Refined Learning Bounds for Kernel and Approximate \(k\)-Means

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Abstract

Kernel \(k\)-means is one of the most popular approaches to clustering and its theoretical properties have been investigated for decades. However, the existing state-of-the-art risk bounds are of order \(O\left(\frac{k}{\sqrt{n}}\right)\), which do not match with the stated lower bound \(\Omega\left(\frac{\sqrt{k}}{n}\right)\) in terms of \(k\), where \(k\) is the number of clusters and \(n\) is the size of the training set. In this paper, we study the statistical properties of kernel \(k\)-means and Nyström-based kernel \(k\)-means, and obtain optimal clustering risk bounds, which improve the existing risk bounds. Particularly, based on a refined upper bound of Rademacher complexity \([21]\), we first derive an optimal risk bound of rate \(O\left(\frac{\sqrt{k}}{n}\right)\) for empirical risk minimizer (ERM), and further extend it to general cases beyond ERM. Then, we analyze the statistical effect of computational approximations of Nyström kernel \(k\)-means, and prove that it achieves the same statistical accuracy as the original kernel \(k\)-means considering only \(\Omega\left(\sqrt{nk}\right)\) Nyström landmark points. We further relax the restriction of landmark points from \(\Omega\left(\sqrt{nk}\right)\) to \(\Omega\left(\sqrt{n}\right)\) under a mild condition. Finally, we validate the theoretical findings via numerical experiments.

1 Introduction

Clustering, a fundamental data mining task, is used in numerous applications including web search, medical imaging, gene expression analysis, social network analysis and recommendation systems \([56,55,23,42]\). \(k\)-means is arguably one of the most popular approaches to clustering, producing clusters with piece-wise linear boundaries. Its kernel version, which employs a nonlinear distance function, has the ability to find clusters of varying densities and distributions, greatly improving the flexibility of the approach \([18,53,38,37,39,60,29,36,35,61]\).

To understand (kernel) \(k\)-means and guide the development of new clustering algorithms, researchers have investigated its theoretical properties for decades. The consistency of the empirical minimizer was demonstrated by \([45,47,1]\). Rates of convergence and non-asymptotic performance bounds were considered by \([46,13,33,7,32,14,20]\). Most of the proposed risk bounds are dependent upon the dimension of the hypothesis space. For example, Bartlett et al. \([7]\) provided, under certain mild assumptions, a clustering risk bound of order \(O(\sqrt{kd/n})\), where \(d\) is the dimension of the hypothesis space and \(n\) is the size of the training set. However, the hypothesis space of kernel \(k\)-means is typically an infinite-dimensional Hilbert space, such as the reproducing kernel Hilbert space (RKHS) associated with Gaussian kernels \([50]\). Thus, the existing theoretical analysis of \(k\)-means are not usually suitable for explaining its kernel version. Recently, \([24,16,10,41,5,27,24,9]\) extended the previous results, and provided dimension-independent bounds for kernel \(k\)-means. As shown in \([16]\), if the feature map associated with the kernel function satisfies \(||\Phi|| \leq 1\), then the clustering risk bounds are of order \(O(k/\sqrt{n})\). These clustering risk bounds for kernel \(k\)-means are usually linearly
dependent on the number of clusters $k$. However, the number of clusters $k$ may be very large in some domains, such as social networks and recommendation systems. Thus, from a theoretical perspective, these existing bounds of $O(k/\sqrt{n})$ do not match with the stated lower bound $\Omega(\sqrt{k/n})$ in $k$ [7].

Although kernel $k$-means is one of the most popular clustering methods, it requires the computation of a $n \times n$ kernel matrix. As for other kernel methods, this becomes unfeasible for large-scale problems, and thus deriving approximate computations, such as partial decompositions [6, 28], random projection [16, 13], Nyström approximations [19, 11, 9, 43, 53, 58, 57], and random feature approximations [48, 12, 5, 49, 34, 31], has become the subject of numerous recent works. However, few of these optimization-based methods focused on the underlying excess risk problem. To the best of our knowledge, the only two results providing excess risk guarantees for approximate kernel $k$-means are [16] and [9]. In [16], Devroye and Lugosi considered the excess clustering risk when the approximate Hilbert space is obtained using Gaussian projections. In [9], Calandrriello and Rosasco showed that, when sampling $\Omega(\sqrt{n})$ Nyström landmarks, the excess risk bound can reach $O(k/\sqrt{n})$. The excess risk bounds of [9] and [16] are both linearly dependent on $k$ and thus do not match with the theoretical lower bound $\Omega(\sqrt{k/n})$.

In the recent work [21], the authors showed that the Rademacher complexity of the $k$-valued function class of Lipschitz continuity with respect to the $L_\infty$ norm can be bounded by the maximum Rademacher complexity of the restriction of the function class along each coordinate, times a factor of $O(\sqrt{k})$. Although it may be not very difficult to use the result of [21] for kernel $k$-means, the optimal bound of $O(\sqrt{k/n})$ for kernel $k$-means has never been given before. Moreover, we creatively extend the results of kernel $k$-means to the approximate one. Our major contributions include two parts:

1) A (nearly) optimal excess clustering risk bound of rate $\tilde{O}(\sqrt{k/n})^1$ is proposed for empirical risk minimization (ERM) (see Theorem 1). To the best of our knowledge, this is the first (nearly) optimal excess risk bound for kernel $k$-means in terms of both $k$ and $n$. Beyond ERM, we further extend the result of Theorem 1 to general cases (see Theorem 2 and Theorem 3).

2) A (nearly) optimal excess risk bound for Nyström kernel $k$-means is also obtained when sampling $\Omega(\sqrt{nk})$ points (see Theorem 4). We further relax the restriction of landmark points from $\Omega(\sqrt{n}k)$ to $\Omega(\sqrt{n})$ (see Theorem 5) and extend it to general cases (see Theorem 6 and Theorem 7). This result shows that we can use the Nyström method to improve the effectiveness of kernel $k$-means, while guaranteeing the optimal generalization performance.

The rest of the paper is organized as follows. In Section 2, we introduce some notations and provide an overview of kernel $k$-means. In Section 3, we provide nearly optimal excess risk bounds. In Section 4, we quantify the statistical effect of computational approximations of the Nyström-based kernel $k$-means. In Section 5, we validate our theoretical findings by performing experiments on both simulated and real data. We end in Section 6 with conclusion. All the detailed proofs are deferred to the Appendix.

2 Background

In this section, we will introduce some notations and provide a brief introduction of kernel $k$-means. Please refer to [18, 9] for more details.

2.1 Notations

Assume $\mathbb{P}$ is a (unknown) distribution on $\mathcal{X}$, and $\mathcal{S} = \{x_i\}_{i=1}^n \in \mathcal{X}$ is a set of $n$ samples drawn i.i.d. from $\mathbb{P}$. The empirical distribution $\mathbb{P}_n$ is denoted as $\mathbb{P}_n(x) = \frac{1}{n}$ if $x \in \mathcal{S}$, otherwise 0. Let $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a Mercer kernel [51], and $\mathcal{H}$ be its associated RKHS [52], which is the completion of the linear span of the set of functions:

$$\mathcal{H} = \text{span}\{\kappa(x, \cdot), x \in \mathcal{X}\}.$$ We denote the Cartesian product of $\mathcal{H}$ by $\mathcal{H}^k = \bigotimes_{i=1}^k \mathcal{H}$. We use the feature map $\psi : \mathcal{X} \to \mathcal{H}$ to map $\mathcal{X}$ into the Hilbert space $\mathcal{H}$, and assume that $\mathcal{H}$ is separable, such that for any $x \in \mathcal{X}$, we have

$^1\tilde{O}$ hides logarithmic terms.
\[ \Phi_x = \psi(x). \] Intuitively, in the rest of the paper, the reader can assume that \( \Phi_x \in \mathbb{R}^d \) with \( d \gg n \) or even infinite. From here on, we will denote the inner product of \( H \) by \( \langle \cdot, \cdot \rangle \), and the associated norm by \( \| \cdot \| \), and assume that \( \| \Phi_x \| \leq 1 \) for any \( x \in X \). We let

\[ D = \{ \Phi_i = \psi(x_i) \}_{i=1}^n, \]

and denote \([K]_{i,j} = \kappa(x_i, x_j) = \langle \Phi_i, \Phi_j \rangle\) as the kernel matrix.

The notations \( \mu = \mathcal{O}(\nu) \) and \( \mu = \Omega(\nu) \) mean that there exist constants \( c, c_1, c_2 \) such that \( \mu \leq c\nu \) and \( c_1\nu \leq \mu \leq c_2\nu \), respectively. We use \( \mathcal{O} \) and \( \Omega \) to hide logarithmic terms.

### 2.2 Kernel k-Means

In this paper, we aim at partitioning the given dataset into \( k \) disjoint clusters, each characterized by its centroid \( c_j \). The Voronoi cell associated with a centroid \( c_j \) is defined as \([9]\)

\[ C_j := \left\{ i : j = \arg \min_{s=1, \ldots, k} \| \Phi_i - c_s \|^2 \right\}. \]

Let \( C = [c_1, \ldots, c_k] \) be a collection of \( k \) centroids from \( H^k \). In this paper, we focus on the so-called *kernel k-means clustering*, by minimizing the empirical squared norm criterion

\[ \mathcal{W}(C, \mathbb{P}_n) := \frac{1}{n} \sum_{i=1}^n \min_{j=1, \ldots, k} \| \Phi_i - c_j \|^2 \]

over all possible choices of cluster centers \( C \in H^k \). From \([18][9]\), we know that \( \mathcal{W}(C, \mathbb{P}_n) \) can be written as

\[
\mathcal{W}(C, \mathbb{P}_n) := \frac{1}{n} \min_{C \in H^k} \sum_{j=1}^k \sum_{i \in C_j} \left( \theta_j - \frac{1}{|C_j|} \sum_{t \in C_j} \theta_t \right)^2 \\
= \frac{1}{n} \min_{C \in H^k} \sum_{j=1}^k \sum_{i \in C_j} \left( \kappa(x_i, x_j) - \frac{2}{|C_j|} \sum_{t \in C_j} \kappa(x_i, x_t) + \frac{1}{|C_j|^2} \sum_{t,t' \in C_j} \kappa(x_t, x_{t'}) \right).
\]

The *empirical risk minimizer* (ERM) is defined as

\[ C_n := \arg \min_{C \in H^k} \mathcal{W}(C, \mathbb{P}_n). \]

The performance of a clustering scheme given by the collection \( C = [c_1, \ldots, c_k] \in H^k \) of cluster centers is usually measured by the *expected squared norm criterion* or *expected clustering risk*

\[ \mathcal{W}(C, \mathbb{P}) := \int \min_{j=1, \ldots, k} \| \Phi_x - c_j \|^2 d\mathbb{P}(x). \]

Given a \( C \in H^k \), let \( f_C = (f_{c_1}, \ldots, f_{c_k}) \) be a \( k \)-valued function of the collection \( C \) with \( f_{c_j}(x) = \| \Phi_x - c_j \|^2 \). Let \( \varphi : \mathbb{R}^k \to \mathbb{R} \) be a minimum function. From the definition of \( \varphi(f_C(x)) = \min(f_{c_1}(x), \ldots, f_{c_k}(x)) \), one can see that the empirical and expected squared norm criteria can be respectively written as

\[
\mathcal{W}(C, \mathbb{P}_n) := \frac{1}{n} \sum_{i=1}^n \varphi(f_C(x_i)) \quad \text{and} \quad \mathcal{W}(C, \mathbb{P}) := \int \varphi(f_C(x)) d\mathbb{P}(x).
\]

In this paper, we consider bounding the *excess clustering risk* \( \mathcal{E}(C_n) \) of the empirical risk minimizer \([16]\):

\[ \mathcal{E}(C_n) := \mathbb{E}_D [\mathcal{W}(C_n, \mathbb{P})] - \mathcal{W}^*(\mathbb{P}), \]

where \( \mathcal{W}^*(\mathbb{P}) = \inf_{C \in H^k} \mathcal{W}(C, \mathbb{P}) \) is the optimal clustering risk. In the following, we will ignore the subscript \( D \) if the input dataset \( D \) is clear.
2.3 The Existing Excess Clustering Risk Bounds

According to [7], we know that there exists a collection of centroids \( C_{lb} \in \mathcal{H}^k \), a constant \( c \), and a distribution \( \mathbb{P} \) with \( \|\Phi_\mathbf{x}\| \leq 1 \) for any \( \mathbf{x} \in \mathcal{X} \), such that

\[
\mathbb{E}[\mathcal{W}(C_{lb}, \mathbb{P})] - \mathcal{W}^*(\mathbb{P}) \geq c\sqrt{\frac{k^{1-4/d}}{n}}.
\]

Note that \( d \) is the dimension of \( \Phi_\mathbf{x} \), which is usually very large or even infinite. Thus, the lower bound of kernel \( k \)-means is \( \Omega(\sqrt{k/n}) \). However, most of the existing risk bounds proposed for kernel \( k \)-means are \( O(k/\sqrt{n}) \) [16 10 41 20 9], for example:

**Lemma 1** ([16, Theorem 2.1]). If \( \|\Phi_\mathbf{x}\| \leq 1 \) for any \( \mathbf{x} \in \mathcal{X} \), then there exists a constant \( c \) such that

\[
\mathbb{E}[\mathcal{W}(C_n, \mathbb{P})] - \mathcal{W}^*(\mathbb{P}) \leq c\sqrt{\frac{k}{n}},
\]

where \( C_n \) is the ERM of \( \mathcal{W}(C, \mathbb{P}) \) defined in [2].

Note that the number of clusters \( k \) may be very large for fine-grained analyses in social networks or recommendation systems. This leaves us with the question: is it possible to prove a bound of rate \( \sqrt{k/n} \), which is (nearly) optimal in terms of both \( k \) and \( n \)? In this paper, we attempt to answer this.

3 Main Results

In this section, we will provide nearly optimal excess risk bounds for kernel \( k \)-means. There are very few works focus on the underlying excess risk problem for kernel \( k \)-means. To the best of our knowledge, there are only two results [16 9] providing excess risk bounds for kernel \( k \)-means or approximate kernel \( k \)-means. However, these bounds of [16 9] are all linearly dependent on \( k \). Based on a recently improvement of the upper bound of Rademacher complexity of \( L \)-Lipschitz with respect to the \( L_\infty \) norm [21], we derive a (nearly) optimal excess risk bound of linearly dependent on \( \sqrt{k} \).

**Theorem 1.** If \( \forall \mathbf{x} \in \mathcal{X}, \|\Phi_\mathbf{x}\| \leq 1 \), then for any \( \delta \in (0, 1) \), there exists a constant \( c \), and with probability at least \( 1 - \delta \), we have,

\[
\mathbb{E}[\mathcal{W}(C_n, \mathbb{P})] - \mathcal{W}^*(\mathbb{P}) \leq c \left( \sqrt{\frac{k}{n} \log^2 (\sqrt{n})} + \sqrt{\frac{\log \frac{1}{\delta}}{n}} \right).
\]

From Theorem[1] we know that

\[
\mathbb{E}[\mathcal{W}(C_n, \mathbb{P})] - \mathcal{W}^*(\mathbb{P}) \leq \tilde{O} \left( \sqrt{\frac{k}{n}} \right),
\]

which matches the theoretical lower bound \( \Omega(\sqrt{k/n}) \) when \( d \) is large [7]. Thus, our proposed bound is (nearly) optimal.

**Remark (Fast Rates).** Some results suggest that the learning rate of kernel \( k \)-means can reach \( O(k/n) \) under certain assumptions on the distribution. Chou [13] pointed out that, if continuous densities of distribution satisfy certain regularity properties, the expected excess risk is of rate \( O(k/n) \). An improved result was obtained by [3], who proved that the learning rate can reach \( O(k/n) \) for any distribution supported on a finite set. Levrard [27] further showed that, if the distribution satisfies a margin condition, the learning rate can also reach \( O(k/n) \). Based on the notion of local Rademacher complexity, the expected excess risk has a rate faster than \( O(k/\sqrt{n}) \) given in [24 30]. However, as pointed out, these conditions are difficult to verify in general. Moreover, these expected excess risk bounds are linearly dependent on \( k \). In the future, we will consider studying whether it is possible to prove a bound of \( O(\sqrt{k/n}) \) under certain strict assumptions.

3.1 Further Results: Beyond ERM

So far we have provided guarantees for \( C_n \), that is, the optimal ERM in \( \mathcal{H}^k \). Note that obtaining the optimal ERM \( C_n \) is a NP-hard problem in general [2]. In the following, we will consider the risk bound for a general \( \tilde{C}_n \), which only requires that its empirical squared norm criterion is not far from that of \( C_n \).
Theorem 2. If \( \forall x \in \mathcal{X}, \| \phi_x \| \leq 1 \) and
\[
\mathbb{E} \left[ W(\mathcal{C}_n, \mathbb{P}_n) - W(\mathcal{C}_n, \mathbb{P}_n) \right] \leq \zeta,
\]
then for any \( \delta \in (0, 1) \), there exists a constant \( c \) and, with probability at least \( 1 - \delta \), we have
\[
\mathbb{E}[W(\tilde{\mathcal{C}}_n, \mathbb{P})] - W^*(\mathbb{P}) \leq c\sqrt{\frac{k}{n}} \log^2 (\sqrt{n}) + c\sqrt{\frac{\log \frac{1}{\delta}}{n}} + \zeta.
\]

From the above theorem, one can see that if the discrepancy between the empirical squared norm criterion of \( \mathcal{C}_n \) and \( \mathcal{C}_n \) is small, that is \( \zeta \leq O(\sqrt{k/n}) \), the risk bound of \( \mathcal{C}_n \) is (nearly) optimal.

3.2 Further Results: \( k \)-means++

Lloyd’s algorithm [40] is the most popular \( k \)-means algorithm and when coupled with a careful \( k \)-means++ seeding [41], a good approximate solution \( \tilde{\mathcal{C}}_n \) can be obtained. Recently, based on a simple combination of \( k \)-means++ sampling and a local search strategy, an improved \( k \)-means++ algorithm was proposed [23]. It was shown that the empirical squared norm criterion of \( \mathcal{C}_n \) can be up to a constant factor from the optimal empirical solution. For the completeness, we briefly describe the improved \( k \)-means++ in the following, please refer to [23] for more details.

1: If \( |C| < k \), add a sampled point \( x \in S \) with probability
\[
\frac{\text{cost}\{\psi(x), C\}}{\sum_{x \in S} \text{cost}\{\psi(x), C\}}, \quad \text{where } \text{cost}(P, C) = \sum_{x_i \in P} \min_{c \in C} \| \phi_{x_i} - c \|,
\]
and add \( \psi(x) \) to \( \mathcal{C} \).

2: If \( |C| \geq k \), sample \( x \in S \) with probability
\[
\frac{\text{cost}\{\psi(x), C\}}{\sum_{x \in S} \text{cost}\{\psi(x), C\}}, \quad \text{check whether there exists a point } c \in C \text{ such that}
\]
\[
\text{cost}(S, C \setminus \{c\} \cup \{\psi(x)\}) < \text{cost}(S, C).
\]
If this is the case, we replace \( c \) by the point in \( C \) that reduces the cost function by the largest amount.

Note that we use the algorithm from [23] for kernel \( k \)-means by replacing the Euclidean distance \( \| x_i - x_j \|^2 \) with \( \| \phi_{x_i} - \phi_{x_j} \|^2_H = \kappa(x_i, x_i) - 2\kappa(x_i, x_j) + \kappa(x_j, x_j) \).

Lemma 2 ([23]). If \( \mathcal{C}^n_A \) is returned by the improved \( k \)-means++ algorithm with a local search strategy [23], then
\[
\mathbb{E}_A[W(\mathcal{C}^n_A, \mathbb{P}_n)] \leq \beta \cdot W(\mathcal{C}_n, \mathbb{P}_n),
\]
where \( \beta \) is a constant and \( A \) is the randomness derived from the \( k \)-means++ initialization.

In the following, we derive a risk bound for \( \mathcal{C}^n_A \).

Theorem 3. If \( \forall x \in \mathcal{X}, \| \phi_x \| \leq 1 \), and \( \mathcal{C}^n_A \) is returned by the improved \( k \)-means++ algorithm with a local search strategy [23], then for any \( \delta \in (0, 1) \), with a probability at least \( 1 - \delta \), we have
\[
\mathbb{E}_D \left[ \mathbb{E}_A[W(\mathcal{C}^n_A, \mathbb{P})] \right] \leq O\left(\sqrt{\frac{k}{n}} + W^*(\mathbb{P})\right).
\]
The above result implies that if the optimal clustering risk \( W^*(\mathbb{P}) \) is small, the risk of \( W(\mathcal{C}^n_A, \mathbb{P}) \) can reach \( O(\sqrt{k/n}) \).

4 Risk Analysis of Nyström Kernel \( k \)-Means

Kernel \( k \)-means is one of the most popular clustering methods. However, it requires the computation of a \( n \times n \) kernel matrix. This renders it non-scalable to large datasets that contain more than a few
We can use any kernel $\tilde{\Phi}$ where $\tilde{\Phi} : \mathcal{X} \rightarrow \mathbb{R}^d$.

The Nyström method [19] is a popular method for approximating the kernel matrix. The properties of Nyström approximations for kernel $k$-means have recently been studied in [11 15 43 9 53 59]. However, most of these works focus on the computation area. To the best of our knowledge, the only study providing excess risk guarantees for the Nyström kernel $k$-means is [9]. However, its excess risk bound is linearly dependent on $k$. In the following, we will improve it from $k$ to $\sqrt{k}$.

### 4.1 Nyström Kernel $k$-Means

To derive the excess risk bound of Nyström kernel $k$-means, we first briefly introduce some notations. Given a dataset $\mathcal{D} = \{\Phi_i\}^n_{i=1}$, we use

$$\mathcal{I} = \{\Phi_i\}^m_{i=1} \subseteq \mathcal{D}$$

as a collection of landmark points to replace $\mathcal{D}$. Let $\mathcal{H}_m$ be a linear span of $\mathcal{I} = \{\Phi_i\}^m_{i=1}$,

$$\mathcal{H}_m = \operatorname{span}\left\{\sum_{i=1}^m \alpha_i \Phi_i, \alpha_i \in \mathbb{R}, \Phi_i \in \mathcal{I}\right\},$$

and $\mathcal{H}^k_m = \otimes_{i=1}^k \mathcal{H}_m$ be its Cartesian product. The Nyström kernel $k$-means, i.e., the approximate kernel $k$-means over $\mathcal{H}^k_m$, can be written as [9]:

$$C_{n,m} = \arg \min_{C \in \mathcal{H}^k_m} \frac{1}{n} \sum_{i=1}^n \min_{j=1,\ldots,k} \|\Phi_i - c_j\|^2. \tag{3}$$

The centroids $C_{n,m}$ are still point in $\mathcal{H}^k_m \subset \mathcal{H}$. Let $K_{m,m} \in \mathbb{R}^{m \times m}$ be the empirical kernel matrix between all points in $\mathcal{I}$, and its eigen-decomposition is $K_{m,m} = U \Lambda U$. From [9], we can search over $C_{n,m} \in \mathbb{R}^{m \times k}$ instead of searching over $C \in \mathcal{H}^k_m$, that is,

$$\tilde{C}_{n,m} = \arg \min_{C \in \mathbb{R}^{m \times k}} \frac{1}{n} \sum_{i=1}^n \min_{j=1,\ldots,n} \|\tilde{\Phi}_i - \tilde{c}_j\|^2, \tag{4}$$

where $\tilde{\Phi}_i := \Lambda^{-1/2} U^T \Phi_i^T \Phi_i$, $\tilde{c}_j := \Lambda^{-1/2} U^T \tilde{\Phi}_i^T c_j$, $\Phi_i^m = \begin{bmatrix} \Phi_{\pi(1)}, \ldots, \Phi_{\pi(m)} \end{bmatrix}$, $\pi(i) \in [1, m]$. We can use any $k$-means algorithms to solve Eq.4 and then use the reverse of the relationship $c_j := \Lambda^{-1/2} U^T \tilde{\Phi}_i^T \tilde{c}_j$ to bring back the solution to $\mathcal{H}_m$, i.e., $C_{n,m} = \Phi_m^U \Lambda^{-1/2} \tilde{C}_{n,m}$. This can be done in $O(nm)$ space and $O(nm^2 + nm^2)$ time using $t$ steps of Lloyd’s algorithm for $k$ clusters [40]. Please refer to [9] for more details.

### 4.2 Excess Risk Bound of Nyström Kernel $k$-Means

Denote with $\Xi = \operatorname{Tr}(K^T(K + I)^{-1})$ the so-called effective dimension of $K$ [49 9]. Note that

$$\operatorname{Tr}(K^T(K + I)^{-1}) \leq \operatorname{Tr}(K^T K)^+,$$

so we can obtain that $\Xi \leq \operatorname{Rank}(K)$. Thus, the effective dimension $\Xi$ can be seen as a soft version of the rank.

**Theorem 4.** If $\forall x \in X$, $\|\Phi_x\| \leq 1$, and the size of a uniform sampling is

$$m \geq \Omega\left(\frac{\sqrt{n} \log(1/\delta) \min(k, \Xi)}{\sqrt{k}}\right),$$

then, with probability at least $1 - \delta$, we have

$$\mathbb{E}[\mathcal{W}(C_{n,m}, P)] - \mathcal{W}^*(P) \leq O\left(\sqrt{\frac{k}{n}} \log \left(\frac{n}{\delta}\right)\right).$$
Note that
\[ \sqrt{n \min(k, \Xi)} \sqrt{k} \leq \sqrt{nk}. \]

Thus, from a statistical point, Theorem 4 shows that when sampling \( \tilde{\Omega}(\sqrt{nk}) \) points, the Nyström kernel \( k \)-means achieves the same excess risk as the exact one does. This result demonstrates that we can improve the computational aspect of kernel \( k \)-means using Nyström embedding, while maintaining optimal generalization guarantees.

**Remark.** Calandriello and Rosasco [9] have reported that if \( m \geq \tilde{\Omega}(\sqrt{n}) \), an excess risk bound of rate \( \tilde{O}(k/\sqrt{n}) \) for Nyström kernel \( k \)-means can be obtained, which seems to be better than our \( \tilde{\Omega}(\sqrt{nk}) \). However, it should be noted that the risk bound in [9] is linearly dependent on \( k \), while ours is linearly dependent on \( \sqrt{k} \). From the proof of Lemma 10, if we want to obtain a risk of linear dependence on \( k \), we only need
\[ m \geq \Omega \left( \sqrt{n \log(1/\delta)} \min(k, \Xi) \right) = \tilde{\Omega}(\sqrt{n}), \]
which is the same as [9]. In the following, we will show that we can relax the restriction of landmark points under a mild condition.

### 4.3 Further Results: Reducing the Sampling Points

From Theorem 4, we know that we need \( \tilde{\Omega}(\sqrt{nk}) \) sampling points to guarantee the nearly optimal rate for approximating kernel \( k \)-means. In the following, we show how to reduce the sampling points from \( \tilde{\Omega}(\sqrt{nk}) \) to \( \tilde{\Omega}(\sqrt{n}) \) under a basic assumption on the eigenvalues of the kernel matrix.

**Theorem 5.** Let \( \lambda_i \) be the \( i \)-th eigenvalue of the kernel matrix \( K \), \( i = 1, \ldots, n \), and \( \lambda_{i+1} \leq \lambda_i \). If \( \forall x \in \mathcal{X}, \|\Phi x\| \leq 1 \), the eigenvalues satisfy the assumption
\[ \exists \alpha > 1, c > 0 : \lambda_i \leq ci^{-\alpha}, \]
and the size of an uniform sampling is
\[ m \geq \Omega \left( \sqrt{n \log(1/\delta)} \right) \left( \frac{\min(k, \Xi)}{k} \right) \]
then, with probability at least \( 1 - \delta \), we have
\[ \mathbb{E}[\mathcal{W}(\tilde{C}_{n,m}, \mathbb{P}_n) - \mathcal{W}^{*}(\mathbb{P})] \leq \tilde{O} \left( \sqrt{\frac{k}{n} \log \left( \frac{n}{\delta} \right)} \right). \]

The assumption of algebraically decreasing eigenvalues of the kernel matrix is a common assumption, and met by the popular finite rank kernels and shift invariant kernel [54], for example. The above results show that we can guarantee the optimal generalization performance when only sampling \( \tilde{\Omega}(\sqrt{n}) \) points, which is much better than \( \tilde{\Omega}(\sqrt{nk}) \) when \( k \) is large.

### 4.4 Further Results: Beyond ERM

In the following, we show that our result can be extended to general cases beyond ERM.

**Theorem 6.** Under the same assumptions as Theorem 5 if
\[ \mathbb{E}[\mathcal{W}(\tilde{C}_{n,m}, \mathbb{P}_n) - \mathcal{W}(C_{n,m}, \mathbb{P}_n)] \leq \zeta, \]
and the size of an uniform sampling is
\[ m \geq \Omega \left( \sqrt{n \log(1/\delta)} \right), \]
then, with probability at least \( 1 - \delta \), we have
\[ \mathbb{E}[\mathcal{W}(\tilde{C}_{n,m}, \mathbb{P}) - \mathcal{W}^{*}(\mathbb{P})] \leq \tilde{O} \left( \sqrt{\frac{k}{n} \log \left( \frac{n}{\delta} \right)} + \zeta \right). \]

The above result demonstrates that the risk bound of \( \tilde{C}_{n,m} \) is optimal when \( \mathbb{E}[\mathcal{W}(\tilde{C}_{n,m}, \mathbb{P}_n) - \mathcal{W}(C_{n,m}, \mathbb{P}_n)] \) is small.
4.5 Further Results: \textit{k}-means ++

If adopting the improved \textit{k}-kernel means++ sampling with a local search strategy \cite{25} for Nyström kernel \textit{k}-means, we can obtain the following results:

**Theorem 7.** Under the same assumptions as Theorem 5, \( C_{n,m}^A \) is returned by the improved \textit{k}-means++ algorithm with a local search strategy \cite{25}, if the size of an uniform sampling is

\[
m \geq \Omega \left( \sqrt{n \log(1/\delta)} \right),
\]

then with probability at least \( 1 - \delta \), we have

\[
\mathbb{E}_D \left[ \mathbb{E}_A[\mathcal{W}(C_{n,m}^A, \mathbb{P})] \right] \leq \tilde{O} \left( \sqrt{\frac{k}{n}} + \mathcal{W}^*(\mathbb{P}) \right),
\]

where \( A \) is the randomness derived from the \textit{k}-means++ initialization.

The above result implies that if the optimal clustering risk \( \mathcal{W}^*(\mathbb{P}) \) is small, i.e. \( \mathcal{W}^*(\mathbb{P}) \leq \tilde{O}(\sqrt{k/n}) \), the risk of \( \mathcal{W}(C_{n,m}^A, \mathbb{P}) \) can reach \( \tilde{O}(\sqrt{k/n}) \).

5 Experiments

In this section, we will validate our theoretical findings by performing experiments on both simulated data and real data for kernel \textit{k}-means and approximate \textit{k}-means.

5.1 Numerical Experiments

In this subsection, we will validate our theoretical findings by performing experiments on simulated data for kernel \textit{k}-means and approximate \textit{k}-means.
Let $c_i^* \in \mathbb{R}^{10}$, $i = 1, \ldots, k$, be the clustering centers, where the values of the 10 dimensions are 1 or $-1$ with equal probability. We generate the $i$th clustering samples $C_i$ from the normal distribution with mean $c_i^*$ and variance 2, $|C_1| = \ldots = |C_k|$. In the experiments, we consider the popular Gaussian kernel

$$
\kappa(x, x') = \exp \left( -\frac{\|x - x'\|^2}{10} \right).
$$

Based on the above construction method, it is easy to verify that the optimal clustering risk is

$$
W^*(P) = \int \min_{j=1, \ldots, k} \|\Phi_x - \Phi_{c_j}\|^2 \, d\mathbb{P}(x) = \int \min_{j=1, \ldots, k} 2(1 - \kappa(x, c_j^*)) \, d\mathbb{P}(x).
$$

**Kernel $k$-Means**

In the first experiment, we validate our theoretical findings of kernel $k$-means. We generate $\sum_{i=1}^k |C_i|$ samples of $k$ clustering centers for training and 10,000 samples for testing. The empirical excess risk of kernel $k$-means on the test set can be written as

$$
\frac{\sum_{x \in D_t} \min_{j=1, \ldots, k} \|\Phi_{x_i} - \Phi_{c_j}\|^2 - \min_{j=1, \ldots, k} \|\Phi_{x_i} - \Phi_{c_j^*}\|^2}{|D_t|},
$$

where $C_n = [c_1, \ldots, c_k]$ is the solution returned by the kernel $k$-means using Lloyd’s algorithm [40], and $D_t$ is the test set.

The empirical excess errors of kernel $k$-means on the test set with different sizes of training data and numbers of $k$ are given in Figure 1. We can see that the line of best fit for empirical excess risks is $\frac{k^0.45}{n^{0.4}}$ for $k = 20$, $\frac{k^{0.52}}{n^{0.49}}$ for $k = 40$, $\frac{k^{0.49}}{n^{0.50}}$ for $k = 80$, and $\frac{k^{0.50}}{n^{0.50}}$ for $k = 160$, achieving the predicted rate $\frac{k^{0.5}}{n^{0.5}}$ (from Theorem 1), which verifies our theoretical findings.

**Approximate Kernel $k$-Means**

In the second experiment, we validate our theoretical findings of approximate kernel $k$-means on simulated data.
The data generation rule is the same as that in the kernel $k$-means. We generate 10,000 samples ($|\mathcal{C}_i| = 10000/k$) for training and 10,000 samples for testing. The empirical excess errors of the approximate kernel $k$-means on the test set with different uniform samplings $m$ are given in Figure 2, which can be summarized as follows:

1) There exists a lower bound of the sampling landmarks $l$ which does not decrease the error when increase its value. This verifies the theoretical statement in Theorem 4.

2) The lower bound of $l$ increases with the number of the clusters $k$. This result confirms Theorem 4 once again.

5.2 Real-World Scenarios

To reflect real-world scenarios, we add more experiments on the real data sets. We use 6 publicly available datasets, dna, segment, mushrooms, mnist, skin-nonskin and covtype, from the LIBSVM Data.

The empirical evaluations with Gaussian kernel

$$
\exp\left(-\frac{\|x - x'\|^2}{\sigma^2}\right), \sigma = \sqrt{\frac{\sum_{ij} \|x_i - x_j\|^2}{d}},
$$

are given in the following table [1] where $d$ is the dimension of $x \in \mathcal{X}$.

Table 1: Experiments on the real data sets with kernel $k$-means and Nyström kernel $k$-means ($m = 100$).

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Datasize</th>
<th>Kernel $k$-means</th>
<th>Nyström Kernel $k$-Means</th>
</tr>
</thead>
<tbody>
<tr>
<td>dna</td>
<td>2000</td>
<td>0.53</td>
<td>0.52</td>
</tr>
<tr>
<td>segment</td>
<td>2310</td>
<td>0.55</td>
<td>0.55</td>
</tr>
<tr>
<td>mushrooms</td>
<td>8124</td>
<td>0.66</td>
<td>0.65</td>
</tr>
<tr>
<td>mnist</td>
<td>60000</td>
<td>–</td>
<td>0.43</td>
</tr>
<tr>
<td>skin-nonskin</td>
<td>245057</td>
<td>–</td>
<td>0.63</td>
</tr>
<tr>
<td>covtype</td>
<td>581012</td>
<td>–</td>
<td>0.32</td>
</tr>
</tbody>
</table>

From the above results on real data sets, we can find that Nyström kernel $k$-means give the similar results as the original one, which also match the theoretical findings.

6 Conclusion

In this paper, we derive nearly optimal risk bounds for both kernel $k$-means and Nyström kernel $k$-means of learning rate of $O(\sqrt{k/n})$, which fills the gap ignoring the optimal risk bounds for (approximate) kernel $k$-means. Furthermore, we extend these results to general cases beyond ERM and $k$-means++. Our result may provide a new perspective to study the optimal statistical properties of unsupervised learning.

In this paper we only derived the risk bounds of learning rate $O(\sqrt{k/n})$ for the basic case. In the future, we will consider studying whether it is possible to prove a bound of $O(\sqrt{k/n})$ under certain strict assumptions.

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[^1]: [http://www.csie.ntu.edu.tw/~cjlin/libsvm](http://www.csie.ntu.edu.tw/~cjlin/libsvm)


References


