Spectral Clustering using Eigenspectrum Shape Based Nyström Sampling

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Abstract—Spectral clustering has shown a superior performance in analyzing the cluster structure. However, its computational complexity limits its application in analyzing large-scale data. To address this problem, many low-rank matrix approximating algorithms are proposed, including the Nyström method—an approach with proven approximate error bounds. There are several algorithms that provide recipes to construct Nyström approximations with variable accuracies and computing times. This paper proposes a scalable Nyström-based clustering algorithm with a new sampling procedure. Centroid Minimum Sum of Squared Similarities (CMS3), and a heuristic on when to use it. Our heuristic depends on the eigenspectrum shape of the dataset, and yields competitive low-rank approximations in test datasets compared to the other state-of-the-art methods.

Keywords—Nyström sampling, clustering, subsampling

I. INTRODUCTION

Clustering is one of the fundamental problems in machine learning [1]. The recent development of data-storage and data-acquisition devices has increased the scale of data sets, which poses a serious computational challenge for the existing offline and online learning algorithms [2], [3], [4], [5], [6], [7], [8], [9], [10], [11], [12], [13], [14], [15], [16], [17], [18], [19], [20], [21], [22], [23], [24], [25], [26], [27]. Spectral clustering techniques are widely used, due to their empirical performance advantages compared to other clustering methods [28]. However, a significant obstacle to scaling up spectral clustering to large datasets is that it requires building an affinity matrix between pairs of data points which becomes computationally prohibitive for large data-sets [29].

To address this computational challenge, a common approach is to use the Nyström method as low-rank matrix approximation [30]. [1]. [31]. The method works by sampling a small set of landmark points from a large instances, to formulate an approximation for the eigen-decomposition of the full dataset using the sampled data. However, the performance of the approach is highly dependent on proper sub-sampling of the input data to include some landmark points, points that capture the inherent complexity and variability of the full dataset. Uniform sampling without replacement is the most used approach for this purpose [1]. [32].

Using local or global properties of the data distribution a leading version of non-uniform sampling has recently been suggested. The authors in [33] propose the ensemble minimum sum of the squared similarity sampling algorithm or ensemble-MS3. This algorithm is based on two works, the first one is the minimum sum of the squared similarity sampling or MS3 proposed in [34], that considers both the variance and the similarity of the dataset to select the landmark points. The second one is the ensemble Nyström methods proposed in [35], which is a meta algorithm that combines the standard Nyström methods with the mixture weights. The ensemble-MS3 gives better results than the standard algorithms by increasing the accuracy compared with the standard Nyström method. However, the lack of speed is still a problem for the ensemble methods since the algorithm need to sample multiple times in order to aggregate the results.

In this paper, we propose two algorithms that perform better than the ensemble MS3 and any existing ensemble Nyström algorithm. The first one, the “Centroid Minimum Sum of Squared Similarities algorithm” or CMS3 is an incremental sampling algorithm for Nyström based-spectral clustering. CMS3 improves the MS3 by adding centroid sampling upon the MS3, increasing the accuracy. In the first step, the algorithm starts sampling with a fixed number of initial landmark points and selects new landmark points one by one, such that the sum of the squared similarities between the previously selected points and the new point is minimized, and as a second step the algorithm selects only the centroid points from this sub-sample. The second one, the CMS3-tuned is deducted from the theoretical analyse of MS3 and leads to adapt the sampling according to the spectrum shape of the dataset.

The rest of the paper is organized as follows: related works are discussed in Section 2. In Section 3, we briefly introduce spectral clustering and the Nyström extension. An error analysis of the approximated matrix is proposed in Section 4, and an incremental sampling method is also proposed. We evaluate the proposed method in Section 5. Finally, we conclude our work in Section 6.

II. RELATED WORK

To apply spectral clustering to large datasets, new efforts have been concentrating on solving issues around algorithm scalability [36], such as using dimension reduction by Nyström approximation [31], a method originally designed for numerical solution of integral equations [37]. However the performance of the approach is highly dependent on proper landmark points that capture the inherent variability of the full dataset [38].

To address this problem, different sampling methods have been proposed, assuming that clusters have an equiprobable distribution, authors in [11] and [22] propose a random sampling (RS). Although, this implicit assumption is not true in all
datasets, it is shown in [39] that it performs better than two proposed alternatives that use diagonal sampling [40] and column-norm sampling [41] algorithms.

In [42] the authors developed a weighted sampling (WS) approach using the determinant of the kernel matrix to select landmark points, where the probability of choosing a new landmark point was in proportion to the determinant of the similarity matrix between landmark points. They analyzed the Nyström reconstruction error using the Schur complement [43], concluding that the larger the determinant, the smaller the error. Although the work provides a solid theoretical basis for measuring the error levels in Nyström approximation, a main drawback of the algorithm provided is in its time complexity.

Assuming that the potential clusters are convex, [43] introduced k-means based sampling (KS) algorithm, as a means to select points near k-means centroids as landmark points. Similarly, [45] also pre-processed the data using k-means clustering, to select a committee of data points near centroids. Although the latter method does not explicitly state the convexity assumption, both methods perform poorly for non-convex clusters.

In [30], the authors proposed an incremental sampling (IS) algorithm that first randomly samples two points from a dataset, to compute a similarity matrix between the sampled points and the remaining points. The algorithm picks the point with the smallest variance, and then iteratively repeats the process until a desired number of landmarks is reached. While promising, [36] showed that IS performs poorly on high-dimensional data, as the variance of the Euclidean distance tends to zero. In such cases IS may pick inappropriate landmark points for dimension reduction, hence for successful clustering.

The minimum similarity sampling (SS) is proposed in [36] for high-dimensional space clustering purpose. The authors studied how the similarity between the sample set and non-sample set influences the approximation error, and observed that their result depends on the dimensionality of the dataset: SS outperforms IS on high-dimensional data, but not on low dimensional data.

Recently, a new sampling algorithm is proposed in [34], named MS3 for Minimum Sum of Squared Similarities. This algorithm approximately maximizes the determinant of the reduced similarity matrix that represents the mutual similarities between sampled data points, and demonstrates the performance of MS3 compared with the standard Nyström method. An ensemble version of MS3 method was proposed in [34]. It treats each approximation generated by the MS3 method for a sample of columns as an expert and combines such experts to derive an improved hypothesis, typically more accurate than any of the original experts, but the drawback of this method is in its computationally time.

In this paper, we propose the CMS3 that performs better than the ensemble MS3 algorithm. The proposed algorithm samples at first using MS3 and after that selects only the centroid points of the MS3 sampling. We have also proposed an improved version based on theoretical analysis of the upper error bound of this algorithm. This tuned version yields more accurate low-rank approximations than the ensemble Nyström methods.

### III. Key Notion

This section focuses on introducing the key notions used in this paper.

#### A. Spectral Clustering

Spectral clustering algorithms employ the first k eigenvectors of a Laplacian matrix to guide clustering. Loosely following the notation in [46], this can be outlined as follows. The algorithm takes as an input a number k of clusters, an affinity matrix $S \in R^{n \times n}$ constructed using the similarity between each pair of data points, and as an output clusters $c_1, \ldots, c_k$. It starts by computing the Laplacian matrix $P = D - S$; where $D$ is an $n \times n$ diagonal matrix defined by $D_{ii} = \sum_{j=1}^{n} S_{ij}$, and after that it computes k eigenvectors $u_1, \ldots, u_k$ corresponding to the first k eigenvalues of the generalized eigenproblem $Pu = \lambda Du$; and let $Z \in R^{n \times k}$ be the matrix containing the vectors $u_1, \ldots, u_k$. Finally, it clusters $y_1, \ldots, y_n$ by k-means algorithm into clusters $c_1, \ldots, c_k$; with $y_i$ corresponding to the i-th row of $Z$.

By analyzing the spectrum of the Laplacian matrix constructed over all data entries, the original data can be compressed into a smaller number of representative points using the Nyström approximation described below.

#### B. Nyström Sampling

If we consider m landmark data points $L = l_1, l_2, \ldots, l_m$ from a given dataset $X = x_1, x_2, \ldots, x_n$ with $x_i \in R^n$ and $m \ll n$, then for any given point $x$ in $X$, Nyström method formulates

$$
\frac{1}{m} \sum_{i=1}^{m} \text{sim}(x, l_i) \hat{\phi}(l_i) = \hat{\lambda} \hat{\phi}(x)
$$

where $\hat{\phi}(x)$ is an approximation to the exact eigenfunction, $\hat{\lambda}$ is the corresponding approximate eigenvalue and $\text{sim}(x, y)$ denotes the similarity between $x$ and $y$.

We can write the Eq[1] in matrix form, $S \hat{\Phi} = m \hat{\Phi} \Lambda$ where $\hat{\Phi} = [\hat{\phi}_1 \hat{\phi}_2 \ldots \hat{\phi}_m]$ are the eigenvectors of $S$ and $\Lambda = \text{diag}\{\lambda_1, \lambda_2, \ldots, \lambda_m\}$ is a diagonal matrix of the corresponding approximate eigenvalues. Then for an unsampled point $x$, the j-th eigenfunction at $x$ can be approximated by $\hat{\phi}_j(x) \approx \frac{1}{m \lambda_j} \sum_{i=1}^{m} \text{sim}(x, l_i) \hat{\phi}_j(l_i)$. With this equation, the eigenvector for any given point $x$ can be approximated through the eigenvectors of the landmark points $L$ [42]. The same idea can be applied to approximate k eigenvectors of $S$ by decomposing and then extending a $k \times k$ principal sub-matrix of $S$. First, let $S$ be partitioned as $S = \begin{bmatrix} A & B^T \\ B & C \end{bmatrix}$ with $A \in R^{k \times k}$. Now, define spectral decompositions $S = U \Lambda U^T$ and $A = U_A \Lambda_A U_A^T$; the Nyström extension then provides an approximation for k eigenvectors in $\tilde{U} = \begin{bmatrix} U_A \\ B U_A \Lambda_A^{-1} \end{bmatrix}$ where the approximations of $\tilde{U} \approx U$ and $\tilde{\Lambda} \approx \Lambda$ may then be composed, yielding an Nyström approximation $\tilde{S} \approx S$, with $\tilde{S} = \tilde{U} \tilde{\Lambda} U^T$. To measure the distance of these approximations, conventionally Frobenius norm is used.
C. Minimum Sum of Squared Similarities

The MS3 algorithm \cite{34} initially randomly chooses two points from the dataset \( X \). It then computes the sum of similarities between the sampled points and a subset, \( T \), selected randomly from the remaining data points. The point with the smallest sum of squared similarities is then picked as the next landmark data point. The procedure is repeated until a total of \( m \) landmark points are picked.

Algorithm 1 The Minimum Sum of Squared Similarities Algorithm

1. **Input:** \( X = \{x_1, x_2, ..., x_n\} \): dataset \( m \): number of landmark data points \( \gamma \): size of the random sub-sampled set from the remaining data, in percentage
2. **Output:** \( S \in R^{m \times m} \): similarity matrix between landmark points
3. **Initialize** \( S = I_0 \)
4. For (i=0 to i<m) do
5. \( \tilde{x}_i = \text{Random}(X) \)
6. \( S := S_{\cup \{ \tilde{x}_i \}} \)
7. \( \tilde{X} := \tilde{X} \cup \{ \tilde{x}_i \} \)
8. \textbf{End For}
9. While \( i < m \) do
10. \( T = \text{Random}(X \backslash \{ \tilde{X} \}) \)
11. Find \( \tilde{x}_i = \arg\min_{x \in T} \sum_{j<i-1} \sim(x, \tilde{x}_j) \)
12. \( \tilde{S} := S_{\cup \{ \tilde{x}_i \}} \)
13. \( \tilde{X} := \tilde{X} \cup \{ \tilde{x}_i \} \)
14. **End While**

IV. CENTROID MINIMUM SUM OF Squared Similarities (CMS3)

The idea of the proposed algorithm CMS3 (described in Algorithm 2) is to sample \( r \) points using MS3 where \( m \leq r \leq X \) with the assumption that this sampling will give an \( r \) convex points, and after that the CMS3 uses k-means \cite{37} to cluster these \( r \) points and select the centroids of these clusters as a global optimal landmark points. We could say that, the proposed algorithm is implemented under the following Hypothesis:

**Hypothesis 1.** Comparing two similarity matrix \( \tilde{S}_m \) and \( \tilde{S'}_m \) corresponding to CMS3 and MS3 approximations, we have the following inequality between their error upper bounds:

\[
\sup(||S - \tilde{S}_m||) \leq \sup(||S - \tilde{S'}_m||)
\]

A. Theoretical Study

We propose here to study under which condition the proposed Hypothesis \cite{37} is valid. In order to do that, we propose at first to compute the the upper bound of the proposed sampling algorithm “CMS3” in Theorem \cite{37} and then compare it to the ”MS3” upper bound in Corollary \cite{37}

**Theorem 1.** For a dataset \( X = \{x_1, x_2, ..., x_n\} \), define the following positive definite similarity matrices:

- \( S \): the \( n \times n \) similarity matrix for the overall dataset with a maximum diagonal entry \( S_{\max} \);

**Algorithm 2 CMS3 Algorithm**

1. **Input:** \( X = \{x_1, x_2, ..., x_n\} \): dataset \( m \): number of landmark data points \( r \): number of landmark data points selected with MS3 \( \gamma \): size of the random sub-sampled set from the remaining data, in percentage
2. **Output:** \( S \in R^{m \times m} \): similarity matrix between landmark points
3. **Initialize** \( S = I_0 \)
4. \( X_r := MS3(X, r, \gamma) \)
5. \( \tilde{r} := \text{kmeans}(X_r, m) \)
6. **For** (i=0 to i\leq m) do
7. \( \tilde{x}_i := \frac{1}{|\tilde{r}|} \sum_{x_j \in \tilde{r}_i} x_j \text{ get centroid of the cluster } \tilde{r}_i \in \tilde{r} \)
8. \( \tilde{S} := S_{\cup \tilde{x}_i} \)
9. **End For**

- \( \tilde{S}_l \): a similarity matrix for \( X_l \) with \( l \) landmark point selected randomly from \( X \);
- \( \tilde{S}_r \): a similarity matrix for \( X_r \) with \( r \) landmark point selected from \( X_l \) using MS3, with \( r \leq l \leq n \);
- \( \tilde{S}_m \): a similarity matrix for \( X_m \) with \( m \) landmark point selected from \( X_r \) using K-means sampling, with \( m \leq r \leq l \leq n \); and
- \( \tilde{S}_k \): the best possible rank-k approximation of \( S \).

Then with some probability \( 1 - p \) or more, we can write

\[
||S - \tilde{S}_m|| \leq 4T \sqrt{mC^{ker}_{mT}e + mC^{ker}_{X}Te||W^{-1}||} + (r + 1) \sum_{i=r+1}^{n} \lambda_i + ||S - \tilde{S}_k||
\]

(2)

where \(||.||\) is the Frobenius norm.

\[
d_{\tilde{S}} = \max_{i,j} (S_{ij} + S_{ji} 2S_{ij})
\]

and

\[
w = \frac{n - 1}{2n - 1} 2 \beta(l, n) \log p
\]

with

\[
\beta(l, n) = 1 - \frac{1}{2 \max(l, n - l)}
\]

**Proof:** Using the above notation, let us introduce some facts.

**Fact 1.** \cite{37} Let \( \lambda_1 \geq ... \geq \lambda_n \) be the eigenvalues of the similarity matrix \( S \), then with some probability \( 1 - p \) or more, we can write

\[
||S - \tilde{S}_r|| \leq (r + 1) \sum_{i=r+1}^{n} \lambda_i + ||S - \tilde{S}_r||
\]

(3)

\[
+ nS_{max} \sqrt{\frac{64k}{T} \left( 1 + \sqrt{\frac{wd_{\tilde{S}}}{S_{max}} \right)^{\frac{1}{2}}}
\]

**Property 1.** \cite{37}

\[
(kern(a, b) - kern(c, d))^2 \leq C^{ker}_{X} ||a - c||^2 + ||d - b||^2,
\]

\( \forall a, b, c, d \in R \)
where \( C^kern \) is a constant depending on, the kernel \( \kern(,\,) \) and the sample set \( X \).

**Fact 2.** [47] Let the whole sample set \( X \) be partitioned into \( g \) disjoint clusters \( \mathcal{S}_{kern} \), \( c(i) \) being the function that maps each sample \( x_i \in X \) to the closest landmark point \( z_{c(i)} \in Z \). Then for some kernel \( kern \) satisfying property (1), the partial approximation error \( ||S - \bar{S}_m|| \) is bounded by

\[
||S - \bar{S}_m|| \leq 4T \sqrt{mC^kern|e|} + mC^kern|e||W^{-1}| \tag{4}
\]

where \( T = \max_k|\mathcal{S}_{kern}| \), and \( e \) is the quantization error induced by coding each sample in \( x_i \in X \) by the closest landmark point in \( Z \). i.e., \( e = \sum_{z_j \in X} ||x_i - z_{c(i)}||^2 \), and \( ||W^{-1}|| \in R^{n \times m} \) where \( w_{ij} = k(z_i, z_j) \).

By adding both sides of Eq\( \mathbf{3} \) and Eq\( \mathbf{4} \), noting that \( \sum_{i=1}^n |c(i)| \geq \sum_{i=r+1}^n |c(i)| \) for positive argument and using the triangle inequality

\[
||S - \bar{S}_m|| \leq ||S - \bar{S}_r|| + ||\bar{S}_r - \bar{S}_m|| \tag{5}
\]

we prove Theorem \( \mathbf{1} \).

**Corollary 1.** The proposed Hypothesis \( \mathbf{7} \) is valid, if and only if

\[
m \leq \frac{\lambda_2 - r \sum_{i=r+1}^n \lambda_i - 4T \sqrt{r - 1} C^kern|e|}{C^kern|e||W^{-1}| - \sum_{i=r}^n \lambda_i} \tag{6}
\]

**Proof:** Assuming the comparison of the upper bounds appears with the inequality,

\[
4T \sqrt{mC^kern|e|} + mC^kern|e||W^{-1}| + (r + 1) \sum_{i=r+1}^n \lambda_i + ||S - S_k|| + nS_{\max} \sqrt{64k \left( 1 + \frac{wd^2}{S_{\max}} \right)^\frac{1}{2}} \leq (m + 1) \sum_{i=m+1}^n \lambda_i + ||S - S_k|| + nS_{\max} \sqrt{64k \left( 1 + \frac{wd^2}{S_{\max}} \right)^\frac{1}{2}} \tag{7}
\]

after simplification we get

\[
4T \sqrt{mC^kern|e|} + mC^kern|e||W^{-1}| \leq (m + 1) \sum_{i=m+1}^n \lambda_i - (r + 1) \sum_{i=r+1}^n \lambda_i \]

Knowing that \( m \leq r \) we can write

\[
4T \sqrt{mC^kern|e|} + mC^kern|e||W^{-1}| \leq (m - r) \sum_{i=r+1}^n \lambda_i + (m + 1) \sum_{i=m+1}^r \lambda_i \tag{8}
\]

which gives

\[
m \leq \frac{\sum_{i=m+1}^r \lambda_i - r \sum_{i=r+1}^n \lambda_i - 4T \sqrt{r - 1} C^kern|e|}{C^kern|e||W^{-1}| - \sum_{i=r}^n \lambda_i} \tag{9}
\]

then replacing \( m \) by \( r - 1 \) gives,

\[
m \leq \frac{\lambda_2 - r \sum_{i=r+1}^n \lambda_i - 4T \sqrt{r - 1} C^kern|e|}{C^kern|e||W^{-1}| - \sum_{i=r}^n \lambda_i} \tag{10}
\]

We note that going from inequality (7) back to (10) is straightforward, and can be achieved by tracing the above steps in reverse.

**B. CMS3-tuned**

We propose here to use the above theoretical results to propose an improved version of the CMS3.

Corollary \( \mathbf{1} \) prescribes a method to select between MS3 and CMS3 methods. However, due to its complexity, the idea here is to relax the “if and only if” of the Corollary \( \mathbf{1} \) as follows:

**Corollary 2.** Comparing the upper bound of MS3 and CMS3, as defined in Hypothesis \( \mathbf{7} \) Assuming that \( m \lambda_{m+1} + r \lambda_n << \lambda_2 \), a necessary condition for \( \sup(||S - \bar{S}_m||) \leq \sup(||S - \bar{S}_n||) \) is

\[
\lambda_2 \leq n \lambda_n \tag{11}
\]

**Proof:** From Eq. \( \mathbf{8} \) a necessary condition for having the Corollary \( \mathbf{1} \) could be the following:

\[
0 \leq (m - r) \sum_{i=r+1}^n \lambda_i + (m + 1) \sum_{i=m+1}^r \lambda_i \]

then the following still hold,

\[
0 \leq (m - r)(n - r)\lambda_n + (m + 1)(r - m)\lambda_{m+1}
\]

which implies

\[
0 \leq (m + 1)\lambda_{m+1} - (n - r)\lambda_n
\]

with \( \lambda_{m+1} \leq \lambda_2 \) we get

\[
0 \leq (m + 1)\lambda_2 - (n - r)\lambda_n
\]

and assuming that \( m \lambda_{m+1} + r \lambda_n << \lambda_2 \), gives us

\[
\lambda_2 \leq n \lambda_n
\]

Following the Corollary \( \mathbf{2} \) the idea in the proposed algorithm (Algorithm \( \mathbf{5} \)), is to use \( \lambda_2 \leq |sm| \times \lambda_{|sm|} \) as a switch condition for using CMS3 or MS3, where \( |sm| \) is the subsampling size. These parameters could be seen as a proxy of the eigenspectrum shape of the data.
**Algorithm 3 CMS3-tuned Algorithm**

1. **Input:** \( X = \{x_1, x_2, \ldots, x_n\} \): dataset
2. **m:** number of landmark data points
3. **r:** number of landmark data points selected with MS3
4. **γ:** size of the random subsampled set from the remaining data, in percentage

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**Theorem 2.** Let \( A \) be an \( n \times n \) symmetric matrix with eigenvalues \( \lambda_1 \geq \ldots \geq \lambda_n \). Let \( B \) be an \((n-k) \times (n-k)\) symmetric minor of \( A \) with eigenvalues \( \mu_1 \geq \ldots \geq \mu_{n-k} \). Then, with probability \( 1-\delta \) and with \( \epsilon = \sqrt{\frac{1}{2|sm|} \ln \left( \frac{k}{\delta} \right)} \), we can write

\[
|\lambda_1 - \lambda_{n-k} - \mu_1| \leq \epsilon
\]

Theorem 2 is proving that behavior of our eigenvalue in our sample set is similar to the original set, with some probability.

**Proof:** We start by introducing the following fact.

**Fact 3.** (Interlacing eigenvalues) Let \( A \) be an \( n \times n \) symmetric matrix with eigenvalues \( \lambda_1 \geq \ldots \geq \lambda_n \). Let \( B \) be an \((n-k) \times (n-k)\) symmetric minor of \( A \) with eigenvalues \( \mu_1 \geq \ldots \geq \mu_{n-k} \). Then \( \lambda_i \leq \mu_i \leq \lambda_{i-k} \)

by using Fact 3 in equation (11) we get:

\[
|\lambda_2 - n\lambda_n - \mu_2 + m\lambda_m| \leq \epsilon
\]

Assuming that \( \lambda_i - \lambda_{i-1} \geq \lambda_j - \lambda_{j-1} \) \((i < j)\) we have:

\[
n\lambda_n < m\lambda_m
\]

then

\[
|\lambda_2 - n\lambda_n - \lambda_{2-k} + m\lambda_m| \leq \epsilon
\]

**Fact 4.** (Chernoff-Hoeffding bound) Let \( X_i \in [0,1] \) an independent random variables with \( \mu = E[X_i] \). \( Pr\left(\frac{1}{n} \sum_{i=1}^{n} X_i - \mu \geq \epsilon\right) \leq e^{-2\epsilon^2 n}\)

First of all, the equation 12 is true if \( Pr(\{\lambda_2 - n\lambda_n\} - (\mu_2 - m\mu_m)) \leq \epsilon \) with \( \epsilon \) small. Then to quantify the \( \epsilon \) we use the Fact 4 that gives us:

\[
Pr(\{\lambda_2 - n\lambda_n\} - (\mu_2 - m\mu_m)) \leq \epsilon \leq e^{-2|sm|\epsilon^2}.
\]

Then with \( e^{-2|sm|\epsilon^2} = \delta \) we get \( \epsilon = \sqrt{\frac{2|sm|\ln \left( \frac{\delta}{2} \right)}{2}} \).

**Corollary 3.** We can write:

\[
sup(|S - \tilde{S}_m|) \leq sup(\{sup(|S - \tilde{S}'_m|), sup(|S - \tilde{S}''_m|)\})
\]

**Proof:** The proof is straightforward, if the Corollary 3 hold then sup(|S - \tilde{S}_m|) = sup(|S - \tilde{S}'_m|) else sup(|S - \tilde{S}_m|) = sup(|S - \tilde{S}'_m|). Then in these both situations the sup(|S - \tilde{S}_m|) is at least smaller then max(sup(|S - \tilde{S}'_m|), sup(|S - \tilde{S}''_m|)) and then prove the Corollary 3.

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**V. Evaluation**

We tested CMS3 and CMS3-tuned, and compared their performance to the results of four leading sampling methods described in Section IV. These are:

- Random sampling (RS).
- K-means sampling (KS) [44].
- Minimum similarity sampling (SS) [36], and
- Minimum sum of squared similarity sampling (SSS) [34].

Notice that, we compare our algorithm to ensemble Nyström rather than the standard Nyström, since it was shown earlier both in [35] and in [33] that ensemble performs better than standard Nyström. We denote these algorithms as ensemble-RS, ensemble-KS, ensemble-SS, and ensemble-MS3, respectively.

We required each algorithm to sample 2%, 4%, 6%, 8% and 10% of the data as landmark points, which are used by Nyström-based spectral clustering methods to cluster the datasets. We have also tested the ensemble Nyström methods with different values of \( p \), going from 2 to 10.

Because sampling algorithms are sensitive to the datasets used, and clustering algorithms contain a degree of randomness, we used various benchmark datasets, and repeated our evaluations 10 times. We measured the clustering quality of each algorithm using their average accuracy across these tests, also recording their standard deviations.

**A. Comparison on Accuracy**

We compared the performance of the seven sampling methods using data from University of California, Irvine (UCI) Machine Learning Repository[1]. We chose nine datasets with different instances, attributes and classes size: Abalone, Breast, Wine, Wdbc, Yeast, Shuttle, Letter, PenDigits and a7a. A brief summary of the datasets is listed in Table I.

Table I reports the average accuracy of each algorithm, along with their standard deviations across 1000 tests on the UCI datasets. As expected, the accuracies depend on the dataset. For example, the accuracy of all algorithms in Haberman problem and Wdbc datasets stay in the range of 50%, while going as high as over 80% for the Abalone dataset. From this observation, we can say that the Haberman problem and Wdbc datasets present difficulties to Nyström method-based spectral clustering.

We note that, on these datasets, all tested algorithms have better performance than the baseline of random sampling. The results show that CMS3-tuned provided better clustering than the other algorithms on seven out of nine datasets, coming only narrowly second to CMS3 on the remaining two, though still within a standard deviation. Ranking the algorithms with

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[1] https://archive.ics.uci.edu/ml/datasets.html
respect to their mean accuracies, we note that the top two performing algorithms were CMS3-tuned and CMS3, in that order. The results on the UCI dataset confirm our heuristics that choosing between CMS3 and MS3 need to be done according to the spectrum shape of the dataset.

### TABLE II. DATASETS USED FOR BENCHMARKING

| UCI Datasets | Instances | Attributes | Classes |
|--------------|-----------|------------|---------|
| Abalone      | 488       | 9          | 3       |
| Breast       | 699       | 9          | 2       |
| Wine         | 178       | 13         | 3       |
| Wine         | 569       | 32         | 2       |
| Yeast        | 1484      | 6          | 8       |
| Shuttle      | 14500     | 9          | 7       |
| Letter       | 20000     | 16         | 26      |
| PenDigits    | 10992     | 16         | 10      |
| a7a          | 16100     | 122        | 2       |

The results of the Ensemble-SS algorithm show overall better performance compared to Ensemble-KS and Ensemble-RS sampling. We also notice that the ensemble-MS3 gave higher performance than the sampling algorithms that are not based on MS3.

### VI. CONCLUSION

In this paper, we introduced a new sampling algorithm for Nyström method-based spectral clustering, CMS3, and a heuristics on how it can be selected over the MS3 algorithm on which it is built. We call the latter CMS3-tuned. What sets CMS3 apart from other algorithms is that it uses the eigenspectrum of the input datasets to choose between sampling algorithms; CMS3 and MS3 in this case. Further, through benchmarking experiments we have demonstrated the favourable performance of our algorithms.

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