Coresets for Kernel Clustering

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Abstract

We devise coresets for kernel $k$-Means with a general kernel, and use them to obtain new, more efficient, algorithms. Kernel $k$-Means has superior clustering capability compared to classical $k$-Means, particularly when clusters are non-linearly separable, but it also introduces significant computational challenges. We address this computational issue by constructing a coreset, which is a reduced dataset that accurately preserves the clustering costs.

Our main result is a coreset for kernel $k$-Means that works for a general kernel and has size $\text{poly}(k\epsilon^{-1})$. Our new coreset both generalizes and greatly improves all previous results; moreover, it can be constructed in time near-linear in $n$. This result immediately implies new algorithms for kernel $k$-Means, such as a $(1 + \epsilon)$-approximation in time near-linear in $n$, and a streaming algorithm using space and update time $\text{poly}(k\epsilon^{-1} \log n)$.

We validate our coreset on various datasets with different kernels. Our coreset performs consistently well, achieving small errors while using very few points. We show that our coresets can speed up kernel $k$-Means++ (the kernelized version of the widely used $k$-Means++ algorithm), and we further use this faster kernel $k$-Means++ for spectral clustering. In both applications, we achieve significant speedup and a better asymptotic growth while the error is comparable to baselines that do not use coresets.

1 Introduction

The $k$-Means problem has proved to be fundamental for unsupervised learning in numerous application domains. Vanilla $k$-Means fails to capture sophisticated cluster structures, e.g., when the clusters are separable non-linearly, but this can be tackled by applying kernel methods [SSM98, Gir02]. This has led to kernel $k$-Means, where data points are first mapped to a high-dimensional feature space (possibly implicitly via a kernel function), and then clustered in this richer space using a classical $k$-Means.

Formally, a kernel for a dataset $X$ is a function $K : X \times X \rightarrow \mathbb{R}$ (intended to measure similarity between elements in $X$) that can be realized by inner products, i.e., there exist a Hilbert space $\mathcal{H}$...
and a map \( \varphi : X \to \mathcal{H} \) (called feature space and feature map) such that
\[
\forall x, y \in X, \quad \langle \varphi(x), \varphi(y) \rangle = K(x, y).
\]

(1)

In kernel \( k \)-MEANS, the input is a dataset \( X \) with weight function \( w_X : X \to \mathbb{R}_+ \) and a kernel function \( K : X \times X \to \mathbb{R} \) as above, and the goal is to find a \( k \)-point center set \( C \subseteq \mathcal{H} \) that minimizes the objective
\[
\text{cost}^\varphi(X, C) = \sum_{x \in X} w_X(x) \cdot \min_{c \in C} \| \varphi(x) - c \|^2.
\]

(2)

(An equivalent formulation asks for a \( k \)-partitioning of \( X \), keeping \( C \) implicit.)

This kernel version has superior clustering capability compared to classical \( k \)-MEANS [ZR02, KLLL05], and has proved useful in different application domains, such as pattern recognition, natural language processing and social networks. In fact, kernel \( k \)-MEANS is useful also for solving other clustering problems, such as normalized cut and spectral clustering [DGK04, DHS05].

**Computational challenges.** As observed in previous work [Gir02, DGK04], the kernel trick can be applied to rewrite kernel \( k \)-MEANS using access only to the kernel \( K(\cdot, \cdot) \) and without computing the very high-dimensional map \( \varphi \) explicitly. However, this approach has outstanding computational challenges (compared to classical \( k \)-MEANS), essentially because of the kernel trick. Consider the special case where \( k = 1 \) and the input is \( n \) unweighted points (i.e., \( 1 \)-MEAN clustering). It is well known that the optimal center \( c^* \) has a closed form \( c^* := \frac{1}{n} \sum_{x \in X} \varphi(x) \). But the kernel trick requires \( \Omega(n^2) \) accesses to \( K \) to evaluate \( \text{cost}^\varphi(X, c^*) \),\(^1\) while in the classical setting such evaluation takes only \( O(n) \) time.

This \( \Omega(n^2) \) barrier can be bypassed at the cost of \((1 + \epsilon)\)-approximation. In particular, let \( S \) be a uniform sample of \( \text{poly}(\epsilon^{-1}) \) points from \( X \), and let \( \hat{c} := \frac{1}{|S|} \sum_{x \in S} \varphi(x) \) be its \( 1 \)-MEAN; then with high probability, \( \text{cost}^\varphi(X, \hat{c}) \leq (1 + \epsilon) \text{cost}^\varphi(X, c^*) \) and evaluating \( \text{cost}^\varphi(X, \hat{c}) \) takes only \( \text{poly}(\epsilon^{-1})n \) time. However, this uniform-sampling approach does not generally work for \( k \geq 2 \), because if the optimal clustering is highly imbalanced, a uniform sample is unlikely to include any point from a small cluster. Alternative approaches, such as dimension reduction, were also proposed to obtain efficient algorithms for kernel \( k \)-MEANS, but they too do not fully resolve the computational issue. We elaborate on these approaches in Section 1.2.

**Our approach.** To tackle this computational challenge, we adapt the notion of coresets [HM04] to kernel \( k \)-MEANS. Informally, a coreset is a tiny reweighted subset of the original dataset on which the clustering cost is preserved within \((1 \pm \epsilon)\)-factor for all candidate centers \( C \subseteq \mathcal{H} \). This notion has proved very useful for classical \( k \)-MEANS, e.g., to design efficient near-linear algorithms. In our context of kernel \( k \)-MEANS, a coreset of size \( s \) for an input of size \( n \) has a huge advantage that each of its \( k \) optimal centers can be represented as a linear combination of only \( s \) points in the feature space. Given these \( k \) optimal centers (as linear combinations), evaluating the distance between a point \( \varphi(x) \) and a center takes merely \( O(s^2) \) time, instead of \( O(n^2) \), and consequently the objective can be \((1 + \epsilon)\)-approximated in time \( O(s^2 kn) \). Moreover, it suffices to use \( k \) centers (again as linear combinations) that are \((1 + \epsilon)\)-approximately optimal for the coreset \( S \).

In addition, coresets are very useful in dealing with massive datasets, since an offline construction of coresets usually implies streaming algorithms [HM04], distributed algorithms [BEL13] and dynamic algorithms [HK20] via the merge-and-reduce method [HM04], and existing (offline) algorithms can run efficiently on the coreset, instead of the original dataset, with minor or no modifications.

\(^1\)In fact, evaluating \( ||c^* - \varphi(u)||^2 \) for a single point \( u \in X \) already requires \( \Theta(n^2) \) accesses, since \( ||c^* - \varphi(u)||^2 = K(u, u) - 2 \frac{1}{s} \sum_{x \in X} K(x, u) + \frac{1}{n^2} \sum_{x, y \in X} K(x, y) \).
Designing coresets for clustering problems has been an active area, but unfortunately only limited results are currently known regarding coresets for kernel clustering. Indeed, all existing results achieve a weaker notion of coreset, apply only to some kernels, and/or have an exponential coreset size (see comparison below). A major recent success in the area has been the design coresets for high-dimensional Euclidean inputs, referring to coresets of size $\text{poly}(k\epsilon^{-1})$, which is independent of the Euclidean dimension [FSS20, SW18, BBC+19, HV20, BJKW21, CSS21, FKW21]. Intuitively, these new coresets are an excellent fit for kernels, which are often high-dimensional, or even infinite-dimensional, but employing these results requires a formal treatment to streamline technical details like infinite dimension or accesses to $K$.

1.1 Our Results

We devise a coreset for kernel $k$-Means that works for a general kernel function and has size $\text{poly}(k\epsilon^{-1})$. Our new coreset significantly improves over the limited existing results, being vastly more general and achieving much improved bounds. (In fact, it also generalizes to kernel $(k, z)$-Clustering, see Section 2 for definitions.) Formally, an $\epsilon$-coreset for kernel $k$-Means with respect to weighted dataset $X$ and kernel function $K : X \times X \rightarrow \mathbb{R}$ is a weighted subset $S \subseteq X$, such that for every feature space $\mathcal{H}$ and feature map $\varphi$ that realize $K$, as defined in (1),

$$\forall C \subseteq \mathcal{H}, |C| = k, \quad \text{cost}^\varphi(S, C) \in (1 \pm \epsilon) \cdot \text{cost}^\varphi(X, C) \quad (3)$$

Throughout, we assume an oracle access to $K$ takes unit time, and therefore our stated running times also bound the number of accesses to $K$. We denote $\tilde{O}(f) = O(f \cdot \text{polylog } f)$ to suppress logarithmic factors.

**Theorem 1.1** (Informal version of Theorem 3.1). Given $n$-point weighted dataset $X$, oracle access to a kernel $K : X \times X \rightarrow \mathbb{R}$, integer $k \geq 1$ and $0 < \epsilon < 1$, one can construct in time $\tilde{O}(nk)$, a reweighted subset $S \subseteq X$ of size $|S| = \text{poly}(k\epsilon^{-1})$, that with high probability is an $\epsilon$-coreset for kernel $k$-Means with respect to $X$ and $K$.

**Comparison to previous coresets.** A weak coreset for kernel $k$-Means was designed in [FMS07]; in this notion, the objective is preserved only for certain candidate centers, whereas (3) guarantees this for all centers. Moreover, that result pertains only to finite-dimensional kernels. Strong coresets of size $k^{\text{poly}(\epsilon^{-1})}$ were designed in [FSS20, Sch14], by computing $k$-Means recursively to obtain a total of $k^{\text{poly}(\epsilon^{-1})}$ clusters, and taking the geometric mean of each cluster. A similar size bound was obtained in [BF20] using a slightly different approach. Compared with our results, their coreset-size bounds are exponentially larger (in $\epsilon$) and their construction time is worse (super-linear in $k$). In addition, their guarantee is weaker as it introduces a fixed shift $D > 0$ such that $\text{cost}^\varphi(S, C) + D \in (1 \pm \epsilon) \cdot \text{cost}^\varphi(X, C)$, whereas in our result $D = 0$. On top of that, all previous results work only for $k$-Means, while our result works for the more general $(k, z)$-Clustering, which in particular includes the well-known variant $k$-Median.

**Technical overview.** Technically, our result builds upon the recent coresets for finite-dimensional Euclidean spaces, which have dimension-independent size bound $\text{poly}(k\epsilon^{-1})$. In particular, we rely on coresets that can be constructed in near-linear time even in the kernel setting (via the kernel trick) [BJKW21]. In contrast, another recent algorithm [SW18] is slow and uses the explicit representation in the feature space. To adapt the coreset of [BJKW21] to the kernel setting, the

\footnote{Some of these results do not explicitly mention kernel $k$-Means, but their method is applicable.}
main technical step is an embedding from (infinite-dimensional) Hilbert space to finite-dimensional Euclidean space, which eliminates any potential dependence on the ambient space (e.g., which points can serve as centers). This step requires a formal treatment, e.g., careful definitions, although its proof is concise. Crucially, we apply this embedding step (which could be computationally heavy) only in the analysis, avoiding any blowup in the running time. In hindsight, all these technical details fit together very smoothly, but this might be less obvious a priori; moreover, the simplicity of our construction is a great advantage for implementation.

**FPT-PTAS for kernel \( k \)-Means.** We can employ our coreset to devise a \((1 + \epsilon)\)-approximation algorithm for kernel \( k \)-Means, that runs in time that is near-linear in \( n \) and parameterized by \( k \). This is stated in Corollary 1.2, whose corresponding algorithm, presented in Algorithm 1, computes a coreset \( S \) and solves \( k \)-Means on \( S \) optimally by straightforward enumeration over all \( k \)-partitions of \( S \). Previously, \((1 + \epsilon)\)-approximation for kernel \( k \)-Means has been achieved by [KSS04], whose algorithm runs in time \( O(n \cdot 2^{\text{poly}(k \epsilon^{-1})}) \). Our algorithm is more efficient, as it isolates the data size \( n \) from the factor \( 2^{\text{poly}(k \epsilon^{-1})} \).

**Corollary 1.2 (FPT-PTAS).** Given \( n \)-point weighted dataset \( X \), oracle access to a kernel \( K : X \times X \to \mathbb{R} \), integer \( k \geq 1 \) and \( 0 < \epsilon < 1 \), one can compute in time \( O(nk + \text{poly}(k \epsilon^{-1})) \), a center set \( C \) of \( k \) points, each represented as a linear combination of at most \( \text{poly}(k \epsilon^{-1}) \) points from \( \varphi(X) \), such that with high probability \( C \) is a \((1 + \epsilon)\)-approximation for kernel \( k \)-Means on \( X \) and \( K \). In particular, given such \( C \), one can find for each \( x \in X \) its closest center in \( C \) in time \( \text{poly}(k \epsilon^{-1}) \).

**Streaming algorithms.** In fact, for the purpose of finding near-optimal solutions, it already suffices to preserve the cost for centers coming from \( \text{span}(\varphi(X)) \) (see Fact 2.1) which is an \( n \)-dimensional subspace. However, our definition of coreset in (3) is much stronger, in that the objective is preserved even for centers coming from a possibly infinite-dimensional feature space. This stronger guarantee ensures that the coreset is composable, and thus the standard merge-and-reduce method can be applied. In particular, our coreset implies the first streaming algorithm for kernel \( k \)-Means.

**Corollary 1.3 (Streaming kernel \( k \)-Means).** There is a streaming algorithm that given a dataset \( X \) presented as a stream of \( n \) points, and oracle access to a kernel \( K : X \times X \to \mathbb{R} \), constructs a reweighted subset \( S \subseteq X \) of \( \text{poly}(k \epsilon^{-1}) \) points using \( \text{poly}(k \epsilon^{-1} \log n) \) words of space and update time, such that with high probability \( S \) is an \( \epsilon \)-coreset for \( k \)-Means with respect to \( X \) and \( K \).

\[\text{Algorithm 1 FPT-PTAS for kernel } k \text{-Means on dataset } X \text{ with kernel } K \]

1. construct \( \epsilon \)-coreset \( S \) of size \( \text{poly}(k \epsilon^{-1}) \) for kernel \( (k, z) \)-CLUSTERING on \( X \) with kernel \( K \)
2. enumerate over all \( k^{\text{poly}(k \epsilon^{-1})} \) \( k \)-partitions of \( S \) to find \( k \)-partition \( P = \{P_1, \ldots, P_k\} \) with smallest \( k \)-Means objective

\[
\sum_{i=1}^{k} \frac{1}{|P_i|} \sum_{x,y \in P_i} \|x - y\|^2
\]

return optimal center set for \( P \), i.e., \( C = \{c_1, \ldots, c_k\} \), where each \( c_i \) is represented as

\[
\frac{1}{|P_i|} \sum_{x \in P_i} \varphi(x)
\]

\[\triangleright \text{use Theorem 1.1} \]

\[\triangleright \text{compute distances using the kernel trick} \]
Experiments and other applications. We validate the efficiency and accuracy of our coresets on various datasets with polynomial and Gaussian kernels, which are frequently-used kernels. For every dataset, kernel, and coreset-size that we test, our coreset performs consistently better than uniform sampling which serves as a baseline. In fact, our coreset achieves less than 10% error using only about 1000 points for every dataset.

We also showcase significant speedup to several applications that can be obtained using our coresets. Specifically, we adapt the widely used $k$-Means++ [AV07] to the kernel setting, and we compare the running time and accuracy of this kernelized $k$-Means++ with and without coresets. In these experiments, we observe a significant speedup and more importantly, a better asymptotic growth of running time of $k$-Means++ when using coresets, while achieving a very similar error. Furthermore, this new efficient version of kernelized $k$-Means++ (based on coresets) is applied to solve spectral clustering, using the connection discoverd by [DGK04]. Compared to the implementation provided by Scikit-learn [PVG+11], our algorithm often achieves a better result and uses significantly less time. Hence, our coreset-based approach can potentially become the leading method for solving spectral clustering in practice.

1.2 Comparison to Other Approaches

The computational issue of kernel $k$-Means is an important research topic and has attracted significant attention. In the following, we compare our result with previous work that is representative of different approaches for the problem.

Uniform sampling of data points is a commonly used technique, which fits well in kernel clustering, because samples can be drawn without any access to the kernel. While the coresets that we use rely on sampling, we employ importance sampling, which is non-uniform by definition. [CJHJ11] employs uniform sampling for kernel $k$-Means, but instead of solving kernel $k$-Means on a sample of data points directly (as we do), their method works in iterations, similarly to Lloyd’s algorithm, that find a center set that is a linear combination of the sample. However, it has no worst-case guarantees on the error or on the running time, which could be much larger than $O(nk)$. Lastly, this method does not generalize easily to other sublinear settings, such as streaming (as our Corollary 1.3).

[RD20] analyze uniform sampling for $k$-Means in a Euclidean space, which could be the kernel’s feature space. In their analysis, the number of samples (and thus running time) crucially depends on the diameter of the dataset and on the optimal objective value, and is thus not bounded in the worse-case. This analysis builds on several earlier papers, for example [CS07] achieve bounds of similar flavor for $k$-Means in general metric spaces.

Another common approach to speed up kernel $k$-Means is to approximate the kernel $K$ using dimension-reduction techniques. In a seminal paper, [RR07] proposed a method that efficiently computes a low (namely, $O(\log n)$) dimensional feature map $\tilde{\varphi}$ that approximates $\varphi$ (without computing $\varphi$ explicitly), and this $\tilde{\varphi}$ can be used in downstream applications. Their method is based on designing random Fourier features, and works for a family of kernels that includes the Gaussian one, but not general kernels. This method was subsequently tailored to kernel $k$-Means by [CJJ12], and another followup work by [CP17] established worst-case bounds for kernel $k$-Means with Gaussian kernels. Despite these promising advances, we are not aware of any work based on dimension reduction that can handle a general kernel function (as in our approach). In a sense, these dimension-reduction techniques are “orthogonal” to our data-reduction approach, and the two techniques can possibly be combined to yield even better results.

An alternative dimension-reduction approach is low-rank approximation of the kernel matrix $K$. Recent works by [MM17] and by [WGM19] present algorithms based on Nyström approximation to compute a low-rank (namely, $O(k/\epsilon)$) approximation $\tilde{K} := UU^T$ to the kernel matrix $K$ in time
near-linear in \( n \), where \( U \in \mathbb{R}^{n \times O(k/\epsilon)} \) defines an embedding of data points into \( \mathbb{R}^{O(k/\epsilon)} \). One might then try to construct a coreset on the subspace of \( U \) via applying \( k \)-MEANS coreset construction after dimension-reduction, however, it does not satisfy our definition, in which we require the objective to be preserved for all centers from any ambient space that realizes \( K \), not only a specific space induced by \( U \). Such a seemingly slight difference plays a great role when designing algorithms for sublinear models, such as streaming, since it ensures the coreset is mergable (i.e. \( \text{coreset}(A) \cup \text{coreset}(B) \) is a coreset of \( A \cup B \)), so that the standard merge-and-reduce technique can be applied.

## 2 Preliminaries

### Notations. A weighted set \( U \) is a finite set \( U \) associated with a weight function \( w_U : U \to \mathbb{R}_+ \). For such \( U \), let \( |U|_0 \) be the number of distinct elements in it. For a weight function as above and a subset \( S \subseteq U \), define \( w_U(S) := \sum_{u \in S} w_U(u) \). For any other map \( f : U \to V \) (not a weight function), we follow the standard definition \( f(S) := \{ f(x) : x \in S \} \). For an integer \( t \geq 1 \), let \( [t] := \{1, \ldots, t\} \).

For \( x > 0 \) and integer \( i \geq 1 \), let \( \log^i x \) be the \( i \)-th iterated log of \( x \), i.e., \( \log^{(1)} x = \log x \) and \( \log^{(i)} x = \log(\log^{(i-1)} x) \) for \( i \geq 2 \).

### Kernel functions. Let \( X \) be a set of \( n \) points. A function \( K : X \times X \to \mathbb{R} \) is a kernel function if the \( n \times n \) matrix \( M \) such that \( M_{ij} = K(x_i, x_j) \) (where \( x_i, x_j \in X \)) is positive semi-definite. Since \( M \) is positive semi-definite, there exists a map \( \varphi \) from \( X \) to some Hilbert space \( \mathcal{H} \), such that all \( x, y \in X \) satisfy \( K(x, y) = \langle \varphi(x), \varphi(y) \rangle \). This above (existence of a map \( \varphi \) of into \( \mathcal{H} \)) can be extended to infinite \( X \), e.g., \( X = \mathbb{R}^d \), by Mercer’s Theorem. The distance between \( x', y' \in \mathcal{H} \) is defined as \( \text{dist}(x', y') := \| x' - y' \| = \sqrt{\langle x' - y', x' - y' \rangle} \). Hence, the distance \( \text{dist}(\varphi(x), \varphi(y)) \) for \( x, y \in X \) can be represented using \( K \) as

\[
\text{dist}(\varphi(x), \varphi(y)) = \| \varphi(x) - \varphi(y) \| = \sqrt{K(x, x) + K(y, y) - 2K(x, y)}.
\]

We refer to a survey by [GGK21] for a more comprehensive introduction to kernel functions.

### Data model. For a dataset \( X \) associated with a kernel (as in Theorem 3.1), it is convenient to assume that \( X = \{1, \ldots, n\} \) and one has oracle access to the kernel function. Our actual requirement is that every point in \( X \) can be stored in \( O(1) \) space and manipulated in \( O(1) \) time, and the kernel can be evaluated on any pair of points from \( X \) in \( O(1) \) time. A similar model is assumed when \( X \) is associated with a distance function (as in Theorem 3.4).

### Kernel \((k, z)\)-Clustering. In the the kernel \((k, z)\)-CLUSTERING problem, the input is a weighted dataset \( X \) of \( n \) objects, a kernel function \( K : X \times X \to \mathbb{R} \), an integer \( k \geq 1 \), and \( z > 0 \). The goal is to find a \( k \)-point center set \( C \subseteq \mathcal{H} \) that minimizes the objective

\[
\text{cost}^z_\mathcal{H}(X, C) := \sum_{x \in X} w_x(x)(\text{dist}(\varphi(x), C))^z,
\]

where \( \mathcal{H} \) is an induced Hilbert space of \( K \) and \( \varphi : X \to \mathcal{H} \) is its feature map, and \( \text{dist}(\varphi(x), C) := \min_{c \in C} \| \varphi(x) - c \| \). The case \( z = 2 \) clearly coincides with kernel \( k \)-MEANS whose objective is (2). The (non-kernel) \((k, z)\)-CLUSTERING problem may be viewed as kernel \((k, z)\)-CLUSTERING with kernel \( K(x, y) = \langle x, y \rangle \) and identity feature map \( \varphi(x) = x \).

While the feature map \( \varphi \) might not be unique, we show below that this kernel \((k, z)\)-CLUSTERING is well defined, in the sense that the optimal value is independent of \( \varphi \). The following two facts are standard and easy to prove.
Fact 2.1. For every map $\varphi$ into $\mathcal{H}$, there is an optimal solution $C^*$ in which every center point $c \in C^*$ lies inside $\text{span}(\varphi(X))$, and is thus a linear combination of $\varphi(X)$.

Corollary 2.2. The optimal value of (4) can be represented as a function of kernel values $K(x, y)$, thus invariant of $\varphi$.

$\epsilon$-Coresets for kernel $(k, z)$-Clustering. For $0 < \epsilon < 1$, an $\epsilon$-coreset for kernel $(k, z)$-CLUSTERING on a weighted dataset $X$ and a kernel function $K$ is a reweighted subset $S \subseteq X$, such that for every Hilbert space $\mathcal{H}$ and map $\varphi : X \to \mathcal{H}$ satisfying (1), we have

$$\forall C \subseteq \mathcal{H}, |C| = k, \quad \text{cost}_z(S, C) \leq (1 + \epsilon) \cdot \text{cost}_z(X, C).$$

The case $z = 2$ clearly coincides with (3).

3 Coresets for Kernel $(k, z)$-Clustering

Theorem 3.1. Given $n$-point weighted dataset $X$, oracle access to a kernel $K : X \times X \to \mathbb{R}$, $z \geq 1$, $0 < \epsilon < 1$, and integer $k \geq 1$, one can construct in time $O(nk)$, a reweighted subset $S \subseteq X$ of size $|S| = 2^{O(z)} \cdot \text{poly}(k^{(e-1)})$, that with high constant probability is an $\epsilon$-coreset for kernel $(k, z)$-CLUSTERING with respect to $X$ and $K$.

At a high level, our proof employs recent constructions of coresets for $(k, z)$-CLUSTERING in Euclidean spaces, in which the coreset size is independent of the Euclidean dimension [SW18, FSS20, HV20, BJKW21]. However, these coresets are designed for finite-dimensional Euclidean spaces, and are thus not directly applicable to our feature space $\mathcal{H}$, which might have infinite dimension.

To employ these coreset constructions, we show that the data points in the feature space $\mathcal{H}$ embed into an $(n+1)$-dimensional (Euclidean) space, without any distortion to distances between data points and centers (Lemma 3.2). This observation is similar to one previously made by [SW18] for a different purpose. Due to this embedding, it suffices to construct coresets in a limited setting where centers come only from $\mathbb{R}^{n+1}$ (Corollary 3.3).

Lemma 3.2. Let $\mathcal{H}$ be a Hilbert space and let $X \subseteq \mathcal{H}$ be a subset of $n$ points. Then there exists a map $f : \mathcal{H} \to \mathbb{R}^{n+1}$ such that $\forall x \in X, c \in \mathcal{H}$, $\|x - c\| = \|f(x) - f(c)\|$.

Proof. Let $S = \text{span}(X)$. Then every point $c \in \mathcal{H}$ can be written (uniquely) as $c = c^\parallel + c^\perp$, where $c^\parallel \in S$ and $c^\perp$ is orthogonal to $S$. Thus, $\|c\|^2 = \|c^\parallel\|^2 + \|c^\perp\|^2$. Note that for all $x \in X$, we have $x^\perp = 0$. Now, for every $c \in \mathcal{H}$, let $f(c) := (c^\parallel; |c^\perp|)$, where we interpret $x^\parallel$ as an $n$-dimensional vector. Then for all $x \in X$ and $c \in \mathcal{H}$,

$$\|x - c\|^2 = \|x^\parallel - c^\parallel\|^2 + \|x^\perp - c^\perp\|^2$$

$$= \|x^\parallel - c^\parallel\|^2 + \|c^\perp\|^2$$

$$= \|f(x) - f(c)\|^2.$$

The claim follows.

Corollary 3.3. Consider $n$-point weighted dataset $X$, kernel function $K : X \times X \to \mathbb{R}$, $z \geq 1$, integer $k \geq 1$, and $0 < \epsilon < 1$. Suppose that a reweighted subset $S \subseteq X$ satisfies that for every $\varphi : X \to \mathbb{R}^{n+1}$ such that for all $x, y \in X$, $\langle \varphi(x), \varphi(y) \rangle = K(x, y)$, for all $C \subseteq \mathbb{R}^{n+1}$ with $|C| = k$ the following holds

$$\text{cost}_z(S, C) \leq (1 + \epsilon) \cdot \text{cost}_z(X, C).$$

Then $S$ is an $\epsilon$-coreset for kernel $(k, z)$-CLUSTERING with respect to $X$ and kernel $K$.
Proof. To verify that $S$ is a coreset with respect to $X$ and $K$, consider some feature space $\mathcal{H}$ and feature map $\varphi'$ be induced by $K$. Apply Lemma 3.2 to obtain $f: \mathcal{H} \to \mathbb{R}^{n+1}$, then for all $C \subseteq \mathcal{H}$, $|C| = k$, we have $\forall Q \subseteq X$, $\text{cost}^\varphi_Q(C) = \text{cost}^{f \circ \varphi'}_K(Q, f(C))$, and using the promise about $S$ with $\varphi = f \circ \varphi'$,
\[
\text{cost}^\varphi_S(C, f(C)) = \text{cost}^{f \circ \varphi'}_K(S, f(C)) \\
\in (1 \pm \epsilon) \cdot \text{cost}^\varphi_S(X, f(C)) \\
\leq (1 \pm \epsilon) \cdot \text{cost}^\varphi_S(X, C).
\]
Thus, $S$ is indeed a coreset with respect to $X$ and $K$. \hfill \Box

Another issue is that some of the existing algorithms, such as [SW18, FSS20], require the explicit representations of points in $\varphi(X)$, which is very expensive to compute. Fortunately, the importance-sampling-based algorithms of [HV20] and [BJKW21] are oblivious to the representation of $\varphi$, and only rely on a distance oracle that evaluates $\forall x, y \in X$, $\|\varphi(x) - \varphi(y)\| = \sqrt{K(x, x) + K(y, y) - 2K(x, y)}$. Now, by Corollary 3.3, executing these algorithms without any modifications (except for plugging in the distance oracle defined by kernel $K$) yields the desired coreset for kernel $(k, z)$-CLUSTERING. We choose to use the coreset construction of [BJKW21], which is arguably simpler. We now recall its statement for completeness.

**Theorem 3.4 ([BJKW21]).** Given $n$-point weighted dataset $X \subseteq \mathbb{R}^m$ for some integer $m$, together with $z \geq 1$, integer $k \geq 1$, and $0 < \epsilon < 1$, one can construct in time $\tilde{O}(mnk)$ a reweighted subset $S \subseteq X$ of size $\|S\|_0 = \tilde{O}(\epsilon^{-1}2^zd^2k^2)$, that with high constant probability is an $\epsilon$-coreset for $(k, z)$-CLUSTERING with respect to $X$. If the explicit representation of $X \subseteq \mathbb{R}^m$ is replaced by oracle access to the distance function $\mathrm{dist}: X \times X \to \mathbb{R}_+$, then the time bound improves to $\tilde{O}(nk)$.

**Proof of Theorem 3.1.** Suppose $f$ is the asserted map from Lemma 3.2. Hence, $f(\varphi(X)) = \{f(\varphi(x)) : x \in X\}$ is a subset of $\mathbb{R}^{n+1}$. Apply Theorem 3.4 on top of this $f(\varphi(X))$, then by the guarantee of Theorem 3.4 and Corollary 3.3, the resulting weighted set is an $\epsilon$-coreset for $X$.

To show that the running time is $\tilde{O}(nk)$, it suffices to verify that the distance between a pair of points in $f(\varphi(X))$ can be evaluated in $O(1)$ time (as required by Theorem 3.4). Indeed, by Lemma 3.2, for all $x, y \in X$, one can evaluate $\mathrm{dist}(f(\varphi(x)), f(\varphi(y))) = \mathrm{dist}(\varphi(x), \varphi(y))$ in $O(1)$ time using 3 queries to the kernel function. \hfill \Box

### 3.1 Description of Coreset Construction Algorithms

For completeness, we present our full algorithm in Algorithm 2 (which depends on the subroutines defined in Algorithm 3 and 4). As can be easily seen in the proof of Theorem 3.1, our algorithm is a black-box application of Theorem 3.4, i.e., it is identical to the algorithm of [BJKW21], except that we use the kernel distance (instead of Euclidean distance), which can be computed efficiently via the kernel trick.

The following notation is needed. For a subset $C \subseteq \mathcal{H}$ and data point $x \in X$, define $\text{NN}_C(x) := \arg\min\{\mathrm{dist}(\varphi(x), y) : y \in C\}$ as the nearest neighbor of $x$ in $C$ with respect to the distances in the feature space (breaking ties arbitrarily). Thus $\text{NN}_C(\cdot)$ defines a $|C|$-partition of $X$, and the cluster that $x$ belongs to (with respect to $C$) is denoted $C(x) := \{x' \in X : \text{NN}_C(x') = \text{NN}_C(x)\}$.

Algorithm 2 is the main procedure for constructing the coreset, and it iteratively executes another importance-sampling-based coreset construction (Algorithm 3). Informally, each invocation of IMPORTANCE-SAMPLING constructs a coreset $X_i$ from the current coreset $X_{i-1}$, to reduce the number of distinct elements in $X_{i-1}$ to roughly $\|X_{i-1}\|_0$. The procedure ends when such size
Algorithm 2 Constructing $\epsilon$-coreset for kernel $(k, z)$-Clustering on dataset $X$ with kernel $K$

1: let $X_0 \leftarrow X$, $i \leftarrow 0$
2: repeat
3: let $i \leftarrow i + 1$ and $\epsilon_i \leftarrow \epsilon / (\log(i) \|X\|_0)^{1/4}$
4: $X_i \leftarrow$ IMPORTANCE-SAMPLING($X_{i-1}, \epsilon_i$)
5: until $\|X_i\|_0$ does not decrease compared to $\|X_{i-1}\|_0$

return $X_i$

Algorithm 3 IMPORTANCE-SAMPLING($X$, $\epsilon$)

1: let $C^* \leftarrow D^2$-SAMPLING($X$)
2: $\forall x \in X$, let $\sigma_x \leftarrow \frac{w_X(x) \cdot \text{dist}(x, C^*)^2}{\text{cost}^2(X, C^*)}$
3: $\forall x \in X$, let $p_x \leftarrow \frac{\sigma_x}{\sum_{y \in X} \sigma_y}$
4: draw $N = O(\epsilon^{-4}2^{2k}z k^2 \log k \|X\|_0)$ i.i.d. samples from $X$, using probabilities $(p_x)_{x \in X}$
5: let $D$ be the sampled set; $\forall x \in D$ let $w_D(x) \leftarrow \frac{w_X(x)}{p_x N}$

return weighted set $D$

reduction cannot be done any more, at which point the size of the coreset reaches the bound in Theorem 3.4, which is independent of $n$.

In fact, subroutine IMPORTANCE-SAMPLING already constructs a coreset, albeit of a worse size that depends on $\log\|X\|_0$. This subroutine is based on the well-known importance sampling approach that was proposed and improved in a series of works, e.g., [LS10, FL11, FSS20]. Its first step is to compute an importance score $\sigma_x$ for every $x \in X$ (lines 1–2), and then draw independent samples from $X$ with probability proportional to $\sigma_x$ (lines 3–4). The final coreset is formed by reweighting the sampled points (lines 5–6). Roughly speaking, the importance score $\sigma_x$ measures the relative contribution of $x$ to the objective function in the worst-case, which here means the maximum over all choices of the center set. It can be computed from an $O(\log k)$-approximate solution for kernel $(k, z)$-Clustering on $X$, which is obtained by the $D^2$-sampling subroutine (Algorithm 4), a natural generalization of the $D^2$-sampling introduced by [AV07].

We stress that our algorithm description uses the feature vectors $\phi(x)$ for clarity of exposition. These vectors do not have to be provided explicitly, because only distances between them are required, and thus all steps can be easily implemented using the kernel trick, and the total time (and number of accesses to the kernel function $K$) is only $O(nk)$.

4 Experiments

We validate the empirical performance of our coreset for kernel $k$-MEANS on various datasets, and show that our coresets significantly speed up a kernelized version of the widely used $k$-MEANS++ [AV07]. In addition, we apply this new coreset-based kernelized $k$-MEANS++ to spectral clustering (via a reduction devised by [DGK04]), showing that it outperforms the well-known Scikit-learn solver in both speed and accuracy.

Experimental setup. Our experiments are conducted on standard clustering datasets that consist of vectors in $\mathbb{R}^d$, and we use the RBF kernel (radial basis function kernel, also known as Gaussian kernel) and polynomial kernels as kernel functions. An RBF kernel $K_G$ is of the form $K_G(x, y) := \exp\left(-\frac{\|x-y\|_2^2}{2\sigma^2}\right)$, where $\sigma > 0$ is a parameter, and a polynomial kernel $K_P$ is of the form...
Algorithm 4 \( D_z - \text{Sampling}(X) \)

1: draw \( x \in X \) uniformly at random, and initialize \( C \leftarrow \{ \varphi(x) \} \)
   \( \triangleright \) we use here the feature vectors for clarity, and the implementation should represent \( \varphi(x) \) by storing \( x \)
2: for \( i = 1, \ldots, k - 1 \) do
3:   draw one sample \( x \in X \), using probabilities \( w_X(x) \cdot \frac{\text{dist}(\varphi(x), C)}{\text{cost}_z(X, C)} \)
4:   let \( C \leftarrow C \cup \{ \varphi(x) \} \)
5: return \( C \)

Table 1: Specifications of datasets

| dataset    | size       | RBF kernel param. | poly. kernel param. |
|------------|------------|-------------------|---------------------|
| Twitter    | 21040936   | \( \sigma = 50 \) | \( c = 0, d = 4 \) |
| Census1990 | 2458284    | \( \sigma = 100 \) | \( c = 0, d = 4 \) |
| Adult      | 48842      | \( \sigma = 200000 \) | \( c = 0, d = 2 \) |
| Bank       | 41188      | \( \sigma = 500 \) | \( c = 0, d = 4 \) |

\( K_F(x, y) := (\langle x, y \rangle + c)^d \) where \( c \) and \( d \) are parameters. Table 1 summarizes the specifications of datasets and our choice of the parameters for the kernel function. We note that the parameters are dataset-dependent, and that for Twitter and Census1990 dataset we subsample to \( 10^5 \) points since otherwise it takes too long to run for some of our inefficient baselines. Unless otherwise specified, we use a typical value \( k = 5 \) for the number of clusters. All experiments are conducted on a PC with Intel Core i7 CPU and 16 GB memory, and algorithms are implemented using C++.

4.1 Size and Empirical Error Tradeoff

Our first experiment evaluates the empirical error versus coreset size. In our coreset implementation, we simplify the construction in Algorithm 2 by running the importance sampling step only once instead of running it iteratively, and it turns out this simplification still achieves excellent performance. As in many previous implementations, instead of setting \( \epsilon \) and solving for the number of samples \( N \) in the Importance-Sampling procedure (Algorithm 3), we simply set \( N \) as a parameter to directly control the coreset size. We construct the coreset with this \( N \) and evaluate its error by drawing 500 random center sets \( C \) (each consisting of \( k \) points) from the dataset, and evaluate the maximum empirical error, defined as

\[
\hat{\epsilon} := \max_{C \in \mathcal{C}} \frac{\text{cost}_z(S, C) - \text{cost}_z(X, C)}{\text{cost}_z(X, C)}.
\]  

(5)

This error is measured similarly as in the definition of coreset, except that it is performed on a sample of center sets. To make the measurement stable, we independently evaluate the empirical error 100 times and report the average.

The tradeoff between the coreset size and empirical error is shown in Figure 1, where we also compare with a baseline that constructs coresets by uniform sampling. These experiments show that our coreset performs consistently well on all datasets and kernels. Furthermore, our coreset admits a similar error curve regardless of dataset and kernel function – for example, one can get \( \leq 10\% \) error using a coreset of 1000 points, – which is perfectly justified by our theory that the size of \( \epsilon \)-coreset only depends on \( \epsilon \) and \( k \). Comparing with the uniform-sampling baseline, our coreset
generally has superior performance, especially when the coreset size is small. We also observe that
the uniform sampling suffers a larger variance compared with our coreset.

4.2 Speeding Up Kernelized $k$-Means++

$k$-Means++ [AV07] is a widely-used algorithm for $k$-Means, and it could easily be adapted to
solve kernel $k$-Means. In particular, kernelized $k$-Means++ is the $k$-Means++ algorithm applied
on the feature space $\mathcal{H}$, where the distances are the kernel distances $\text{dist}(\varphi(x), \varphi(y))$. This kernel
distance between a pair of points may be evaluated using the kernel trick efficiently, however, as
mentioned earlier, implementing $k$-Means++ using the kernel trick can take $\Omega(n^2)$ time in total.
We use our coreset to speed up this kernelized $k$-Means++ algorithm, by first computing the
coreset and then running kernelized $k$-Means++ on top of it; this yields an implementation of
kernelized $k$-Means++ with near-linear running time.

In Figure 2, we demonstrate the running time and the error achieved by kernelized $k$-Means++
with and without coresets, experimented with varying coreset sizes. We measure the relative error
of our coreset-based kernelized $k$-Means++ by comparing the objective value it achieves with
that of vanilla (i.e., without coreset) kernelized $k$-Means++. These experiments show that the
error decreases significantly as the coreset size increases, and it stabilizes around size $N = 100$,
achieving merely $< 5\%$ error. Naturally, the running time of our coreset-based approach increases
with the coreset size, but even the slowest one is still several orders of magnitude faster than vanilla
kernelized $k$-Means++.

4.3 Speeding Up Spectral Clustering

In the spectral clustering problem, the input is a set of $n$ objects $X$ and an $n \times n$ matrix $A$ that
measures the similarity between every pair of elements in $X$, and the goal is to find a $k$-partition of
$X$ such that a certain objective function with respect to $A$ is minimized. [DGK04] shows a way to
write spectral clustering as a (weighted) kernel $k$-Means problem, and use the kernel $k$-Means
solution to produce a spectral clustering. Specifically, let $D$ be an $n \times n$ diagonal matrix such that
Figure 2: Speedup of kernelized \( k \)-MEANS++ using our coreset. This experiment is conducted on the Twitter dataset with RBF and polynomial kernels. We run each algorithm 10 times, and report the average running time and the minimum objective value (in relative-error evaluation).

\[
D_{ii} = \sum_{j \in [n]} A_{ij}.
\]

Then according to [DGK04], spectral clustering can be written as a weighted kernel \( k \)-MEANS problem with weights \( w_i := D_{ii} \) and kernel function \( K := D^{-1}AD^{-1} \), provided that \( A \) is positive semidefinite (which could be viewed as a kernel). We apply this reduction, and use the abovementioned coreset-based kernelized \( k \)-MEANS++ to solve kernel \( k \)-MEANS. We experiment on the subsampled Twitter dataset with varying number of points, and we use the polynomial and RBF kernels as the similarity matrix \( A \).

However, it takes \( \Theta(n^2) \) time if we evaluate \( D_{ii} \) naively. To resolve this issue, we draw a uniform sample \( S \) from \([n] \), and use \( \hat{D}_{ii} := \frac{n}{|S|} \sum_{j \in S} A_{ij} \) as an estimate for \( D_{ii} \). The accuracy of \( \hat{D} \) is justified by previous work on kernel density estimation [JKPV11], and for our application we set \(|S| = 1000\) which achieves good accuracy.

We compare our implementation with the spectral clustering solver from the well-known Scikit-learn library [PVG+11]. The experimental results, reported in Figure 3, show that our approach has a much better asymptotic growth of running time than that of Scikit-learn’s, and achieves more than 1000x of speedup already for moderately large datasets (\( n = 40000 \)). Although the difference of absolute running time might be partially caused by efficiency issues of the Python language used in the Scikit-learn implementation (recall that our implementation is in C++), the outperformance in asymptotic growth suggests that our improvement in running time is fundamental, not only due to the programming language. We also observe that our approach yields better objective values than Scikit-learn. One possible reason is that Scikit-learn might be conservative in using more iterations to gain better accuracy, due to the expensive computational cost that we do not suffer. We also observe that our approach yields better objective values than Scikit-learn. One possible reason is that Scikit-learn might be conservative in using more iterations to gain better accuracy, due to the expensive computational cost that we do not suffer.

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Figure 3: Speedup of spectral clustering using coreset-based kernelized \textit{k}-\textsc{Means++}, with coreset size $N = 2000$. Similar to Figure 2, we run each algorithm 10 times, report the average running time and the minimum objective value.

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