Efficient Algorithms and Error Analysis for the Modified Nyström Method

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Abstract

Many kernel methods suffer from high time and space complexities and are thus prohibitive in big-data applications. To tackle the computational challenge, the Nyström method has been extensively used to reduce time and space complexities by sacrificing some accuracy. The Nyström method speedups computation by constructing an approximation of the kernel matrix using only a few columns of the matrix. Recently, a variant of the Nyström method called the modified Nyström method has demonstrated significant improvement over the standard Nyström method in approximation accuracy, both theoretically and empirically. In this paper, we propose two algorithms that make the modified Nyström method practical. First, we devise a simple column selection algorithm with a provable error bound. Our algorithm is more efficient and easier to implement than and nearly as accurate as the state-of-the-art algorithm. Second, with the selected columns at hand, we propose an algorithm that computes the approximation in lower time complexity than the approach in the previous work. Furthermore, we prove that the modified Nyström method is exact under certain conditions, and we establish a lower error bound for the modified Nyström method.

1 Introduction

The kernel method is an important tool in machine learning, computer vision, and data mining (Schölkopf and Smola, 2002; Shawe-Taylor and Cristianini, 2004). However, many kernel methods require matrix computations of high time and space complexities. For example, let $m$ be the number of data instances. The Gaussian process regression computes the inverse of an $m \times m$ matrix which takes time $O(m^3)$ and space $O(m^2)$; the kernel PCA, Isomap, and Laplacian eigenmaps all perform the truncated singular value decomposition which takes time $O(m^2k)$ and space $O(m^2)$, where $k$ is the target rank of the decomposition. When $m$ is large, it is challenging to store the $m \times m$ kernel matrix in RAM to perform these matrix computations. Therefore, these kernel methods are prohibitive when $m$ is large.

To overcome the computational challenge, Williams and Seeger (2001) employed the Nyström method (Nyström, 1930) to generate a low-rank approximation to the original symmetric positive semidefinite (SPSD) kernel matrix. By using the Nyström method, eigenvalue decomposition and some matrix inverse can be approximately done on only a few columns of the SPSD matrix instead of on the entire matrix, and the time and space costs are reduced to $O(m)$. The Nyström method has been widely used to speedup various kernel methods, such as the Gaussian process regression (Williams and Seeger, 2001), spectral clustering (Fowlkes et al., 2004; Li et al., 2011), kernel SVMs (Zhang et al., 2008; Yang et al., 2012), kernel PCA (Zhang et al., 2008; Zhang and Kwok, 2010; Talwalkar et al., 2013), kernel ridge regression (Cortes et al., 2010; Yang et al., 2012), determinantal processes (Affandi et al., 2013), etc.

To construct a low-rank matrix approximation, the Nyström method requires a small number of columns (say, $c$ columns) to be selected from the kernel matrix by a column sampling technique. The approximation accuracy is largely determined by the sampling technique; that is, a better sampling technique can result in a Nyström approximate with a lower approximation error. In the previous work, much attention has been made on improving the error bounds of the Nyström method: additive-error bound has been explored by Drineas and Mahoney (2005); Shawe-Taylor et al. (2005); Kumar et al. (2012); Jin et al. (2012); etc. Very recently, Gittens and Mahoney (2013) established...
the first relative-error bound which is more interesting than additive-error bound (Mahoney, 2011).

However, the approximation quality cannot be arbitrarily improved by devising a very good sampling technique. As shown theoretically by Wang and Zhang (2013), no matter what sampling technique is used to construct the Nyström approximation, the incurred error (in the spectral norm or the squared Frobenius norm) must grow with matrix size $m$ at least linearly. Thus, the Nyström approximation can be very rough when $m$ is large, unless large number columns are selected. As was pointed out by Cortes et al. (2010), the tighter kernel approximation leads to the better learning accuracy, so it is useful to find a kernel approximation model that is more accurate than the Nyström method.

To improve the approximation accuracy, Wang and Zhang (2013) proposed a new alternative called the modified Nyström method and a sampling algorithm for the modified Nyström method. The modified Nyström method can be applied in the same way exactly as the standard Nyström method keeps till open. In this paper we seek to make the modified Nyström method efficient and much easier to implement than the uniform+adaptive algorithms. For an $m \times n$ matrix $A = [a_{ij}]$, we let $\hat{a}^{(i)}$ be its $i$-th row, $a_j$ be its $j$-th column, $\|A\|_F = \left(\sum_{i,j} a_{ij}^2\right)^{1/2}$ be its Frobenius norm, and $\|A\|_2 = \max_{x \neq 0} \|Ax\|_2/\|x\|_2$ its spectral norm.

Letting $\rho = \text{rank}(A)$, we write the condensed singular value decomposition (SVD) of $A$ as $A = U_A \Sigma_A V_A^T$, where the $(i,j)$-th entry of $\Sigma_A \in \mathbb{R}^{p \times p}$ is the $i$-th largest singular value of $A$. We also let $U_{A,k}$ and $V_{A,k}$ be the first $k$ ($< \rho$) columns of $U_A$ and $V_A$, respectively, and $\Sigma_{A,k} = \Sigma_{A,k} \Sigma_{A,k} V_{A,k}^T$ is the “closest” rank-$k$ approximation to $A$.

Based on SVD, the matrix coherence of the columns of $A$ relative to the best rank-$k$ approximation to $A$ is defined by $\mu_k = \frac{n}{k} \max_j \|V^{(j)}_{A,k}\|_2^2$. Let $A^! = V_A \Sigma_A^{-1} U_A^T$ be the Moore-Penrose inverse of $A$. When $A$ is nonsingular, the Moore-Penrose inverse is identical to the matrix inverse. Given another $m \times c$ matrix $C$, we define $\mathcal{P}_C A = CC^T A$ as the projection of $A$ onto the column space of $C$ and $\mathcal{P}_{C,k} A = C \cdot \arg\min_{\mathcal{X}, \mathcal{X} \subseteq \mathcal{C}} \|A - \mathcal{X}\|_F$ as the rank restricted projection. It is obvious that $\|A - \mathcal{P}_C A\|_F \leq \|A - \mathcal{P}_{C,k} A\|_F$.

Finally, we discuss the time complexities of the matrix operations mentioned above. For an $m \times n$ general matrix $A$ (assume $m \geq n$), it takes $O(mn^2)$ flops to compute the full SVD and $O(mnk)$ flops to compute the truncated SVD of rank $k$ ($< n$). The computation of $A^!$ takes $O(mn^2)$ flops. It is worth mentioning that although multiplying an $m \times n$ matrix by an $n \times p$ matrix takes $mnp$ flops, it can be performed in full parallel by partitioning the matrices into blocks. Thus, the time and space expense of large-scale matrix multiplication is not a challenge in real-world applications. We denote the time complexity of such a matrix multiplication by $T_{\text{Multiply}}(mnp)$, which

2 Notation

The notation used in this paper follows that of Wang and Zhang (2013). For an $m \times n$ matrix $A = [a_{ij}]$, we let $\hat{a}^{(i)}$ be its $i$-th row, $a_j$ be its $j$-th column, $\|A\|_F = \left(\sum_{i,j} a_{ij}^2\right)^{1/2}$ be its Frobenius norm, and $\|A\|_2 = \max_{x \neq 0} \|Ax\|_2/\|x\|_2$ its spectral norm.
can be tremendously smaller than $O(mnp)$ in parallel computing environment (Halko et al., 2011). An algorithm can still be efficient even if it demands large-scale matrix multiplications.

## 3 Previous Work

In Section 3.1 we introduce the standard and modified Nyström methods and discuss their advantages and disadvantages. In Section 3.2 we describe some commonly used column sampling algorithms.

### 3.1 The Nyström Methods

Given an $m \times m$ symmetric matrix $A$, one needs to select $c (\ll m)$ columns of $A$ to form a matrix $C \in \mathbb{R}^{m \times c}$ to construct the standard or modified Nyström approximation. Without loss of generality, $A$ and $C$ can be permuted such that

\[
A = \begin{bmatrix} W & A_{21}^T \\ A_{21} & A_{22} \end{bmatrix} \quad \text{and} \quad C = \begin{bmatrix} W \\ A_{21} \end{bmatrix},
\]

where $W$ is of size $c \times c$. The standard Nyström approximation is defined by

\[
\hat{A}^\text{nys} \triangleq \text{CU}^\text{nys} C^T = CW^\dagger C^T,
\]

and the modified Nyström approximation is

\[
\hat{A}^\text{mod} \triangleq \text{CU}^\text{mod} C^T = C(C^\dagger A(C^\dagger)^T)C^T.
\]

Here the $c \times c$ matrices $U^\text{nys} \triangleq W^\dagger$ and $U^\text{mod} \triangleq C(C^\dagger A(C^\dagger)^T)$ are called the intersection matrices. We see that the only difference between the two models is their intersection matrices.

For the approximation $\text{CU} C^T$ constructed by either of the methods, given a target rank $k$, we hope the error ratio

\[
f = \|A - \text{CU} C^T\|_\xi / \|A - A_k\|_\xi, \quad (\xi = F \text{ or } 2),
\]

is as small as possible. However, Wang and Zhang (2013) showed that for the standard Nyström method, whatever a column selection algorithm is used, the ratio $f$ must grow with the matrix size $m$ when $c$ is fixed.

**Lemma 1** (Lower Error Bound of the Standard Nyström Method (Wang and Zhang, 2013)). Whatever a column sampling algorithm is used, there exists an $m \times m$ SPSD matrix $A$ such that the error incurred by the standard Nyström method obeys:

\[
\|A - \text{CU} C^T\|_F \geq \Omega \left( 1 + \frac{mk}{\epsilon^2} \right) \|A - A_k\|_F,
\]

\[
\|A - \text{CU} C^T\|_2 \geq \Omega \left( \frac{m}{\epsilon^2} \right) \|A - A_k\|_2.
\]

Here $k$ is an arbitrary target rank, and $c$ is the number of selected columns. Thus, when the matrix size $m$ is large, the standard Nyström approximation is very inaccurate unless a large number of columns are selected. By comparison, when using an algorithm in Wang and Zhang (2013) for the modified Nyström method, the error ratio $f$ remains constant for a fixed $c$ and a growing $m$. Therefore, the modified Nyström method is more accurate than the standard Nyström method.

However, the accuracy gained by the modified Nyström method is at the cost of higher time and space complexities. Computing the intersection matrix $U^\text{nys} = W^\dagger$ only takes time $O(c^3)$ and space $O(c^2)$, while computing $U^\text{mod} = C(C^\dagger A(C^\dagger)^T)^T$ naively takes time $O(m^2c^2) + T_{\text{Multiply}}(m^2c)$ and space $O(mc)^2$.

### 3.2 Sampling Algorithms for the Nyström Methods

The column selection problem has been widely studied in the theoretical computer science community (Boutsidis et al., 2011; Mahoney, 2011; Guruswami and Sinop, 2012) and the numerical linear algebra community (Gu and Eisenstat, 1996; Stewart, 1999), and numerous algorithms have been devised and analyzed. Here we focus on some theoretically guaranteed algorithms studied in the theoretical computer science community.

In the previous work much attention has been paid on improving column sampling algorithms such that the Nyström approximation is more accurate. Uniform sampling is the simplest and most time-efficient column selection algorithm, and it has provable error bounds when applied to the standard Nyström method (Gittens, 2011; Jin et al., 2012; Kumar et al., 2012; Gittens and Mahoney, 2013). To improve the approximation accuracy, many importance sampling algorithms have been proposed, among which the adaptive sampling of Deshpande et al. (2006) (see Algorithm 2) and the leverage score based sampling of Drineas et al. (2008); Ma et al. (2014) are widely studied. The leverage score based sampling has provable bounds when applied to the standard Nyström method (Gittens and Mahoney, 2013), and the adaptive sampling has provable bounds when applied to the modified Nyström method (Wang and Zhang, 2013). Besides, quadratic Rényi entropy based active subset selection (De Brabanter et al., 2010) and $k$-means clustering based selection (Zhang and Kwok, 2010) are also effective algorithms, but they do not have additive-error or relative-error bound.

Particularly, Wang and Zhang (2013) proposed an algorithm for the modified Nyström method by combining the near-optimal column sampling algorithm (Boutsidis et al., 2011). The matrix multiplication can be done blockwisely, that is, loading two small blocks into RAM to perform multiplication at a time. So the space cost of the matrix multiplication is $O(mc)$ rather than $O(m^2c)$ (Wang and Zhang, 2013).
Algorithm 1 The Uniform+Adaptive² Algorithm.
1: Input: an $m \times m$ symmetric matrix $A$, target rank $k$, error parameter $\epsilon \in (0, 1)$, matrix coherence $\mu$.
2: Uniform Sampling. Uniformly sample $c_1 = 8.7\mu k \log (\sqrt{5}k)$ columns of $A$ without replacement to construct $C_1$.
3: Adaptive Sampling. Sample $c_2 = 10k^{\epsilon^{-1}}$ columns of $A$ to construct $C_2$ using adaptive sampling algorithm² according to the residual $A - PC_1A$.
4: Adaptive Sampling. Sample $c_3 = 2\epsilon^{-1}(c_1 + c_2)$ columns of $A$ to construct $C_3$ using adaptive sampling algorithm² according to the residual $A - PC_1C_2A$.
5: return $C = [C_1, C_2, C_3]$ and $U = C^T(A(C^T)^T)^T$.

Algorithm 2 The Adaptive Sampling Algorithm.
1: Input: a residual matrix $B \in \mathbb{R}^{m \times n}$ and number of selected columns $c (< n)$.
2: Compute sampling probabilities $p_j = \|b_j\|_2^2/\|B\|_F^2$ for $j = 1, \ldots, n$.
3: Select $c$ indices in $c$ i.i.d. trials, in each trial the index $j$ is chosen with probability $p_j$.
4: return an index set containing the indices of the selected columns.

The idea behind the uniform+adaptive² algorithm is quite intuitive. Since the modified Nyström method is the simultaneous projection of $A$ onto the column space of $C$ and the row space of $C^T$, the approximation error will get lower if span($C$) better approximates span($A$). After the initialization by uniform sampling, the columns of $A$ far from span($C_1$) have large residuals and are thus likely to get chosen by the adaptive sampling. After two rounds of adaptive sampling, columns of $A$ are likely to be near span($C$).

It is worth mentioning that our uniform+adaptive² algorithm is similar to the adaptive-full algorithm of (Kumar et al., 2012, Figure 3). The adaptive-full algorithm consists of a random initialization followed by multiple adaptive sampling steps. Obviously, using multiple adaptive sampling steps can surely reduce the approximation error. However, the update of sampling probability in each step is expensive, so we choose to do only two steps. Importantly, the adaptive-full algorithm of (Kumar et al., 2012, Figure 3) is merely a heuristic scheme without theoretical guarantee, whereas our uniform+adaptive² algorithm has a strong error bound which is nearly as good as the state-of-the-art algorithm of (Wang and Zhang, 2013) (See Theorem 3).

Theorem 3 (The Uniform+Adaptive² Algorithm.). Given an $m \times m$ symmetric matrix $A$ and a target rank $k$, we let $\mu_k$ denote the matrix coherence of $A$. Algorithm² samples totally $c = O(k\epsilon^{-2} + \mu_k\epsilon^{-1}k \log k)$ columns of $A$ to construct the approximation. We run Algorithm⁷ $t \geq (20\epsilon^{-1} + 18)(1/p)$ times (independently in parallel) and choose the sample that minimizes $\|A - C(C^T)^T\|_F$, then the inequality $\|A - C(C^T)^T\|_F \leq (1 + \epsilon)\|A - A_k\|_F$ holds with probability at least $1 - \rho$. The algorithm costs $O(m^2 + m^2\epsilon^{-2}) + T_{\text{Multiply}}(m^2\epsilon)$ time and $O(m^2)$ space in computing $C$ and $U$.

Remark 1. Theoretically, Algorithm⁷ requires to compute the matrix coherence of $A$ in order to determine $c_1$, $c_2$, and $c_3$. However, computing the matrix coherence...
Table 1: Comparisons between the two sampling algorithms in time complexity, space complexity, the number of selected columns, and the hardness of implementation.

| Algorithm          | Uniform+Adaptive | Near-Optimal+Adaptive |
|--------------------|-------------------|-----------------------|
| Time               | $O(mc^2) + T_{Multiply}(m^2c)$ | $O(mc^2 + mk^2c^2/3)$ + $T_{Multiply}(m^2c)$ |
| Space              | $O(mc)$           | $O(mc)$               |
| #columns           | $O(ke^{-2} + \mu k^{-1}k \log k)$ | $O(ke^{-2})$          |
| Implement          | Easy to implement | Hard to implement     |

Table 2: A summary of the datasets for the Nyström approximation.

| Dataset          | #Instance | #Attribute | Source               |
|------------------|-----------|------------|----------------------|
| Letters          | 15,000    | 16         | Michie et al. (1994) |
| Abalone          | 4,177     | 8          | Frank and Asuncion (2010) |
| Wine Quality     | 4,898     | 12         | Cortez et al. (2009)  |

The following formula:

$$U = C^{-1}A(C^{-1})^T = T_1(W + T_2 + T_2^T + T_3)T_1^T,$$

where the intermediate matrices are computed by

$$T_0 = A_{21}^TA_{21}, \quad T_1 = W^{-1}(I_c + W^{-1}T_2)^{-1},$$

$$T_2 = T_0W^{-1}, \quad T_3 = W^{-1}(A_{21}^TA_{22}A_{21})W^{-1}.$$

The four intermediate matrices are all of size $c \times c$, and the matrix inverse operations are on $c \times c$ small matrices.

Remark 2. Since the submatrix $W$ is not in general nonsingular, before using the algorithm, the user should first test the rank of $W$, which takes time $O(c^3)$.

Empirically, for graph Laplacian and the radial basis function (RBF) kernel (Genton, 2001), the submatrix $W$ is usually nonsingular, and the algorithm is useful; for the linear kernel, $W$ is often singular, so the algorithm does not work.

6 Experiments

In this section we empirically evaluate our two algorithms proposed in Section 4 and 5. In Section 6.1 we compare the sampling algorithms for the modified Nyström method in terms of approximation error and time expense. In Section 6.2 we illustrate the effect of our algorithm for computing the intersection matrix $U = C^{-1}A(C^{-1})^T$.

We implement all of the compared algorithms in MATLAB and conduct experiments on a workstation with Intel Xeon 2.40GHz CPUs, 24GB RAM, and 64bit Windows Server 2008 system. To compare the running time, all the computations are carried out in a single thread in MATLAB.

6.1 Comparisons among the Sampling Algorithms

We mainly compare our uniform+adaptive$^2$ algorithm (Algorithm 1) with the near-optimal+adaptive algorithm (Wang and Zhang, 2013); the two algorithms are the only provable algorithms for the modified Nyström method. We also employ the uniform sampling and the leverage-score based sampling (Drineas et al., 2008; Gittens and Mahoney, 2013) as baselines (they are widely used but not provable for the modified Nyström method).
Efficient Algorithms and Error Analysis for the Modified Nyström Method

Figure 1: Results on the RBF kernel of the Letters dataset. Here the matrix coherence of the kernel matrix is $\mu_{10} = 62.05$, $\mu_{20} = 34.87$, and $\mu_{50} = 19.16$.

Figure 2: Results on the RBF kernel of the Abalone dataset. Here the matrix coherence of the kernel matrix is $\mu_{10} = 3.28$, $\mu_{20} = 3.02$, and $\mu_{50} = 2.64$.

For all of the four algorithms, columns are sampled without replacement.

The experiment settings follow Wang and Zhang (2013). We report the approximation error and running time of each algorithm on each dataset. The approximation error is defined by

$$\text{Approximation Error} = \frac{\| A - \text{CUC}^T \|_F}{\|A - A_k\|_F},$$

where $k$ is a fixed target rank and $U$ is the intersection matrix.

We test the algorithms on three datasets summarized in Table 2. For each dataset we generate an RBF kernel matrix $A$ with $a_{ij} = \exp \left( -\frac{1}{2\sigma^2} \| x_i - x_j \|_2^2 \right)$, where $x_i$ and $x_j$ are data instances and $\sigma$ is the parameter defining the scale of the kernel. We set $\sigma = 0.2$ in our experiments. For each dataset we fix a target rank $k = 10, 20, \text{or } 50$, and vary $c$ in a very large range. We run each algorithm for 20 times and report the the minimum approximation error of the 20 repeats. We also report the average elapsed time of column selection and the computation of the $c \times c$ intersection matrix, respectively. Here we report the average elapsed time rather than the total time of the 20 repeats because the
20 repeats can be performed in parallel. The results are depicted in Figures 1, 2 and 3.

The empirical results in the figures show that our uniform+adaptive² algorithm achieves accuracy comparable with the state-of-the-art algorithm—the near-optimal+adaptive algorithm of Wang and Zhang (2013). Especially, when c is large, these two algorithms have virtually the same accuracy, which is in accordance with our analysis in the last paragraph of Section 4. Large c implies small error term ĉ, and the error bounds of the two algorithms coincide when c is small. We can also see that our uniform+adaptive² algorithm works nearly as good as the near-optimal+adaptive algorithm when the matrix coherence µ_k is small (e.g. Figure 2) when the matrix coherence is large (e.g. Figure 1), the error of our algorithm is a little worse than the near-optimal+adaptive algorithm. Furthermore, our uniform+adaptive² algorithm is much more accurate than uniform sampling and the leverage-score based sampling in most cases.

As for the running time, we can see that our algorithm performs column selection very efficiently and the elapsed time grows slowly in c. By comparison, our algorithm is much more efficient than the other two nonuniform sampling algorithms.

6.2 Effect of the Fast Computation of the Intersection Matrix

To illustrate the effect of our algorithm for computing the intersection matrix \( U = C^T A (C^T)^T \), we generate a kernel matrix of the Letters Dataset (Michie et al., 1994) which has 15, 000 instances and 16 attributes. We first generate a dense RBF kernel matrix with scale parameter \( \sigma = 0.2 \), and then obtain a sparse symmetric matrix by by truncating the entries with small magnitude such that 1% entries are nonzero. We illustrate in Figure 3 the speedup induced by our algorithm. In both cases, our algorithm is faster than the naive approach, and the speedup is particularly significant when A is sparse.

7 Theoretical Analysis for the Modified Nyström Method

In Section 7.1 we show that the modified Nyström approximation is exact when A is low-rank. In Section 7.2 we provide a lower error bound of the modified Nyström method.

7.1 Theoretical Justifications

Kumar et al. (2009); Talwalkar and Rostamizadeh (2010) showed that the standard Nyström method is exact when \( \text{rank}(W) = \text{rank}(A) \). We show in Theorem 5 a similar result for the modified Nyström approximations.

Theorem 5. For a symmetric matrix A defined in (7), the following three statements are equivalent: (i) \( \text{rank}(W) = \text{rank}(A) \), (ii) \( A = CW^TC^T \), (iii) \( A = CC^TA(C^T)^T C^T \).

Theorem 5 shows that the standard and modified Nyström methods are equivalent when \( \text{rank}(W) = \text{rank}(A) \). However, it holds in general that \( \text{rank}(A) \gg c \geq \text{rank}(W) \), where the two models are not equivalent.

Furthermore, \( U^{\text{mod}} = C^T A (C^T)^T \) is the minimizer of the following minimization problem

\[
\min_U \| A - U C U^T \|_F,
\]
Efficient Algorithms and Error Analysis for the Modified Nyström Method

Figure 4: Effect of our fast computation of the intersection matrix. The two matrices are both of size 15,000 × 15,000, and we sample c columns uniformly to compute the intersection matrix \( U = C^TA(C^T)^T \) (the modified Nyström) and \( U = W^\dagger \) (the standard Nyström). The time for computing \( U \) is plotted in the figures.

so we have that

\[
\|A - C(C^TA(C^T)^T)C\|_F \leq \|A - CW^\dagger C\|_F.
\]

This shows that in general the modified Nyström method is more accurate than the standard Nyström method.

7.2 Lower Error Bound of the Modified Nyström Method

We establish in Theorem 6 a lower error bound of the modified Nyström method. Theorem 6 shows that whatever a column sampling algorithm is used to construct the modified Nyström approximation, at least \( c \geq 2k\epsilon^{-1} \) columns must be chosen to attain the \( 1 + \epsilon \) bound.

Theorem 6 (Lower Error Bound of the Modified Nyström Method). Whatever a column sampling algorithm is used, there exists an \( m \times m \) SPSD matrix \( A \) such that the error incurred by the modified Nyström method obeys:

\[
\|A - CUC^T\|_F^2 \geq \frac{m - c}{m - k} \left( 1 + \frac{2k}{c} \right) \|A - A_k\|_F^2.
\]

Here \( k \) is an arbitrary target rank, \( c \) is the number of selected columns, and \( U = C^TA(C^T)^T \).

Boutsidis et al. (2011) established a lower error bound for the column selection problem, and the lower error bound is tight because it is attained by the optimal column selection algorithm of Guruswami and Sinop (2012). Boutsidis et al. (2011) showed that whatever column sampling algorithm is used, there exists an \( m \times n \) matrix \( A \) such that the error incurred by the projection of \( A \) onto the column space of \( C \) is lower bounded by

\[
\|A - CC^TA\|_F^2 \geq \frac{n - c}{n - k} \left( 1 + \frac{k}{c} \right) \|A - A_k\|_F^2. \tag{2}
\]

where \( k \) is an arbitrary target rank, \( c \) is the number of selected columns.

Interestingly, the modified Nyström approximation is the projection of \( A \) onto the column space of \( C \) and the row space of \( C^T \) simultaneously, so there is a strong resemblance between the modified Nyström approximation and the column selection problem. As we see, the lower error bound of the modified Nyström approximation in Theorem 6 differs from (2) only by a factor of 2. So it is a reasonable conjecture that the lower bound in Theorem 6 is tight, as well as the lower bound of the column selection problem in (2). We leave it as an open problem.

8 Conclusions and Future Work

In this paper we have proposed two algorithms to make the modified Nyström method more practical. First, we have proposed a column selection algorithm called uniform+adaptive\(^2\) and provided an relative-error bound for the algorithm. The algorithm is highly efficient and effective and very easy to implement. The error bound of the algorithm is nearly as strong as that of the state-of-the-art algorithm—the near-optimal+adaptive algorithm—which is complicated. The experimental results have shown that our uniform+adaptive\(^2\) algorithm is more efficient than the near-optimal+adaptive algorithm, while their accuracies are comparable. Second, we have devised an algorithm for computing the intersection matrix of the modified Nyström approximation; under certain conditions, our algorithm can significantly improve the time complexity. The speedup induced by this algorithm has also been verified empirically.

Furthermore, we have proved that the modified Nyström approximation can be exact when the original matrix is low-rank. We have also established a lower error bound for the modified Nyström method: at least \( c \geq 2k\epsilon^{-1} \) columns must be chosen to attain the \( 1 + \epsilon \) bound. We have conjectured this lower error bound to be tight. Notice that the best known algorithm for the modified Nyström method requires at most \( c = k\epsilon^{-2} \) columns to attain the \( 1 + \epsilon \) bound, so there is a gap between the lower and upper error bounds. It remains an open problem that if there exists an algorithm attaining the lower error bound.
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A Proof of Theorem 3

The error analysis for the uniform+adaptive algorithm relies on Lemma 7 which guarantees the error incurred by its uniform sampling step. The proof of Lemma 7 essentially follows Gittens (2011). We prove Lemma 7 using probability inequalities and some techniques of Boutsidis et al. (2011); Gittens (2011); Gittens and Mahoney (2013); Tropp (2011); the proof is in Appendix A.1.

Lemma 7 (Uniform Column Sampling). Given an \( m \times n \) matrix \( A \) and a target rank \( k \), let \( \mu_k \) denote the matrix coherence of \( A \). By sampling \( c = \frac{\mu_k k \log(k/\delta)}{\theta \log \theta - \theta + 1}, \)
columns uniformly without replacement to construct \( C \), the following inequality
\[
\|A - PC_kA\|_F^2 \leq (1 + \delta^{-1} \theta^{-1}) \|A - A_k\|_F^2.
\]
holds with probability at least \( 1 - 2\delta \). Here \( \delta \in (0, 0.5) \) and \( \theta \in (0, 1) \) are arbitrary real numbers.

The error analysis for the two adaptive sampling steps of the uniform+adaptive algorithm relies on Lemma 8 which follows immediately from Wang and Zhang (2013) Corollary 7 and Section 4.5.

Lemma 8. Given an \( m \times m \) symmetric matrix \( A \) and a target rank \( k \), we let \( C_1 \) contain the \( c_1 \) columns of \( A \) selected by a column sampling algorithm such that the following inequality holds:
\[
\|A - PC_1A\|_F^2 \leq f \|A - A_k\|_F^2.
\]

Then we select \( c_2 = \epsilon f c_1 \) columns to construct \( C_2 \) and \( c_3 = (c_1 + c_2)\epsilon^{-1} \) columns to construct \( C_3 \), both using the adaptive sampling according to the residual \( B_1 = A - PC_1A \) and \( B_2 = A - PC_1C_2A \), respectively. Let \( C = [C_1, C_2, C_3] \), we have that
\[
\mathbb{P}\left\{ \frac{\|A - C(C^T A (C^T)^T)C\|^2}{\|A - A_k\|^2 F} \geq 1 + s \epsilon \right\} \leq \frac{1 + \epsilon}{1 + s \epsilon},
\]
where \( s \) is an arbitrary constant greater than 1.

Finally Theorem 3 is proved by combining Lemma 7 and Lemma 8. The proof is in Appendix A.2.

A.1 Proof of Lemma 7

Proof. We use uniform column sampling to select \( c \) column of \( A \) to construct \( C = AS \). Here the \( n \times c \) random matrix \( S \) has one entry equal to one and the rest equal to zero in each column, and at most one nonzero entry in each row, and \( S \) is uniformly distributed among \( 2^n \) such kind of matrices. Applying Lemma 7 of Gittens et al. (2011), we get
\[
\|A - PC_{c,k}A\|^2_F \leq \|A - A_k\|^2_F + \| (A - A_k) S \|^2_F \| (V_{A_k}^T S)^\dagger \|^2_2. \quad (3)
\]

Now we bound \( \| (A - A_k) S \|^2_F \) and \( \| (V_{A_k}^T S)^\dagger \|^2_2 \) respectively using the techniques of Gittens (2011); Gittens and Mahoney (2013); Tropp (2011).

Let \( I \subset [n] \) be a random index set corresponding to \( S \). The support of \( I \) is uniformly distributing among all the index sets in \( 2^n \) with cardinality \( c \). According to Gittens and Mahoney (2013), the expectation of \( \| (A - A_k) S \|^2_F \) can be written as
\[
\mathbb{E}\| (A - A_k) S \|^2_F = \mathbb{E}\| (A - A_k) X \|^2_F = c \mathbb{E}\| (A - A_k) \|^2_F = \frac{c}{n} \|A - A_k\|^2_F.
\]

Applying Markov’s inequality, we have that
\[
\mathbb{P}\{ \| (A - A_k) S \|^2_F \geq \frac{c}{n \delta} \|A - A_k\|^2_F \} \leq \frac{\mathbb{E}\| (A - A_k) S \|^2_F}{\frac{c}{n \delta} \|A - A_k\|^2_F} = \delta. \quad (4)
\]

Here \( \delta \in (0, 0.5) \) is a real number defined later.

Now we establish the bound for \( \mathbb{E}\| \Omega \|^2_2 \) as follows. Let \( \lambda_i(X) \) be the \( i \)-th largest eigenvalue of \( X \). Following the proof of Lemma 1 of Gittens (2011), we have
\[
\| (V_{A_k}^T S)^\dagger \|^2_2 = \lambda_k^{-1} \| V_{A_k}^T S S^T V_{A_k} \|^2 \leq \lambda_k^{-1} \left( \sum_{i=1}^c X_i \right) \leq \lambda_{\min}^{-1} \left( \sum_{i=1}^c X_i \right). \quad (5)
\]

where the random matrices \( X_1, \cdots, X_c \) are chosen uniformly at random from the set \( \{ (V_{A_k}^T)_{i} (V_{A_k}^T)_{i}^T \}_{i=1}^n \) without replacement. The random matrices are of size \( k \times k \). We accordingly define
\[
R = \max_i \lambda_{\max}(X_i) = \max_i \| (V_{A_k}^T)_{i} \|^2_2 = \frac{k}{n} \mu_k,
\]
where \( \mu_k \) is the matrix coherence of \( A \), and define
\[
\beta_{\min} = c \lambda_{\min}(\mathbb{E} X_1) = \lambda_{\min} \left( \sum_{i=1}^c X_i \right) = \frac{c}{n},
\]
Then we apply Lemma 8 and obtained the following inequality:

\[ \mathbb{P}\left[ \lambda_{\min}\left( \sum_{i=1}^{c} X_i \right) \leq \frac{\theta c}{n} \right] \leq k \left[ \frac{e^{\theta - 1}}{\theta^\theta} \right] ^{\frac{n}{\theta c}} \triangleq \delta. \tag{6} \]

where \( \theta \in (0, 1) \) is a real number, and it follows that

\[ c = \frac{\mu_k k \log(k/\delta)}{\theta \log \theta - \theta + 1}. \]

Applying (5) and (6), we have

\[ \mathbb{P}\left\{ \left\| (V_{A,k}^T S)^* \right\|_2^2 \geq \frac{n}{\theta c} \right\} \leq \delta. \tag{7} \]

Combining (4) and (7) and applying the union bound, we have the following inequality:

\[ \mathbb{P}\left\{ \left\| (A - A_k) S \right\|_F^2 \geq \frac{c}{n^d} \left\| A - A_k \right\|_F^2 \right\} \]

or

\[ \left\| (V_{A,k}^T S)^* \right\|_2^2 \geq \frac{n}{\theta c} \leq 2 \delta. \tag{8} \]

Finally, from (8) and (9) we have that the inequality

\[ \left\| A - \mathcal{P}_{C,k} A \right\|_F^2 \leq (1 + \delta^{-1} \theta^{-1}) \left\| A - A_k \right\|_F^2 \]

holds with probability at least 1 - 2\( \delta \), by which the lemma follows.

**Lemma 9** (Theorem 2.2 of Tropp [2011]). We are given \( l \) independent random \( d \times d \) SPSD matrices \( X_1, \cdots, X_l \) with the property

\[ \lambda_{\max}(X_i) \leq R \quad \text{for} \quad i = 1, \cdots, l. \]

We define \( Y = \sum_{i=1}^{l} X_i \) and \( \beta_{\min} = \lambda_{\min}(E X_1) \). Then for any \( \theta \in (0, 1) \), the following inequality holds:

\[ \mathbb{P}\left\{ \lambda_{\min}(Y) \leq \theta \beta_{\min} \right\} \leq d \left[ \frac{e^{\theta - 1}}{\theta^\theta} \right] ^{\frac{\lambda_{\min}}{\theta \beta_{\min}}}. \]

### A.2 Proof of the Theorem

**Proof.** The matrix \( C_1 \) consists of \( c_1 \) columns selected by uniform sampling, and \( C_2 \in \mathbb{R}^{m \times c_2} \) and \( C_3 \in \mathbb{R}^{m \times c_3} \) are constructed by adaptive sampling. We set \( \delta = 1/\sqrt{5} \) and \( \theta = \sqrt{5}/4 \) for Lemma 7, then we have

\[ f = 1 + \delta^{-1} \theta^{-1} = 5, \]

\[ c_1 = \frac{\mu_k k \log(k/\delta)}{\theta \log \theta - \theta + 1} = 8.7 \mu_k k \log(\sqrt{5}k). \]

Then we set

\[ c_2 = kf \epsilon^{-1} = 5k \epsilon^{-1}, \]

\[ c_3 = (c_1 + c_2) \epsilon^{-1} = (1 + \epsilon^{-1})(8.7 \mu_k k \log(\sqrt{5}k)) \epsilon^{-1}. \]

According to Lemma 8. Letting \( s > 1 \) be an arbitrary constant, we have that

\[ \mathbb{P}\left\{ \frac{\left\| A - C^T C \right\|_F}{\left\| A - A_k \right\|_F} \leq 1 + s \right\} \]

\[ \geq \mathbb{P}\left\{ \frac{\left\| A - C^T C \right\|_F}{\left\| A - A_k \right\|_F} \leq 1 + s \right\} \left\{ \frac{\left\| A - \mathcal{P}_{C_1} A \right\|_F^2}{\left\| A - A_k \right\|_F^2} \leq f \right\} \]

\[ \cdot \mathbb{P}\left\{ \left\| A - \mathcal{P}_{C_1} A \right\|_F^2 \leq f \right\} \]

\[ \geq \left( 1 - \frac{1 + \epsilon}{1 + s \epsilon} \right) (1 - 2\delta). \]

where the last inequality follows from Lemma 7 and Lemma 8.

Repeating the sampling procedure for \( t \) times and letting \( C_{[i]} \) and \( U_{[i]} \) be the \( i \)-th sample, we obtain an upper error bound on the failure probability:

\[ \mathbb{P}\left\{ \min_{i \in [t]} \left\{ \frac{\left\| A - C_{[i]} U_{[i]} C_{[i]}^T \right\|_F}{\left\| A - A_k \right\|_F} \right\} \geq 1 + s \epsilon \right\} \]

\[ \leq \left( 1 - \frac{1 + \epsilon}{1 + s \epsilon} \right)^t \left( 1 - 2\delta \right) \]
\( T_{\text{Multiply}}(m^2c) \) time in general. So the total time complexity is \( \mathcal{O}(mc^2) + T_{\text{Multiply}}(m^2c) \) without using Theorem \( \text{I} \) or \( \mathcal{O}(m(c_1 + c_2)^2) + T_{\text{Multiply}}(m^2c) \) using Theorem \( \text{II} \). As for the space complexity, the Moore-Penrose inverse of an \( m \times c \) matrix demands \( \mathcal{O}(mc) \) space, and multiplying a \( c \times m \) matrix \( C^\dagger \) by an \( m \times m \) matrix \( A \) costs \( \mathcal{O}(mc) \) space by partitioning \( A \) into small blocks of size smaller than \( m \times c \) and loading one block into RAM at a time to perform matrix multiplication. □

**B Proof of Theorem 4**

**Proof.** Let \( C \in \mathbb{R}^{m \times c} \) consists of a subset of columns of \( A \). By row permutation \( C \) can be expressed as

\[
PC = \begin{bmatrix} W \ A_{21} \end{bmatrix}.
\]

Then according to Lemma 10, the Moore-Penrose inverse of \( C \) can be written as

\[
C^\dagger = W^{-1}(I_c + S^T S)^{-1} \begin{bmatrix} I_c & S^T \end{bmatrix} P A_{21} P^T.
\]

where \( S = A_{21} W^{-1} \). Then the intersection matrix of modified Nyström approximation to \( A \) can be expressed as

\[
U = C^\dagger A(C^\dagger)^T = W^{-1}(I_c + S^T S)^{-1} \begin{bmatrix} I_c & S^T \end{bmatrix} P A_{21} P^T
\]

Then we show that \( T_1(W + T_2 + T_3)T_1^T \).

Here the intermediate matrices are computed by

\[
T_0 = A_{21}^T A_{21},
\]

\[
T_1 = W^{-1}(I_c + S^T S)^{-1} - W^{-1}(I_c + W^{-1} T_0 W^{-1})^{-1},
\]

\[
T_2 = A_{21}^T S = A_{21} A_{21} W^{-1} = T_0 W^{-1},
\]

\[
T_3 = S^T A_{22} S = W^{-1} (A_{21}^T A_{22} A_{21}) W^{-1}.
\]

\[
\text{Lemma 10 (The Moore Penrose Inverse of Partitioned Matrices [Ben-Israel and Greville 2003 Page 179])}. \text{Given a matrix } X \in \mathbb{R}^{m \times n} \text{ of rank of at least } c \text{ which has a nonsingular } c \times c \text{ submatrix } X_{11}. \text{By rearrangement of columns and rows by permutation matrices } P \text{ and } Q, \text{the submatrix } X_{11} \text{ can be bought to the top left corner of } X, \text{that is,}
\]

\[
PXQ = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix}.
\]

Then the Moore-Penrose inverse of \( X \) is

\[
X^\dagger = Q \begin{bmatrix} I_c \\ T^T \end{bmatrix} (I_c + TT^T)^{-1} X_{11}^{-1}(I_c + SS^T)^{-1} \begin{bmatrix} I_c & S^T \end{bmatrix} P,
\]

where \( T = X_{11}^{-1} X_{12} \) and \( S = X_{21} X_{11}^{-1} \).

**C The Proof of Theorem 5**

**Proof.** Suppose that \( \text{rank}(W) = \text{rank}(A) \). We have that \( \text{rank}(W) = \text{rank}(C) = \text{rank}(A) \) because

\[
\text{rank}(A) \geq \text{rank}(C) \geq \text{rank}(W).
\]

Thus there exists a matrix \( X \) such that

\[
\begin{bmatrix} A_{21}^T \\ A_{22} \end{bmatrix} = CX^T = \begin{bmatrix} WX^T \\ A_{21} X^T \end{bmatrix},
\]

and it follows that \( A_{21} = XW \) and \( A_{22} = A_{21} X^T = XWX^T \). Then we have that

\[
A = \begin{bmatrix} W & (XW)^T \\ XX & WWX^T \end{bmatrix}
\]

\[
= \begin{bmatrix} I & X \\ W \end{bmatrix} W \begin{bmatrix} I & X^T \end{bmatrix},
\]

\[
C W^T C^T = \begin{bmatrix} W \\ WX \end{bmatrix} W^T \begin{bmatrix} W & (XW)^T \end{bmatrix}
\]

\[
= \begin{bmatrix} I & X \\ W \end{bmatrix} W \begin{bmatrix} I & X^T \end{bmatrix}.
\]

Here the second equality in (11) follows from \( WW^T W = W \). We obtain that \( A = \frac{1}{C} C W^T C \). Then we show that

\[
A = CC^\dagger A(C^\dagger)^T C^T.
\]

Since \( C^\dagger = (C^T C)^\dagger C^T \), we have that

\[
C^\dagger = (W(I + X^T X) W)^\dagger W [I, X^T],
\]

and thus

\[
C^\dagger A(C^\dagger)^T W
\]

\[
= \langle W(I + X^T X) W \rangle^\dagger W \langle I + X^T X \rangle [W(I + X^T X) W]
\]

\[
W \langle W(I + X^T X) W \rangle^\dagger W
\]

\[
= \langle W(I + X^T X) W \rangle^\dagger W \langle I + X^T X \rangle W.
\]
where the second equality follows from Lemma 11 because $(I + X^T X)$ is positive definite. Similarly we have

\[ WC^T A(C^t)^T W = W(W(I + X^T X)W)^\dagger W(I + X^T X)W = W. \]

Thus we have

\[ CC^T A(C^t)^T C = \begin{bmatrix} 1 & X \\ X & I \end{bmatrix} WC^T A(C^t)^T W \begin{bmatrix} 1 & X^T \\ X & I \end{bmatrix} = \begin{bmatrix} 1 & X \\ X & I \end{bmatrix} W \begin{bmatrix} 1 & X^T \\ X & I \end{bmatrix}. \] (12)

It follows from Equations (10) (11) (12) that $A = CW^T C^T = CC^T A(C^t)^T C^T$.

Conversely, when $A = CW^T C^T$, we have that $\text{rank}(A) \leq \text{rank}(W) = \text{rank}(W)$. By applying (9) we have that $\text{rank}(A) = \text{rank}(W)$.

When $A = CC^T A(C^t)^T C^T$, we have $\text{rank}(A) \leq \text{rank}(C)$. Thus there exists a matrix $X$ such that

\[ \begin{bmatrix} A_{21}^T \\ A_{22} \end{bmatrix} = CX^T = \begin{bmatrix} WX^T \\ A_{21}X\end{bmatrix}, \]

and therefore $A_{21} = XW$. Then we have that

\[ C = \begin{bmatrix} W \\ A_{21} \end{bmatrix} = \begin{bmatrix} I & X \end{bmatrix} W, \]

so $\text{rank}(C) \leq \text{rank}(W)$. Apply (9) again we have $\text{rank}(A) = \text{rank}(W)$. \( \square \)

**Lemma 11.** $X^T VX(X^TVX)^\dagger X^T = X^T$ for any positive definite matrix $V$.

**Proof.** Since the positive definite matrix $V$ have a decomposition $V = B^T B$ for some nonsingular matrix $B$, so we have

\[ X^T VX(X^TVX)^\dagger X^T = (BX)^T((BX)^T(BX))^\dagger(BX)^T(B^T)^{-1} = (BX)^T((BX)^T)^\dagger(BX)^T(B^T)^{-1} = (BX)^T(B^T)^{-1} = X^T. \]

\( \square \)

**D  Proof of Theorem 6**

In Section D.1 we provide two key lemmas, and then in Section D.2 we prove Theorem 6 using the two lemmas.

### D.1 Key Lemmas

**Lemma 12.** For an $m \times m$ matrix $B$ with diagonal entries equal to one and off-diagonal entries equal to $\alpha$, the error incurred by the modified Nyström method is lower bounded by

\[ \|B - \hat{B}^\text{mod}\|^2_F \geq (1 - \alpha)^2(m - c) \left(1 + \frac{2}{\alpha} - (1 - \alpha)^{1+o(1)/\alpha cm/2} \right). \]

**Proof.** Without loss of generality, we assume the first $c$ column of $B$ are selected to construct $C$. We partition $B$ and $C$ as:

\[ B = \begin{bmatrix} W & B_{21}^T \\ B_{21} & B_{22} \end{bmatrix} \quad \text{and} \quad C = \begin{bmatrix} W \\ B_{21} \end{bmatrix}. \]

Here the matrix $W$ can be expressed by $W = (1 - \alpha)I_c + \alpha 1_c 1_c^T$. We apply the Sherman-Morrison-Woodbury formula

\[(A + BCD)^{-1} = A^{-1} - A^{-1}B(C^{-1} + DA^{-1}B)^{-1}DA^{-1} \]

to compute $W^{-1}$, yielding

\[ W^{-1} = \frac{1}{1 - \alpha^2} I_c - \frac{\alpha}{(1 - \alpha)(1 - \alpha + \alpha^2)} 1_c 1_c^T. \] (13)

We expand the Moore-Penrose inverse of $C$ by Lemma [10] and obtain

\[ C^\dagger = W^{-1} (I_c + S^T S)^{-1} \begin{bmatrix} I_c \\ S^T \end{bmatrix} \]

where

\[ S = B_{21} W^{-1} = \frac{\alpha}{1 - \alpha + \alpha^2} 1_{m-c} 1_c^T. \]

It is easily verified that $S^T S = (\frac{\alpha}{1 - \alpha + \alpha^2})^2 (m - c) 1_c 1_c^T$.

Now we express the matrix constructed by the modified Nyström method in a partitioned form:

\[ \hat{B}_c^\text{mod} = CC^T B(C^t)^T C^T = \begin{bmatrix} W \\ B_{21} \end{bmatrix} W^{-1} (I_c + S^T S)^{-1} \begin{bmatrix} I_c \\ S^T \end{bmatrix} B \]

\[ = \begin{bmatrix} I_c \\ S \end{bmatrix} (I_c + S^T S)^{-1} W^{-1} \begin{bmatrix} W \\ B_{21} \end{bmatrix}^T \]

\[ = \begin{bmatrix} I_c \\ S \end{bmatrix} (B_{21} W^{-1} (I_c + S^T S)^{-1}) \begin{bmatrix} I_c \\ S^T \end{bmatrix} B \]

\[ = \begin{bmatrix} I_c \\ S \end{bmatrix} \begin{bmatrix} I_c \\ B_{21} W^{-1} (I_c + S^T S)^{-1} \end{bmatrix} \begin{bmatrix} I_c \\ S^T \end{bmatrix} B \]

\[ = \begin{bmatrix} I_c \\ S \end{bmatrix} \begin{bmatrix} I_c \\ B_{21} W^{-1} (I_c + S^T S)^{-1} \end{bmatrix} \begin{bmatrix} I_c \\ S^T \end{bmatrix} B. \] (14)

We then compute the submatrices $(I_c + S^T S)^{-1}$ and $B_{21} W^{-1} (I_c + S^T S)^{-1}$ respectively as follows. We apply
the Sherman-Morrison-Woodbury formula to compute 
\((I_e + S^T S)^{-1}\), yielding

\[
(I_e + S^T S)^{-1} = \left( I_e + \left( \frac{\alpha}{1 - \alpha + c} \right)^2 (m - c)I_c 1_c^T \right)^{-1} = I_e - \gamma_1 I_c 1_c^T,
\]

where

\[
\gamma_1 = \frac{m - c}{mc + \left( \frac{1 - \alpha}{\alpha} \right)^2 + \frac{2(1 - \alpha)c}{\alpha}}.
\]

It follows from (13) and (15) that

\[
W^{-1}(I_e + S^T S)^{-1} = \left( \gamma_1 I_c 1_c^T \right)(I_e - \gamma_1 I_c 1_c^T) = \gamma_2 I_e + \left( \gamma_1 \gamma_3 - \gamma_1 \gamma_2 - \gamma_3 \right)I_c 1_c^T
\]

where

\[
\gamma_2 = \frac{1}{1 - \alpha} \quad \text{and} \quad \gamma_3 = \frac{\alpha}{(1 - \alpha)(1 - \alpha + \alpha c)}.
\]

Then we have that

\[
B_{21} W^{-1}(I_e + S^T S)^{-1} = \alpha \left( \gamma_1 \gamma_3 c^2 - \gamma_3 c - \gamma_1 \gamma_2 c + \gamma_2 \right) I_{m - c} 1_c^T = \gamma_1 I_{m - c} 1_c^T,
\]

where

\[
\gamma = \alpha \left( \gamma_1 \gamma_3 c^2 - \gamma_3 c - \gamma_1 \gamma_2 c + \gamma_2 \right) = \frac{\alpha(\alpha c - \alpha + 1)}{2 \alpha c - 2 \alpha - 2 \alpha^2 c + \alpha^2 c^2 + \alpha^2 c^2 m + 1}.
\]

Since \(B_{21} = \alpha 1_{m - c} 1_c^T\) and \(B_{22} = (1 - \alpha)I_{m - c} + \alpha 1_{m - c} 1_{m - c}^T\), it is easily verified that

\[
\begin{bmatrix}
  I_e & S^T
\end{bmatrix}
\begin{bmatrix}
  I_e & S
\end{bmatrix}^{-1}
= \begin{bmatrix}
  I_e & S^T
\end{bmatrix}
\begin{bmatrix}
  B_{21} & B_{22}
\end{bmatrix}
\begin{bmatrix}
  I_e & S
\end{bmatrix}^{-1}
= (1 - \alpha)I_e + \lambda I_c 1_c^T,
\]

where

\[
\lambda = \frac{\alpha(3\alpha m - \alpha - 2\alpha + 2 \alpha^2 c - 3 \alpha^2 m + \alpha + \alpha^2 m^2 + 1)}{(\alpha c - \alpha + 1)^2}.
\]

It follows from (14), (15), (17), and (19) that

\[
\tilde{B}^\text{mod}_{e} = \begin{bmatrix}
  I_e - \gamma_1 I_c 1_c^T & \gamma_1 I_{m - c} 1_c^T
\end{bmatrix}
\begin{bmatrix}
  (1 - \alpha)I_e + \lambda I_c 1_c^T & I_e - \gamma_1 I_c 1_c^T
\end{bmatrix}^T
\]

where

\[
\tilde{B}_{11} = (1 - \alpha)I_e + \left[ (1 - \gamma_1 c) \right] (\lambda - \lambda \gamma_1 c - (1 - \alpha)\gamma_1) - (1 - \alpha)\gamma_1 I_c 1_c^T,
\]

\[
\tilde{B}_{12} = \tilde{A}_{12}^T = \gamma_1 (1 - \gamma_1 c)(1 - \alpha + \lambda c)I_{m - c} 1_c^T
\]

\[
\tilde{B}_{22} = \gamma_2 c(1 - \alpha + \lambda c)I_{m - c} 1_{m - c}^T
\]

where

\[
\eta_1 = (1 - \gamma_1 c)(\lambda - \lambda \gamma_1 c - (1 - \alpha)\gamma_1) - (1 - \alpha)\gamma_1,
\]

\[
\eta_2 = \gamma_1 (1 - \gamma_1 c)(1 - \alpha + \lambda c),
\]

\[
\eta_3 = \gamma_2 c(1 - \alpha + \lambda c),
\]

By dealing with the four blocks of \(\tilde{B}^\text{mod}_{e}\) respectively, we finally obtain that

\[
\|B - \tilde{B}^\text{mod}_{e}\|_F^2
= \|W - \tilde{B}_{11}\|_F^2 + 2\|B_{21} - \tilde{B}_{21}\|_F^2 + \|B_{22} - \tilde{B}_{22}\|_F^2
= c^2(\alpha - \eta_1)^2 + 2c(m - c)(\alpha - \eta_2)^2 + (m - c)(\alpha m - 1)(\alpha - \eta_3)^2
= (m - c)(\alpha - 1)^2(\alpha^4 c^2 m^2 - 4\alpha^4 c^2 m + 4\alpha c^2 + 2\alpha^4 c m - 4\alpha^4 c^2 m + \alpha^4 c m + \alpha^4 c m + 4\alpha^4 c^2 m - 8\alpha^3 c^2 + 2\alpha^3 c m + 2\alpha^3 c - 2\alpha^3 m + 2\alpha^3 c - 4\alpha^4 c^2 m + 2\alpha^2 c - 7\alpha^2 c + \alpha^2 m + 4\alpha c - 2\alpha + 1)/(2\alpha c - 2\alpha - 2\alpha^2 c + \alpha^2 c^2 + 4\alpha^2 c^2 m + 1)
= (m - c)(\alpha - 1)^2 \left( 1 + \frac{2}{c} - \left( \frac{1 - \alpha}{c} \right)(6\alpha c - 6\alpha - 12\alpha^2 c + 6\alpha^3 c + 6\alpha^2 - 2\alpha^3 + 3\alpha^4 c^2 - 3\alpha^3 c^2 + 2\alpha^3 c m + 3\alpha^2 c m - 3\alpha^3 c m + 2)/(2\alpha c - 2\alpha - 2\alpha^2 c + \alpha^2 c^2 + 4\alpha^2 c^2 m + 1)^2 \right)
= (m - c)(\alpha - 1)^2 \left( 1 + \frac{2}{c} - \left( 1 + (1 - \alpha) \frac{1 - \alpha}{\alpha c m / 2} \right) \right).
\]

\[
\text{\square}
\]

Lemma 13 (Lemma 19 of [Wang and Zhang (2013)]. Given \(m \) and \(k \), we let \(B\) be an \(\frac{m}{k} \times \frac{m}{k} \) matrix whose diagonal entries equal to one and off-diagonal entries equal to \(\alpha \in [0, 1)\). We let \(A\) be an \(m \times m\) block-diagonal matrix

\[
A = \text{diag}(B, \cdots, B).
\]

Let \(A_k\) be the best rank-\(k\) approximation to the matrix \(A\), then we have that

\[
\|A - A_k\|_F = (1 - \alpha)\sqrt{m - k}.
\]
D.2 Proof of the Theorem

Now we prove Theorem 6 using Lemma 12 and Lemma 13.

Proof. Let $C$ consist of $c$ column sampled from $A$ and $\hat{C}_i$ consist of $c_i$ columns sampled from the $i$-th block diagonal matrix in $A$. Without loss of generality, we assume $\hat{C}_i$ consists of the first $c_i$ columns of $B$. Then the intersection matrix $U$ is computed by

$$U = C^T A (C^T)^T \hat{C}_i$$

$$= \begin{bmatrix} \text{diag}(\hat{C}_1, \ldots, \hat{C}_k) \end{bmatrix} A \begin{bmatrix} \text{diag}(\hat{C}_1, \ldots, \hat{C}_k) \end{bmatrix}^T$$

$$= \text{diag}(\hat{C}_1^T B \hat{C}_1^T, \ldots, \hat{C}_k^T B \hat{C}_k^T).$$

The modified Nyström approximation to $A$ is

$$\tilde{A}_{c}^{\text{mod}} = C U C^T$$

$$= \text{diag}(\hat{C}_1^T B \hat{C}_1^T, \ldots, \hat{C}_k^T B \hat{C}_k^T),$$

and thus the approximation error is

$$\|A - \tilde{A}_{c}^{\text{mod}}\|_F^2 = \sum_{i=1}^{k} \|B - \hat{C}_i \hat{C}_i^T \hat{C}_i^T \hat{C}_i^T \|_F^2$$

$$\geq (1-\alpha)^2 \sum_{i=1}^{k} \left( \frac{p}{c_i} - \frac{1}{\alpha c_i p/2} \right)$$

$$= (1-\alpha)^2 \left( \sum_{i=1}^{k} \frac{p}{c_i} \right)$$

$$+ \sum_{i=1}^{k} \frac{2(p - c_i)}{c_i} \left( 1 - \frac{(1-\alpha)(1+o(1))}{\alpha p} \right)$$

$$\geq (1-\alpha)^2 \left( m - c \right) \left( 1 + \frac{2k}{c} \left( 1 - \frac{k(1-\alpha)(1+o(1))}{\alpha m} \right) \right),$$

where the former inequality follows from Lemma 12 and the latter inequality follows by minimizing over $c_1, \ldots, c_k$. Finally we apply Lemma 13 and the theorem follows by setting $\alpha \to 1$. □

E Supplementary Experiments

We have mentioned in Remark 1 that the resulting approximation accuracy is insensitive to the parameter $\mu$ in Algorithm 1 and setting $\mu$ to be exactly the matrix coherence does not give in general large increase to the highest accuracy. To demonstrate this point of view, we conduct experiments on an RBF kernel matrix of the Letters Dataset with $\sigma = 0.2$, and we set $k = 10$.

We compare the uniform+adaptive^2 algorithm with different settings of $\mu$; we also employ the adaptive-full algorithm of Kumar et al. (2012), the near-optimal-adaptive algorithm of Wang and Zhang (2013), and the uniform sampling algorithm for comparison. The experiment settings are the same to Section 6. Here the adaptive-full algorithm also has three steps: one uniform sampling and two adaptive sampling steps, and we set $c_1 = c_2 = c_3 = c/3$ according to Kumar et al. (2012). We plot the approximation errors in Figure 5.

![Figure 5: Effect of the parameter $\mu$ in Algorithm 1](image)

We can see from Figure 5 that different settings of $\mu$ does not have big influence on the approximation accuracy. We can also see that it is unnecessary to set $\mu$ to be exactly the matrix coherence; in this set of experiments, the uniform+adaptive^2 algorithm achieves the higher accuracy when $\mu = 0.5$ (the actual matrix coherence is $\mu_{10} = 0.05$).