Scalable Kernel Clustering: Approximate Kernel \(k\)-means

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Abstract—Kernel-based clustering algorithms have the ability to capture the non-linear structure in real world data. Among various kernel-based clustering algorithms, kernel \(k\)-means has gained popularity due to its simple iterative nature and ease of implementation. However, its run-time complexity and memory footprint increase quadratically in terms of the size of the data set, and hence, large data sets cannot be clustered efficiently. In this paper, we propose an approximation scheme based on randomization, called the Approximate Kernel \(k\)-means. We approximate the cluster centers using the kernel similarity between a few sampled points and all the points in the data set. We show that the proposed method achieves better clustering performance than the traditional low rank kernel approximation based clustering schemes. We also demonstrate that its running time and memory requirements are significantly lower than those of kernel \(k\)-means, with only a small reduction in the clustering quality on several public domain large data sets. We then employ ensemble clustering techniques to further enhance the performance of our algorithm.

Index Terms—Clustering, Large Scale Clustering, Kernel Clustering, \(k\)-means, scalability, ensemble clustering, meta-clustering.

1 INTRODUCTION

Recent advances in data generation, collection and storage technologies have resulted in a digital data explosion. A study by IDC and EMC Corp \[1\] predicted the creation of 8 trillion gigabytes of digital data by the year 2015. Massive amounts of data are generated through online services like blogs, e-mails and social networks in the form of text, images, audio and video. Clustering is one of the principal tools to efficiently organize such large amounts of data and to enable convenient access. It has found use in a multitude of applications such as web search, social network analysis, image retrieval, medical imaging, gene expression analysis, recommendation systems and market analysis \[2\].

Most algorithms capable of clustering large data sets assume that the clusters in the data set are linearly separable and group the objects based on their pairwise Euclidean distances. On the other hand, kernel-based clustering algorithms employ a non-linear distance measure, defined in terms of a positive-definite kernel, to compute the similarity. The kernel function embeds the objects in a high-dimensional feature space, in which the clusters are more likely to be separable. Kernel clustering algorithms, therefore, have the ability to capture the non-linear structure in real world data sets and, thus, usually perform better than the Euclidean distance based clustering algorithms \[3\].

A number of kernel-based clustering methods such as spectral clustering \[4\], kernel Self-Organizing Maps (SOM) \[5\] and kernel neural gas \[6\] have been proposed. In this study, we focus on kernel \(k\)-means \[7\], \[8\] due to its simplicity and efficiency. In addition, several studies have established the equivalence of kernel \(k\)-means and other kernel-based clustering methods, suggesting that they yield similar results \[9\]–[11].

Kernel \(k\)-means \[7\], a non-linear extension of the classical \(k\)-means algorithm, replaces the Euclidean distance function \(d^2(x_a, x_b) = \|x_a - x_b\|^2\) employed in the \(k\)-means algorithm with a non-linear kernel distance function defined as

\[
d^2_k(x_a, x_b) = \kappa(x_a, x_a) + \kappa(x_b, x_b) - 2\kappa(x_a, x_b),
\]

where \(x_a \in \mathbb{R}^d\) and \(x_b \in \mathbb{R}^d\) are two data points and \(\kappa(\cdot, \cdot) : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}\) is the kernel function. While the kernel distance function enables the clustering algorithm to capture the non-linear structure in...
data, it requires computation and storage of an $n \times n$ kernel matrix in memory, where $n$ is the number of data points to be clustered. This renders kernel k-means non-scalable to data sets with more than a few thousands of data points, on a standard workstation. In this paper, we address the challenge posed by the large kernel matrix.

The Nystrom method for kernel approximation has been successfully employed in several learning problems [12]–[15]. The naive Nystrom approximation method [16] randomly samples a small number of points from the data set and computes a low rank approximation of the kernel matrix using the similarity between all the points and the sampled points. The spectral clustering algorithm was adapted to use this low rank approximate kernel [14], [17]–[19]. The clusters are found by approximating the top eigenvectors of the kernel using the similarity between a subset of randomly selected data points. The proposed algorithm, named Approximate kernel k-means (aKKm), follows along the idea of the Nystrom approximation and avoids computing the full $n \times n$ kernel matrix. We randomly select a subset of $m$ data points ($m \ll n$), and approximate the cluster centers using vectors in the subspace spanned by this subset. This approximation requires the computation and storage of only the $n \times m$ portion of the kernel matrix, leading to a significant speedup of kernel k-means. We demonstrate, both theoretically and empirically, that aKKm yields similar clustering performance as kernel k-means using the full kernel matrix. Unlike the spectral clustering algorithm based on the naive Nystrom extension [14], our method uses information from all the eigenvectors of the approximate kernel matrix (without explicitly computing them), thereby yielding more accurate clustering results. We further improve the efficacy of our algorithm through ensemble clustering methods.

2 BACKGROUND

We first briefly describe some of the related work on large scale clustering and kernel-based clustering, and then outline the kernel k-means algorithm.

2.1 Large scale clustering

A number of methods have been developed to efficiently cluster large data sets. Incremental clustering [20], [21] and divide-and-conquer based clustering algorithms [22], [23] were designed to operate in a single pass over the data points, thereby reducing the time required for clustering. Sampling based methods, such as CLARA [24] and CURE [25], reduce the computation time by finding the cluster centers based on a small number of randomly selected data points. The coreset algorithms [26] represent the data set using a small set of core data points and find the cluster centers using only these core data points. Clustering algorithms such as BIRCH [27] and CLARANS [28] improve the clustering efficiency by summarizing the data set into data structures like trees and graphs, thus enabling efficient data access.

With the evolution of cloud computing, parallel processing techniques for clustering are gaining popularity [29], [30]. These techniques speedup the clustering process by first dividing the task into a number of independent sub-tasks that can be performed simultaneously, and then efficiently merging these solutions into the final solution. For instance, in [30], the MapReduce framework [31] is employed to speedup the k-means and the k-median clustering algorithms. The data set is split among many processors and a small representative data sample is obtained from each of the processors. These representative data points are then clustered to obtain the cluster centers or medians.

2.2 Kernel-based clustering

Most of the existing methods for large scale clustering compute the pairwise dissimilarities between the data points using the Euclidean distance measure. As a result, they cannot accurately cluster data sets that are not linearly separable. Kernel based clustering techniques address this limitation by employing a non-linear kernel distance function to capture the non-linear structure in data [3]. Various kernel-based clustering algorithms have been developed, including kernel k-means [7], [8], spectral clustering [4], kernel SOM [5] and kernel neural gas [6].

Scalability is a major challenge faced by all the kernel-based algorithms, as they require computation of the full kernel matrix whose size is quadratic in the number of data points. To the best of our knowledge, only a few attempts have been made to scale kernel clustering algorithms to large data sets. In [32], the memory requirement is reduced by dividing the kernel matrix into blocks and using one block of the kernel matrix at a time. Although this technique handles the memory complexity, it still requires the computation of the full kernel matrix. The leaders clustering algorithm is integrated with kernel k-means to reduce its computational complexity in [33]. However, this method is data order-dependent and does not always produce accurate
results. Sampling methods, such as the Nyström method \cite{15}, have been employed to obtain low rank approximation of the kernel matrix to address this challenge \cite{14, 18}. In \cite{34}, random projection is combined with sampling to further improve the clustering efficiency. However, these methods rely on the approximation of the top eigenvectors of the kernel matrix. In our method, we propose to use the approximate kernel matrix directly to find the clusters and show that this leads to more accurate clustering of the data.

2.3 Kernel k-means

Let $X = \{x_1, x_2, ..., x_n\}$ be the input data set consisting of $n$ data points, where $x_i \in \mathbb{R}^d$, $C$ be the number of clusters and $K \in \mathbb{R}^{n \times n}$ be the kernel matrix with $K_{ij} = \kappa(x_i, x_j)$, where $\kappa(\cdot, \cdot)$ is the kernel function. Let $\mathcal{H}_K$ be the Reproducing Kernel Hilbert Space (RKHS) endowed by the kernel function $\kappa(\cdot, \cdot)$, and $\| \cdot \|_{\mathcal{H}_K}$ be the functional norm for $\mathcal{H}_K$. The objective of kernel k-means is to minimize the clustering error, defined as the sum of squared distances between the data points and the center of the cluster to which each point is assigned. Hence, the kernel k-means problem can be cast as the following optimization problem \cite{11}:

$$
\min_{U} \max_{\{c_k(\cdot) \in \mathcal{H}_K\}_{k=1}^C} \sum_{i=1}^n \sum_{k=1}^C U_{ki}^2 \kappa(x_i, \cdot) - \kappa(x_i, c_k(\cdot))_{\mathcal{H}_K}, \tag{1}
$$

where $U = (u_1, \ldots, u_C)^\top$ is the cluster membership matrix, $c_k(\cdot) \in \mathcal{H}_K$, $k \in [C]$ are the cluster centers, and domain $\mathcal{P} = \{U \in \{0,1\}^{C \times n} : U^\top 1 = 1\}$, where 1 is a vector of all ones. Let $n_k = u_k^\top 1$ be the number of data points assigned to the $k$th cluster, and

$$
\hat{U} = (\hat{u}_1, \ldots, \hat{u}_C)^\top = [\text{diag}(n_1, \ldots, n_C)]^{-1} U,
$$

$$
\tilde{U} = (\hat{u}_1, \ldots, \hat{u}_C)^\top = [\text{diag}(\sqrt{n_1}, \ldots, \sqrt{n_C})]^{-1} U,
$$

denote the $\ell_1$ and $\ell_2$ normalized membership matrices, respectively.

The problem in (1) can be relaxed to the following optimization problem over $U$ \cite{11}:

$$
\min_{U} \text{tr}(K) - \text{tr}(UKK^\top), \tag{2}
$$

and the optimal cluster centers found using

$$
c_k(\cdot) = \sum_{i=1}^n \hat{U}_{ki} \kappa(x_i, \cdot), k \in [C]. \tag{3}
$$

As indicated in (2), a naive implementation of kernel k-means requires computation and storage of the full $n \times n$ kernel matrix $K$, restricting its scalability. The objective of our work is to reduce the computational complexity and the memory requirements of kernel k-means.

3 Approximate Kernel k-means

A simple and naive approach for reducing the complexity of kernel k-means is to randomly sample $m$ points from the data set to be clustered, and find the cluster centers based only on the sampled points; then assign every unsampled data point to the cluster whose center is nearest. We refer to this two-step process as the two-step kernel k-means (tKKm), detailed in Algorithm \ref{algorithm}. Though this approach has reduced run-time complexity and memory requirements, its performance does not match that of the kernel k-means algorithm, unless it is provided with a sufficiently large sample of data points.

We propose a superior approach for reducing the complexity of kernel k-means based on the fact that kernel k-means requires the full $n \times n$ kernel matrix $K$ only because the the cluster centers $\{c_k(\cdot), k \in [C]\}$ are represented as linear combinations of all the data points to be clustered (see (3)) \cite{35}. In other words, the cluster centers lie in the space spanned by all the data points, i.e., $c_k(\cdot) \in \mathcal{H}_K = \text{span}(\kappa(x_1, \cdot), \ldots, \kappa(x_n, \cdot)), k \in [C]$. We can avoid computing the full kernel matrix if we restrict the cluster centers to a smaller subspace $\mathcal{H}_b \subset \mathcal{H}_K$. $\mathcal{H}_b$ should be constructed such that (i) $\mathcal{H}_b$ is small enough to allow efficient computation, and (ii) $\mathcal{H}_b$ is rich enough to yield similar clustering results as those obtained using $\mathcal{H}_K$. We employ a simple approach of randomly sampling $m$ data points ($m \ll n$), denoted by $\tilde{X} = \{\tilde{x}_1, \ldots, \tilde{x}_m\}$, and construct the subspace $\mathcal{H}_b = \text{span}(\tilde{x}_1, \ldots, \tilde{x}_m)$. Given the subspace $\mathcal{H}_b$, we modify (1) as

$$
\min_{U} \max_{\{c_k(\cdot) \in \mathcal{H}_b\}_{k=1}^C} \sum_{i=1}^n \sum_{k=1}^C U_{ki}^2 \kappa(x_i, \cdot) - \kappa(x_i, c_k(\cdot))_{\mathcal{H}_b}, \tag{4}
$$

Let $K_B \in \mathbb{R}^{m \times m}$ represent the kernel similarity matrix between data points in $X$ and the sampled data points in $\tilde{X}$, and $\hat{K}_B \in \mathbb{R}^{m \times m}$ represent the kernel similarity between the sampled data points. The following lemma allows us to reduce (4) to an optimization problem involving only the cluster membership matrix $U$.

**Lemma 1.** Given the cluster membership matrix $U$, the optimal cluster centers in (4) are given by

$$
c_k(\cdot) = \sum_{i=1}^m \alpha_{ki} \kappa(\tilde{x}_i, \cdot), \tag{5}
$$

where $\alpha = \hat{U} K_B \hat{K}_B^{-1}$. The optimization problem for $U$ is given by

$$
\min_{U} \text{tr}(K) - \text{tr}(\tilde{U} K_B \hat{K}_B^{-1} \hat{K}_B \tilde{U}^\top), \tag{6}
$$

Proof: Let $\phi_i = (\kappa(x_i, \tilde{x}_1), \ldots, \kappa(x_i, \tilde{x}_m))$ and $\alpha_i = (\alpha_{i1}, \ldots, \alpha_{im})$ be the $i$-th rows of matrix-
By minimizing over $\alpha$ respectively. As $c_k(\cdot) \in \mathcal{H}_b = \text{span}(\tilde{x}_1, \ldots, \tilde{x}_m)$, we can write $c_k(\cdot)$ as

$$c_k(\cdot) = \sum_{i=1}^{m} \alpha_k \kappa(\tilde{x}_i, \cdot).$$

and write the objective function in (9) as

$$\sum_{k=1}^{C} \sum_{i=1}^{n} \hat{U}_{ki} |c_k(\cdot) - \kappa(x_i, \cdot)|^2 = \text{tr}(K) + \sum_{k=1}^{C} \left( \alpha_k \alpha_k^\top \hat{K} \alpha_k - 2 \alpha_k^\top K_B \alpha_k \right).$$

By minimizing over $\alpha_k$, we have

$$\alpha_k = (\hat{K}^{-1}K_B \hat{\alpha}_k, k \in [C])$$

and therefore, $\alpha = \hat{U}K_B \hat{K}^{-1}$. We complete the proof by substituting the expression for $\alpha$ into (7).

As indicated by Lemma 1, we need to compute only $K_B$ for finding the cluster memberships. When $m \ll n$, this computational cost is significantly smaller than that of computing the full kernel matrix. On the other hand, when $m = n$, i.e., all the data points are selected for constructing the subspace $\mathcal{H}_b$, we have $\hat{K} = K_B = K$ and the problem in (6) reduces to (2). We refer to the proposed algorithm as Approximate Kernel k-means (aKKm), outlined in Algorithm 2. Fig. 4 illustrates and compares this algorithm with tKKm on a 2-dimensional synthetic data set. Note that the problem in (6) can also be viewed as approximating the kernel matrix $K$ in (4) by $K_B \hat{K}^{-1}K_B^*$, which is essentially the Nyström method for low rank matrix approximation. However, our method offers two advantages over previous learning methods which employ the Nyström approximation. Firstly, we do not need to explicitly compute the top eigenvectors of the approximate kernel matrix, resulting in a higher speedup over kernel k-means. Secondly, our method uses the approximate kernel matrix directly to estimate the clusters instead of the top eigenvectors. We demonstrate through our analysis that this leads to a more accurate solution than that obtained by the earlier methods.

2. $\hat{K}$ is part of $K_B$ and therefore does not need to be computed separately.

Algorithm 1 Two-step Kernel k-means (tKKm)

Input:
- $X = (x_1, \ldots, x_n)$: the set of $n$ data points to be clustered
- $\kappa(\cdot, \cdot) : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$: kernel function
- $m$: the number of randomly sampled data points ($m \ll n$)
- $C$: the number of clusters

Output: Cluster membership matrix $U \in \{0,1\}^{C \times n}$

1: Randomly select $m$ data points from $X$, denoted by $\tilde{X} = (\tilde{x}_1, \ldots, \tilde{x}_m)$.
2: Compute the cluster centers, denoted by $c_k(\cdot), k \in [C]$, by applying kernel k-means to $\tilde{X}$.
3: for $i = 1, \ldots, n$ do
4: Update the $i^{th}$ column of $U$ by $U_{ki} = 1$ where $k_i = \arg\min_{k \in [C]} |c_k(\cdot) - \kappa(x_i, \cdot)|$
5: end for

Algorithm 2 Approximate Kernel k-means (aKKm)

Input:
- $X = (x_1, \ldots, x_n)$: the set of $n$ data points to be clustered
- $\kappa(\cdot, \cdot) : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$: kernel function
- $m$: the number of randomly sampled data points ($m \ll n$)
- $C$: the number of clusters
- MAXITER: maximum number of iterations

Output: Cluster membership matrix $U \in \{0,1\}^{C \times n}$

1: Randomly sample $m$ data points from $X$, denoted by $\hat{X} = (\hat{x}_1, \ldots, \hat{x}_m)$.
2: Compute $K_B = [\kappa(x_i, \hat{x}_j)]_{n \times m}$ and $\hat{K} = [\kappa(\hat{x}_i, \hat{x}_j)]_{m \times m}$.
3: Compute $T = K_B \hat{K}^{-1}$.
4: Randomly initialize the membership matrix $U$.
5: Set $t = 0$.
6: repeat
7: Set $t = t + 1$.
8: Compute the $\ell_1$ normalized membership matrix $\hat{U}$ by $\hat{U} = \text{diag}(U^\top)^{-1} U$.
9: Calculate $\alpha = \hat{U} T$.
10: for $i = 1, \ldots, n$ do
11: Update the $i^{th}$ column of $U$ by $U_{ki} = 1$ where $k_i = \arg\min_{k \in [C]} |\alpha_k - \kappa(x_i, \cdot)|$
where $\alpha_j$ and $\kappa$ are the $j^{th}$ rows of matrices $\alpha$ and $K_B$, respectively.
12: end for
13: until the membership matrix $U$ does not change or $t > \text{MAXITER}$

4 Ensemble Approximate Kernel k-means

We improve the quality of the aKKm solution by using ensemble clustering.

The objective of ensemble clustering [36] is to combine multiple partitions of the given data set. A popular ensemble clustering algorithm is the Meta-Clustering algorithm (MCLA) [37], which maximizes the average normalized mutual information. It is based on hypergraph partitioning. Given $r$ cluster membership matrices, $\{U^1, \ldots, U^r\}$, where $U^q = (u^q_1, \ldots, u^q_n)^\top$, the objective of this algorithm is to find a consensus membership matrix $U^{(e)}$ that maximizes the Average Normalized Mutual
Information, defined as

\[ ANMI = \frac{1}{r} \sum_{q=1}^{r} NMI(U^{(c)}, U^{(q)}) , \]  

where \( NMI(U^a, U^b) \), the Normalized Mutual Information (NMI) [39] between two partitions \( a \) and \( b \), represented by the membership matrices \( U^a \) and \( U^b \) respectively, is defined by

\[ NMI(U^a, U^b) = \frac{\sum_{i,j=1}^{C} \sum_{b} n_{i,j} \log \left( \frac{n_{i,j} n_{i,j}}{n_i n_j} \right)}{\sqrt{\left( \sum_{i=1}^{C} n_i \log \frac{n_i}{n} \right) \left( \sum_{j=1}^{C} n_j \log \frac{n_j}{n} \right)}}. \]  

In equation (9), \( n_i \) represents the number of data points that have been assigned label \( i \) in partition \( a \), and \( n_{i,j} \) represents the number of data points that have been assigned label \( i \) in partition \( a \) and label \( j \) in partition \( b \). NMI values lie in the range \([0, 1]\). An NMI value of 1 indicates perfect matching between the two partitions whereas 0 indicates perfect mismatch.

Maximizing (8) is a combinatorial optimization problem and solving it exhaustively is computationally infeasible. MCLA obtains an approximate consensus solution by representing the set of partitions as a hypergraph. Each vector \( u_k^q, k \in [C], q \in [r] \) represents a vertex in a regular undirected graph, called the meta-graph. Vertex \( u_i \) is connected to vertex \( u_j \) by an edge whose weight is proportional to the Jaccard similarity between the two vectors \( u_i \) and \( u_j \):

\[ s_{i,j} = \frac{u_i \cdot u_j}{\|u_i\|^2 + \|u_j\|^2 - u_i \cdot u_j} \]  

This meta-graph is partitioned using a graph partitioning algorithm such as METIS [39] to obtain \( C \) balanced meta-clusters \( \pi_1, \pi_2, \ldots, \pi_C \). Each meta-cluster \( \pi_k \) is obtained. For each sample \( x_i \) is assigned to the meta-cluster with which it is associated the most, breaking ties randomly, i.e.

\[ U^{(c)}_{k,i} = \begin{cases} 1 & \text{if } k_a = \arg \max_{k \in [C]} \mu_{k_i} \\ 0 & \text{otherwise} \end{cases} \]  

The \( \text{aKKm} \) algorithm is combined with MCLA to enhance its accuracy. We execute the \( \text{aKKm} \) algorithm \( r \) times with different samples from the data set and MCLA is used to integrate the partitions obtained from each execution into a consensus partition.

More specifically, we independently draw \( r \) samples \( \{ \tilde{X}^1, \ldots, \tilde{X}^r \} \), where each \( \tilde{X}^i = \{ \tilde{x}_1, \ldots, \tilde{x}_m \} \) contains \( m \) data points. Each \( \tilde{x}_j \) is uniformly sampled without replacement. After the sampling of \( \tilde{X}^i \) is performed, the samples are replaced and the next sample \( \tilde{X}^j \) is obtained. For each sample \( \tilde{X}^i \), we first compute the kernel matrices \( K_{i,j}^k = [k(x_a, \tilde{x}_b)]_{n \times m} \) and \( \tilde{K}^i = [k(\tilde{x}_a, \tilde{x}_b)]_{m \times m} \), and then execute \( \text{aKKm} \) to obtain the cluster membership matrix \( U_i^c \). We then combine the partitions \( \{U_i^c\}_{i=1}^r \) using MCLA to obtain the consensus cluster membership \( U^{(c)} \).

This ensemble clustering algorithm is described in Algorithm 3 and illustrated in Fig. 2. On the synthetic data set in Fig. 1(a), we obtain the partitions similar to Fig. 1(e) by using a sample of 20 data points instead of 50 data points. This illustrates that the efficiency of the algorithm is improved by using...
ensemble clustering.

Algorithm 3 Ensemble aKKm

Input:
- \( X = \{x_1, \ldots, x_n\} \): the set of \( n \) data points to be clustered
- \( \kappa(\cdot, \cdot): \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R} \): kernel function
- \( m \): the number of randomly sampled data points (\( m \ll n \))
- \( C \): number of clusters
- \( r \): number of ensemble partitions
- \( \text{MAXITER} \): maximum number of iterations

Output: Consensus cluster membership matrix \( U^{(c)} \in \{0, 1\}^{C \times n} \)

1: for \( i = 1, \ldots, r \) do
  2: Randomly select \( m \) data points from \( X \), denoted by \( \hat{X}^i \).
  3: Run Algorithm 2 using \( \hat{X}^i \) as the sampled points and obtain the cluster membership matrix \( U^i \).
4: end for

MCLA:
5: Concatenate the membership matrices \( \{U^i\}_{i=1}^r \) to obtain an \( rC \times n \) matrix \( U = (u_1, u_2, \ldots, u_{rC})^\top \).
6: Compute the Jaccard similarity \( s_{i,j} \) between the vectors \( u_i \) and \( u_j \), \( i, j \in [rC] \) using (15).
7: Construct a complete weighted meta-graph \( G = (V, E) \), where vertex set \( V = \{u_1, u_2, \ldots, u_{rC}\} \) and each edge \( (u_i, u_j) \) is weighted by \( s_{i,j} \).
8: Partition \( G \) into \( C \) meta-clusters \( \{\pi_k\}_{k=1}^C \) and compute the mean vectors \( \{\mu_k\}_{k=1}^C \) using (11).
9: for \( i = 1, \ldots, n \) do
  10: Update the \( i^{th} \) column of \( U^{(c)} \) in accordance with (12).
11: end for

5 Analysis of Approximate Kernel K-means

In this section, we first show that the computational complexity of the aKKm algorithm is less than that of the kernel k-means algorithm and then we derive bounds on the difference in the clustering error achieved by our algorithm and the kernel k-means algorithm.

5.1 Computational complexity

Approximate kernel k-means: The aKKm algorithm consists of two parts: kernel computation and clustering. As only an \( n \times m \) portion of the kernel needs to be computed and stored, the cost of kernel computation is \( O(ndm) \), a dramatic reduction over the \( O(n^2d) \) complexity of classical kernel k-means. The memory requirement also reduces to \( O(mn) \). The most expensive clustering operation is the matrix inversion \( \hat{K}^{-1} \) and calculation of \( T = K_B \hat{K}^{-1} \), which has a computational cost of \( O(m^3 + m^2n) \).

The cost of computing \( \alpha \) and updating the membership matrix \( U \) is \( O(mnCl) \), where \( l \) is the number of iterations needed for convergence. Hence, the overall cost of clustering is \( O(m^3 + m^2n + mnCl) \). We can further reduce this cost by avoiding the matrix inversion \( \hat{K}^{-1} \) and formulating the calculation of \( \alpha = \bar{U}T = \bar{U}K_B \hat{K}^{-1} \) as the following optimization problem:

\[
\min_{\alpha \in \mathbb{R}^n} \frac{1}{2} \text{tr}(\alpha \hat{K} \alpha) - \text{tr}(\hat{U}K_B \alpha^\top) \tag{13}
\]

If \( \hat{K} \) is well conditioned (i.e., the minimum eigenvalue of \( \hat{K} \) is significantly larger than zero), we can solve the optimization problem in (13) using the simple gradient descent method with a convergence rate of \( O(\log(1/\varepsilon)) \), where \( 1 - \varepsilon \) is the desired accuracy. As the cost of each step in the gradient descent method is \( O(m^2C) \), the overall computational cost is only \( O(m^2C\log(1/\varepsilon)) \ll O(m^3) \) when \( Cl \ll m \). Using this approximation, we can reduce the overall computational cost to \( O(m^2Cl + mnCl + m^2n) \sim O(n) \) when \( m \ll n \).

Ensemble aKKm: In the ensemble aKKm algorithm, an additional cost of \( O(nC^2r^2) \) is incurred for combining the partitions using MCLA [37]. However, we empirically observed that the sample size \( m \) required to achieve a satisfactory clustering accuracy is reduced considerably when compared to aKKm. This leads to a further reduction in the running time.

5.2 Clustering error

Let binary random variables \( \xi = (\xi_1, \xi_2, \ldots, \xi_n)^\top \in \{0, 1\}^n \) represent the random sampling process, where \( \xi_i = 1 \) if \( x_i \in \hat{X} \) and 0 otherwise. The following proposition allows us to write the clustering error in terms of the random variable \( \xi \).

Proposition 1. Given the cluster membership matrix \( U = (u_1, \ldots, u_C)^\top \), the clustering error can be expressed as

\[
L(U, \xi) = \text{tr}(K) + \sum_{k=1}^C L_k(U, \xi), \tag{14}
\]

where \( L_k(U, \xi) \) is

\[
L_k(U, \xi) = \min_{\alpha_k \in \mathbb{R}^n} -2u_k^\top K(\alpha_k \circ \xi) + n_k(\alpha_k \circ \xi)^\top K(\alpha_k \circ \xi).
\]

Note that \( \xi = 1 \), where 1 is a vector of all ones, implies that all the data points are chosen for constructing the subspace \( H_k \), which is equivalent to kernel k-means using the full kernel matrix. As a result, \( L(U, 1) \) is the clustering error of the standard kernel k-means algorithm.

The following theorem bounds the expectation of the clustering error.

Theorem 1. Given the membership matrix \( U \), we have
the expectation of $L(U, \xi)$ bounded as follows

$$\mathbb{E}_\xi[L(U, \xi)] \leq L(U, 1)$$

$$\quad + \tr\left( \bar{U} \left[ K^{-1} + \frac{m}{n} \text{diag}(K) \right]^{-1} \right)\bar{U}^\top$$

where $L(U, 1) = \tr(K) - \tr(UKU^\top)$.

**Proof:** We first bound $\mathbb{E}_\xi[L_k(U, \xi)]$ as

$$\mathbb{E}_\xi[L_k(U, \xi)] = \mathbb{E}_\xi\left[ k \right] \leq \mathbb{E}_\xi\left[ k^2 \right]$$

$$\quad \leq \mathbb{E}_\xi\left[ k^2 + \frac{1}{n} \right]$$

$$\quad = \mathbb{E}_\xi\left[ k - 2 \bar{u}_k^\top K (\alpha \odot \xi) + (\alpha \odot \xi)^\top K (\alpha \odot \xi) \right]$$

$$\quad \leq \mathbb{E}_\xi\left[ k^2 + \frac{1}{n} \right]$$

$$\quad = \mathbb{E}_\xi\left[ k^2 - 2 \bar{u}_k^\top K (\alpha \odot \xi) + (\alpha \odot \xi)^\top K (\alpha \odot \xi) \right]$$

$$\quad \leq \mathbb{E}_\xi\left[ k^2 + \frac{1}{n} \right]$$

$$\quad = \mathbb{E}_\xi\left[ k - 2 \bar{u}_k^\top K (\alpha \odot \xi) + (\alpha \odot \xi)^\top K (\alpha \odot \xi) \right]$$

By minimizing over $\alpha$, we obtain

$$\alpha_\ast = \left( \frac{n}{n} K + \text{diag}(K) \right)^{-1} K \bar{u}_k.$$  

Thus, $\mathbb{E}_\xi[L_k(U, \xi)]$ is bounded as

$$\mathbb{E}_\xi[L_k(U, \xi)] \leq \frac{1}{n} \mathbb{E}_\xi[L_k(U, \xi)] + n_k \bar{u}_k^\top K \bar{u}_k$$

$$\quad \leq n_k \bar{u}_k^\top \left( K - K \left[ K + \frac{m}{n} \text{diag}(K) \right]^{-1} K \right) \bar{u}_k$$

$$\quad = \bar{u}_k^\top \left( K - 2 \bar{u}_k^\top K (\alpha \odot \xi) + (\alpha \odot \xi)^\top K (\alpha \odot \xi) \right)$$

We complete the proof by adding up $\mathbb{E}_\xi[L_k(U, \xi)]$ and using the fact that

$$L_k(U, 1) = \min_{\alpha} -2 \bar{u}_k^\top K (\alpha \odot \xi) + (\alpha \odot \xi)^\top K (\alpha \odot \xi) = -\bar{u}_k^\top K \bar{u}_k.$$

The following corollary interprets the result of the above theorem in terms of the eigenvalues of $K$.

**Corollary 1.** Given the membership matrix $U$, we have

$$\mathbb{E}_\xi[L(U, \xi)] \leq 1 + \frac{\sum_{i=1}^{C+1} \lambda_i}{n} \left[ 1 + \frac{m}{n} \text{diag}(K)^{-1} \right]^{-1} \bar{U}\bar{U}^\top$$

$$\quad \leq 1 + \frac{\sum_{i=1}^{C+1} \lambda_i}{n} \left[ 1 + \frac{m}{n} \text{diag}(K)^{-1} \right]^{-1} \bar{U}\bar{U}^\top$$

$$\quad \leq \frac{C}{m} \sum_{i=1}^{C+1} \lambda_i \leq \frac{Cn}{m}$$

and

$$L(U, 1) = \tr(K - UKU^\top) \geq \tr(K) - \sum_{i=1}^{C} \lambda_i.$$

We complete the proof by combining the above inequalities.

As an illustration of the result of Corollary 1, consider a special kernel matrix $K$ that has its first $a$ eigenvalues equal to $n/a$ and the remaining eigenvalues equal to zero; i.e. $\lambda_1 = \ldots = \lambda_a = n/a$ and $\lambda_{a+1} = \ldots = \lambda_n = 0$. Assuming $a > 2C$, i.e. the number of non-zero eigenvalues of $K$ is larger than twice the number of clusters, we have

$$\mathbb{E}_\xi[L(U, \xi)] - L(U, 1) \leq 1 + \frac{Ca}{m(a - C)} \leq 1 + \frac{2C}{m}.$$  

This indicates that when the number of non-zero eigenvalues of $K$ is significantly larger than the number of clusters, the difference in the clustering errors between the standard kernel $k$-means and our approximation scheme decreases at the rate of $O(1/m)$.

### 5.3 Parameter sensitivity

One of the important factors that determines the performance of the approximate kernel $k$-means algorithm is the sample size $m$. Sampling introduces a trade-off between clustering quality and efficiency. As $m$ increases, the clustering quality improves but the speedup achieved by the algorithm suffers. The following theorem gives an estimate of $m$.

**Theorem 2.** Let $\Sigma_1 = \text{diag}(\lambda_1, \ldots, \lambda_C)$, $\Sigma_2 = \text{diag}(\lambda_{C+1}, \ldots, \lambda_n)$, $Z_1 = (z_1, z_2, \ldots, z_C)$ and $Z = (z_{C+1}, \ldots, z_n)$. Let

$$\tau = n \max_{1 \leq i \leq n} |Z(i)_i|^2$$

denote the coherence of the kernel matrix $K$ (adapted from [16]). For any $\epsilon \in (0, 1)$, the spectral norm of the approximation error is bounded above, with probability $1 - \delta$, as

$$\|K - KBK^{-1}_B\|_2 \leq \lambda_{C+1} \left( 1 + 8 \tau \ln \frac{2}{\delta} \sqrt{\frac{Cn}{m}} \right),$$

provided $m \geq \tau C \max(C_1 \ln p, C_2 \ln(3/\delta))$, for some positive constants $C_1$ and $C_2$.

A small sample size $m$ suffices if the coherence measure $\tau$ is low and there is a large gap in the eigenspectrum. The approximation error reduces at a rate of $O(1/\sqrt{m})$. The reader is referred to the appendix for the proof of this theorem.

In our experiments, we examined the performance of our algorithm for different sample sizes

3. This improves over the approximation error bound of the naive Nyström method presented in [16].
| Data set         | Size   | Dimensionality | Kernel function |
|-----------------|--------|----------------|-----------------|
| Imagenet        | 20,000 | 7,000          | Pyramid         |
| MNIST           | 70,000 | 784            | Neural          |
| Forest Cover Type | 381,012 | 54        | RBF             |
| Network Intrusion | 1,898,431 | 50    | Polynomial      |

TABLE 1: Data set summary

(m) ranging from 0.001% to 15% of the data set size n, and observed that setting m equal to 0.01% to 0.05% of n leads to a satisfactory performance.

6 EXPERIMENTAL RESULTS

In this section, we show that aKKm is an efficient and scalable variant of the kernel k-means algorithm. It has lower run-time and memory requirements but is on par with kernel k-means in terms of the clustering error and clustering quality. We tested our algorithm on four data sets with varying sizes: Imagenet, MNIST, Forest Cover Type, and Network Intrusion data sets (Table 1). Using small and medium-sized data sets (Imagenet and MNIST) for which the full kernel calculation is feasible on a single processor, we demonstrate that our algorithm’s clustering performance is similar to that of the kernel k-means algorithm. We then demonstrate scalability using the large Forest Cover Type and Network Intrusion data sets. Finally, we show that the performance can be improved by using the ensemble aKKm algorithm.

All algorithms were implemented in MATLAB\(^4\) and run on an 2.8 GHz processor. The memory used was explicitly limited to 40 GB.

6.1 Performance comparison with kernel k-means

We use the Imagenet and MNIST data sets to demonstrate that the approximate kernel k-means algorithm’s clustering performance is similar to that of the kernel k-means algorithm.

6.1.1 Datasets

- **Imagenet**: The Imagenet data set \([41]\) consists of over 1.2 million images that are organized according to the WordNet hierarchy. Each node in this hierarchy represents a concept (known as the “synset”). We chose 20,000 images from 12 synsets. We extracted keypoints from each image using the VLFeat library \([42]\) and represented each keypoint as a 128 dimensional SIFT descriptor; an average of 3,055 keypoints were extracted from each image.

- **MNIST**: The MNIST data set \([43]\) is a subset of the database of handwritten digits available from NIST. It contains 60,000 training images and 10,000 test images from 10 classes. Each image is represented using a 784-dimensional feature vector. For the purpose of clustering, we combined the training and test images to form a data set with 70,000 images.

6.1.2 Experimental setup

We first compare the approximate kernel k-means (aKKm) algorithm with the kernel k-means algorithm to show that they achieve similar performance. We then compare it to the two-step kernel k-means (tKKm) algorithm and demonstrate that aKKm is superior. We also gauge it’s performance against that of (i) the Nystrom spectral clustering algorithm (nysSC) \([14]\), which clusters the top \(C\) eigenvectors of a low rank approximate kernel obtained through the Nystrom approximation technique, (ii) the leaders based kernel k-means algorithm (lKKm) \([33]\) which finds a few representative patterns (called leaders) based on a user-defined distance threshold and then runs kernel k-means on the leaders, and (iii) the k-means algorithm to show that it achieves a better clustering accuracy.

For the Imagenet data set, we employ the spatial pyramid kernel \([44]\) to calculate the pairwise similarity with the number of pyramid levels set to 4. This has been shown to be effective for object recognition and image retrieval. It took 24,236 seconds to compute the multi-resolution histograms and the pyramid representation of the data.

On the MNIST data set, we use the neural kernel defined as \(\kappa(x, y) = \tanh(ax^\top y + b)\), with the parameters \(a\) and \(b\) set to 0.0045 and 0.11 respectively, as suggested in \([32]\).

We evaluate the efficiency of the aKKm algorithm for different sample sizes ranging from 100 to 5,000. We directly compute \(\hat{K}^{-1}\) instead of using the approximation method in \([13]\) to demonstrate that our algorithm is efficient in spite of a naive implementation. The number of clusters \(C\) is set equal to the number of true classes in the data set.

We measure the time taken for computing the kernel matrix (when applicable) and clustering the data points. We measure the clustering performance using error reduction, defined as the ratio of the difference between the initial clustering error (on random initialization) and the final clustering error (after running the clustering algorithm) to the initial
6.1.3 Experimental results

Imagenet: Tables 2(a) and 3 and Figs. 4(a) and 5(a) compare the performance of the aKKm algorithm on the Imagenet data set with the kernel $k$-means, $k$-means, IKKm, tKKm, and nysSC clustering algorithms.

Table 2(a) lists the running time of all the algorithms. The kernel computation time is common to both the aKKm and tKKm algorithms. We observe that a significant speedup (over 90%) is achieved by both the algorithms in kernel computation when compared to kernel $k$-means. tKKm is the most efficient in terms of the clustering speedup. aKKm takes longer as it needs to compute the inverse matrix $K^{-1}$. However, when the algorithms are compared with the requirement that they yield the same clustering performance, we will see later that aKKm is more efficient. For $m \leq 1,000$, aKKm is even faster than the $k$-means algorithm executed on the pyramid features. This is due to the high dimensionality of the pyramid features, which plays an important role in the complexity of $k$-means.

In Table 3 (columns 2-3), we observe that the ARI values of the aKKm algorithm are much higher than those of the tKKm algorithm. This shows that aKKm obtains partitions that are similar to the kernel $k$-means partitions. When $m = 5,000$, the partitions obtained by aKKm are, on an average, 84% similar to the partitions generated by kernel $k$-means.

Figs. 4(a) and 5(a) show the error reduction and NMI plots, respectively. We again observe that the aKKm algorithm achieves performance similar to that of the kernel $k$-means. The tKKm algorithm achieves much lower error reduction. The tKKm, IKKm and nysSC algorithms yield lower NMI values. With just 100 sampled points, aKKm significantly outperforms tKKm provided with 1,000 sampled points, and achieves the same performance as the nysSC algorithm. This observation indicates that it is insufficient to estimate the cluster centers using only the randomly sampled data points as in the tKKm method, further justifying the design of the aKKm algorithm. As expected, all the kernel-based algorithms perform better than the $k$-means algorithm.

MNIST: Table 2(b) shows the results for the MNIST data set using the neural kernel. Unlike the Imagenet data set, more time is spent in clustering than in kernel calculation due to the simplicity of the kernel function. As observed in the Imagenet data set, a significant amount of time was saved by the aKKm algorithm as well as by the tKKm algorithm, when compared to the kernel $k$-means algorithm. When the sample size is small ($m < 5,000$), the aKKm algorithm is also faster than the $k$-means algorithm.

Though the tKKm algorithm is more efficient than the aKKm algorithm, the ARI values in Table 3 (columns 4-5) indicate that the tKKm algorithm produces inferior partitions. The partitions generated by the aKKm algorithm are more similar to those generated by the kernel $k$-means even for small sample sizes. The aKKm algorithm achieves similar performance as kernel $k$-means when $m = 500$, whereas the tKKm algorithm cannot achieve this until $m \geq 5,000$.

As seen in Fig. 4(b), approximately equal amounts of error reduction are achieved by both the kernel $k$-means and the aKKm algorithm for $m \geq 500$. In the NMI plot shown in Fig. 5(b) we first observe that all the kernel-based algorithms, except tKKm and IKKm, perform better than the $k$-means algorithm. The aKKm algorithm’s performance is better than that of the IKKm and nysSC algorithms, and comparable to that of kernel $k$-means, when $m \geq 500$.

6.2 Performance of Approximate kernel $k$-means using different sampling strategies

Table 4(a) and Figs. 3(a) and 3(b) compare the diagonal sampling, column norm sampling, and $k$-means sampling strategies with the uniform random sampling technique. In Table 4(a) we assume that the $n \times n$ kernel matrix is pre-computed and only include the time taken for sorting the diagonal entries (for diagonal sampling), or computing the column norms (for column norm sampling), and the time taken for choosing the first $m$ indices, in the sampling time. For the $k$-means sampling, we show the time taken to execute $k$-means and find the representative sample. As expected, the
### Table 2: Comparison of running time in seconds on the four data sets

| Sample size | Full Kernel calculation time | Kernel k-means clustering time | nysSC |
|-------------|------------------------------|---------------------------------|-------|
|             | aKKm                         | IKKm                            |       |
| 100         | 203.65 (±20.87)              | 4.33 (±1.32)                    | 0.02  |
|             | (613.26)                     | (643.30)                        | (600.67) |

### Table 3: Adjusted Rand Index (ARI) with respect to the kernel k-means partitions

| Data set   | ImageNet | MNIST |
|------------|----------|-------|
| Sample size | aKKm     | IKKm   | aKKm | IKKm |
| 100        | 0.71     | 0.28   | 0.47  | 0.37 |
| 200        | 0.71     | 0.36   | 0.61  | 0.36 |
| 500        | 0.75     | 0.51   | 0.69  | 0.48 |
| 1,000      | 0.70     | 0.58   | 0.70  | 0.58 |
| 2,000      | 0.78     | 0.59   | 0.71  | 0.61 |
| 5,000      | 0.84     | 0.68   | 0.71  | 0.70 |

### 6.3 Scalability

Using the large Forest Cover Type and Network Intrusion data sets, we demonstrate that the proposed algorithm is scalable to large data sets. The aKKm algorithm uses less than 40 GB of memory, thereby dramatically reducing the memory requirements of clustering.

#### 6.3.1 Datasets

- **Forest Cover Type**: This data set [46] is composed of cartographic variables obtained from the US Geological Survey (USGS) and the US Forest Service (USFS) data. Each of the 581,012 data points represents the attributes of a 30 × 30 meter cell of the forest floor. There are a total of 12 attributes, including qualitative...
measures like soil type and wilderness area, and quantitative measures like slope, elevation, and distance to hydrology. These 12 attributes are represented using 54 features. The data are grouped into 7 classes, each representing a different forest cover type. The true cover type was determined from the USFS Region 2 Resource Information System (RIS) data.

- **Network Intrusion:** The Network Intrusion data set [47] contains 4,889,431 50-dimensional patterns representing TCP dump data from seven weeks of local-area network traffic. The data are classified into 23 classes, one class representing legitimate traffic and the remaining 22 classes representing different types of illegitimate traffic.

### 6.3.2 Experimental setup

For these data sets, it is currently infeasible to compute and store the full kernel on a single system due to memory and computational time constraints. The aKKm algorithm alleviates this complexity issue.

We compare the performance of the aKKm algorithm on these data sets in terms of the running time, error reduction and NMI, with that of the $k$-means, the tKKm, and the nysSC algorithms. We found that the IKKm algorithm takes longer than 24 hours to find the leaders for these large data sets, clearly demonstrating its non-scalability. Therefore, we eliminated this algorithm from the set of baseline algorithms.

We evaluate the efficiency of the aKKm algorithm for different sample sizes ranging from 100 to 5,000. On the Network Intrusion data set, the value of $m$ is increased only up to 2,000, as greater values of $m$ require more than 40 GB memory. On the Cover Type data set, we employ the RBF kernel to compute the pairwise similarity, with the parameter $\sigma$ set to 0.35. The 3-degree polynomial kernel is employed for the Network Intrusion data set. The kernels and their parameters are tuned to achieve optimal performance. The number of clusters is again set equal to the true number of classes in the data set.

### 6.3.3 Experimental results

**Forest Cover Type:** We compare the running time of the algorithms in Table 2(c). As in the MNIST data set, kernel calculation time is minimal when compared to clustering time and the aKKm algorithm is less efficient than the tKKm algorithm in terms of the clustering time. When compared to the nysSC algorithm, its running time is higher when the sample size $m$ is small, but as the time taken by the nysSC algorithm increases cubically with $m$, the aKKm algorithm becomes more efficient as $m$ is increased. It is faster than the $k$-means algorithm when $m < 500$.

Figs. 4(c) and 5(c) show the effectiveness of our algorithm in terms of error reduction and NMI,
We employ the ensemble aKKm algorithm to combine 10 ensemble partitions. The times taken for combining the partitions (averaged over 10 runs), for each of the data sets, are shown in Table 5. We find that these times are small when compared to the clustering times and hence, do not significantly impact the overall running time. Fig. 4 shows the improvement in NMI achieved through the use of ensembles on the four data sets. A significant improvement is observed, especially when the sample size \( m \) is small. For example, in Fig. 6(b) an NMI of around 0.48 is obtained on the MNIST data set, even for a small sample size of \( m = 100 \). The NMI increases by about 15% and becomes almost equal to the average NMI obtained for a sample size \( m = 1,000 \). On the Cover Type and Network Intrusion data sets, there are significant improvements in the NMI values. We obtain a good clustering accuracy for small values of \( m \), thereby enhancing the efficiency of the approximate kernel \( k \)-means algorithm.

### 7 Conclusions

We have proposed an efficient approximation for the kernel \( k \)-means algorithm, suitable for large data sets. The key idea is to avoid computing the full kernel matrix by restricting the cluster centers to a subspace spanned by a small set of randomly sampled data points. We show theoretically and empirically that the proposed algorithm is efficient in terms of both computational complexity and memory requirement, and is able to yield similar clustering results as the kernel \( k \)-means algorithm using the full kernel matrix. In most cases, the performance of our algorithm is better than that of other popular large scale kernel clustering algorithms. By integrating ensemble clustering meth-
ods with the proposed algorithm, its efficiency is further enhanced. In the future, we plan to further enhance the scalability of kernel clustering by devising more efficient kernel approximation techniques. We also plan to extend these ideas to semi-supervised clustering.

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APPENDIX

Proof of Theorem 2

To prove this theorem, we use the following results from [16], [49], and [49]:

Lemma 2. (Theorem 1 from [16]) Let \( A \) be a \( n \times n \) positive semi-definite matrix and \( S \in \{0, 1\}^{n \times m} \) be a random sampling matrix. Let \( A \) be partitioned as

\[
A = \begin{bmatrix} Z_1 & Z_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} Z_1^\top \\ Z_2^\top \end{bmatrix},
\]

where \( Z_1 \in \mathbb{R}^{n \times C} \), \( Z_2 \in \mathbb{R}^{n \times (n-C)} \), \( \Sigma_1 \in \mathbb{R}^{C \times C} \) and \( \Sigma_2 \in \mathbb{R}^{(n-C) \times (n-C)} \). Define \( \Omega_1 = Z_1^\top S \) and \( \Omega_2 = Z_2^\top S \). Assume \( \Omega_1 \) has full row rank. Then the spectral approximation error of the Nyström extension of \( A \) using \( S \) as the column sampling matrix satisfies

\[
\|A - AS(S^\top AS)^{\dagger}S^\top A\| \leq \|\Sigma_2\|_2 \left( 1 + \|\Omega_2\Omega_1^{\dagger}\|_2 \right).
\]

Lemma 3. (Theorem 1.2 from [49]) Let \( Z \in \mathbb{R}^{n \times n} \) include the eigenvectors of a positive semi-definite \( A \) with coherence \( \tau \), where coherence is defined in [16]. Let \( Z_1 \in \mathbb{R}^{n \times C} \) represent the first \( C \) columns of \( Z \), containing the first \( C \) eigenvectors of \( A \), and \( S \in \{0, 1\}^{n \times m} \) represent the first \( m \) columns of a random permutation matrix of size \( n \). We have, with probability at least \( 1 - \delta \),

\[
\left\| \frac{1}{m} Z_1^\top SS^\top Z_1 - I \right\|_2 < \frac{1}{\sqrt{2}},
\]

provided that \( m \geq C \tau \max(C_1 \ln k, C_2 \ln(3/\delta)) \), for some fixed positive constants \( C_1 \) and \( C_2 \).

Lemma 4. (Lemma 2 from [49]) Let \( H \) be a Hilbert space and \( \xi \) be a random variable on \( (Z, \rho) \) with values in \( H \). Assume \( \|\xi\| \leq M < \infty \) almost surely. Denote \( \sigma^2(\xi) = E(\|\xi\|^2) \). Let \( \{z_i\}_{i=1}^m \) be independent random draws of \( \rho \). For any \( 0 < \delta < 1 \), with confidence \( 1 - \delta \),

\[
\left\| \frac{1}{m} \sum_{i=1}^m (\xi_i - E[\xi_i]) \right\|_2 \leq \frac{2M \ln(2/\delta)}{m} + \sqrt{2\sigma^2(\xi) \ln(2/\delta) / m}.
\]

Proof: Let \( a_i \) and \( b_i \) represent the \( i \)-th rows of \( Z_1 \) and \( Z_2 \) respectively. Let \( \Delta \) be the subset of rows of \( Z_1 \) and \( Z_2 \) selected by \( S \). Using Lemma 4, we have

\[
\left\| Z_2^\top SS^\top Z_1 \right\|_2 \leq \sum_{k \in \Delta} (b_k a_k^\top - E[b_k a_k^\top]) \right\|_2 \leq 2M \ln(2/\delta) + \sqrt{2\sigma^2(\xi) \ln(2/\delta) / m},
\]

where \( M = \max_j \|b_j a_j^\top\|_2 \leq \max_j \sqrt{|b_j|^2 |a_j|^2} \leq \tau \sqrt{C/n} \) and \( \sigma^2 = E \left[ \|b_j a_j^\top\|_2 \right] \leq \tau \sqrt{C/n} \). Substituting \( \Omega_2\Omega_1^{\dagger} = Z_2^\top SS^\top Z_1(Z_1^\top SS^\top Z_1)^{-1} \)

in the result of Lemma 2, we have with probability \( 1 - \delta \),

\[
\left\| A - AS(S^\top AS)^{\dagger}S^\top A \right\| \leq \lambda_{C+1} \left( 1 + \|Z_2^\top SS^\top Z_1\|_2^2 \right) \|Z_1^\top SS^\top Z_1\|_2^{-2}.
\]

We obtain the result in the theorem by combining the result of Lemma 3 with equations (17) and (18), and substituting \( A, AS \) and \( S^\top AS \) with \( K, KB \) and \( K \) respectively.

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