Abstract—K-means is one of the most widely used algorithms for clustering in Data Mining applications, which attempts to minimize the sum of square of Euclidean distance of the points in the clusters from the respective means of the clusters. The simplicity and scalability of K-means makes it very appealing. However, K-means suffers from local minima problem, and comes with no guarantee to converge to the optimal cost. K-means++ tries to address the problem by seeding the means using a distance based sampling scheme. However, seeding the means in K-means++ needs \( O(K) \) passes through the entire dataset. This could be very costly in large amount of dataset. Here we propose a method of seeding initial means based on factorizations of higher order moments for bounded data. Our method takes \( O(1) \) passes through the entire dataset to extract the initial set of means, and its final cost can be proven to be within \( O(\sqrt{K}) \) of the optimal cost. We demonstrate the performance of our algorithm in comparison with the existing algorithms on various benchmark datasets.

1. Introduction

K-means has been used over a wide range of Data Mining Applications for years. It is the most common algorithm for extracting clusters from datasets containing real attributes. In recent times it has also been used for feature extraction purpose, which is further used for classification using Neural Networks in [1]. K-means is an NP hard problem even for \( K = 2 \) [2], and only heuristic solutions exist. Perhaps the most common of such heuristics is the Lloyd’s algorithm, which uses an EM style approach; it first assigns the points to different clusters according to their distance from the means of the clusters, and then updates the cluster means by averaging out the points in each cluster. The algorithm uses a random initialization, and comes with no guarantee to reach the global minima.

The K-means++ in [3] addresses the problem by using an initial seeding of the means. The expected optimal cost of K-means++ over different executions is bounded by \( O(\log K) \) of the optimal cost. However, the algorithm uses \( K \) passes through the entire dataset to seed the means, which makes it very expensive for large amount of data. K-means++ over different executions is bounded by \( O(K) \) of the optimal cost. The oversampling strategy also improves accuracy in case there are outliers present in the dataset, by reducing the number of passes in the seeding phase. The oversampling strategy also improves accuracy in case there are outliers present in the dataset, by reducing the number of passes in the seeding phase. The oversampling strategy also improves accuracy in case there are outliers present in the dataset, by reducing the number of passes in the seeding phase. The oversampling strategy also improves accuracy in case there are outliers present in the dataset, by reducing the number of passes in the seeding phase. There are other variants of K-means algorithm, such as [5] and [6].

Most of these algorithms build on K-means++ and aim to reduce the computational burden, rather than improving accuracy. Hence, we limit our discussion on K-means++ and K-means++.

There have been recent developments on clustering algorithms based on Method of Moments (MoM), also referred to as Spectral Methods in the literature. Unlike traditional clustering algorithms which rely on EM or similar algorithms to maximize the likelihood of the data, MoM tries to learn the parameters from the higher order moments of the data, and has been successfully applied for Hidden Markov Model in [7] and [8], for Topic Modeling in [9], for various Natural Language Processing applications in [10], [11], for Mixtures of Gaussian in [12] and for Spectral Experts of Linear Regression in [13].

Here we propose a method to extract a set of K-Means based on Method of Moments, and use the means to seed K-Means algorithm. We assume the norm of the data instances to be bounded. This assumptions holds true for real datasets, since any datasets generated from real life applications is always bounded. We show the derivation of our algorithm, and the theoretical bounds, and then show the competitive performance of our algorithm on various datasets with respect to the existing algorithm [1].

2. Problem Formulation

Given a dataset \( X \subseteq \mathbb{R}^D \), K-means algorithm tries to find a set \( C \subseteq \mathbb{R}^D \) of \( K \) centres \( (K > 0) \) which optimizes the following cost function:

\[
\phi(C) = \sum_{x \in X} \min_{c \in C} ||x - c||^2
\]

The algorithm is usually started with a random initialization, but fails to converge to global minima of the objective. K-means++ tries to alleviate the problem using an initial mean seeding, as described in Algorithm [1]. K-means++ (described as Algorithm [2]) introduces a method to reduce the number of passes during the seeding phase, by oversampling seeding points during each pass. In our algorithm, we propose a probabilistic method to extract the means of the cluster based on the covariance and third order central moment of the data, which we outline in this section. Please note that we do not try to find a non-parametric version of K-means unlike [14], although our model is probabilistic, we assume a fixed value of \( K \).
2.1. Method of Moments

Here we formulate a generative model for K-means, where we select a cluster $h$ randomly based on the probability $P[h = k] = \pi_k, k \in 1 \ldots K$, and choose a data point in the vicinity of the mean of the cluster.

\[ h \sim \text{Discrete}(\pi) \]
\[ \varepsilon \sim \mathcal{E}_h, \quad \mathbb{E}[\mathcal{E}_h] = \mu_h \]  
\[ x = \mu_X + \varepsilon \quad (2) \]

where, $\mu_X = \mathbb{E}[x], x \in X$, and can be estimated as the mean of the entire dataset. $\mathcal{E}_h$ is the p.d.f of $h$th cluster of the centred data, i.e., $\mathcal{E}_h = p[x - \mu_X | h = k], x \in X$, and $\mu_h \in \mathbb{R}^D$ is the mean of the $h$th cluster of the centred data, i.e., $\mu_h = \mathbb{E}[\mathcal{E}_h] = \mathbb{E}[x - \mu_X | h = k], \forall k \in 1 \ldots K$.

We assume the resulting data instances are bounded, i.e. $||x|| \leq B$ for some $B > 0$. We further assume $p[x - \mu_X | h], \forall x \in X$ are conditionally independent given $h$. Also, by the definition of K-Means, the dimensions of the data are independent. This is similar to the assumptions in [12]. Following the assumption,

\[ \mathcal{E}_h = p[x - \mu_X | h = k] = \prod_{d=1}^{D} p[x_d - [\mu_X]_d | h = k] \quad (3) \]

where $x = [x_1, x_2 \ldots x_D]^\top$, i.e. $D$ is the dimension of the $x$, and $[\mu_X]_d$ is the $d$th element of the vector $\mu_X$. Similarly, individual element the conditional mean $\mu_k$ can be expressed as,

\[ [\mu_k]_d = \mathbb{E}[x_d - [\mu_X]_d | h = k], \forall d \in 1 \ldots D \quad (4) \]

Following the generative model in Equation (2) the expectation of the centred data takes the form,

\[ M_1 = \mathbb{E}[x - \mu_X] = \mathbb{E}_h[\mathbb{E}[x - \mu_h | h]] = \sum_{k=1}^{K} \pi_k \mu_k = 0 \quad (5) \]

if the covariance matrix is $M_2 \subset \mathbb{R}^{D \times D}$, then any element of $M_2$ can be expressed as,

\[ [M_2]_{ij} = \mathbb{E}[(x_i - [\mu_X]_i)(x_j - [\mu_X]_j)] \]
\[ = \mathbb{E}_h \mathbb{E}[(x_i - [\mu_X]_i)(x_j - [\mu_X]_j) | h] \]
\[ = \mathbb{E}_h [\mathbb{E}[x_i - [\mu_X]_i | h][x_j - [\mu_X]_j | h]] \]
\[ = \mathbb{E}_h [[\mu_h]_i][\mu_h]_j \]
\[ = \sum_{k=1}^{K} [\mu_k]_i[\mu_k]_j \pi_k, \quad \forall i,j \in 1 \ldots D \quad (6) \]

where $[\mu_k]_i$ is the mean along the $i$th dimension of the data, and so on.

Therefore, the covariance matrix $M_2$ can be expressed as,

\[ M_2 = \mathbb{E}[(x - \mu_X) \otimes (x - \mu_X)] \]
\[ = \sum_{k=1}^{K} \pi_k \mu_k \mu_k^\top \]
\[ = \sum_{k=1}^{K} \pi_k \mu_k \otimes \mu_k \otimes \mu_k \quad (7) \]

Similarly, the third order central moment $M_3$ can be expressed as,

\[ M_3 = \mathbb{E}[(x - \mu_X) \otimes (x - \mu_X) \otimes (x - \mu_X)] \]
\[ = \sum_{k=1}^{K} \pi_k \mu_k \otimes \mu_k \otimes \mu_k \quad (8) \]

The aim of our algorithm is to retrieve the cluster means $\{\mu_k\}_{K}^{1}$ from the covariance $M_2$ and third order moment $M_3$. We first compute a matrix $W$ of rank $K$ to whiten $M_2$, such that $W^\top M_2 W = I$. This is similar to whitening in Independent Component Analysis (ICA), and is usually done through eigenvalue decomposition. If the $K$ maximum eigenvalues of $M_2$ are $\{\nu_k\}_{K}^{1}$, and the corresponding eigenvectors are $\{u_k\}_{K}^{1}$, then the whitening matrix is computed as $W = U \Sigma^{-1/2}$, where $U = [u_1 | u_2 | \ldots | u_K]$, and $\Sigma = \text{diag}(\nu_1, \nu_2, \ldots, \nu_K)$. 

---

**Algorithm 1** K-means++ Seeding

**Input:** A set of points $X \subseteq \mathbb{R}^D$ and $K$

**Output:** A set $C \subseteq \mathbb{R}^D$ containing $K$ centres

Choose the first centre $c_1$ uniformly at random from $X$, $C \leftarrow c_1$

for $k = 2$ to $K$

Sample a point $x$ from $X$ with the probability $p_x = \frac{D(x)^2}{\sum_{x \in X} D(x)^2}$, where $D(x) = \min_{c \in C} ||x - c||$

$C \leftarrow C \cup x$

end for

return $C$

---

**Algorithm 2** K-means|| Seeding

**Input:** A set of points $X \subseteq \mathbb{R}^D$, number of clusters $K$, oversampling factor $l$

**Output:** A set $C \subseteq \mathbb{R}^D$ containing $K$ centres

$C \leftarrow$ sample a point $c$ uniformly at random from $X$

$p(X) \leftarrow \sum_{x \in X} ||x - c||^2$

for $O(\log p(X))$ times do

$C' \leftarrow$ sample each point $x$ from $X$ with the probability $p_x = \frac{D(x)^2}{\sum_{x \in X} D(x)^2}$, where $D(x) = \min_{c \in C} ||x - c||$

Assign $C' \leftarrow C' \cup C'$

end for

For $x \in C$, set $w_x$ to be the number of points in $X$ closer to $x$ than any other point in $C$

return $K$ cluster means from weighted clustering of $C$ with the weights $w_x$
Algorithm 3 Method of Moments for K-means Seeding

Input: $X \in \mathbb{R}^{N \times D}$, Number of Clusters $K$
Output: $\{\mu_k\}_{k=1}^K$

1) Compute $\hat{X} = X - \mu \tilde{I}^T_N$
2) If $N > D$ Compute the top $K$ eigenvalues of $M_2 = \frac{1}{N} \hat{X}^T \hat{X}$ as $\Sigma$, and corresponding eigenvectors as $U$
   Else Compute the top $K$ eigenvalues $\Sigma$ and the corresponding eigenvectors $P$ of $\frac{1}{N} \hat{X} \hat{X}^T$
3) Estimate the whitening matrix $W = U \Sigma^{-1/2}$
4) Compute $\tilde{M}_3 = \frac{1}{N} \hat{X} W \otimes \hat{X} W$
5) Compute eigenvalues $\{\lambda_k\}_{k=1}^K$ and eigenvectors $\{v_k\}_{k=1}^K$ of $\tilde{M}_3$
6) Estimate $\mu_k = \lambda_k W^T v_k$, where $W^T = W(W^T W)^{-1}$, $\forall k \in 1, 2 \ldots K$
return $\{\mu_k\}_{k=1}^K$

Let us note that, upon whitening, $M_2$ takes the form:

\[
W^T M_2 W = W^T \left( \sum_{k=1}^K \pi_k \mu_k \mu_k^T \right) W
= \sum_{k=1}^K (\sqrt{\pi_k} W^T \mu_k) \left( \sqrt{\pi_k} W^T \mu_k \right)^T
= \sum_{k=1}^K \tilde{\mu}_k \tilde{\mu}_k = I
\]

Hence $\tilde{\mu}_k = \sqrt{\pi_k} W^T \mu_k$ are orthonormal vectors. Multiplying $\tilde{M}_3$ by $W$ across all three dimensions, we get

\[
\tilde{M}_3 = M_3(W, W, W)
= \sum_{k=1}^K \pi_k (W^T \mu_k) \otimes (W^T \mu_k) \otimes (W^T \mu_k)
= \sum_{k=1}^K \frac{1}{\sqrt{\pi_k}} \tilde{\mu}_k \otimes \tilde{\mu}_k \otimes \tilde{\mu}_k
\]

Upon canonical decomposition of $\tilde{M}_3$, if the eigenvalues and eigenvectors are $\{\lambda_k\}_{k=1}^K$ and $\{v_k\}_{k=1}^K$ respectively, then $\lambda_k = 1/\sqrt{\pi_k}$, i.e., $\pi_k = \lambda_k^2$, and,

\[
v_k = \tilde{\mu}_k = \sqrt{\pi_k} W^T \mu_k = \frac{1}{\lambda_k} W^T \mu_k
\]

The means $\{\mu_k\}_{k=1}^K$ can be retrieved from $\{\tilde{\mu}_k\}_{k=1}^K$ as, $\mu_k = \frac{1}{\lambda_k} W^T \tilde{\mu}_k$, where $W^T$ is the pseudo-inverse of $W^T$, i.e., $W^T = W (W^T W)^{-1}$. The final cluster means of the data (non-centered) can be further computed as $\mu_X + \mu_k$, $\forall k = 1 \ldots K$.

2.2. Related Works and Implementation Detail

[12] uses method of moments to extract the parameters of Mixtures of Gaussians. It assumes the presence of $K$ dominant eigenvalues in $M_2$, and assigns the $K$th largest eigenvalue to the variance $\sigma^2$ of each Gaussian component, and uses $\sigma^2$ for subsequent computation of the means of Gaussian Components. Although this assumption may hold true for synthetic datasets generated from Gaussian Mixtures, for real datasets, the covariance matrix ($M_2$) in real datasets does not have $K$ dominant eigenvalues; rather the eigenvalues decrease steadily. Therefore assignment of $K$th eigenvalue of $M_2$ to $\sigma^2$ will lead into error that will propagate to the subsequent computation of the means. We do not compute any variance term. Also, the Mixture of Gaussians algorithm needs number of data instances $N \geq \text{poly}(D)$ (Theorem 3 in [12]). This can be difficult to attain especially for high dimensional datasets where $N < D$. Our algorithm does not have any such requirements, and can work well with high dimensional datasets, as explained here.

The covariance $M_2$ can be estimated as $M_2 = \frac{1}{N} \hat{X} \otimes \hat{X}$, where $\hat{X} = X - \mu \tilde{I}^T_N$. The size of $M_2$ can be very high for high-dimensional datasets. For such datasets, the condition $N \ll D$ usually holds. We can compute the singular value decomposition $\frac{1}{\sqrt{N}} \hat{X} = P_N \Sigma K \hat{Q}_D \otimes K$. If $\Sigma$ & $U$ are the top $K$ eigenvalues and corresponding eigenvectors of $M_2$, then it can be easily checked that $\Sigma = S^2$ & $U = Q$. The top $K$ eigenvalues of $\frac{1}{\sqrt{N}} \hat{X} \hat{X}^T$ are also $\Sigma$, whereas $P$ contains the corresponding eigenvectors.

We first compute the top $K$ eigenvalues $\Sigma$ and corresponding eigenvectors $P$ of $\frac{1}{\sqrt{N}} \hat{X} \hat{X}^T$. Since $\Sigma^T = P^T \Sigma^{-1/2} P^T = I$, the matrix $Q$ can be computed as,

\[
Q^T = S^{-1} P^T \left( \frac{1}{\sqrt{N}} \hat{X} \right) = \frac{1}{\sqrt{N}} \Sigma^{-1/2} P^T \hat{X}
\]

\[
\Rightarrow U = Q = \frac{1}{\sqrt{N}} \hat{X}^T \Sigma^{-1/2}
\]

Also, we do not need to explicitly compute $M_3$. Since $M_3$ can be estimated as $M_3 = \frac{1}{N} \hat{X} \otimes \hat{X} \otimes \hat{X}$, $\tilde{M}_3 = M_3(W, W, W)$ can be estimated as,

\[
\tilde{M}_3 = \frac{1}{N} \hat{X} W \otimes \hat{X} W \otimes \hat{X} W
\]

where $\hat{X} = X - \mu \tilde{I}^T_N$.

The overall algorithm is described as Algorithm 3. Beyond the storage of the data, the whitening step takes $O(\text{min}(N, D)^2)$ space, and the rest of the algorithm $O(K^2 + DK)$. The whitening step is the main bottleneck of the algorithm, and we carried it out using eig function in Matlab, which uses Arnoldi’s iterations for $K$ largest eigenvalues in $M_2$. The whitening process has complexity $O(\text{min}(N, D)DK)$, $O(D^2 K)$ if $N > D$, or $O(N^2 K + NDK) = O(NDK)$ if $N < D$; the term $O(NDK)$ comes from the step in Equation (12). The computation of $M_2$ and whitening takes a single pass through the entire dataset. Even if the dataset
Theorem 1. Let us assume that for a bounded data with the Robust Power Method in [16]. for tensor decomposition, which gives very similar result to discussed in detail in [16]. We used the Tensor Toolbox [17] on a distributed system with clusters are can be computed as \( \sum_{p=1}^{P} \hat{M}_{3p} \), where \( \hat{M}_{3} \) is the covariance matrix computed from the data located at node \( p \). \( \hat{M}_{3} \) can be constructed by another pass through the entire dataset, resulting in \( O(1) \) passes for the entire seeding process. Again, for a distributed system with \( P \) nodes, \( \hat{M}_{3} \) can be computed using \( \hat{M}_{3} = \sum_{p=1}^{P} \hat{M}_{3p} \). The complexity of forming \( \hat{M}_{3} \) using equation [13] is \( O(NK^3) \), making the overall complexity \( O(\min(N,D)DK + NK^3) \). The tensor factorization does not require any more pass through the data. The complexity the tensor computation and factorization are discussed in detail in [16]. We used the Tensor Toolbox [17] for tensor decomposition, which gives very similar result to the Robust Power Method in [16].

### TABLE 1: Description of the datasets

| Dataset     | N    | D    | K    |
|-------------|------|------|------|
| Synthetic   | 5000 | 20   | 10   |
| Wine        | 178  | 13   | 3    |
| Isolet      | 7800 | 617  | 26   |
| HAPT        | 7767 | 561  | 12   |
| MNIST       | 60,000 | 784  | 10   |
| Yale-B      | 2414 | 32256 | 38   |
| CIFAR       | 50,000 | 3072 | 10   |
| CIFAR-100   | 50,000 | 3072 | 100  |

We choose real datasets with known cluster labels; this enables us to evaluate the performance in terms of clustering indices like Normalized mutual information (NMI), Rand Index & Purity. For K-means\(^{\dagger}\), we use \( r = 5 \) and \( l = 2K \), since these settings usually give the best results as described in [4]. For each method of initialization, we run the K-means iterations until \( \phi^{t-1}(C) - \phi^t(C) < \eta \phi^{t-1}(C) \), where \( \phi^t(C) \) is the cost defined in Equation 1 at iteration \( t \). We carry out our experiments on Unix Platform on a single machine with Intel i5 Processor (2.4GHz) and 8GB memory, and no multithreading or any other performance enhancement method is used in the code.

#### 3.1. Case: D > K

We first show our results on synthetic dataset generated from Gaussian Mixture model. We generate 5000 points from 10 component Gaussian Mixture with dimension \( D = 20 \) and with \( \sigma = 1 \) along each dimension. The convergence threshold \( \eta \) is kept at 0.001. Method of Moments produces the best clustering indices in competitive execution time.

Thereafter, we show the performance of different K-Means method on real life datasets, namely Wine dataset for classifying wine quality, Isolet dataset for speaker recognition, a dataset for Smartphone-Based Recognition of Human Activities and Postural Transitions (HAPT [18]), MNIST dataset for OCR recognition, Yale-B dataset for face recognition and CIFAR datasets for generic image recognition. The experiment for each K-Means algorithm is repeated for 10 executions. The detail of the datasets are listed in Table [1] and the aggregated results are shown in Table [2]. We used \( \eta = .01 \) for Wine dataset, and \( \eta = .001 \) for the rest. The variation in different clustering indices for each algorithm is shown in Figure [I].

MoM produces very competitive results compared to the rest of the methods. Its results are distinctly better than the rest for MNIST and Yale-B datasets. It produces better Rand Index for all the datasets except one. MoM also takes the least time to complete than K-Means++ or K-Means\(^{\dagger}\). Although K-Means takes less time than MoM in a number of cases, MoM almost always produces better clustering than K-Means. K-Means\(^{\dagger}\) takes a lot more time that the rest in a single node environment, since the algorithm has computational benefit only in distributed frameworks.

#### 3.2. Case: D ≤ K

The only limitation of our algorithm is the requirement \( D > K \). This can be easily overcome by synthesizing new features to increase the dimension of the training dataset. For example, we used Iris dataset (150 instance, 4 features, \( K = 3 \)) that has \( D \sim K \), and Method of Moments did not perform well on the original features. We synthesized additional 6 features as \( x_i - [\mu_{x_i}] \), \( x_j - [\mu_{x_j}] / \sqrt{\sigma_{x_j}} \), where \( x = [x_1, x_2, \ldots, x_D] \in X & i, j \in \{1, \ldots D\}, i \neq j \) and \( \sigma_{x_j} \) is the standard deviation along \( i \)th dimension of the data and so on. We used \( \eta = .01 \) for convergence threshold of K-Means iterations, and aggregated the results over
excluding the case when all the
possible to find
ferent K-Means methods for Iris dataset with synthesized
TABLE 3: NMI, Adjusted Rand Index and Purity for differ-
| Dataset | Method | NMI      | Rand Index | Purity | Time (sec) |
|---------|--------|----------|------------|--------|------------|
| Synthetic | K-M | 0.4363 ± 0.2066 | 0.1471 ± 0.1483 | 0.9042 ± 0.0564 | 0.275 ± 0.1458 |
|         | K-M++ | 0.8711 ± 0.0464 | 0.8064 ± 0.0696 | 0.9172 ± 0.0456 | 2.875 ± 0.1496 |
|         | KM|| | 0.8558 ± 0.0369 | 0.8067 ± 0.0643 | 0.9107 ± 0.0303 | 2.555 ± 0.1154 |
|         | MoM | 0.9351 ± 0.0006 | 0.9444 ± 0.0006 | 0.9744 ± 0.0003 | 1.815 ± 0.142 |
| Wine    | K-M | 0.4242 ± 0.0960 | 0.3645 ± 0.0663 | 0.6910 ± 0.0661 | 0.01 ± 0.0662 |
|         | K-M++ | 0.4288 ± 0.0119 | 0.3645 ± 0.0307 | 0.7079 ± 0.0382 | 0.01 ± 0.0654 |
|         | KM|| | 0.4378 ± 0.0128 | 0.3719 ± 0.0096 | 0.7079 ± 0.0205 | 0.925 ± 0.1154 |
|         | MoM | 0.4430 ± 0.0006 | 0.3728 ± 0.0006 | 0.7023 ± 0.0001 | 2.015 ± 1.719 |
| Isolet  | K-M | 0.604 ± 0.0453 | 0.2868 ± 0.0569 | 0.519 ± 0.0483 | 36 ± 18.2647 |
|         | K-M++ | 0.709 ± 0.0075 | 0.4562 ± 0.0272 | 0.6152 ± 0.0314 | 88 ± 5.6634 |
|         | KM|| | 0.627 ± 0.0221 | 0.3217 ± 0.0210 | 0.7518 ± 0.0403 | 112 ± 8.0709 |
|         | MoM | 0.709 ± 0.0045 | 0.4474 ± 0.0099 | 0.6484 ± 0.0103 | 46 ± 12.6826 |
| HAPT    | K-M | 0.5552 ± 0.0537 | 0.3125 ± 0.0759 | 0.3848 ± 0.0941 | 12 ± 9.3119 |
|         | K-M++ | 0.5887 ± 0.0176 | 0.3848 ± 0.0474 | 0.5415 ± 0.0498 | 41 ± 5.1546 |
|         | KM|| | 0.281 ± 0.0430 | 0.3450 ± 0.0702 | 0.7770 ± 0.0664 | 45 ± 4.2039 |
|         | MoM | 0.6057 ± 0.0028 | 0.4523 ± 0.003 | 0.5912 ± 0.0049 | 25 ± 2.0674 |
| MNIST   | K-M | 0.463 ± 0.0187 | 0.3334 ± 0.0299 | 0.5446 ± 0.0341 | 155 ± 21.9898 |
|         | K-M++ | 0.478 ± 0.0092 | 0.3571 ± 0.0083 | 0.5696 ± 0.0145 | 166 ± 32.0633 |
|         | KM|| | 0.481 ± 0.0192 | 0.3494 ± 0.0284 | 0.5614 ± 0.0204 | 437 ± 25.0438 |
|         | MoM | 0.494 ± 0.0108 | 0.3775 ± 0.0160 | 0.6064 ± 0.0155 | 83 ± 13.1723 |
| Yale-B  | K-M | 0.1015 ± 0.0113 | 0.012 ± 0.0009 | 0.1237 ± 0.0081 | 370 ± 51.6615 |
|         | K-M++ | 0.1409 ± 0.0062 | 0.0131 ± 0.0013 | 0.1315 ± 0.0070 | 470 ± 27.6560 |
|         | KM|| | 0.1302 ± 0.0066 | 0.0112 ± 0.0020 | 0.1359 ± 0.0061 | 2040 ± 147.8753 |
|         | MoM | 0.1688 ± 0.0038 | 0.0201 ± 0.0011 | 0.1437 ± 0.0042 | 396 ± 11.4195 |
| CIFAR   | K-M | 0.0748 ± 0.0039 | 0.0401 ± 0.0024 | 0.2263 ± 0.0085 | 232 ± 30.3556 |
|         | K-M++ | 0.0734 ± 0.0026 | 0.0365 ± 0.0063 | 0.2335 ± 0.0142 | 419 ± 63.6475 |
|         | KM|| | 0.0770 ± 0.0027 | 0.0384 ± 0.0047 | 0.2404 ± 0.0124 | 1132 ± 211.0498 |
|         | MoM | 0.0792 ± 0.0022 | 0.0451 ± 0.0023 | 0.2382 ± 0.0126 | 269 ± 19.6842 |
| CIFAR-100 | K-M | 0.1496 ± 0.0016 | 0.0165 ± 0.0038 | 0.101 ± 0.0107 | 385 ± 441 |
|         | K-M++ | 0.1529 ± 0.0012 | 0.0197 ± 0.0004 | 0.0963 ± 0.0035 | 519 ± 3800 |
|         | KM|| | 0.1520 ± 0.0014 | 0.0205 ± 0.0004 | 0.1035 ± 0.0027 | 1172 ± 836 |
|         | MoM | 0.1504 ± 0.0009 | 0.0238 ± 0.0007 | 0.117 ± 0.004 | 3780 ± 602 |

TABLE 2: NMI, Adjusted Rand Index, Purity and Computation Time for different K-Means methods for the datasets

100 executions. MoM produces best results with minimal variation of the results across different executions (Table 3).
We can synthesize features \( \propto \prod_{d=1}^{D}(x_d - [\mu_X]_d)^{m_d} \) with \( m_d = 0, 1 \ldots M \). When \( m_d = 1 \) for \( d \)th feature, and 0 elsewhere, we get back the original centered data. The total number of features we can synthesize this way is \( M^D - 1 \), excluding the case when all the \( m_d \)s are 0. Since it is always possible to find \( M \in \mathbb{Z}^+ \) such that \( M^D - 1 > K \), we can always use Method of Moments for any dataset.

4. Conclusion and Further Extension

Here we present a probabilistic K-means algorithm based on factorization of higher order moments of the data. The existing algorithms are heuristic in nature, whereas here we introduce a probabilistic interpretation of K-means algorithm based on latent variables. Latent Variable modeling has been used in various applications. However, these algorithms assume that the clusters are generated from a particular probability distribution. K-means, on the other hand, imposes no such assumption, and is a much more versatile algorithm for clustering real datasets. Here, we show how the latent variable model can be incorporated in K-means without assuming the clusters to follow any particular distribution. The only assumption needed is the bounded norm of the data, which holds well for real life datasets.

We establish the competitive performance of our model through various experiments. Method of Moments requires \( O(1) \) passes through the entire dataset to compute the second and third order moments to extract the initial means for most practical datasets, and is therefore very suitable for Large Scale datasets. In practice, it will require only two passes to compute the moments. Also, Method of Moments takes less number of K-means or Lloyd’s iterations to converge after the mean initialization. For smaller datasets, the tensor factorization takes a lot more time compared to the K-Means iterations through the dataset. As the size of datasets and \( K \) increase, the K-Means iterations become significantly costlier than tensor factorization. A higher seeding time of MoM is well compensated by lower number of K-Means iterations following it. For CIFAR-100 dataset, MoM
finishes in minimum time of all.

References

[1] A. Coates, A. Y. Ng, and H. Lee, “An analysis of single-layer networks in unsupervised feature learning,” in International conference on artificial intelligence and statistics, 2011, pp. 215–223.

[2] D. Aloise, A. Deshpande, P. Hansen, and P. Popat, “Np-hardness of euclidean sum-of-squares clustering,” Machine Learning, vol. 75, no. 2, pp. 245–248, 2009. [Online]. Available: http://dx.doi.org/10.1007/s10994-009-5103-0

[3] D. Arthur and S. Vassilvitskii, “k-means++: The advantages of careful seeding,” in Proceedings of the eighteenth annual ACM-SIAM symposium on Discrete algorithms. Society for Industrial and Applied Mathematics, 2007, pp. 1027–1035.

[4] B. Bahmani, B. Moseley, A. Vattani, R. Kumar, and S. Vassilvitskii, “Scalable k-means++,” Proceedings of the VLDB Endowment, vol. 5, no. 7, pp. 622–633, 2012.

[5] N. Ailon, R. Jaiswal, and C. Monteleoni, “Streaming k-means approximation,” in Advances in Neural Information Processing Systems, 2009, pp. 10–18.

[6] M. Shindler, A. Wong, and A. W. Meyerson, “Fast and accurate k-means for large datasets,” in Advances in neural information processing systems, 2011, pp. 2375–2383.

[7] D. Hsu, S. M. Kakade, and T. Zhang, “A spectral algorithm for learning hidden markov models,” Journal of Computer and System Sciences, vol. 78, no. 5, pp. 1460–1480, 2012.

[8] L. Song, B. Boots, S. M. Siddiqui, G. J. Gordon, and A. J. Smola, “Hilbert space embeddings of hidden markov models,” in Proceedings of the 27th international conference on machine learning (ICML-10), 2010, pp. 991–998.

[9] A. Anandkumar, Y.-k. Liu, D. J. Hsu, D. P. Foster, and S. M. Kakade, “A spectral algorithm for latent dirichlet allocation,” in Advances in Neural Information Processing Systems, 2012, pp. 917–925.

[10] S. B. Cohen, K. Stratos, M. Collins, D. P. Foster, and L. Ungar, “Spectral learning of latent-variable pcfgs: Algorithms and sample complexity,” The Journal of Machine Learning Research, vol. 15, no. 1, pp. 2399–2449, 2014.

[11] P. S. Dhillon, J. Rodu, M. Collins, D. P. Foster, and L. H. Ungar, “Spectral dependency parsing with latent variables,” in Proceedings of the 2012 joint conference on empirical methods in natural language processing and computational natural language learning. Association for Computational Linguistics, 2012, pp. 205–213.
The LHS is the cost incurred keeping the cluster assignments $C_{1:k}$ but changing the means to $\{\hat{\mu}_k\}_{k=1}^K$. Now, if we keep running the Lloyd’s iterations seeding the means with $\{\hat{\mu}_k\}_{k=1}^K$, at each iteration the cost with decrease, and the LHS will converge to a local minima. If the final cluster assignment is $\hat{C}_{1:k}$, then $\phi(C_{1:k}, \hat{\mu}_{1:k}) \leq \phi(C_{1:k}, \hat{\mu}_{1:k})$.

Therefore, we can write,

$$
\phi(C_{1:k}, \hat{\mu}_{1:k}) \leq \phi(C_{1:k}, \hat{\mu}_{1:k}) + \sum_{k=1}^K |C_k|(\mu_k - \hat{\mu}_k)^2
$$

Next, we will establish a bound on $||\mu_k - \hat{\mu}_k||$ for $k = 1, 2 \ldots K$.

Appendix B.

Vector Norms

Let us assume that we draw samples from a distribution which satisfies $||x|| \leq B$. Let the true covariance matrix and the third order moment of the population be $M_2$ and $M_3$. Let us assume that we select $N$ i.i.d. samples $x_1, \ldots x_N$ from the population such that $N \gg K$, and the covariance and the third order moment estimates are $M_2$ and $M_3$. Let $\varepsilon_{M_2} = ||M_2 - M_2||_2$. We use the second order operator norm of the matrices here. Let us assume $\varepsilon_{M_2} \leq \sigma_K(M_2)/2$, where $\sigma_K$ is the $K$th largest eigenvalue of $M_2$. We will derive the conditions which satisfies this later.

If $\Sigma = diag(\sigma_1, \sigma_2 \ldots \sigma_K)$ are the top-$K$ eigenvalues of $M_2$, and $U$ are the corresponding eigenvectors, then the whitening matrix $W = U\Sigma^{-1/2}$. Also, $W^TM_2KW = I_{K \times K}$, where $M_{2K}$ is the $K$ rank approximation of $M_2$.

Then,

$$
||W||_2 = \sqrt{\max \text{eig}(W^TW)} = \sqrt{\max \text{eig}(\Sigma^{-1})}
= \frac{1}{\sqrt{\sigma_K(M_2)}}
$$

Similarly, if $W^W = W(W^W)^{-1}$, then $W^W = W\Sigma = U\Sigma^{1/2}$. Therefore,

$$
||W^W||_2 = \sqrt{\max \text{eig}(\Sigma)} = \sqrt{\sigma_1(M_2)}
$$

Let $\hat{W}$ be the whitening matrix for $\hat{M}_2$, i.e., $\hat{W}^TM_2K\hat{W} = I_{K \times K}$. Then by Weyl’s inequality, $\sigma_k(M_2) - \sigma_k(\hat{M}_2) \leq ||M_2 - \hat{M}_2||, \forall k = 1, 2 \ldots K$. Therefore,

$$
||\hat{W}||_2^2 = \frac{1}{\sigma_K(M_2)} \leq \frac{1}{\sigma_K(M_2) - ||M_2 - \hat{M}_2||} \leq \frac{2}{\sigma_K(M_2)}
$$

Appendix A.

General Outline of the Bound

If the optimal set of clusters are $C_1, C_2 \ldots C_K$ with means $\mu_1, \mu_2 \ldots \mu_K$, then the optimal cost is $\phi(C_{1:k}, \mu_{1:k}) = \sum_{k=1}^K \sum_{x \in C_k} (x - \mu_k)^2$. Without loss of generality, we can assume that the means corresponding to the latent variable model in Equation (3) are the optimal means. Now, let us assume that we run MoM on $N$ i.i.d. samples, and the resulting means are $\hat{\mu}_1, \hat{\mu}_2 \ldots \hat{\mu}_K$. Then, if we change the mean of $k$th cluster from $\mu_k$ to $\hat{\mu}_k$ keeping the cluster assignment of the points same,

$$
\phi(C_k, \hat{\mu}_k) = \sum_{x \in C_k} (x - \hat{\mu}_k)^2
= \sum_{x \in C_k} (x - \mu_k + \mu_k - \hat{\mu}_k)^2
= \sum_{x \in C_k} (x - \mu_k) + |C_k|(\mu_k - \hat{\mu}_k)^2
= \phi(C_k, \mu_k) + |C_k|(\mu_k - \hat{\mu}_k)^2
$$

Taking into account all the $K$ clusters,

$$
\phi(C_{1:k}, \hat{\mu}_{1:k}) = \phi(C_{1:k}, \mu_{1:k}) + \sum_{k=1}^K |C_k|(\mu_k - \hat{\mu}_k)^2
$$

(14)
Also, by Weyl's Theorem,
\[
\|\hat{W}^\top\|^2 = \sigma_1^2(M_2) \leq \sigma_1(M_2) + \varepsilon M_2 \leq 1.5 \sigma_1(M_2) \\
\implies \|\hat{W}^\top\|_2 \leq \sqrt{1.5} \sigma_1(M_2) \leq 1.5 \sqrt{\sigma_1(M_2)} \quad (18)
\]

Let \( D \) be the eigenvectors of \( \hat{W} M_2 \hat{W} \), and \( A \) be the corresponding eigenvalues. Then we can write, \( W M_2 \hat{W} = ADA^\top \). Then \( W = W A D^{-1/2} A^\top \) whitens \( M_2 \), i.e., \( W^\top M_2 W = I \). Therefore,
\[
\|I - D\|_2 = \|I - ADA^\top\|_2 \\
= \|I - \hat{W} M_2 \hat{W}\|_2 \\
= \|\hat{W} M_2 \hat{W} - \hat{W} M_2 \hat{W}\|_2 \\
\leq \|\hat{W}\|_2^2 \|M_2 - \hat{M}_2\| \\
\leq \frac{2}{\sigma_K(M_2)^{3/2}} \varepsilon M_2 
\]

\( \varepsilon_W = \|W - \hat{W}\|_2 \\
= \|W - W A D^{1/2} A^\top\|_2 \\
= \|W\|_2 \|D^{1/2}\|_2 \|I - D^{1/2}\|_2 \\
= \|W\|_2 \|D^{1/2}\|_2 \|I + D^{1/2}\|_2 \\
\leq \frac{2}{\sigma_K(M_2)^{3/2}} \varepsilon M_2 
\]

\( \varepsilon_{W^\top} = \|W^\top - \hat{W}^\top\|_2 \\
= \|W^\top A D^{1/2} A^\top - \hat{W}^\top\|_2 \\
= \|W^\top\|_2 \|D^{1/2}\|_2 \|I - D^{1/2}\|_2 \\
\leq \frac{2}{\sigma_K(M_2)^{3/2}} \varepsilon M_2 
\]

**Appendix C. Tensor Norm**

Let us define the second operator norm of a tensor \( T \in \mathbb{R}^{D \times D \times D} \) as,
\[
\|T\|_2 = \sup\{\|T(v, v, v)\|_2 : v \in \mathbb{R}^{D} \& ||v|| = 1\} \quad (21)
\]

**Lemma 1.** For a tensor \( T \in \mathbb{R}^{D \times D \times D} \), \( \|T\|_2 \leq \|T\|_F \), where \( \|T\|_F \) is the Frobenius norm defined as,
\[
\|T\|_F = \sqrt{\sum_{i,j,k} (T_{i,j,k})^2} \quad (22)
\]

**Proof:** For any real matrix \( A \), \( \|A\|_2 \leq \|A\|_F \). Let us unfold the tensor \( T \) as the collection of \( D \) matrices, as, \( T = \{T_1, T_2 \ldots T_D\} \). Then,
\[
T(v, v, v) = v^\top [T_1 v | T_2 v | \ldots | T_K v] v \\
= \langle [v^\top T_1 v, v^\top T_2 v, \ldots, v^\top T_K v], v \rangle 
\]

Therefore,
\[
\|T\|_2 = \sup\{\|T(v, v, v)\|_2 : v \in \mathbb{R}^{D} \& ||v|| = 1\} \\
= \sup\{\|v^\top T_1 v, v^\top T_2 v, \ldots, v^\top T_K v\|_2 : v \in \mathbb{R}^{D} \& ||v|| = 1\} 
\]

Using Holder's inequality,
\[
\|T\|_2 \leq \sup\{\|v^\top T_1 v, v^\top T_2 v, \ldots, v^\top T_K v\|_2 \|v\|_2 \} \\
= \sup\{\|v^\top T_1 v, v^\top T_2 v, \ldots, v^\top T_K v\|_F \} \\
= \sqrt{\left(\sum_{i=1}^{K} \|T_i\|_F^2 \right)} \\
= \|T\|_F 
\]

Let us define \( \varepsilon_{M_3} = \|M_3 - \hat{M}_3\|_2 \). Then from Appendix B in [13].

\[
\varepsilon_{tw} = \|M_3(W, W, W) - \hat{M}_3(\hat{W}, \hat{W}, \hat{W})\|_2 \\
\leq \|M_3\|_2 \left(\|\hat{W}\|_2^2 + \|\hat{W}\|_2 \|W\|_2 + \|W\|_2^2\right) \varepsilon_W \\
+ \|\hat{W}\|^3 \varepsilon_{M_3} \\
\leq \|M_3\|_2 \left(\frac{2 + \sqrt{2} + 1}{\sigma_K(M_2)}\right) \varepsilon_W + \frac{2\sqrt{2}}{\sigma_K(M_2)^{3/2}} \varepsilon_{M_3} \\
\leq \|M_3\|_2 \left(\frac{3 + \sqrt{2}}{\sigma_K(M_2)}\right) \frac{2}{\sigma_K(M_2)^{3/2}} \varepsilon_{M_2} + \frac{2\sqrt{2}}{\sigma_K(M_2)^{3/2}} \varepsilon_{M_3} \\
\leq \frac{10\|M_3\|_2}{\sigma_K(M_2)^{3/2}} \varepsilon_{M_2} + \frac{2\sqrt{2}}{\sigma_K(M_2)^{3/2}} \varepsilon_{M_3} 
\]

**Lemma 2.** (Robust Power Method from [16]) If \( \hat{T} = T + E \in \mathbb{R}^{K \times K \times K} \), where \( T \) is an symmetric tensor with orthogonal decomposition \( T = \sum_{k=1}^{K} \lambda_k v_k \otimes v_k \otimes v_k \) with each \( \lambda_k > 0 \), and \( E \) has operator norm \( ||E|| \leq \epsilon \). Let \( \lambda_{\text{min}} = \min_{k \geq 1} \{\lambda_k\} \) and \( \lambda_{\text{max}} = \max_{k \geq 1} \{\lambda_k\} \). Let there exist constants \( c_1, c_2 \) such that \( \epsilon \leq c_1 \cdot (\lambda_{\text{min}}/K) \), and \( N \geq c_2(\log K + \log \log (\lambda_{\text{max}}/\epsilon)) \). Then if Algorithm 1 in [16] is called for \( K \) times, with \( L = \text{poly}(K) \log(1/\eta) \) restarts each time for some \( \eta \in (0, 1) \), then with probability at least \( 1 - \eta \), there exists a permutation \( \pi \in [K] \), such that,
\[ \|v_{\pi(k)} - \hat{v}_k\| \leq 8 \frac{\epsilon}{\lambda_{\pi(k)}} , \|\lambda_k - \lambda_{\pi(k)}\| \leq 5\epsilon \ \forall k \in [K] \] (27)

If the original K clusters are \( C_{1,K} \), then,
\[ \lambda_k = \frac{1}{\sqrt{\pi_k}} = \frac{1}{\sqrt{|C_k|/N}} = \sqrt{\frac{N}{|C_k|}} , \ k \in [K] \] (28)

Therefore, we need,
\[ N \geq c_2 \left( \log K + \log \left( \frac{K\lambda_{\text{max}}}{c_1\lambda_{\text{min}}} \right) \right) \]
\[ \geq c_2 \left( \log K + \log \left( \frac{K}{c_1} \cdot \sqrt{\frac{\max_k |C_k|}{\min_k |C_k|}} \right) \right) \] (29)

This contributes in the first lower bound (\( n_1 \)) of \( N \) in Theorem 1.

Next, we will derive the bound for the reconstruction error for the means from these bounds. Since \( \mu_k = \lambda_k W^* v_k \) (Algorithm 3),
\[ ||\mu_k - \hat{\mu}_k|| \]
\[ = ||\lambda_k W^* v_k - \hat{\lambda}_k \hat{W}^* \hat{v}_k|| \]
\[ = ||\lambda_k W^* v_k - \lambda_k W^* \hat{v}_k + \lambda_k W^* \hat{v}_k - \hat{\lambda}_k \hat{W}^* \hat{v}_k|| \]
\[ \leq ||\lambda_k W^*||_2 ||v_k - \hat{v}_k|| + ||\lambda_k W^* - \hat{\lambda}_k \hat{W}^*||_2 \|\hat{v}_k|| \]
\[ \leq ||\lambda_k W^*||_2 ||v_k - \hat{v}_k|| + ||\lambda_k W^* - \hat{\lambda}_k \hat{W}^*|| \]
\[ + ||\lambda_k \hat{W}^* - \hat{\lambda}_k \hat{W}^*|| \]
\[ \leq ||\lambda_k(||W^*||_2 ||v_k - \hat{v}_k|| + \epsilon W^*|| + ||W^*||_2 \lambda_k - \hat{\lambda}_k|| \]
\[ \leq \lambda_k \left( ||W^*||_2 \frac{8\epsilon}{\lambda_k} + \epsilon W^*|| + ||W^*||_2 \cdot 5\epsilon \right) \]
\[ \leq \left( 8\sqrt{\sigma_1(M_2)} + \frac{3}{2} \sqrt{\sigma_1(M_2)} \right) \epsilon + \lambda_k \epsilon W^* \]
\[ \leq 16\sqrt{\sigma_1(M_2)} \epsilon + \lambda_k \frac{2\sqrt{\sigma_1(M_2)}}{\sigma_K(M_2)} \epsilon M_2 \] (30)

Setting \( \epsilon \) as the upper-bound of \( \epsilon_{tw} = ||M_3(W, W, W) - \hat{M}_3(W, W, W)||_2 \), we get
\[ ||\mu_k - \hat{\mu}_k|| \]
\[ \leq 16\sqrt{\sigma_1(M_2)} \left( \frac{10||M_2||}{\sigma_K(M_2)^{5/2}} \epsilon M_2 + \frac{2\sqrt{2}}{\sigma_K(M_2)^{3/2}} \epsilon M_2 \right) \]
\[ + \lambda_k \frac{2\sqrt{\sigma_1(M_2)}}{\sigma_K(M_2)} \epsilon M_2 \] (31)

### Appendix D.

#### Tail Inequality

If we draw \( N \) i.i.d. samples \( x_1, x_2 \ldots x_N \) from a distribution with bounded support such that \( ||x|| \leq B \), then with probability at least \( 1 - \delta \) with \( \delta \in (0,1) \),
\[ \left| \left| \frac{1}{N} \sum_{i=1}^{N} x_i - \mathbb{E}[x] \right| \right|_F \leq \frac{2}{\sqrt{N}} \left( 1 + \sqrt{\log(1/\delta)} \right) \] (32)

This is proven as Lemma 5 in [13]. To keep the equations simple, we assume \( ||x|| \leq 1 \). Please note that we can simply replace \( x \) by \( x/B \) to get back the original equations.

If \( ||x|| \leq 1 \), then \( ||x \otimes x|| \) and \( ||x \otimes x \otimes x||_F \) are also bounded by 1. Therefore, we can say that with probability at least \( 1 - \delta \) (Lemma 7 in [21]),
\[ \left| \left| \frac{1}{N} \sum_{i=1}^{N} x_i \otimes x_i - \mathbb{E}[x \otimes x] \right| \right|_F \leq \frac{2}{\sqrt{N}} \left( 1 + \sqrt{\log(1/\delta)} \right) \] (33)

and,
\[ \left| \left| \frac{1}{N} \sum_{i=1}^{N} x_i \otimes x_i \otimes x_i - \mathbb{E}[x \otimes x \otimes x] \right| \right|_F \leq \frac{2}{\sqrt{N}} \left( 1 + \sqrt{\log(1/\delta)} \right) \] (34)

Let us define \( \mu_X = \mathbb{E}[x] \), and \( \hat{\mu}_X = \frac{1}{N} \sum_{i=1}^{N} x_i \). Then \( M_2 = \mathbb{E}[(x - \mu_X) \otimes (x - \mu_X)] = \mathbb{E}[x \otimes x] - \mu_X \otimes \mu_X \), and \( M_2 = \frac{1}{N} \sum_{i=1}^{N} x_i \otimes x_i - \mu_X \otimes \mu_X \). Therefore,
\[ M_2 - \hat{M}_2 = \mathbb{E}[x \otimes x] - \frac{1}{N} \sum_{i=1}^{N} x_i \otimes x_i \]
\[ + \mu_X \otimes (\hat{\mu}_X - \mu_X) + (\hat{\mu}_X - \mu_X) \otimes \mu_X \]

Each of the terms of RHS can be bounded with a probability of \( \delta \), resulting in a total probability of \( 3\delta \) (using union-bond principle), i.e., with a probability of \( 1 - 3\delta \),
\[ \left| \left| M_2 - \hat{M}_2 \right| \right|_F \leq \frac{6}{\sqrt{N}} \left( 1 + \sqrt{\log(3/\delta)} \right) \] (35)

Replacing \( \delta \) by \( \delta/3 \), we can say with probability at least \( 1 - \delta \),
\[ \left| \left| M_2 - \hat{M}_2 \right| \right|_F \leq \frac{6}{\sqrt{N}} \left( 1 + \sqrt{\log(3/\delta)} \right) \] (36)

Also, since \( \epsilon_{M_2} = ||M_2 - \hat{M}_2||_2 \leq ||M_2 - \hat{M}_2||_F \), to satisfy \( \epsilon_{M_2} \leq \sqrt{\sigma_K(M_2)/2} \), we need,
\[ N \geq \left( \frac{12}{\sigma_K(M_2)} \left( 1 + \sqrt{\log(3/\delta)} \right)^2 \right) \] (37)

This contributes in the second lower bound (\( n_2 \)) of \( N \) in Theorem 1.
Please note that,
\[
M_3 = E[(x - \mu_X) \otimes (x - \mu_X) \otimes (x - \mu_X)] \\
= E[x \otimes x \otimes x] - E[x \otimes x] \otimes \mu_X - \mu_X \otimes E[x \otimes x] \\
- E[x \otimes x] \otimes x + 2\mu_X \otimes \mu_X \otimes x
\]
Therefore, using (34),
\[
M_3 - \hat{M}_3 \\
= E[x \otimes x \otimes x] - \frac{1}{N} x_i \otimes x_i \otimes x_i \\
+ E[x \otimes x] \otimes (\hat{\mu}_X - \mu_X) \\
+ \left( \frac{1}{N} x_i \otimes x_i - E[x \otimes x] \right) \otimes \hat{\mu}_X \\
+ (\hat{\mu}_X - \mu_X) \otimes E[x \otimes x] \\
+ \hat{\mu}_X \otimes \left( \frac{1}{N} x_i \otimes x_i - E[x \otimes x] \right) \\
+ E[x \otimes (\hat{\mu}_X - \mu_X) \otimes x] \\
+ \left( \frac{1}{N} x_i \otimes \hat{\mu}_X - \mu_X \right) \otimes x_i - E[x \otimes \hat{\mu}_X \otimes x] \\
+ 2(\mu_X \otimes \mu_X \otimes \hat{\mu}_X - \mu_X \otimes \mu_X \otimes \mu_X) \\
+ 2(\mu_X \otimes \mu_X \otimes \mu_X - \mu_X \otimes \mu_X \otimes \mu_X) \\
+ 2(\mu_X \otimes \mu_X \otimes \hat{\mu}_X - \mu_X \otimes \hat{\mu}_X \otimes \mu_X)
\]
(38)
Combining all the terms results in a bounding probability of 10δ using union-bound principle, and 13 units of bounding norm, i.e., with probability at least 1 - 10δ,
\[
||M_3 - \hat{M}_3||_F \leq \frac{26}{\sqrt{N}} \left( 1 + \sqrt{\frac{\log(1/\delta)}{2}} \right)
\]
Replacing δ with δ/10, with probability at least 1 - δ,
\[
||M_3 - \hat{M}_3||_F \leq \frac{26}{\sqrt{N}} \left( 1 + \sqrt{\frac{\log(10/\delta)}{2}} \right)
\]
(39)

Appendix E.
Completing the Proof

From Lemma 1 we get \( \varepsilon_{M_3} \leq ||M_3 - \hat{M}_3||_F \). Also, \( ||M_3||_2 \leq ||M_3||_F \leq ||x \otimes x \otimes x|| \leq 1 \). Therefore, from equation (31)
\[
||\mu_k - \hat{\mu}_k|| \leq 160 \frac{\sigma_1(M_2)}{\sigma_K(M_2)^{3/2}} \cdot \frac{6}{\sqrt{N}} \left( 1 + \sqrt{\frac{\log(3/\delta)}{2}} \right) \\
+ 32 \frac{2\sigma_1(M_2)}{\sigma_K(M_2)^{3/2}} \cdot \frac{26}{\sqrt{N}} \left( 1 + \sqrt{\frac{\log(10/\delta)}{2}} \right) \\
+ 2 \frac{\sigma_1(M_2)}{\sigma_K(M_2)^{3/2}} \cdot \frac{6}{\sqrt{|C_k|}} \left( 1 + \sqrt{\frac{\log(3/\delta)}{2}} \right)
\]
(40)
Since \( \lambda_k = \frac{1}{\sqrt{\theta_K}} = \sqrt{\frac{N}{|C_k|}} \), where \( |C_k| \) is the size of kth cluster, with \( k \in [K] \).
Assigning \( c_3 = 960 \sqrt{\frac{\sigma_1(M_2)}{\sigma_K(M_2)^{3/2}}} \), \( c_4 = 832 \sqrt{2\sigma_1(M_2)} \), \( c_5 = 12 \frac{\sqrt{\sigma_1(M_2)}}{\sqrt{\sigma_K(M_2)^{3/2}}} \), \( \varepsilon_1 = 1 + \sqrt{\frac{\log(3/\delta)}{2}} \) and \( \varepsilon_2 = 1 + \sqrt{\frac{\log(10/\delta)}{2}} \), we get
\[
||\mu_k - \hat{\mu}_k|| \leq c_3\varepsilon_1 \sqrt{\frac{N}{N}} + c_4 \varepsilon_2 \sqrt{\frac{N}{N}} + c_5 \varepsilon_1 \sqrt{\frac{N}{|C_k|}}
\]
(41)
\[
\sum_{k=1}^{K} |C_k| (\mu_k - \hat{\mu}_k)^2 \\
\leq \sum_{k=1}^{K} \frac{|C_k|}{N} (c_3\varepsilon_1^2 + c_4\varepsilon_2^2 + 2c_3c_4\varepsilon_1\varepsilon_2) \\
+ 2\sum_{k=1}^{K} \sqrt{\frac{|C_k|}{N}} (c_3c_5\varepsilon_1^2 + c_4c_5\varepsilon_1\varepsilon_2) \\
+ \sum_{k=1}^{K} |C_k| \left( \sqrt{\frac{c_5\varepsilon_1^2}{|C_k|}} \right)
\]
(42)
The quantity \( \sum_{k=1}^{K} \frac{|C_k|}{N} \) reaches its maximum value when \( |C_k| = N/K \) for all \( k = 1, 2 \ldots K \), and the maximum value is \( \sqrt{K} \). Therefore,
\[
\sum_{k=1}^{K} |C_k| (\mu_k - \hat{\mu}_k)^2 \\
\leq (c_3\varepsilon_1^2 + c_4\varepsilon_2^2 + 2c_3c_4\varepsilon_1\varepsilon_2) + 2\sqrt{K} (c_3c_5\varepsilon_1^2 + c_4c_5\varepsilon_1\varepsilon_2)
\]
(43)
The proof of Theorem 1 is completed by substituting the value of \( \sum_{k=1}^{K} |C_k| (\mu_k - \hat{\mu}_k)^2 \) in Equation 15.
Also, to satisfy the conditions in Lemma 2, we need \( \varepsilon_{tw} \leq \varepsilon \leq c_1 \lambda_{min}^2 \). Since \( \lambda_{min} = 1/\sqrt{\pi_{max}} \), from equation 26 we need,
\[
\varepsilon_{tw} \leq \frac{c_3}{16 \sqrt{\sigma_1(M_2)}} \cdot \frac{\varepsilon_1}{\sqrt{N}} + \frac{c_4}{16 \sqrt{\sigma_1(M_2)}} \cdot \frac{\varepsilon_2}{\sqrt{N}} \\
\leq c_1 \lambda_{min}^2 = c_1 \frac{1}{K \sqrt{\pi_{max}}}
\]
(44)
Therefore, we require,
\[
N \geq \frac{\pi_{max} K^2}{(16c_1)^2 \sigma_1(M_1)^2 (c_3\varepsilon_1 + c_4\varepsilon_2)^2}
\]
or,
\[
N \geq \frac{K^2}{(16c_1)^2 \sigma_1(M_1)^2 (c_3\varepsilon_1 + c_4\varepsilon_2)^2}
\]
since \( \pi_{max} \leq 1 \). This contributes to \( n_3 \) in Theorem 1.