our classical algorithm (i.e., that arithmetic is exact). For instance, the quantum state $|x\rangle$ can be thought of as the *bit-encoding* of x:

$$|x\rangle = |x_1\rangle|x_2\rangle\cdots|x_b\rangle,\tag{3.2}$$

where $x_i \in \{0,1\}$ is the *i*-th bit of a *b*-bit binary finite-precision representation of x. Classical fixed and floating-point arithmetic circuits have analogs which can be implemented on quantum computers. Hence, Assumption 3.2 essentially states that we use enough bits of precision that the impacts of finite precision are negligible compared to other errors. More efficient circuits designed specifically for quantum computing are also a topic of study [TGA10, RPGE17, WLL⁺25]

3.2 Core primitives

The first main tool we use is the fixed-point amplitude amplification algorithm, which boosts the amplitude of a "good state" to a large probability with a quadratic improvement in the complexity over classical analogue [BHMT02, NC10, GSLW19].

⁷There are several proposals for data structures which efficiently implement QRAM [GLM08, KP17], and hence it would be possible to measure the cost in terms of something like the gate complexity. However, quantum query models (such as the one used here) are popular because they allow natural and simple analyses of many core quantum algorithms, as well as fine-grained lower-bounds [BdW02, Aar21].

Imported Theorem 3.3 (Fixed-point amplitude amplification [GSLW19, Theorem 27]). Assume access to a unitary *Q* which performs the map

$$|0,0\rangle \mapsto \sum_{\ell \in [n]} \alpha_{\ell} |\psi_{\ell}\rangle |\ell\rangle.$$

Fix $j \in [n]$. Given parameter $\Delta \in (0,1)$ and $0 < \alpha < \alpha_j$, there is a quantum algorithm that uses $O(\alpha^{-1}\log(1/\Delta))$ queries to Q and Q^{\dagger} to construct a unitary that performs the map

$$|0,0\rangle \mapsto \sqrt{1-\delta}|\psi_i\rangle|j\rangle + \sqrt{\delta}|G\rangle$$
,

for some $\delta \leq \Delta$, where $|G\rangle$ is orthogonal to $|\psi_i\rangle|j\rangle$. The state $|\psi_i\rangle$ need not be known.

Proof. Let $|\psi_0\rangle = |0,0\rangle$ and $|\psi\rangle = U|\psi_0\rangle$. Denote C_P NOT = $X\otimes P + I\otimes (I-P)$ for an orthogonal projector P (where X is the Pauli X matrix), $\Pi_j = I\otimes |j\rangle\langle j|$, and $P_0 = |\psi_0\rangle\langle\psi_0|$. Observe that $\Pi_j|\psi\rangle = \alpha_j|\psi_j\rangle|j\rangle$. Then, by [GSLW19, Theorem 27], there is a unitary \tilde{Q} that can be constructed using $O(\alpha^{-1}\log(1/\Delta))$ queries to Q, Q^{\dagger} , C_{Π_j} NOT, C_{P_0} NOT, and $e^{i\varphi Z}$ (where Z is the Pauli Z matrix), such that

$$\| |\psi_j\rangle |j\rangle - \tilde{Q}|\psi_0\rangle \| \le \sqrt{\Delta}. \tag{3.3}$$

Note that we don't count the queries to C_{Π_j} NOT, C_{P_0} NOT, and $e^{i\phi Z}$ since they are straightforward to implement for the given choice of Π_j and P_0 . Thus, writing $\tilde{Q}|\psi_0\rangle = \beta |\psi_j\rangle |j\rangle + \alpha |G'\rangle$ with $\beta \geq 0$ and $|G'\rangle$ orthogonal to $|\psi_j\rangle |j\rangle$ (up to a global phase), we can see that $\beta \geq \sqrt{1-\Delta}$. Writing $\beta = \sqrt{1-\delta}$ for $\delta \leq \Delta$, $\alpha = e^{i\theta}\sqrt{\delta}$ for some phase θ , and $|G\rangle = e^{i\theta}|G'\rangle$ completes the proof.

The second important tool we use is a quantum mean estimation algorithm.⁸

Imported Theorem 3.4 (Quantum mean estimation [CHJ22, Theorem 3.5]). Let Ω be a finite sample space and \mathbf{X} a d-dimensional random variable taking value $\mathbf{X}(\omega)$ with probability $p(\omega)$. Define the mean and covariance

$$\boldsymbol{\mu} = \sum_{\omega \in \Omega} p(\omega) \mathbf{X}(\omega) \qquad \boldsymbol{\Sigma} = \sum_{\omega \in \Omega} p(\omega) (\mathbf{X}(\omega) - \boldsymbol{\mu}) (\mathbf{X}(\omega) - \boldsymbol{\mu})^{\mathsf{T}}.$$

Assume access to unitaries U and B that implement the maps

$$|0,0\rangle \mapsto \sum_{\omega \in \Omega} \sqrt{p(\omega)} |\omega\rangle |G_{\omega}\rangle \qquad |\omega\rangle |0\rangle \mapsto |\omega\rangle |\mathbf{X}(\omega)\rangle,$$

respectively. Here $|G_{\omega}\rangle$ can be any state.

Fix $\delta > 0$. For $\varepsilon < \log(d/\delta)/\sqrt{d}$, there is a quantum algorithm that uses $\tilde{O}(\sqrt{d}/\varepsilon)$ queries to U and B to output an estimate $\hat{\mu}$ of μ such that, with probability at least $1 - \delta$,

$$\|\boldsymbol{\mu} - \widehat{\boldsymbol{\mu}}\|^2 \le \varepsilon^2 \operatorname{tr}(\boldsymbol{\Sigma}).$$

⁸While [CHJ22, Theorem 3.5] gives an improvement over classical estimators for small ε , no improvement over classical estimators is possible for large ε [CHJ22, Theorems 3.7].

⁹The probability $p(\omega)$ is recovered by the projective measurement $\|\Pi_{\omega}U(0,0)\|^2$, where $\Pi_{\omega} = |\omega\rangle\langle\omega| \otimes I$ are the orthogonal projectors corresponding to a measurement (in the standard basis) of the first register.

3.3 Algorithm

Algorithm 3 describes the quantum algorithm for performing one-step of the *k*-means algorithm.

Algorithm 3 (Quantum uniform k-means (one iteration)).

Input: Data $\mathbf{v}_1, ..., \mathbf{v}_n \in \mathbb{R}^d$, initial centers $\mathbf{c}_1^0, ..., \mathbf{c}_k^0 \in \mathbb{R}^d$ (both with quantum query access)

1: **for** j = 1, ..., k **do**

2: Use Algorithm 5 to construct unitary \widetilde{U}_i (approximately) implementing the map:

$$|0,0\rangle \mapsto \sum_{i \in C_j^0} \frac{1}{\sqrt{|C_j^0|}} |i\rangle |j\rangle.$$

3: Use Algorithm 6 to construct unitary B_i implementing the map:

$$|i\rangle|\mathbf{0}\rangle \mapsto |i\rangle|\mathbf{X}_{i}(i)\rangle$$
,

where

$$\mathbf{X}_{j}(i) = \begin{cases} \mathbf{v}_{i} - \mathbf{c}_{j}^{0} & \ell_{i} = j \\ \mathbf{0} & \text{otherwise} \end{cases},$$

and $\ell_i = \operatorname{argmin}_{j' \in [k]} \{ \| \mathbf{v}_i - \mathbf{c}_{j'}^0 \| \}.$

4: Use mean estimation (Imported Theorem 3.4) with \tilde{U}_i and B_i to obtain estimate $\hat{\mu}_i$.

5: Set $\widehat{\mathbf{c}}_j = \mathbf{c}_i^0 + \widehat{\boldsymbol{\mu}}_j$.

Output: Updated centers $\hat{\mathbf{c}}_1, ..., \hat{\mathbf{c}}_k \in \mathbb{R}^d$

3.4 Main result

Our main result theoretical result is the following.

Theorem 3.5. Given QRAM access (Assumption 3.1) to data points $\mathbf{v}_1, ..., \mathbf{v}_n$ and cluster centers $\mathbf{c}_1^0, ..., \mathbf{c}_k^0$ such that the quantum data encoding satisfies Assumption 3.2, Then, for $\varepsilon < \sqrt{k_C \min_j \phi_j \log(d/\delta)} / \sqrt{d}$, using

$$\tilde{O}\left(\frac{k^{3/2}k_C\sqrt{d}}{\varepsilon}\sqrt{\phi}\right) \tag{3.4}$$

with probability at least 9/10, the output $(\hat{\mathbf{c}}_1,...,\hat{\mathbf{c}}_k)$ of Algorithm 3 satisfies

$$\forall j \in [j]: \|\mathbf{c}_j - \widehat{\mathbf{c}}_j\| \le \varepsilon$$

where k_C is defined in (1.13).

In particular, assuming the balanced cluster size assumption $k_C = \Theta(k)$ [KLLP19, DLT25], we get the bound (1.11) from the introduction. We note that the $\tilde{O}(\cdot)$ in Theorem 3.5 hides a logarithmic factors in n, d, and $\mathcal{L}(\mathbf{c}_1^0,\ldots,\mathbf{c}_k^0)$. The exact dependencies, which are suppressed in the theorem statement, can be seen in the proof.

 $^{^{10}\}mathcal{L}(\mathbf{c}_1^0,\ldots,\mathbf{c}_k^0)$ is incomparable to the quantities terms $\bar{\eta}$ and η appearing in past work. However, for any reasonable initialization (i.e., better than $\mathbf{c}_j^0 = \mathbf{0}$), we expect $\mathcal{L}(\mathbf{c}_1^0,\ldots,\mathbf{c}_k^0)$ to be small relative to these quantities.

Remark 3.6. As noted in Section 1.2, the precise access model and way of measuring costs for the quantum algorithms in [KLLP19], [DLT25], and our work are all slightly different. In particular, [KLLP19] assumes the the data is prepared in quantum states using amplitude encoding. This is a weaker assumption than we make in the current paper, since a bit-encoding can be efficiently converted to an amplitude encoding. [DLT25] uses bit-encoding, similar to the present paper, and additionally assumes that the QRAM can efficiently prepare row-norm weighted superpositions over the data. While the time-complexity is reported, as noted in Footnote 3, it seems that the analysis omits the time cost of mean estimation and rather reports its QRAM query complexity.

3.5 Subroutines of the algorithm

Note that the centers output by the k-means algorithm Algorithm 1 are simply the mean of the points within each cluster C_j^0 . Therefore, in order to perform a similar mean estimation step in Algorithm 3 over a given cluster $j \in [k]$, we would like access to a unitary U_j which performs the map

$$|0\rangle \mapsto \sum_{i \in C_j^0} \frac{1}{\sqrt{|C_j^0|}} |i\rangle,\tag{3.5}$$

and additionally access to a unitary B_i implementing the map

$$|i\rangle|\mathbf{0}\rangle\mapsto|i\rangle|\mathbf{X}_i(i)\rangle$$
,

where

$$\mathbf{X}_{j}(i) = \begin{cases} \mathbf{v}_{i} - \mathbf{c}_{j}^{0} & \ell_{i} = j \\ \mathbf{0} & \text{otherwise} \end{cases},$$

and $\ell_i = \operatorname{argmin}_{j' \in [k]} \{ \| \mathbf{v}_i - \mathbf{c}_{j'}^0 \| \}.$

As with past work [KLLP19, DLT25], the starting point of algorithm is implementing a unitary which provides labels to the data points.

Theorem 3.7 (Cluster assignment). Algorithm 4 uses O(k) QRAM queries to construct a unitary U which performs the map:

$$|0,0\rangle \mapsto |i,\ell_i\rangle, \qquad \ell_i = \underset{j \in [k]}{\operatorname{argmin}} \|\mathbf{v}_i - \mathbf{c}_j^0\|.$$

Algorithm 4, which we describe explicitly in Section 3.7, simply uses the QRAM to load \mathbf{v}_i and $\mathbf{c}_1^0, \dots, \mathbf{c}_k^0$, and then applies reversible analogs of classical operations to identify the nearest cluster. We note that it may be possible to get a better k dependence by using a quantum minimization algorithm that can approximately compute the argmin of k numbers using $O(\sqrt{k})$ QRAM queries, compared to an exact classical algorithm that uses O(k) queries. Such an approach was used in [DLT25], although the impact of the error was not analyzed. We leave such an analysis to future work.

In Algorithm 5 we describe how to approximately implement U_j . The key observation is that a uniform superposition of the labeled data can be used to obtain an approximation to U_j . Indeed,

$$\sum_{i \in [n]} \frac{1}{\sqrt{n}} |i, \ell_i\rangle = \sum_{j \in [k]} \sum_{i \in C_j^0} \frac{1}{\sqrt{n}} |i, j\rangle = \sum_{j \in [k]} \sqrt{\frac{|C_j^0|}{n}} \left(\sum_{i \in C_j^0} \frac{1}{\sqrt{|C_j^0|}} |i\rangle \right) |j\rangle. \tag{3.6}$$

Since we know the "good state" has the form $|\psi_j\rangle|j\rangle$, we can use fixed point amplitude amplification guarantee Imported Theorem 3.3 to implement a unitary performing an approximate version of the map (3.5).

Corollary 3.8. Fix $\Delta \in (0, 1)$. Assume access to a unitary *U* that performs

$$|0,0\rangle \mapsto |i,\ell_i\rangle, \qquad \text{where } \ell_i = \mathop{\rm argmin}_{j \in [k]} \|\mathbf{v}_i - \mathbf{c}_j^0\|.$$

For all $j \in [k]$, Algorithm 5 uses at most $O(\sqrt{k_C} \log(1/\Delta))$ queries to U and U^{\dagger} to construct a unitary \tilde{U}_j which performs the map:

$$|0\rangle|0\rangle \mapsto \sqrt{1-\delta} \sum_{i \in C_i^0} \frac{1}{\sqrt{|C_i^0|}} |i\rangle|j\rangle + \sqrt{\delta}|G\rangle,$$

for some $\delta \leq \Delta$ and garbage state $|G\rangle$ orthogonal to the desired state.

In Algorithm 6 we describe how to implement B_j Here, we observe that using QRAM to $|i,\ell_i\rangle$ allows to load $|\mathbf{v}_i\rangle|\mathbf{c}_{\ell_i}^0\rangle$. Subsequently, we can use exact quantum arithmetic Assumption 3.2 to implement the target unitary.

Corollary 3.9. Assume access to a unitary U that performs

$$|0,0\rangle \mapsto |i,\ell_i\rangle, \quad \text{where } \ell_i = \operatorname*{argmin}_{j \in [k]} \|\mathbf{v}_i - \mathbf{c}_j^0\|.$$

For each $j \in [k]$, Algorithm 6 uses O(k) calls to the QRAM to prepare the unitary B_j .

3.6 Proof of the main theorem

We now provide the proof of Theorem 3.5 which essentially amounts to applying the quantum mean estimation guarantee Imported Theorem 3.4 while controlling the impact of using \tilde{U}_i in place of U_i .

Throughout, it will be useful to consider the per-cluster cost

$$\mathcal{L}_j(\mathbf{c}_1^0, \dots, \mathbf{c}_k^0) := \frac{1}{n} \sum_{i \in C_j^0} \|\mathbf{v}_i - \mathbf{c}_j^0\|^2.$$
(3.7)

Since C_1^0, \dots, C_k^0 forms a partition of [n], we have that $\mathcal{L}_1(\mathbf{c}_1^0, \dots, \mathbf{c}_k^0) + \dots + \mathcal{L}_k(\mathbf{c}_1^0, \dots, \mathbf{c}_k^0) = \mathcal{L}(\mathbf{c}_1^0, \dots, \mathbf{c}_k^0)$.

Proof of Theorem 3.5. Fix $j \in [k]$. We will use the sample space

$$\Omega = [n] \tag{3.8}$$

and consider the random variable

$$\mathbf{X}_{j}(i) = \begin{cases} \mathbf{v}_{i} - \mathbf{c}_{j}^{0} & \ell_{i} = j \\ \mathbf{0} & \text{otherwise} \end{cases}, \tag{3.9}$$

which is encoded by the unitary B_j of Algorithm 3 Line 3. Recall here that $\ell_i = \operatorname{argmin}_{j' \in [k]} \{ \| \mathbf{v}_i - \mathbf{c}_{j'} \| \}$. As noted in Corollary 3.9, Algorithm 6 used to construct B_j , requires O(k) QRAM queries.

Before proceeding, it is informative to consider what would happen if we had a unitary U_j performing (3.5). Let $\Pi_i = |i\rangle\langle i| \otimes I$ be the orthogonal projector onto the subspace corresponding to $|i\rangle$ in the first register. Applying U_i and performing the measurement $\{\Pi_i\}$ gives the probability distribution

$$p_{j}(i) = \|\Pi_{i}(U_{j} \otimes I)|0,0\rangle\|^{2} = \begin{cases} |C_{j}^{0}|^{-1} & \ell_{i} = j\\ 0 & \text{otherwise} \end{cases}, \quad i \in [n]$$
(3.10)

on the sample space (3.8). Mean estimation with U_i and B_i therefore produces an approximation of

$$\mu_{j} = \mathbb{E}[\mathbf{X}_{j}] = \sum_{i} p_{j}(i)\mathbf{X}_{j}(i) = \sum_{i \in C_{j}^{0}} \frac{1}{|C_{j}^{0}|} (\mathbf{v}_{i} - \mathbf{c}_{j}^{0}) = \mathbf{c}_{j} - \mathbf{c}_{j}^{0},$$
(3.11)

from which we could obtain an approximation to \mathbf{c}_i . The corresponding variance term is

$$\operatorname{tr}(\mathbf{\Sigma}_{j}) = \mathbb{E}[\|\mathbf{X}_{j} - \boldsymbol{\mu}_{j}\|^{2}] = \sum_{i \in [n]} p_{j}(i) \|\mathbf{X}_{j}(i) - (\mathbf{c}_{j} - \mathbf{c}_{j}^{0})\|^{2}$$
(3.12)

$$= \sum_{i \in C_i^0} \frac{1}{|C_j^0|} \|\mathbf{v}_i - \mathbf{c}_j\|^2$$
 (3.13)

$$=\frac{n}{|C_j^0|}\phi_j,\tag{3.14}$$

where the last equality is by our definition of the per-cluster cost (2.1).

Of course, we do not have access to U_j . Instead, we have access to \widetilde{U}_j , which corresponds to a perturbed version of the distribution described in (3.10), which we will write as $\widetilde{p}_j(i)$. As guaranteed by Corollary 3.8, Algorithm 5 constructs \widetilde{U}_j using $O(\sqrt{k_C}\log(1/\Delta))$ queries to the unitary U and U^\dagger that performs $|0,0\rangle \mapsto \sum_{i\in[n]}\frac{1}{\sqrt{n}}|i,\ell_i\rangle$, where $\ell_i= \operatorname{argmin}_{j\in[k]}\|\mathbf{v}_i-\mathbf{c}_j^0\|$. Since we need O(k) QRAM queries to construct U (and also U^\dagger), as shown in Theorem 3.7, we need a total of

$$O\left(k\sqrt{k_C}\log\left(\frac{1}{\Delta}\right)\right)$$
 QRAM queries (3.15)

to construct \widetilde{U}_j . Here, Δ is an accuracy parameter, to be determined, which controls the nearness of $\widetilde{p}_j(i)$ to $p_j(i)$.

From Corollary 3.8, we know that $\widetilde{U}_i|0,0\rangle = \sqrt{1-\delta}(U_i\otimes I)|0,0\rangle + \sqrt{\delta}|G\rangle$ for some $\delta \leq \Delta$, and therefore,

$$\widetilde{p}_{j}(i) = \|\Pi_{i}\widetilde{U}_{j}|0,0\rangle\|^{2} = \|\sqrt{1-\delta}\Pi_{i}(U_{j}\otimes I)|0,0\rangle + \sqrt{\delta}\Pi_{i}|G\rangle\|^{2}, \qquad i \in [n].$$
(3.16)

Thus, since $\|\Pi_i(U_i \otimes I)|0,0\rangle\| \le 1$ and $\|\Pi_i|G\rangle\| \le 1$, we have

$$\forall i \in [n]: \quad |p_j(i) - \widetilde{p}_j(i)| = \left| \left(\sqrt{p_j(i)} + \sqrt{\widetilde{p}_j(i)} \right) \left(\sqrt{p_j(i)} - \sqrt{\widetilde{p}_j(i)} \right) \right| \tag{3.17}$$

$$\leq \left(\sqrt{p_{j}(i)} + \sqrt{\widetilde{p}_{j}(i)}\right) \left\| (\sqrt{1-\delta} - 1)\Pi_{i}(U_{j} \otimes I)|0,0\rangle + \sqrt{\delta}\Pi_{i}|G\rangle \right\| \tag{3.18}$$

$$\leq 4\sqrt{\delta} \tag{3.19}$$

$$\leq 4\sqrt{\Delta}$$
, (3.20)

where we used reverse triangle inequality in the second inequality.

Now, define $\widetilde{\mu}_j = \widetilde{\mathbb{E}}[\mathbf{X}_j] = \sum_{i \in [n]} \widetilde{p}_j(i) \mathbf{X}_j(i)$ to be the expected value of \mathbf{X}_j with respect to the probabilities induced by \widetilde{U}_j . Let $\widehat{\mu}_j$ denote the output of mean estimation in Line 4 of Algorithm 3. By the triangle inequality and definition of $\widehat{\mathbf{c}}_j$ in Algorithm 3,

$$\|\mathbf{c}_{j} - \widehat{\mathbf{c}}_{j}\| = \|(\mathbf{c}_{j} - \mathbf{c}_{j}^{0}) - \widehat{\boldsymbol{\mu}}_{j}\| \le \|\widetilde{\boldsymbol{\mu}}_{j} - (\mathbf{c}_{j} - \mathbf{c}_{j}^{0})\| + \|\widetilde{\boldsymbol{\mu}}_{j} - \widehat{\boldsymbol{\mu}}_{j}\|.$$
(3.21)

We will now bound each of these terms by $2\varepsilon_j \cdot \sqrt{k_C \phi_j}$ for ε_j to be determined. Subsequently, we choose ε_j such that the sum of errors is bounded above by ε .

With the benefit of foresight, we set

$$\varepsilon_{j} = \frac{\varepsilon}{3\sqrt{k_{C}\phi_{j}}}, \qquad \Delta_{j} = \frac{\min\{1, \varepsilon_{j}^{2}\}}{16n^{2}k_{C}^{2}} \frac{(\phi_{j})^{2}}{\mathcal{L}_{j}(\mathbf{c}_{1}^{0}, \dots, \mathbf{c}_{k}^{0})^{2}}, \tag{3.22}$$

and

$$\Delta = \min_{j \in [k]} \Delta_j. \tag{3.23}$$

Bound for $\|\widetilde{\boldsymbol{\mu}}_j - (\mathbf{c}_j - \mathbf{c}_j^0)\|$: From (3.11) we know $\mathbb{E}[\mathbf{X}_j] = \mathbf{c}_j - \mathbf{c}_j^0$. Since the distributions p_j and \widetilde{p}_j are close, we expect $\widetilde{\mathbb{E}}[\mathbf{X}_j]$ to be close to $\mathbb{E}[\mathbf{X}_j]$.

Note that $\mathbf{X}_{j}(i) = \mathbf{v}_{i} - \mathbf{c}_{i}^{0}$ if $i \in C_{j}^{0}$ and $\mathbf{0}$ otherwise. Therefore, we have

$$\widetilde{\boldsymbol{\mu}}_{j} = \sum_{i \in [n]} (p_{j}(i) + \widetilde{p}_{j}(i) - p_{j}(i)) \mathbf{X}_{j}(i) = (\mathbf{c}_{j} - \mathbf{c}_{j}^{0}) + \sum_{i \in C_{j}^{0}} (\widetilde{p}_{j}(i, j) - p_{j}(i, j)) (\mathbf{v}_{i} - \mathbf{c}_{j}^{0}).$$
(3.24)

Let **A** be the $d \times |C_j^0|$ size matrix with columns given by $\mathbf{v}_i - \mathbf{c}_j^0$ for $i \in C_j^0$, and **b** to be the $|C_j^0|$ -dimension vector with entries given by $\widetilde{p}_j(i) - p_j(i)$ for $i \in C_j^0$. Then, we can write

$$\sum_{i \in |C_j^0|} (\widetilde{p}_j(i) - p_j(i))(\mathbf{v}_i - \mathbf{c}_j^0) = \mathbf{Ab}.$$
(3.25)

Then, using submultiplicativity, $\|\mathbf{A}\mathbf{b}\| \leq \|\mathbf{A}\|_{\mathsf{F}} \|\mathbf{b}\|$, we obtain

$$\|\widetilde{\boldsymbol{\mu}}_j - (\mathbf{c}_j - \mathbf{c}_j^0)\|^2 = \left\| \sum_{i \in C_i^0} (\widetilde{p}_j(i, j) - p_j(i, j))(\mathbf{v}_i - \mathbf{c}_j^0) \right\|^2$$
(3.26)

$$\leq \left(\sum_{i \in C_{i}^{0}} |\widetilde{p}_{j}(i,j) - p_{j}(i,j)|^{2}\right) \left(\sum_{i \in C_{i}^{0}} \|\mathbf{v}_{i} - \mathbf{c}_{j}^{0}\|^{2}\right)$$
(3.27)

$$\leq 16n^2 \Delta \mathcal{L}_j(\mathbf{c}_1^0, \dots, \mathbf{c}_k^0) \tag{3.28}$$

$$\leq \varepsilon_j^2 k_C \phi_j, \tag{3.29}$$

where in the second-last step we used (3.20) and the definition of per-cluster cost given in (3.7). The last step follows from the choice of Δ in (3.23), $k_C \ge 1$, and the fact that $\phi_j / \mathcal{L}_j(\mathbf{c}_1^0, \dots, \mathbf{c}_k^0) \le 1$.

Bound for $\|\widetilde{\boldsymbol{\mu}}_j - \widehat{\boldsymbol{\mu}}_j\|$: Recall that $\widehat{\boldsymbol{\mu}}_j$ is the output of mean estimator for \mathbf{X}_j with respect to the $\widetilde{p}_j(i)$ probabilities. Let $\widetilde{\boldsymbol{\Sigma}}_j$ be the covariance of the random variable \mathbf{X}_j with respect to these probabilities.

The condition on ε guarantees $\varepsilon_i < \log(d/\delta)/\sqrt{d}$, and hence, by Imported Theorem 3.4,

$$\|\widetilde{\boldsymbol{\mu}}_{j} - \widehat{\boldsymbol{\mu}}_{j}\| \le \varepsilon_{j} \sqrt{\operatorname{tr}(\widetilde{\boldsymbol{\Sigma}}_{j})},\tag{3.30}$$

with probability at least 1-1/(10k), using $\tilde{O}(\sqrt{d}/\varepsilon_i)$ queries to \tilde{U}_i and B_i , and therefore

$$\tilde{O}\left(\frac{k\sqrt{dk_C}}{\varepsilon_i}\log\left(\frac{1}{\Delta}\right)\right) = \tilde{O}\left(\frac{kk_C\sqrt{d\phi_j}}{\varepsilon}\log\left(\frac{1}{\Delta}\right)\right) \text{ QRAM queries.} \tag{3.31}$$

We now bound $\operatorname{tr}(\widetilde{\boldsymbol{\Sigma}}_j)$. Using that $\operatorname{tr}(\widetilde{\boldsymbol{\Sigma}}_j) = \widetilde{\mathbb{E}}[\|\mathbf{X}_j - \widetilde{\boldsymbol{\mu}}_j\|^2] \leq \widetilde{\mathbb{E}}[\|\mathbf{X}_j - \mathbf{c}\|^2]$ for all vectors \mathbf{c} , we obtain

$$\operatorname{tr}(\widetilde{\boldsymbol{\Sigma}}_{j}) = \widetilde{\mathbb{E}}\big[\|\mathbf{X}_{j} - \widetilde{\boldsymbol{\mu}}_{j}\|^{2}\big] \leq \widetilde{\mathbb{E}}\big[\|\mathbf{X}_{j} - \boldsymbol{\mu}_{j}\|^{2}\big] = \sum_{i \in C_{j}^{0}} \widetilde{p}_{j}(i)\|\mathbf{X}_{j}(i) - \boldsymbol{\mu}_{j}\|^{2} + \sum_{i \in [n] \setminus C_{j}^{0}} \widetilde{p}_{j}(i)\|\mathbf{X}_{j}(i) - \boldsymbol{\mu}_{j}\|^{2}. \tag{3.32}$$

The first term in (3.32) is bounded as

$$\sum_{i \in C_j^0} \widetilde{p}_j(i) \|\mathbf{X}_j(i) - \boldsymbol{\mu}_j\|^2 = \sum_{i \in C_j^0} \widetilde{p}_j(i) \|(\mathbf{v}_i - \mathbf{c}_j^0) - (\mathbf{c}_j - \mathbf{c}_j^0)\|^2$$
(3.33)

$$\leq \sum_{i \in C_i^0} \left(\frac{1}{|C_j^0|} + 4\sqrt{\Delta} \right) \|\mathbf{v}_i - \mathbf{c}_j\|^2 \tag{3.34}$$

$$= \left(\frac{n}{|C_j^0|} + 4n\sqrt{\Delta}\right)\phi_j,\tag{3.35}$$

where the inequality follows from the bound (3.20).

The second term in (3.32) is bounded by

$$\sum_{i \in [n] \setminus C_j^0} \widetilde{p}_j(i) \|\mathbf{X}_j(i) - \boldsymbol{\mu}_j\|^2 = \sum_{i \in [n] \setminus C_j^0} \widetilde{p}_j(i) \|\mathbf{0} - (\mathbf{c}_j - \mathbf{c}_j^0)\|^2$$
(3.36)

$$\leq \sum_{i \in [n] \setminus C_j^0} 4\sqrt{\Delta} \|\mathbf{c}_j - \mathbf{c}_j^0\|^2 \tag{3.37}$$

$$\leq 4n\sqrt{\Delta}\|\mathbf{c}_{i} - \mathbf{c}_{i}^{0}\|^{2},\tag{3.38}$$

where the inequality also follows from the bound (3.20). Finally, observe that by a "bias-variance" type identity,

$$n\mathcal{L}_{j}(\mathbf{c}_{1}^{0},...,\mathbf{c}_{k}^{0}) = \sum_{i \in C_{j}^{0}} \|\mathbf{v}_{i} - \mathbf{c}_{j}^{0}\|^{2} = \sum_{i \in C_{j}^{0}} \|\mathbf{v}_{i} - \mathbf{c}_{j}\|^{2} + |C_{j}^{0}| \|\mathbf{c}_{j} - \mathbf{c}_{j}^{0}\|^{2} \ge |C_{j}^{0}| \|\mathbf{c}_{j} - \mathbf{c}_{j}^{0}\|^{2}.$$
(3.39)

Plugging (3.39) into (3.38), and then plugging (3.35) and (3.38) into (3.32), we get the bound

$$\operatorname{tr}(\widetilde{\mathbf{\Sigma}}_{j}) \leq \left(\frac{n}{|C_{j}^{0}|} + 4n\sqrt{\Delta}\right)\phi_{j} + \frac{n}{|C_{j}^{0}|} 4n\sqrt{\Delta}\mathcal{L}_{j}(\mathbf{c}_{1}^{0}, ..., \mathbf{c}_{k}^{0})$$

$$\leq k_{C}\phi_{j} + 8nk_{C}\sqrt{\Delta}\mathcal{L}_{j}(\mathbf{c}_{1}^{0}, ..., \mathbf{c}_{k}^{0})$$

$$\leq 4k_{C}\phi_{j},$$
(3.40)

where we used the fact that $1 \le n/|C_j^0| \le k_C$ and $\phi_j \le \mathcal{L}_j(\mathbf{c}_1^0, \dots, \mathbf{c}_k^0)$ in the second step, and the choice of Δ in (3.23) in the last step. Therefore, (3.30) becomes

$$\|\widetilde{\boldsymbol{\mu}}_{j} - \widehat{\boldsymbol{\mu}}_{j}\| \le 2\sqrt{k_{C}\phi_{j}}\varepsilon_{j}. \tag{3.41}$$

Using this with (3.29) and (3.21), we obtain

$$\|\mathbf{c}_{j} - \widehat{\mathbf{c}}_{j}\| \le 3\sqrt{k_{C}\phi_{j}}\varepsilon_{j} \le \varepsilon \tag{3.42}$$

with probability at least 1 - 1/(10k), where the last inequality follows from the definition of ε_j in (3.22).

Putting it together: Finally, using the union bound, we obtain $\|\mathbf{c}_j - \hat{\mathbf{c}}_j\| \le \varepsilon$ simultaneously for all $j \in [k]$ with probability at least 9/10. We sum (3.31) over $j \in [k]$ to get a total cost of

$$\tilde{O}\!\left(\frac{k^{3/2}k_{C}\sqrt{d}}{\varepsilon}\sqrt{\phi}\log\!\left(\frac{1}{\Delta}\right)\!\right) \text{QRAM queries,} \tag{3.43}$$

where we use the fact that $\sum_{i=1}^k \sqrt{\phi_i} \le \sqrt{k \sum_{i=1}^k \phi_i} = \sqrt{k \phi}$ by concavity of square-root.

3.7 Additional supporting algorithms

We now explicitly describe Algorithms 4 to 6 which are used to construct unitaries U_j (approximately) and B_j respectively.

Algorithm 4 (Quantum cluster assignment).

Input: Data $\mathbf{v}_1, ..., \mathbf{v}_n \in \mathbb{R}^d$, initial centers $\mathbf{c}_1^0, ..., \mathbf{c}_k^0 \in \mathbb{R}^d$ (both with quantum query access)

1: Use k + 1 calls to the QRAM to load the data:

$$|i\rangle|\mathbf{0},\ldots,\mathbf{0}\rangle\mapsto|i\rangle|\mathbf{v}_i\rangle|\mathbf{c}_1^0,\ldots,\mathbf{c}_k^0\rangle.$$

2: Use quantum arithmetic to perform:

$$|i\rangle|\mathbf{v}_i\rangle|\mathbf{c}_1^0,\ldots,\mathbf{c}_k^0\rangle|0,\ldots,0\rangle\mapsto|i\rangle|\|\mathbf{c}_1^0-\mathbf{v}_i\|^2,\ldots,\|\mathbf{c}_k^0-\mathbf{v}_i\|^2\rangle.$$

3: Use classical minimization circuit to perform:

$$|i\rangle|\|\mathbf{c}_1^0 - \mathbf{v}_i\|^2, \dots, \|\mathbf{c}_k^0 - \mathbf{v}_i\|^2\rangle|0\rangle \mapsto |i\rangle|\ell_i\rangle,$$

where $\ell_i = \operatorname{argmin}_{j' \in [k]} \{ \| \mathbf{v}_i - \mathbf{c}_{j'}^0 \| \}.$

Output: Unitary to perform:

$$\forall i \in [n]: |i\rangle|0\rangle \mapsto |i\rangle|\ell_i\rangle.$$

Proof of Theorem 3.7. In Line 1, we use k+1 calls to the QRAM. The rest of the operations are implemented by quantum analogs of classical circuits, and we uncompute the ancilla registers afterwards. Note that the arithmetic operations and minimum finding are agnostic to the value of i because they act on whatever data is loaded by the QRAM. Since each line of Algorithm 4 is a unitary operation and the product of unitary maps is unitary, the resulting map that takes $|i\rangle|0\rangle$ to $|i\rangle|\ell_i\rangle$ for all $i \in [n]$ is unitary.

Next, we show how to construct \widetilde{U}_j , which gives an approximate uniform superposition over the data points within C_j^0 . To do this, we make use of fixed point amplitude amplification Imported Theorem 3.3.

Algorithm 5 (Approximate sampling unitary preparation).

Input: Index $j \in [k]$, parameter $\Delta \in (0, 1)$

1: Create the uniform superposition:

$$|0\rangle \mapsto \sum_{i\in[n]} \frac{1}{\sqrt{n}} |i\rangle.$$

2: Use Algorithm 4 to construct a unitary U that performs:

$$\sum_{i \in [n]} \frac{1}{\sqrt{n}} |i\rangle |0\rangle \mapsto \sum_{i \in [n]} \frac{1}{\sqrt{n}} |i\rangle |\ell_i\rangle,$$

where $\ell_i = \operatorname{argmin}_{j' \in [k]} \{ \| \mathbf{v}_i - \mathbf{c}_{j'}^0 \| \}$.

3: Perform amplitude amplification (see Imported Theorem 3.3) with $O(\sqrt{n/|C_j^0|}\log(1/\Delta))$ queries to U and U^{\dagger} to obtain unitary V_i which performs the map

$$\sum_{i \in [n]} \frac{1}{\sqrt{n}} |i\rangle |\ell_i\rangle \mapsto \sqrt{1-\delta} \sum_{i \in C_j^0} \frac{1}{\sqrt{|C_j^0|}} |i\rangle |j\rangle + \sqrt{\delta} |G\rangle$$

for some $\delta \leq \Delta$ and garbage state $|G\rangle$ orthogonal to the desired state.

Output: Unitary \tilde{U}_i to (approximately) perform:

$$|0\rangle|0\rangle \mapsto \sum_{i\in C_j^0} \frac{1}{\sqrt{|C_j^0|}} |i\rangle|j\rangle.$$

Proof of Corollary 3.8. The uniform superposition over $i \in [n]$ can be created using a unitary map [SV24]. Next, note that the state created after the application of the unitary U constructed by Algorithm 4 on this uniform superposition can be expressed as

$$\sum_{i \in [n]} \frac{1}{\sqrt{n}} |i\rangle |\ell_i\rangle = \sum_{j \in [k]} \sqrt{\frac{|C_j^0|}{n}} \sum_{i \in C_j^0} \frac{1}{\sqrt{|C_j^0|}} |i\rangle |j\rangle. \tag{3.44}$$

Then, amplitude amplification (see Imported Theorem 3.3) of the state $|j\rangle$ (in the second register) with $O(\sqrt{n/|C_j^0|}\log(1/\Delta)) \le O(\sqrt{k_C}\log(1/\Delta))$ queries to U, U^\dagger gives a unitary V_j that acts on $\sum_{i\in[n]}(1/\sqrt{n})|i\rangle|\ell_i\rangle$ to produce

$$\sqrt{1-\delta} \sum_{i \in C_i^0} \frac{1}{\sqrt{|C_i^0|}} |i\rangle |j\rangle + \sqrt{\delta} |G\rangle, \tag{3.45}$$

where $|G\rangle$ is some state orthogonal to $\sum_{i \in C_j^0} |i\rangle |j\rangle$. We need a total of $O(\sqrt{k_C} \log(1/\Delta))$ calls to U to construct the map \widetilde{U}_j . Note that we uncompute the ancilla registers. Since the composition of unitary maps is unitary, the map \widetilde{U}_j is unitary.

Finally we show how to construct B_j .

Algorithm 6 (Random variable access unitary preparation).

Input: Data $\mathbf{v}_1, ..., \mathbf{v}_n \in \mathbb{R}^d$ and initial centers $\mathbf{c}_1^0, ..., \mathbf{c}_k^0 \in \mathbb{R}^d$ (with quantum query access), index $j \in [k]$

1: Use Algorithm 4 on to perform the map:

$$|i\rangle|0\rangle \mapsto |i\rangle|\ell_i\rangle$$
,

where $\ell_i = \operatorname{argmin}_{j' \in [k]} \{ \| \mathbf{v}_i - \mathbf{c}_{j'}^0 \| \}.$

2: Use 2 calls to the QRAM to load the data:

$$|i\rangle|\ell_i\rangle|\mathbf{0}\rangle|\mathbf{0}\rangle\mapsto|i\rangle|\ell_i\rangle|\mathbf{v}_i\rangle|\mathbf{c}_{\ell_i}^0\rangle.$$

3: Use quantum arithmetic to perform:

$$|i\rangle|\ell_i\rangle|\mathbf{v}_i\rangle|\mathbf{c}_{\ell_i}^0\rangle|\mathbf{0}\rangle \mapsto |i\rangle|\ell_i\rangle|\mathbf{v}_i\rangle|\mathbf{c}_{\ell_i}^0\rangle|(\mathbf{v}_i - \mathbf{c}_{\ell_i}^0)\mathbb{1}[\ell_i = j]\rangle.$$

Output: Unitary B_i to perform:

$$\forall i \in [n]: \quad |i\rangle |\mathbf{0}\rangle \mapsto |i\rangle |(\mathbf{v}_i - \mathbf{c}_{\ell_i}^0)\mathbb{1}[\ell_i = j]\rangle.$$

Proof of Corollary 3.9. By Theorem 3.7, Algorithm 6 uses O(k) queries to the QRAM to construct a unitary that maps $|i\rangle|0\rangle$ to $|i\rangle|\ell_i\rangle$. It follows that the we make a total of O(k) QRAM queries in Algorithm 6. Since all the lines in Algorithm 6 are unitary operations, and the composition of unitary maps is unitary, the map B_i is unitary. Note that we uncompute the ancilla registers at the end of the computation.

4 Outlook

We have described and analyzed classical (randomized) and quantum algorithms for the k-means problem. Our analysis shows that these algorithms produce cluster centers near to those produced by the classical k-means algorithm (over one iteration) with query complexity bounds depending on the parameter ϕ (1.9). This a notable improvement over past work [KLLP19, DLT25] which incur dependency on $\eta = \max_i \|\mathbf{v}_i\|^2$ and $\bar{\eta} = n^{-1} \sum_i \|\mathbf{v}_i\|^2$ respectively; indeed $\phi \leq \bar{\eta} \leq \eta$ always holds.

This improvement is due to a more fine-grained analysis of the algorithms described in this paper and a key observation that the algorithms proposed by [KLLP19, DLT25] are sensitive to rigid-body transforms of the data, and can therefore fail to produce good centers even on intuitively easy to cluster datasets. The algorithms we study, whose core is *uniform sampling*, are invariant to such transforms leading to the improved bounds.

There are a number of directions for future work. For instance, it would be interesting to understand the behavior of the algorithms studied in this paper over multiple iterations. The primary difficulty limiting this extension is that the k-means algorithm is not smooth; a tiny change to the initialization can produce very different centers, even after one step. However, for certain types of problems, it may be possible to derive guarantees on the centers or the cost. It would also be interesting to derive quantum algorithms for other clustering objectives, including on spaces other than \mathbb{R}^d (e.g., on the space of probability distributions).

Acknowledgements

We thank our colleagues at the Global Technology Applied Research center of JPMorganChase for support and helpful feedback. Special thanks to Brandon Augustino, Shouvanik Chakrabarti, Jacob Watkins, and Jamie Heredge for their valuable discussions regarding the manuscript.

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A Useful facts

A.1 k-means cost function

We use the following bounds for the cost function throughout.

Lemma A.1 (Local optimality). The k-means steps are locally optimal in the sense that the following hold:

(i) Given centers $(\mathbf{c}_1, \dots, \mathbf{c}_k)$, define $C_j = \{i \in [n] : j = \operatorname{argmin}_{j' \in [k]} \|\mathbf{v}_i - \mathbf{c}_{j'}\|\}$. Then

$$\sum_{j \in [k]} \sum_{i \in C_j} \|\mathbf{v}_i - \mathbf{c}_j\|^2 \leq \sum_{j \in [k]} \sum_{i \in C_i'} \|\mathbf{v}_i - \mathbf{c}_j\|^2, \text{ where } (C_1', \dots, C_k') \text{ is a partition of } [n].$$

(ii) Given a partition $C_1, ..., C_k$ of [n], define $\mathbf{c}_j = |C_j|^{-1} \sum_{i \in C_i} \mathbf{v}_i$. Then

$$\sum_{j \in [k]} \sum_{i \in C_j} \|\mathbf{v}_i - \mathbf{c}_j\|^2 \leq \sum_{j \in [k]} \sum_{i \in C_j} \|\mathbf{v}_i - \mathbf{c}_j'\|^2, \text{ where } \mathbf{c}_1', \dots, \mathbf{c}_k' \in \mathbb{R}^d.$$

Proof. Item (i) follows from the fact that if $i \in C_j$, then $\|\mathbf{v}_i - \mathbf{c}_j\| \le \|\mathbf{v}_i - \mathbf{c}_{j'}\|$, for any j', and Item (ii) follows from the fact that a function of the form $\sum_{i \in C} \|\mathbf{v}_i - \mathbf{c}\|^2$ is is minimized at $|C|^{-1} \sum_i \mathbf{v}_i$.

As mentioned in the introduction, the parameter ϕ (see (1.13)) appearing in our analysis is bounded above by the quantities $\bar{\eta}$ and η appearing in past work. The following result exactly quantifies how much smaller ϕ is than $\bar{\eta}$.

Lemma A.2. For any $(\mathbf{c}_1^0, ..., \mathbf{c}_k^0)$,

$$\phi = \bar{\eta} - \frac{1}{n} \sum_{j \in [k]} |C_j^0| \|\mathbf{c}_j\|^2.$$

where $\bar{\eta} = n^{-1} \sum_{i} \|\mathbf{v}_{i}\|^{2} = n^{-1} \|\mathbf{V}\|_{\mathsf{F}}^{2}$

Proof. Observe that

$$\phi = \frac{1}{n} \sum_{j \in [k]} \sum_{i \in C_i^0} \|\mathbf{v}_i - \mathbf{c}_j\|^2$$
(A.1)

$$= \frac{1}{n} \sum_{j \in [k]} \left(\sum_{i \in C_i^0} \|\mathbf{v}_i\|^2 + \|\mathbf{c}_j\|^2 - 2\mathbf{v}_i^\mathsf{T} \mathbf{c}_j \right)$$
(A.2)

$$= \frac{1}{n} \sum_{i \in [n]} \|\mathbf{v}_i\|^2 - \frac{1}{n} \sum_{j \in [k]} |C_j^0| \|\mathbf{c}_j\|^2.$$
(A.3)

where we have used that $\sum_{i \in C_j^0} \mathbf{v}_i = |C_j^0| \mathbf{c}_j$.

A.2 Approximate matrix multiplication

Lemma A.3 (Approximate matrix multiplication). Consider a matrix $\mathbf{A} \in \mathbb{R}^{n \times d}$ and vector $\mathbf{b} \in \mathbb{R}^d$. Independently sample random indices s_1, \ldots, s_b such that $\Pr(s_i = i) = p_i$ and define the estimator

$$\widehat{\mathbf{y}} = \frac{1}{b} \sum_{i \in [b]} \frac{1}{p_{s_i}} \mathbf{A}_{:,s_i} \mathbf{b}_{s_i}.$$

Then $\mathbb{E}[\widehat{\mathbf{y}}] = \mathbf{Ab}$ and

$$\mathbb{E}[\|\widehat{\mathbf{y}}\|^2] = \frac{1}{b} \sum_{i \in [n]} \frac{1}{p_i} \|\mathbf{A}_{:,i}\|^2 |\mathbf{b}_i|^2.$$

Proof. The mean computation is straightforward; since s_1, \ldots, s_b are identically distributed,

$$\mathbb{E}[\widehat{\mathbf{y}}] = \mathbb{E}\left[\frac{1}{p_{s_1}}\mathbf{A}_{:,s_1}\mathbf{b}_{s_1}\right] = \sum_{i \in [n]} p_i \frac{1}{p_i}\mathbf{A}_{:,i}\mathbf{b}_i = \sum_{i \in [n]} \mathbf{A}_{:,i}\mathbf{b}_i = \mathbf{Ab}.$$
(A.4)

We now compute the variance. Using that $s_1, ..., s_b$ are independent and identically distributed, and that $\mathbb{E}[p_{s_i}^{-1}\mathbf{A}_{:,s_i}\mathbf{b}_{s_i}] = \mathbf{A}\mathbf{b}$ so that cross-terms vanish,

$$\mathbb{E}[\|\widehat{\mathbf{y}}\|^2] = \mathbb{E}\left[\left\|\frac{1}{b}\sum_{i\in[b]}\left(\frac{1}{p_{s_i}}\mathbf{A}_{:,s_i}\mathbf{b}_{s_i}\right)\right\|^2\right]$$
(A.5)

$$= \frac{1}{b} \mathbb{E} \left[\left\| \frac{1}{p_{s_i}} \mathbf{A}_{:,s_i} \mathbf{b}_{s_i} \right\|^2 \right] \tag{A.6}$$

$$= \frac{1}{b} \mathbb{E} \left[\frac{1}{p_{S_i}^2} \| \mathbf{A}_{:,s_i} \|^2 |\mathbf{b}_{s_i}|^2 \right]$$
 (A.7)

$$= \frac{1}{b} \sum_{i \in [n]} \frac{1}{p_i} \|\mathbf{A}_{:,i}\|^2 |\mathbf{b}_i|^2.$$
(A.8)

This is the desired result.

A.3 Concentration inequalities

We also state two standard concentration bounds which we have used.

Imported Theorem A.4 (Markov inequality). Let X be a non-negative random variable. Then, for any $\alpha > 0$,

$$\Pr(X > \alpha) \le \frac{\mathbb{E}[X]}{\alpha}.$$

Imported Theorem A.5 (Chernoff bound). Let $X_1, ..., X_b$ be independent copies of a Bernoulli random variable with success probability p and let $X = X_1 + \cdots + X_n$. Then, for any $\delta \in (0,1)$

$$\Pr(X \le (1 - \delta)bp) \le \exp\left(-\frac{\delta^2 bp}{2}\right).$$

A.4 Median trick in high dimension

We now describe how to efficiently turn an estimator which produces a ε -approximation to some highdimensional quantity with constant probability into one which produces an $O(\varepsilon)$ -approximation with arbitrary probability.

Algorithm 7 (High dimensional median trick).

Input: Random vector $\mathbf{X} \in \mathbb{R}^d$, parameter $t \in \mathbb{N}$

- 1: Make independent copies $X_1, ..., X_t$ of X
- 2: For all $i, j \in [t]$, define $d(i, j) = ||\mathbf{X}_i \mathbf{X}_i||$
- 3: For all $i \in [t]$, define c(i) = median(d(i, 1), ..., d(i, t))
- 4: $i^* = \operatorname{argmin}_{i \in [t]} c(i)$
- 5: $\mathbf{X}^* = \mathbf{X}_{i^*}$

Output: X*

Theorem A.6. Let $\mathbf{X} \in \mathbb{R}^d$ be a random vector, and suppose there is some vector $\boldsymbol{\mu}$ such that $\Pr(\|\boldsymbol{\mu} - \mathbf{X}\| > \varepsilon) < 1/3$. Then, for $t = O(\log(1/\delta))$ the output \mathbf{X}^* of Algorithm 7 satisfies

$$\Pr(\|\boldsymbol{\mu} - \mathbf{X}^*\| > 3\varepsilon) < \delta.$$

Proof. Let $G = \{i : \|\boldsymbol{\mu} - \mathbf{X}_i\| \le \varepsilon\}$. Denoting $\mathbbm{1}[A]$ to be the indicator function of the event A (i.e., $\mathbbm{1}[A](\omega) = 1$ if $\omega \in A$ and 0 otherwise), we can write $|G| = \sum_{i=1}^t \mathbbm{1}[\|\boldsymbol{\mu} - \mathbf{X}_i\| \le \varepsilon]$. Since $\mathbb{E}[|G|] > 2t/3$, it follows from Imported Theorem A.5 that $\Pr(|G| \le t/2) \le \delta$ for $t = O(\log(1/\delta))$. Therefore, it suffices to show that if |G| > t/2, then $\|\boldsymbol{\mu} - \mathbf{X}^*\| < 3\varepsilon$.

Suppose |G| > t/2. By the triangle inequality, for each $i, j \in [t]$,

$$d(i, j) = \|\mathbf{X}_i - \mathbf{X}_i\| \le \|\boldsymbol{\mu} - \mathbf{X}_i\| + \|\boldsymbol{\mu} - \mathbf{X}_i\|. \tag{A.9}$$

Therefore, for each $i \in G$

$$\left| \{ j \in [t] : d(i,j) \le 2\varepsilon \} \right| > t/2, \tag{A.10}$$

and hence,

$$c(i) = \text{median}(d(i, 1), \dots, d(i, t)) \le 2\varepsilon.$$

It follows that $c(i^*) = \min_i c(i) \le 2\varepsilon$, and since $c(i^*) = \operatorname{median}(d(i^*, 1), \dots, d(i^*, t))$, we have

$$|\{j \in [t] : d(i^*, j) \le 2\varepsilon\}| \ge t/2.$$
 (A.11)

But also |G| > t/2. So, by the pigeonhole principle, there is at lest one index $j^* \in G$ for which

$$d(i^*, j^*) \le 2\varepsilon. \tag{A.12}$$

Therefore, by the triangle inequality

$$\|\mu - X_{i^*}\| \le \|\mu - X_{j^*}\| + \|X_{i^*} - X_{j^*}\| \le \varepsilon + 2\varepsilon = 3\varepsilon,$$
 (A.13)

as desired. \Box

B Bounds for the *k*-means cost function

The following shows that Theorem 2.1 also implies the cost the final cluster centers output by Algorithm 2 is not much larger than the cost of the initial clusters.

Corollary B.1. Suppose

$$b \ge k_C \cdot \max \left\{ \frac{40}{\varepsilon}, 8\log(20k) \right\}.$$

Then, with probability at least 9/10, the output $(\hat{\mathbf{c}}_1, ..., \hat{\mathbf{c}}_k)$ of Algorithm 2 satisfies

$$\mathscr{L}(\widehat{\mathbf{c}}_1,\ldots,\widehat{\mathbf{c}}_k) \le (1+\varepsilon)\phi \le (1+\varepsilon)\mathscr{L}(\mathbf{c}_1^0,\ldots,\mathbf{c}_k^0).$$

The following (standard) lemma provides a quantitative bound on how the cost function behaves for centers near the k-means centers.

Lemma B.2. For any cluster centers $(\hat{\mathbf{c}}_1, \dots, \hat{\mathbf{c}}_k)$,

$$\mathcal{L}(\widehat{\mathbf{c}}_1, \dots, \widehat{\mathbf{c}}_k) \leq \phi + \frac{1}{n} \sum_{j \in [k]} |C_j^0| \|\mathbf{c}_j - \widehat{\mathbf{c}}_j\|^2.$$

Proof. Define $\widehat{C}_j = \{i \in [n] : j = \operatorname{argmin}_{j' \in [k]} \|\mathbf{v}_i - \widehat{\mathbf{c}}_{j'}\|\}$. Then

$$\mathcal{L}(\widehat{\mathbf{c}}_1, \dots, \widehat{\mathbf{c}}_k) = \frac{1}{n} \sum_{j \in [k]} \sum_{i \in \widehat{C}_j} \|\mathbf{v}_i - \widehat{\mathbf{c}}_j\|^2 \le \frac{1}{n} \sum_{j \in [k]} \sum_{i \in C_j^0} \|\mathbf{v}_i - \widehat{\mathbf{c}}_j\|^2, \tag{B.1}$$

where the last inequality follows from the optimality of the partition $(\widehat{C}_1,...,\widehat{C}_k)$ for centers $(\widehat{\mathbf{c}}_1,...,\widehat{\mathbf{c}}_k)$.

Next, observe that for any $\hat{\mathbf{c}}_i \in \mathbb{R}^d$,

$$\|\mathbf{v}_i - \widehat{\mathbf{c}}_i\|^2 = \|\mathbf{v}_i - \mathbf{c}_i + \mathbf{c}_j - \widehat{\mathbf{c}}_i\|^2 = \|\mathbf{v}_i - \mathbf{c}_i\|^2 + \|\mathbf{c}_j - \widehat{\mathbf{c}}_i\|^2 + 2(\mathbf{v}_i - \mathbf{c}_i)^{\mathsf{T}}(\mathbf{c}_i - \widehat{\mathbf{c}}_i). \tag{B.2}$$

Since, by definition $\mathbf{c}_j = |C_j^0|^{-1} \sum_{i \in C_i^0} \mathbf{v}_i$, by linearity

$$\sum_{i \in C_i^0} 2(\mathbf{v}_i - \mathbf{c}_j)^{\mathsf{T}} (\mathbf{c}_j - \widehat{\mathbf{c}}_j) = \mathbf{0}.$$
(B.3)

Therefore, since $(\mathbf{c}_1,\ldots,\mathbf{c}_k)$ are the optimal cluster center with respect to the partition (C_1^0,\ldots,C_k^0) ,

$$\frac{1}{n} \sum_{j \in [k]} \sum_{i \in C_j^0} \|\mathbf{v}_i - \widehat{\mathbf{c}}_j\|^2 = \sum_{j \in [k]} \sum_{i \in C_j^0} \left(\|\mathbf{v}_i - \mathbf{c}_j\|^2 + \|\mathbf{c}_j - \widehat{\mathbf{c}}_j\|^2 \right)$$
(B.4)

$$= \phi + \frac{1}{n} \sum_{i \in [k]} |C_j^0| \|\mathbf{c}_j - \widehat{\mathbf{c}}_j\|^2.$$
 (B.5)

Plugging (B.5) into (B.1) gives the result.

Proof of Corollary B.1. The first result follows by plugging Theorem 2.1 into Lemma B.2 and scaling ε appropriately. The second is due to the optimality of $(\mathbf{c}_1, ..., \mathbf{c}_k)$ for the clusters $(C_1^0, ..., C_k^0)$.

C Damping

Both the mini-batch and quantum algorithms described above perform an approximate k-means step. While the variance in these updates can be controlled by decreasing the accuracy parameter ε , an alternative approach to decreasing the variance is to damp the iterates by interpolating between the initial

cluster center and the approximate update. In particular, given damping coefficients $\alpha_1, ..., \alpha_k \in (0, 1]$, we might aim to emulate a damped k-means update

$$\mathbf{c}_{j}^{\alpha} = (1 - \alpha_{j})\mathbf{c}_{j}^{0} + \alpha_{j}\mathbf{c}_{j}. \tag{C.1}$$

In the case that $\alpha_i = 1$ then this recovers the standard k-means update.

C.1 Damped mini-batch algorithm and bound

The damped k-means update naturally gives rise to a generic damped minimatch k-means algorithm which we describe in Algorithm 8. This variant is closely related to the MiniBatchKMeans method implemented in scikit-learn [PVG+11].

Algorithm 8 (Generic damped mini-batch *k*-means (one iteration)).

Input: Initial centers $\mathbf{c}_1^0, \dots, \mathbf{c}_k^0 \in \mathbb{R}^d$, data $\mathbf{v}_1, \dots, \mathbf{v}_n \in \mathbb{R}^d$, damping coefficients $\alpha_1, \dots, \alpha_k \in [0, 1]$

1: Sample *b* indices $B = (s_1, ..., s_b) \in [n]^b$, each independently such that $\Pr(s_\ell = i) = 1/n$.

2: **for** $j \in [k]$ **do**

3:
$$\widehat{C}_j^0 = \{i \in B : j = \operatorname{argmin}_{j' \in [k]} \|\mathbf{v}_i - \mathbf{c}_{j'}^0\|\}$$

4:
$$\widehat{\mathbf{c}}_j = \frac{1}{|\widehat{C}_j^0|} \sum_{i \in \widehat{C}_j^0} \mathbf{v}_i$$

5:
$$\widehat{\mathbf{c}}_{j}^{\alpha} = (1 - \alpha_{j})\mathbf{c}_{j}^{0} + \alpha_{j}\widehat{\mathbf{c}}_{j}$$

Output: updated centers $\widehat{\mathbf{c}}_1^{\alpha}, \dots, \widehat{\mathbf{c}}_k^{\alpha} \in \mathbb{R}^d$

Our main result for Algorithm 8 is a generalization of Corollary B.1.

Corollary C.1. Let $\alpha_{\max} = \max_i \alpha_i$ and $\alpha_{\min} = \min_i \alpha_i$, and suppose

$$b \ge k_C \cdot \max\left\{\frac{40}{\varepsilon}, 8\log(20k)\right\}.$$

Then, with probability at least 9/10, the output $(\hat{\mathbf{c}}_1^{\alpha},...,\hat{\mathbf{c}}_k^{\alpha})$ of Algorithm 8 satisfies

$$\mathscr{L}(\widehat{\mathbf{c}}_{1}^{\alpha},...,\widehat{\mathbf{c}}_{k}^{\alpha}) \leq \left((1-\alpha_{\min})+(\alpha_{\max})\sqrt{1+\varepsilon}\right)^{2}\phi.$$

In particular, if $\alpha_j = \alpha$ are constant, then

$$\mathcal{L}(\widehat{\mathbf{c}}_{1}^{\alpha},...,\widehat{\mathbf{c}}_{k}^{\alpha}) \leq (1+\varepsilon)\phi \leq (1+\varepsilon)\mathcal{L}(\mathbf{c}_{1}^{0},...,\mathbf{c}_{k}^{0}), \tag{C.2}$$

which also generalizes Corollary B.1.

C.2 Proofs

We begin by proving a generalization of Lemma B.2.

Lemma C.2. Let $\alpha_{\max} = \max_j \alpha_j$ and $\alpha_{\min} = \min_j \alpha_j$. For data points $\mathbf{v}_1, \dots, \mathbf{v}_n \in \mathbb{R}^d$ and given centers $\mathbf{c}_1^0, \dots, \mathbf{c}_k^0 \in \mathbb{R}^d$, define $C_j^0 = \{i \in [n] : j = \operatorname{argmin}_{j' \in [k]} \|\mathbf{v}_i - \mathbf{c}_{j'}^0\|\}$. For any cluster centers defined as $\hat{\mathbf{c}}_j^\alpha = (1 - \alpha_j) \mathbf{c}_j^0 + \alpha_j \hat{\mathbf{c}}_j$, we have

$$\mathscr{L}(\widehat{\mathbf{c}}_1^{\alpha},\ldots,\widehat{\mathbf{c}}_k^{\alpha})^{1/2} \leq (1-\alpha_{\min})\phi^{1/2} + (\alpha_{\max})\left(\phi + \frac{1}{n}\sum_{j \in [k]}|C_j^0|\|\mathbf{c}_j - \widehat{\mathbf{c}}_j\|^2\right)^{1/2}.$$

Proof. From (1.1) for centers $\hat{\mathbf{c}}_1^{\alpha},...,\hat{\mathbf{c}}_k^{\alpha} \in \mathbb{R}^d$, and induced clusters $\hat{C}_1^{\alpha},...,\hat{C}_k^{\alpha}$ we have

$$\mathcal{L}(\widehat{\mathbf{c}}_{1}^{\alpha},...,\widehat{\mathbf{c}}_{k}^{\alpha}) = \frac{1}{n} \sum_{j \in [k]} \sum_{i \in \widehat{C}_{j}^{\alpha}} \|\mathbf{v}_{i} - \widehat{\mathbf{c}}_{j}^{\alpha}\|^{2} \le \frac{1}{n} \sum_{j \in [k]} \sum_{i \in C_{j}^{0}} \|\mathbf{v}_{i} - \widehat{\mathbf{c}}_{j}^{\alpha}\|^{2}, \tag{C.3}$$

where for the inequality we use Lemma A.1 Item (i). Then, from the definition of $\hat{\mathbf{c}}_i^{\alpha}$ we have

$$\sum_{j \in [k]} \sum_{i \in C_j^0} \|\mathbf{v}_i - \widehat{\mathbf{c}}_j^{\alpha}\|^2 = \sum_{j \in [k]} \sum_{i \in C_j^0} \|(1 - \alpha_j)(\mathbf{v}_i - \mathbf{c}_j^0) + \alpha_j(\mathbf{v}_i - \widehat{\mathbf{c}}_j)\|^2$$
(C.4)

$$= \sum_{j \in [k]} \sum_{i \in C_i^0} \left((1 - \alpha_j)^2 \| \mathbf{v}_i - \mathbf{c}_j^0 \|^2 + (\alpha_j)^2 \| \mathbf{v}_i - \widehat{\mathbf{c}}_j \|^2 + 2\alpha_j (1 - \alpha_j) (\mathbf{v}_i - \widehat{\mathbf{c}}_j)^\mathsf{T} (\mathbf{v}_i - \mathbf{c}_j^0) \right). \quad (C.5)$$

Define

$$A_j = \sum_{i \in C_i^0} \|\mathbf{v}_i - \mathbf{c}_j^0\|^2, \qquad B_j = \sum_{i \in C_i^0} \|\mathbf{v}_i - \widehat{\mathbf{c}}_j\|^2.$$
 (C.6)

Also observe that by Cauchy-Schwarz, 11

$$\left(\sum_{j \in [k]} \sum_{i \in C_j^0} \alpha_j (1 - \alpha_j) (\mathbf{v}_i - \widehat{\mathbf{c}}_j)^\top (\mathbf{v}_i - \mathbf{c}_j^0)\right)^2 \le \left(\sum_{j \in [k]} \sum_{i \in C_j^0} (\alpha_j)^2 \|\mathbf{v}_i - \widehat{\mathbf{c}}_j\|^2\right) \left(\sum_{j \in [k]} \sum_{i \in C_j^0} (1 - \alpha_j)^2 \|\mathbf{v}_i - \mathbf{c}_j^0\|^2\right). \quad (C.7)$$

Then, using (C.6) and (C.7) in (C.5), and noting that α_j is invariant under the sum over $i \in C_i^0$, we have

$$\sum_{j \in [k]} \sum_{i \in C_j^0} \|\mathbf{v}_i - \widehat{\mathbf{c}}_j^{\alpha}\|^2 \le \sum_{j \in [k]} (1 - \alpha_j)^2 A_j + \sum_{j \in [k]} (\alpha_j)^2 B_j + 2\sqrt{\left(\sum_{j \in [k]} (1 - \alpha_j)^2 A_j\right) \left(\sum_{j \in [k]} (\alpha_j)^2 B_j\right)}$$
(C.8)

$$= \left(\left(\sum_{j \in [k]} (1 - \alpha_j)^2 A_j \right)^{1/2} + \left(\sum_{j \in [k]} (\alpha_j)^2 B_j \right)^{1/2} \right)^2$$
 (C.9)

$$\leq \left((1 - \alpha_{\min}) \left(\sum_{j \in [k]} A_j \right)^{1/2} + \alpha_{\max} \left(\sum_{j \in [k]} B_j \right)^{1/2} \right)^2. \tag{C.10}$$

By definition,

$$\frac{1}{n} \sum_{j \in [k]} A_j = \frac{1}{n} \sum_{j \in [k]} \sum_{i \in C_j^0} \|\mathbf{v}_i - \mathbf{c}_j^0\|^2 = \phi, \tag{C.11}$$

and as in the proof of Lemma B.2,

$$\frac{1}{n} \sum_{j \in [k]} B_j = \frac{1}{n} \sum_{j \in [k]} \sum_{i \in C_j^0} \|\mathbf{v}_i - \widehat{\mathbf{c}}_j\|^2 = \phi + \frac{1}{n} \sum_{j \in [k]} |C_j^0| \|\mathbf{c}_j - \widehat{\mathbf{c}}_j\|^2.$$
 (C.12)

Putting everything back in (C.10) and taking a square-root gives us the lemma.

Proof of Corollary C.1. This follows from plugging Theorem 2.1 into Lemma C.2. □

¹¹ Specifically, we use that $|\sum_i \mathbf{x}_i^\mathsf{T} \mathbf{y}_i|^2 = \operatorname{tr}(\mathbf{X}^\mathsf{T} \mathbf{Y})^2 \le (\sum_i ||\mathbf{x}_i||^2)(\sum_i ||\mathbf{y}_i||^2)$.