Towards More Efficient Nyström Approximation and CUR Matrix Decomposition

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Abstract
Matrix sketching schemes and the Nyström method have both been extensively used to speed up large-scale eigenvalue computation and kernel learning methods. Matrix sketching methods produce accurate matrix approximations, but they are only computationally efficient on skinny matrices where one of the matrix dimensions is relatively small. In particular, they are not efficient on large square matrices. The Nyström method, on the other hand, is highly efficient on symmetric (and thus square) matrices, but can only achieve low matrix approximation accuracy. In this paper we propose a novel combination of the sketching method and the Nyström method to improve their efficiency/effectiveness, leading to a novel approximation which we call the Sketch-Nyström method. The Sketch-Nyström method is computationally nearly as efficient as the Nyström method on symmetric matrices with approximation accuracy comparable to that of the sketching method. We show theoretically that the Sketch-Nyström method can potentially solve eigenvalue problems and kernel learning problems in linear time with respect to the matrix size to achieve $1 + \epsilon$ relative-error, whereas the sketch methods and the Nyström method cost at least quadratic time to attain comparable error bound. Our technique can be straightforwardly applied to make the CUR matrix decomposition more efficiently computed without much affecting the accuracy. Empirical experiments demonstrate the effectiveness of the proposed methods.

Keywords: Kernel approximation, matrix factorization, the Nyström method, CUR matrix decomposition
1. Introduction

In modern large scale data matrix applications, exact matrix inversion and decomposition become impossible due to the limitation of computational resources. Consequently, in the past decade matrix approximation techniques have been extensively studied by the theoretical computer science community (Woodruff, 2014), machine learning community (Mahoney, 2011), and the numerical linear algebra community (Halko et al., 2011).

In machine learning, many graph analysis techniques and kernel methods require expensive matrix computations on symmetric matrices. The truncated eigenvalue decomposition (that is, approximate matrix decomposition with top eigenvectors) is widely used in graph analysis such as spectral clustering, link prediction in social networks (Shin et al., 2012), graph matching (Patro and Kingsford, 2012), etc. Kernel methods (Schölkopf and Smola, 2002) such as kernel PCA and many manifold learning methods also require truncated eigenvalue decomposition. Some other kernel methods such as Gaussian process regression, least squares SVM, kernel ridge regression require solving the $n \times n$ linear systems in the form $(K + \alpha I_n)w = y$ to obtain the model parameter $w$, where $K$ is the $n \times n$ kernel matrix and $y$ contains the $n$ labels. The rank $k$ ($k \ll n$) truncated eigenvalue decomposition (k-eigendecomposition for short) of an $n \times n$ matrix cost time $O(n^2k)$ in general, while solving the above linear system costs time $O(n^3)$. Thus the standard matrix computation approaches are infeasible when $n$ is large.

For kernel methods, we are typically given $n$ data points of dimension $d$, while the $n \times n$ kernel matrix is unknown beforehand and need to be computed. This adds to an additional $O(n^2d)$ time cost. When $n$ and $d$ are both large, computing the kernel matrix is prohibitively expensive. Thus a good kernel approximation method should avoid the computation of the entire kernel matrix.

The Nyström method and the matrix sketching methods can both speed up matrix computation using a fast low-rank decomposition $K \approx CUC^T$ where $C \in \mathbb{R}^{n \times c}$ is a sketch of $K$ (e.g. randomly sampled $c$ columns of $K$) and $U \in \mathbb{R}^{c \times c}$ is called the intersection matrix. Using such a low-rank approximation of $K$, it takes only $O(nc^2)$ additional time to approximately compute the rank $k$ ($k \leq c$) eigenvalue decomposition or approximately solve the aforementioned $n \times n$ linear system. Therefore, if $C$ and $U$ are obtained in linear time (w.r.t. $n$) and $c$ is independent of $n$, then the aforementioned eigenvalue decomposition and linear system can all be approximately solved in linear time.

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The Nyström method is perhaps the most widely used kernel approximation method. Let $P$ be an $n \times c$ sketching matrix such as the uniform sampling matrix (Williams and Seeger, 2001, Gittens, 2011), adaptive sampling matrix (Kumar et al., 2012), leverage score sampling matrix (Gittens and Mahoney, 2013), etc. The Nyström method computes $C$ by $C = KP \in \mathbb{R}^{n \times c}$ and $U$ by $U = (P^TC)^{\dagger} \in \mathbb{R}^{c \times c}$. This method of computing $U$ is computationally very efficient, but it incurs relatively large matrix approximation error even if $C$ is a good sketch of $K$. For such reason, the Nyström method is reported to have low approximation accuracy in real-world applications (Dai et al., 2014, Hsieh et al., 2014, Si et al., 2014b). In fact, using the Nyström method it is impossible to obtain a $1 + \epsilon$ bound relative to $\|K - K_k\|_F^2$ unless $c \geq \Omega(\sqrt{nk/\epsilon})$ (Wang and Zhang, 2013). Here $K_k$ denotes the best rank-$k$ approximation of $K$. The requirement that $c$ grows at least linearly with $\sqrt{n}$ is a very pessimistic result. It implies that in order to attain $1 + \epsilon$ relative-error bound, the
time requirement of the Nyström method is $O(nc^2) \geq \Omega(n^2k/\epsilon)$ for solving the $k$-eigenvalue decomposition or linear system, which is quadratic in $n$. Therefore, the Nyström method is in fact not a linear time method.

The main reason for the low accuracy of Nyström method is due to the way that $U$ is calculated. In fact, much higher accuracy can be obtained if $U$ is calculated by solving the minimization problem $\min_U \|K - UCUT\|_F^2$, which is a standard way to sketching symmetric square matrix (Halko et al., 2011, Section 5.3). This approach is called the projective sketching model by Gittens and Mahoney (2013). Wang and Zhang (2013) called this approach the modified Nyström method when $C$ contains a subset of columns of $K$, and later Wang et al. (2014a) provided an algorithm that samples $c = O(k/\epsilon)$ columns of $K$ to form $C$ such that $\min_U \|K - CUC^T\|_F^2 \leq (1 + \epsilon)\|K - K_k\|_F^2$. The modified Nyström method is far more accurate than the standard Nyström method because $c$ is independent of $\epsilon$. However, it requires visiting every entry of $K$, and the time complex of computing $U$ in this approach is $O(n^2c)$. Therefore when applied to kernel approximation, the computational cost is no less than $O(n^2d + n^2c)$. To reduce the computational cost, this paper considers the problem of efficient calculation of $U$ with fixed $C$ while achieving an accuracy comparable to that of the modified Nyström method.

We note that there are many other kernel approximation approaches; however, they do not directly address the issue we consider here, and thus are complementary to this work. These studies are either less effective or inherently rely on the Nyström method. The random feature approaches are popular kernel approximation methods, but they are known to be noticeably less effective than the Nyström method (Yang et al., 2012). The kernel approximation models such as MEKA (Si et al., 2014a) and the ensemble Nyström method (Kumar et al., 2012) are reported to significantly outperform the Nyström method in terms of approximation accuracy, but their key components are still the Nyström method and the component can be replaced by any other methods such as the method studied in this work. The spectral shifting Nyström method (Wang et al., 2014b) also outperforms the Nyström method in certain situations, but the spectral shifting strategy can be used for any other kernel approximation models beyond the standard/modified Nyström methods. We do not compare with such methods in this paper because MEKA, the ensemble Nyström method, and the spectral shifting Nyström method can all be improved if we replace the underlying standard/modified Nyström methods using the new method considered here.

The key question we try to answer in this paper can be described as follows.

**Question 1** Given an $n \times n$ symmetric matrix $K$, a target rank $k$, and error parameter $\gamma$. Assume that

A1 We are given a sketch matrix $C \in \mathbb{R}^{n \times c}$ of $K$, which is obtained in time $\text{Time}(C)$.

A2 The matrix $C$ is a good sketch of $K$ in that $\min_U \|K - CUC^T\|_F^2 \leq (1 + \gamma)\|K - K_k\|_F^2$.

Then we would like to know whether for an arbitrary error parameter $\epsilon$, it is possible to compute $C$ and $\hat{U}$ such that the following two requirements are satisfied:

R1 The matrix $\hat{U}$ has the following approximation error bound:

$$\|K - CUC^T\|_F^2 \leq (1 + \epsilon)(1 + \gamma)\|K - K_k\|_F^2.$$  

R2 The procedure of computing $C$ and $\hat{U}$ and approximately solving the aforementioned $k$-eigenvalue decomposition or the linear system runs in time $O(n \cdot \text{poly}(k, \gamma^{-1}, \epsilon^{-1})) + \text{Time}(C)$.  

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This paper gives an affirmative answer to the above question, and this has the following consequences. First, the overall approximation has high accuracy in the sense that $\|K - C\tilde{U}C^T\|_F^2$ is comparable to $\min_U \|K - CUC^T\|_F^2$, and is thereby comparable to the best rank $k$ approximation. Second, with $C$ at hand, the intersection matrix $\tilde{U}$ is obtained efficiently (linear in $n$). Third, with $C$ and $\tilde{U}$ at hand, it takes extra time which is linear in $n$ to compute the aforementioned eigenvalue decomposition or linear system. Therefore with a good $C$, we can use time linear in $n$ to obtain desired solutions comparable to that of the modified Nyström method.

Unfortunately, the following theorem shows that the standard/modified Nyström methods do not enjoy such desirable properties. We prove the theorem in the appendix.

**Theorem 1** Neither the standard Nyström method nor the modified Nyström method satisfies both requirements in Question 1. To make requirement $R1$ hold, both of the standard and modified Nyström methods cost time no less than $O\left(n^2 \cdot \text{poly}(k, \gamma^{-1}, \epsilon^{-1})\right) + \text{Time}(C)$ which is at least quadratic in $n$.

As mentioned earlier, the standard Nyström method efficiently computes an intersection matrix that is sub-optimal, and the modified Nyström method computes a good intersection matrix but the computation is not efficient. This motivates us to find an efficient method to compute a good intersection matrix.

The CUR matrix decomposition is closely related to the modified Nyström method and troubled by the same computational problem. The CUR matrix decomposition is an extension of the modified Nyström method from symmetric matrices to general matrices, and it has attracted much attentions in recent years (Mahoney and Drineas, 2009). Given an $m \times n$ matrix $A$, the CUR matrix decomposition selects $c$ columns of $A$ to form $C \in \mathbb{R}^{m \times c}$ and $r$ rows of $A$ to form $R \in \mathbb{R}^{r \times n}$, and computes an intersection matrix $U \in \mathbb{R}^{c \times r}$ such that $\|A - CUR\|_F^2$ is small. Traditionally, it costs time

$$O(mn \cdot \min\{c, r\})$$

to compute the optimal intersection matrix $U^* = C^\dagger AR^\dagger$ (Stewart, 1999, Wang and Zhang, 2013, Boutsidis and Woodruff, 2014). How to efficiently compute a high-quality intersection matrix for CUR is also unsolved.

### 1.1 Contributions and Organization

This work is motivated by an intrinsic connection of the intersection matrix computation between the Nyström method and the modified Nyström method. Based on a generalization of this observation, we propose a called Sketch-Nyström method for approximating any symmetric matrix. We show that the Sketch-Nyström method satisfies both requirements in Question 1. Given $n$ data points of dimension $d$, the Sketch-Nyström method computes $C$ and $U^\text{sn}$ and approximately solve the truncated eigenvalue decomposition or linear system in time

$$O\left(nc^3/\epsilon + nc^2d/\epsilon\right) + \text{Time}(C).$$

Here $\text{Time}(C)$ is defined in Question 1.
The Sketch-Nyström method achieves the desired properties in Question 1 by solving \( \min_U \| K - CUC^T \|_F \) approximately rather than exactly while ensuring 
\[
\| K - CUC^T \|_F^2 \leq (1 + \epsilon) \min_U \| K - CUC^T \|_F^2.
\]
In this way, the time complexity for computing the intersection matrix will be linear in \( n \), which is far less than the time complexity of \( O(n^2 c) \) for the modified Nyström method. Our method also avoids computing the entire kernel matrix \( K \); instead, it computes a block of \( K \) of size \( \frac{\sqrt{nc}}{\epsilon} \times \frac{\sqrt{nc}}{\epsilon} \), which is far smaller than \( n \times n \).

Our method can also be applied to improve the CUR matrix decomposition of the general matrices which are not necessarily square. Given an \( m \times n \) matrix \( A \) and its subsampled columns \( C \in \mathbb{R}^{m \times c} \) and rows \( R \in \mathbb{R}^{r \times n} \), it costs time \( O(mn \cdot \min\{c, r\}) \) to compute the intersection matrix \( U = C^T A R^\dagger \). Applying our technique, the time cost drops to only
\[
O(c r \cdot \min\{m, n\} \cdot \min\{c, r\}),
\]
while the approximation quality is nearly the same.

The remainder of this paper is organized as follows. Section 2 defines the notation used in this paper. Section 3 introduces the related work of matrix sketching and two symmetric matrix approximation methods. Section 4 describes the Sketch-Nyström method and analyze the time complexity and approximation error bound. Section 5 applies the technique of Sketch-Nyström to compute the CUR matrix decomposition more efficiently. Section 6 conducts empirical comparisons to show the effect of the intersection matrix. The proofs of the theorems are in the appendix.

2. Notation

The notation used in this paper are defined as follows. Let \([n] = \{1, \ldots, n\}\), \( I_n \) be the \( n \times n \) identity matrix, and \( I_1 \) be the \( n \times 1 \) vector of all ones. We let \( x = y \pm z \) denote \( y - z \leq x \leq y + z \). For an \( m \times n \) matrix \( A = [A_{ij}] \), we let \( a(i) \) be its \( i \)-th row, \( a_j \) be its \( j \)-th column, \( \text{nnz}(A) \) be the number of nonzero entries of \( A \), \( \|A\|_F = (\sum_{i,j} A_{ij}^2)^{1/2} \) be its Frobenius norm, and \( \|A\|_2 = \max_{x \neq 0} \|Ax\|_2 / \|x\|_2 \) be its spectral norm.

Let \( \rho = \text{rank}(A) \), we can 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 \( \Sigma_A \in \mathbb{R}^{\rho \times \rho} \) is the \( i \)-th largest singular value of \( A \) (denoted as \( \sigma_i(A) \)). We also let \( U_{A,k} \) and \( V_{A,k} \) be the first \( k \) \((< \rho)\) columns of \( U_A \) and \( V_A \), respectively, and \( \Sigma_{A,k} \) be the \( k \times k \) top sub-block of \( \Sigma_A \). Then the \( m \times n \) matrix \( A_k = U_{A,k} \Sigma_{A,k} V_{A,k}^T \) is the best rank-\( k \) approximation of \( A \). Let \( A^\dagger = V_A \Sigma_A^{-1} U_A^T \) be the Moore-Penrose inverse of \( A \).

The row leverage scores of an \( n \times c \) matrix \( C \) are defined by \( \ell_i = (U_C U_C^T)_{ii} \) for all \( i \in [n] \). The leverage scores reflects the importance of the corresponding rows. The exact computation of the leverage scores costs \( O(nc^2) \) time, while the approximate computation of leverage scores within \( 1 \pm \frac{1}{2} \) relative error costs \( O(nc \log n) \) (Drineas et al., 2012) or \( O(\text{nnz}(C) \log n + \text{poly}(c)) \) (Clarkson and Woodruff, 2013).

We also list some frequently used notation in Table 1. Given a rank-\( c \) decomposition \( \tilde{K} = CUC^T \approx K \), it takes \( O(nc^2) \) time to compute the eigenvalue decomposition of \( \tilde{K} \) and \( O(nc^2) \) time to solve the linear system \((\tilde{K} + cI_n)w = y\) to obtain \( w \). (See Appendix A for more discussions.) The truncated eigenvalue decomposition and linear system are the bottleneck.
Table 1: A summary of the notation.

| Notation | Description |
|----------|-------------|
| \( n \)  | number of data points |
| \( d \)  | dimension of the data point |
| \( K \)  | \( n \times n \) kernel matrix |
| \( P \)  | \( n \times c \) sketching matrix |
| \( S \)  | \( n \times s \) sketching matrix |
| \( C \)  | \( n \times c \) sketch computed by \( C = KP \) |
| \( U_{\text{mys}} \) | \((P^T K)\dagger \in \mathbb{R}^{c \times c}\) |
| \( U_{\text{mod}} \) | \((C^T K (C^T)\dagger) \in \mathbb{R}^{c \times c}\) |
| \( U_{\text{sn}} \) | \((S^T C)\dagger (S^T K S) (C^T S)\dagger \in \mathbb{R}^{c \times c}\) |

of many kernel methods, and thus an accurate and efficient low-rank approximation can help accelerating the computation of many kernel learning methods.

3. Related Work

In Section 3.1 we review some of the popular matrix sketching algorithms. In Section 3.2 we describe two symmetric matrix approximation methods. In Section 3.3 we briefly introduce the CUR matrix decomposition.

3.1 Matrix Sketching Algorithms

Matrix sketching algorithms are extensively studied in the literature. Given an \( m \times n \) matrix \( A \), we find an \( n \times c \) sketching matrix \( P \) and compute \( C = AP \). Here \( P \) may or may not depend on \( A \), and the matrix \( C \) is a good sketch of \( A \) if the top \( k \) \((k \leq c)\) left singular vectors of \( A \) are almost contained in the column space of \( C \).

Uniform sampling is the most efficient approach and is widely used for kernel approximation. The performance of uniform sampling relies on matrix coherence (proportional to the largest leverage score) (Gittens and Mahoney, 2013). When the leverage scores are uniform, uniform sampling is nearly as effective as non-uniform sampling algorithms. The popular non-uniform sampling algorithms include the leverage score sampling (Drineas et al., 2008), adaptive sampling (Deshpande et al., 2006, Kumar et al., 2012, Wang and Zhang, 2013), and \( k \)-means clustering sampling (Zhang and Kwok, 2010).

Another class of sketching methods is the data independent random projection algorithms. Gaussian random projection is very widely used for its simplicity, but multiply a matrix with a dense Gaussian matrix is expensive, and the sparseness is destroyed after projection. The more efficient random projection techniques include the fast Johnson-Lindenstrauss transform, the sparse subspace embedding, etc. Woodruff (2014) provided an excellent review of these sketching methods.

Applying sketching to any general matrix \( A \in \mathbb{R}^{m \times n} \), the approximate \( k \)-SVD \( A \approx \tilde{U} \tilde{\Sigma} \tilde{V}^T \) can be computed quite efficiently, especially on skinny matrices, and \( 1 + \epsilon \) relative-error bound are guaranteed. However, when applied to symmetric or SPSD matrix \( K \), the \( 1 + \epsilon \) bound on \( \|K - \tilde{U} \tilde{\Sigma} \tilde{V}^T\|_F \) does not directly imply near \( 1 + \epsilon \) bound on \( \|K - \tilde{U} \tilde{\Sigma} \tilde{U}^T\|_F \) or \( \|K - \tilde{U}^T \tilde{K} \tilde{U} \tilde{U}^T\|_F \). The analysis of \( k \)-eigenvalue decomposition is much more difficult than the \( k \)-SVD.
When applied to large-scale kernel approximation, computing the full kernel matrix $K$ is expensive. Thus, sketching algorithms that do need to access all entries of $K$ are preferable. For example, uniform sampling and the $k$-means clustering sampling avoid computing the entire kernel matrix.

### 3.2 The Standard/Modified Nyström Methods

Given an $n \times n$ matrix $K$ and an $n \times c$ column selection matrix $P$, we let $C = KP$ and $W = P^T C = P^T K P$. Without loss of generality, we assume that $P$ selects the first $c$ columns. We can thus write $K$ and $C$ as

$$K = \begin{bmatrix} W & K_{21}^T \\ K_{21} & K_{22} \end{bmatrix} \quad \text{and} \quad C = \begin{bmatrix} W \\ \hline K_{21} \end{bmatrix}. \quad (1)$$

The standard Nyström method is defined by

$$\tilde{K}^n_{\text{nys}} \triangleq C U_{\text{nys}}^T C^T = C W^T C^T = C (P^T C)^\dagger (P^T K P) (C^T P)^\dagger C^T, \quad (2)$$

and the modified Nyström method (Wang and Zhang, 2013) is defined by

$$\tilde{K}^m_{\text{mod}} \triangleq C U_{\text{mod}}^T C^T = C C^\dagger K (C^\dagger)^T C^T. \quad (3)$$

The only difference between the two models is their intersection matrices, and the difference leads to big difference in their approximation accuracies. Wang and Zhang (2013) provided a lower error bound of the standard Nyström method, which shows that no algorithm can select less than $\Omega(\sqrt{n k/\epsilon})$ columns of $K$ to form $C$ such that

$$\|K - C U_{\text{nys}}^T C^T\|_F^2 \leq (1 + \epsilon)\|K - K_k\|_F^2.$$

In contrast, the modified Nyström method can attain the $1 + \epsilon$ relative-error bound with $c = \text{poly}(k, \epsilon^{-1})$. Wang et al. (2014a) provided an algorithm that attains the error bound with $c = O(k/\epsilon)$, which is optimal up to a constant factor.

While we have mainly discussed the time complexities of kernel approximation in the previous sections, the space complexity is often a more important issue in large scale problems due to the limitation of computer memory. Either the standard or the modified Nyström method requires $O(nc)$ space to hold $C$ and $U$ to approximately solve the aforementioned eigenvalue decomposition or the linear system.\footnote{The space costs of the modified Nyström method and the Sketch-Nyström method are both $O(nc + nd)$ rather than $O(n^2)$ or $O(nc + s^2)$. This is because we can hold the $n \times d$ data matrix in RAM, and compute a small block of $K$ each time, and then compute $C^i K$ or $S^j K$ block by block.} Therefore, we hope to make $c$ as small as possible while achieving a low approximation error. There are two elements: (1) a good sketch $C = KP$, and (2) a high-quality intersection matrix $U$. We focus on the latter in this paper.

### 3.3 The CUR Matrix Decomposition

Given an arbitrary $m \times n$ matrix $A$, the CUR matrix decomposition is computed by selecting $c$ columns of $A$ to form $C \in \mathbb{R}^{m \times c}$ and $r$ rows of $A$ to form $R \in \mathbb{R}^{r \times n}$ and computing an intersection matrix $U$ such that $\|A - CUR\|_F^2$ is small. CUR preserves the sparsity and non-negativity properties of $A$, and it is thus more attractive than SVD in certain
applications (Mahoney and Drineas, 2009). In addition, with CUR of $A$ at hand, the truncated SVD of $A$ can be very efficiently computed.

At present the most accurate CUR algorithm is developed by Boutsidis and Woodruff (2014), which selects $c = \mathcal{O}(k/\epsilon)$ column and $r = \mathcal{O}(k/\epsilon)$ rows to form $C$ and $R$ by adaptive sampling, respectively, and form the intersection matrix $U^* = C^\dagger A R^\dagger$. The approximation error is bounded by

$$\|A - CU^* R\|_F^2 \leq (1 + \epsilon)\|A - A_k\|_F^2.$$ 

This result matches the theoretical lower bound up to a constant factor. Therefore their CUR algorithm is near optimal. Though efficient algorithms have been developed by Boutsidis and Woodruff (2014) to select columns and rows to form $C$ and $R$, computing the intersection matrix $U^*$ costs time linear in $mn$, which make CUR decomposition inefficient.

4. The Sketch-Nyström Method

In Section 4.1 we present the motivation behind the Sketch-Nyström method. In Section 4.2 we provide an alternative perspective on the standard/sketch Nyström methods by formulating them as approximate solutions to an optimization problem. In Section 4.3 we describe the implementation of the Sketch-Nyström method and analyze the time complexity. In Section 4.4 we analyze the error bound of the Sketch-Nyström method. Theorem 3 is the main theorem, which shows that the approximation error of the Sketch-Nyström method is only $\epsilon$ worse than the modified Nyström method. In Section 4.5 we mention some implementation details that help improving the approximation quality. In Section 4.6 we provide a lower error bound of the Sketch-Nyström method.

4.1 Motivation

The Sketch-Nyström method is defined by

$$K_{c,s}^{m,n} \triangleq C(S^T C)^\dagger (S^T K S) (C^T S)^\dagger C^T,$$

where $S$ is also an $n \times s$ column selection matrix.

From (2) and (3) we can see that the standard Nyström method is a special case of the Sketch-Nyström method where $S$ is defined as $P$ and that the modified Nyström method is a special case where $S$ is defined as $I_n$.

Let $P$ be the set of the indices selected by $P$ and $S$ be the set of the indices selected by $S$. Intuitively, when $P \subset S \subset [n]$, the accuracy of the Sketch-Nyström method should be between the standard and modified Nyström methods. We will show that when $s = \mathcal{O}(c\sqrt{n}/\epsilon) \ll n$, the performance of the Sketch-Nyström method is nearly as good as the modified Nyström method. Especially, the fact $s \ll n$ makes the Sketch-Nyström method much cheaper to compute than the modified Nyström method. When applied to the kernel methods, the Sketch-Nyström method avoids computing the entire kernel matrix. We show a very intuitive comparison in Figure 1.

4.2 An Alternative Interpretation

With the sketch $C = KP \in \mathbb{R}^{n \times c}$ at hand, we want to find the intersection matrix $U$ such that $C U C^T \approx K$. It is very intuitive to solve the following problem to make the
Figure 1: The yellow blocks denote the submatrices of $K$ that must be computed by the kernel approximation models. The standard Nyström method computes an $n \times c$ block of $K$; the modified Nyström method computes the entire $n \times n$ matrix $K$; the Sketch-Nyström method computes an $n \times c$ block and an $(s-c) \times (s-c)$ block of $K$ (due to the symmetry of $K$).

approximation tight:

$$U^{\text{mod}} = \arg\min_U \|CUC^T - K\|_F^2 = C^\dagger K(C^\dagger)^T. \quad (4)$$

The solution is the modified Nyström method (Wang and Zhang, 2013). Since solving this system is time expensive, we propose to find a sketching matrix $S \in \mathbb{R}^{n \times s}$ and solve the following problem instead:

$$U^{\text{sn}} = \arg\min_U \|S^T(CUC^T - K)S\|_F^2 = (S^T C)^\dagger (S^T K S) (C^T S)^\dagger, \quad (5)$$

which yields the Sketch-Nyström method. Similar ideas has been exploited to efficiently solve the least squares regression problem (Drineas et al., 2006, 2011, Clarkson and Woodruff, 2013), but their analysis does not directly applied to the more complicated system (5).

This approximate linear system interpretation offers a new perspective on the standard Nyström method. The intersection matrix of the Nyström method is in fact an approximate solution to the problem $\min_U \|CUC^T - K\|_F^2$. The Nyström method use $S = P$ as the embedding matrix, which leads to the solution

$$U^{\text{nys}} = \arg\min_U \|P^T(CUC^T - K)P\|_F^2 = (P^T K P)^\dagger.$$

This gives a new interpretation of the Nyström method and helps to relate the Nyström method to the symmetric matrix sketching method.
Algorithm 1 The Sketch-Nyström Method.

1: **Input:** an $n \times n$ symmetric matrix $K$ and the number of selected columns or target dimension of projection $c (< n)$.
2: **Sketching:** $C = KP$ using an arbitrary $n \times c$ sketching matrix $P$ (not studied in this work);
3: Optional: replace $C$ by any orthonormal bases of the columns of $C$;
4: Compute another $n \times s$ sketching matrix $S$, e.g. the leverage score sampling in Algorithm 2;
5: Compute the sketches $S^T C \in \mathbb{R}^{s \times c}$ and $S^T KS \in \mathbb{R}^{s \times s}$;
6: Compute $U_{sn} = (S^T C) (S^T KS)^\dagger (C^T S)^\dagger \in \mathbb{R}^{c \times c}$;
7: **Output:** $C$ and $U_{sn}$ such that $K \approx CU_{sn}C^T$.

Algorithm 2 The Leverage Score Sampling Algorithm.

1: **Input:** an $n \times c$ matrix $C$, an integer $s$.
2: Orthogonalize the columns of $C$ (by SVD or QR) to obtain its orthonormal bases $U_C \in \mathbb{R}^{n \times c}$;
3: Compute the sampling probabilities $p_i = s\ell_i / c$, where $\ell_i = \|e_i^T U_C\|_2^2$ is the $i$-th leverage score;
4: Initialize $S$ to be an matrices of size $n \times 0$;
5: for $i = 1$ to $n$ do
6: With probability $p_i$, add $\sqrt{c / \ell_i} e_i$ to be a new column of $S$, where $e_i$ is the $i$-th standard basis of size $n \times 1$;
7: end for
8: **Output:** $S$, whose expected number of columns is $s$.

4.3 Algorithm

We describe the whole procedure of the Sketch-Nyström method in Algorithm 1. We are particularly interested in the random selection matrix $S$ corresponding to the row leverage scores of $C$. The matrix $S$ is computed according to Algorithm 2.

Table 2 compares the time complexities of the standard Nyström method (Williams and Seeger, 2001), the modified Nyström method (Wang and Zhang, 2013), and the Sketch-Nyström method (Theorem 3). In Table 2, the medial column lists the time cost for computing the intersection matrices given $C$ and $K$, and the right column lists the time cost for evaluating the kernel function. The time complexities are analyzed in the following.

- In Algorithm 1, suppose $S$ is the leverage score sample matrix. Step 3 and 4 requires SVD or QR of $C$ and costs $O(nc^2)$ time. Step 5 is in negligible time. Step 6 costs $O(sc^2)$ time for pseudo-inverse and $O(s^2c)$ time for matrix multiplication. Thus it takes totally $O(nc^2 + s^2c)$ time to compute $U_{sn}$ given $C$ and $K$.

- Suppose $S$ is a Gaussian projection matrix. Step 5 in Algorithm 1 takes $O(nmz(K)s + ns^2)$ time. Thus the total time cost is $O(nmz(K)s + ns^2 + s^2c) = O(nmz(K)s + ns^2)$.

- In the kernel approximation problems, suppose that we are given $n$ data points of $d$ dimension and that the kernel matrix $K$ is unknown beforehand. Also suppose that computing the sketching matrix $P$ in step 2 in Algorithm 1 does not need to access the kernel matrix. If $S$ is a leverage score sampling matrix, it takes extra $O(ncd + s^2d)$ time to compute an $n \times c$ block and an $s \times s$ block of $K$. Unfortunately, if $S$ is a Gaussian projection matrix, we have to cost $O(n^2d)$ time to compute the entire kernel matrix $K$ in order to compute $S^T KS$. 


Table 2: A summary of the time cost of the approximation models—the standard/modified/sketch Nyström methods (excluding the time for computing $C$). The notation is defined previously in Table 1. Suppose that computing the sketching matrix $R$ in step 2 in Algorithm 1 needs not to see the kernel matrix.

| Intersection Matrix | Kernel Function |
|---------------------|-----------------|
| Standard Nyström    | $c^3$           |
| Modified Nyström    | $\text{nnz}(K)c + nc^2$ |
| Sketch-Nyström      | $nc^2 + s^2c$   |

**Remark 2** If $S$ is a leverage score sampling matrix, we will spend $O(nc^2)$ time to compute the SVD of $C$ to compute the leverage scores. In fact, this does not incur extra computational cost. If our goal is to approximately compute the eigenvalue decomposition of $K$, the SVD of $C$ must be computed in order to compute the eigenvalue decomposition of $\tilde{K} = CUC^T$. If our goal is to approximately solve the $n \times n$ linear system, with the SVD of $C$ at hand, it costs time only $O(c^3 + nc)$ rather than $O(nc^2)$ to obtain the solution. See Appendix A for more discussions.

### 4.4 Error Analysis

Let $U^{\text{mod}}$ and $U^{\text{sn}}$ be the intersection matrices of the modified/sketch Nyström methods defined in (4) and (5), respectively. In the following we show that the Sketch-Nyström method offers a better choice in that it takes time only linear in $n$ to compute $U^{\text{sn}}$ and that $U^{\text{sn}}$ is nearly as good as $U^{\text{mod}}$. Our theoretical analysis is motivated by Drineas et al. (2006, 2011), which analyzed the approximate solution to the (ordinal) least square regression problem. However, our analysis is more sophisticated.

**Theorem 3 (Main Result)** Let $K$ be an $n \times n$ symmetric matrix, $C$ be any $n \times c$ matrix, $S$ be an $n \times s$ leverage score sampling matrix corresponding to the rows of $C$, and $U^{\text{sn}}$ be a $c \times c$ matrix defined in (5). When $s = \mathcal{O}(\epsilon^{-1/2}n^{1/2}c)$, the inequality

$$
\|K - CU^{\text{sn}}C\|_F^2 \leq \|K - CC^TK(C^T)^T\|_F^2 + \epsilon\|K - CC^TK\|_F^2 \\
\leq (1 + \epsilon)\|K - CC^TK(C^T)^TC^T\|_F^2
$$

holds with probability at least 0.7.

**Remark 4** Table 2 indicates that it takes time $O(nc^2/\epsilon)$ (excluding the time of computing $C = KP$) to compute $U^{\text{sn}}$. For the kernel approximation problem, we assume that computing $P$ does not need to access the entire kernel matrix $K$. Then it takes at most $O(nc^2d/\epsilon)$ additional time to evaluate the kernel function.

**Remark 5** Wang et al. (2014a) showed that there exists an algorithm (though not linear-time algorithm) attaining the error bound

$$
\|K - CC^TK(C^T)^T\|_F^2 \leq (1 + \epsilon)\|K - K_k\|_F^2
$$
with high probability by sampling }c = O(k/\epsilon)\text{ columns of }K \text{ to form } C. \text{ Using this algorithm to form } C, \text{ the Sketch-Nyström method attains } 1 + \epsilon \text{ relative-error bound with } c = O(k/\epsilon) \text{ and } s = O(n^{1/2}k\epsilon^{-3/2}).

The next theorem shows that a similar result can be obtained using Gaussian random projection. However, we note that the Gaussian random projection approach costs time } O(\text{nnz}(K)s + ns^2) \text{ to compute } U^\text{nn} \text{ and } O(n^2d) \text{ time to compute the entire kernel matrix. Therefore it is a less practical solution. We only state the result here due to recent interests in Gaussian random projection methods in the literature.}

**Theorem 6 (Gaussian Projection)** Under the assumptions of Theorem 3 except for that } S \text{ is an } n \times s \text{ random projection matrix with each entry sampled independently from } \mathcal{N}(0,1/s). \text{ When }

\[ s = O(\epsilon^{-1/2}n^{1/2}c\log n), \]

the error bound (6) holds with probability } 1 - O(1/n). \text{ When } K \text{ is a low-rank matrix, the standard and modified Nyström methods are guaranteed to exactly recover } K \text{ (Kumar et al., 2009, Talwalkar and Rostamizadeh, 2010, Wang et al., 2014a). We show in the following theorem that the Sketch-Nyström method has the same property.}

**Theorem 7 (Exact Recovery)** Let } K \text{ be an } n \times n \text{ symmetric matrix, } P \text{ and } S \text{ be respectively } n \times c \text{ and } n \times s \text{ column selection matrices, } C = KP \text{, and } W = P^T C. \text{ Let } \mathcal{P} \text{ and } \mathcal{S} \text{ be the index sets formed by } P \text{ and } S \text{, respectively, and suppose that } \mathcal{P} \subset \mathcal{S} \subset [n]. \text{ Then } K = C(S^T C)^\dagger K(C^T S)^\dagger C^T \text{ if and only if } \text{rank}(K) = \text{rank}(W).

4.5 Implementation Details

In practice, the approximation accuracy and numerical stability can be significantly improved by the following techniques and tricks.

When } P \text{ and } S \text{ are both random sampling matrices, empirically enforcing } \mathcal{P} \subset \mathcal{S} \text{ significantly improves the approximation accuracy. Here } \mathcal{P} \text{ and } \mathcal{S} \text{ are the subsets of } [n] \text{ selected by } P \text{ and } S, \text{ respectively. Instead of directly sampling } s \text{ indices from } [n] \text{ by Algorithm 2, it is better to sample } s - c \text{ indices from } [n] \setminus \mathcal{P} \text{ to form } \mathcal{S}' \text{ and let } \mathcal{S} = \mathcal{S}' \cup \mathcal{P}. \text{ Whether the requirement } \mathcal{P} \subset \mathcal{S} \text{ improves the approximation accuracy remains an open problem.}

**Corollary 8** Theorem 3 still holds when we restrict } \mathcal{P} \subset \mathcal{S}.

When } S \text{ is the leverage score sampling matrix, we find it better not to scale the entries of } S, \text{ i.e., letting } S \text{ be a zero-one matrix, although the scaling is necessary for theoretical analysis. According to our observation, the scaling sometimes makes the approximation numerically unstable.
4.6 Lower Error Bound

We establish a lower error bound of the Sketch-Nyström method, which implies that to attain the $1 + \epsilon$ relative-error bound, the Sketch-Nyström method must satisfy $c \geq \Omega(k/\epsilon)$ and $s \geq \Omega(\sqrt{nk/\epsilon})$.

**Theorem 9** Let $P \in \mathbb{R}^{n \times c}$ and $S \in \mathbb{R}^{n \times s}$ be any two column selection matrices satisfying that $P \subset S \subset [n]$, where $P$ and $S$ be the index sets formed by $P$ and $S$, respectively. There exists an $n \times n$ symmetric matrix $K$ such that

\[
\frac{\|K - \tilde{K}_{c,s}^{\text{sn}}\|_F^2}{\|K - K_k\|_F^2} \geq \frac{n - c}{n - k} \left(1 + \frac{2k}{c}\right) + \frac{n - s k(n - s)}{n - k} \frac{k}{s^2},
\]

where $k$ is an arbitrary positive integer less than $n$, $C = KP \in \mathbb{R}^{n \times c}$, and

\[
\tilde{K}_{c,s}^{\text{sn}} = C(S^T C)^\dagger (S^T K S)(C^T S)^\dagger C^T
\]

is the Sketch-Nyström approximation of $K$.

Interestingly, Theorem 9 matches the lower bounds of the standard and modified Nyström method. When $s = c$, the righthand side of (7) becomes $\Omega(1 + kn/c^2)$, which is the lower error bound of the standard Nyström method given by Wang and Zhang (2013). When $s = n$, the righthand side of (7) becomes $\Omega(1 + k/c)$, which is the lower error bound of the modified Nyström method given by Wang et al. (2014a).

Corollary 8 and Remark 5 show that our algorithm can achieve $1 + \epsilon$ relative-error bound with $c = O(k/\epsilon)$ and $s = O(\sqrt{nk/\epsilon} \cdot k/\epsilon^2)$. From the lower error bound we can see that in our algorithm $c$ is optimal up to a constant factor and that $s$ matches the lower bound in terms of $n$, but $s$ is sub-optimal in terms of $k$ and $\epsilon$.

5. Extension to CUR Matrix Decomposition

The CUR matrix decomposition is an extension of the Nyström method, and it also requires computing an intersection matrix. Traditionally, computing the intersection matrix $U^* = C^\dagger A R^\dagger$ requires visiting every entry of $A$ and costs time $O(mn \cdot \min\{c, r\})$.

Fortunately, using the same technique as the Sketch-Nyström method, it takes only

$O(c r \epsilon^{-1} \cdot \min\{m, n\} \cdot \min\{c, r\})$.

time to compute an intersection matrix $\tilde{U}$ which is nearly as good as $U^*$. Our proposed method avoids visiting every entry of $A$.

5.1 Algorithm

With $C$ and $R$ at hand, the optimal intersection matrix is computed by

\[
U^* = \arg\min_U \|A - \text{CUR}\|_F^2 = C^\dagger A R^\dagger,
\]

(8)
which is used by Stewart (1999), Wang and Zhang (2013), Boutsidis and Woodruff (2014). This approach costs time $O(mc^2 + nr^2)$ to compute the Moore-Penrose inverse and $O(mn \cdot \min\{c, r\})$ to compute the matrix product. Therefore, even if $C$ and $R$ are uniformly sampled from $A$, the time cost of CUR is $O(mn \cdot \min\{c, r\})$.

Analogous to our proposed Sketch-Nyström method, the computation of the intersection matrix can be sped up while preserving its accuracy. Let the $m \times s_c$ matrix $S_C$ and the $n \times s_r$ matrix $S_R$ be respectively the leverage score sampling matrices corresponding to the columns of $C^T$ and $R$, which can be computed in time $O(mc^2 + nr^2)$. We propose to compute $U$ more efficiently by

$$
\hat{U} = \arg\min_U \|S_C^T A S_R - (S_C^T C)(RS_R)^{\dagger}\|_F^2
$$

which costs time $O(s_r r^2 + s_c c^2 + s_c s_r \cdot \min\{c, r\})$. By setting $s_r$ and $s_c$ according to Theorem 10, the intersection matrix $\hat{U}$ can be computed in time

$$
O(c r \epsilon^{-1} \cdot \min\{m, n\} \cdot \min\{c, r\}),
$$

which is only linear in $\min\{m, n\}$. In comparison, the traditional approach takes time quadratic in $\min\{m, n\}$.

5.2 Error Analysis

The following theorem shows that the computed intersection matrix $\hat{U}$ is nearly as good as the best possible intersection matrix.

**Theorem 10** Let $A$, $C$, $R$ be any given $m \times n$, $m \times c$, $r \times n$ matrices with $c \leq n$ and $r \leq m$. The $m \times s_c$ matrix $S_C$ and the $n \times s_r$ matrix $S_R$ are leverage score sampling matrices corresponding to the columns of $C^T$ and $R$, respectively. The intersection matrix $\hat{U}$ is defined in (9). When

$$
s_c \geq O(\sqrt{qc}\epsilon^{-1/2}) \quad \text{and} \quad s_r \geq O(\sqrt{qr}\epsilon^{-1/2}),
$$

where $q = \min\{m, n\}$, the following inequality holds with probability at least 0.6:

$$
\|A - C \hat{U} R\|_F^2 \leq (1 + \epsilon) \min_U \|A - CUR\|_F^2.
$$

We establish in Theorem 11 an improved error bound for the adaptive sampling based CUR algorithm of Wang and Zhang (2013), and the constants in the theorem are better than the those in (Boutsidis and Woodruff, 2014). Theorem 11 is obtained by following the idea of Boutsidis and Woodruff (2014) and slightly changing the proof of Wang and Zhang (2013).

**Theorem 11** Let $A$ be any given $m \times n$ matrix, $k$ be any positive integer less than $m$ and $n$, and $\epsilon \in (0, 1)$ be an arbitrary error parameter. Let $C \in \mathbb{R}^{m \times c}$ and $R \in \mathbb{R}^{r \times n}$ be columns
Table 3: A summary of the datasets for kernel approximation.

| Dataset   | Letters | PenDigit | Cpusmall | Mushrooms | WineQuality |
|-----------|---------|----------|----------|-----------|-------------|
| #Instance | 15,000  | 10,992   | 8,192    | 8,124     | 4,898       |
| #Attribute| 16      | 16       | 12       | 112       | 12          |

and rows of \( \mathbf{A} \) selected by the near-optimal column selection algorithm of Boutsidis et al. (2011). When \( c \) and \( r \) are both greater than \( 4k\epsilon^{-1}(1 + o(1)) \), the following inequality holds:

\[
E\|\mathbf{A} - \mathbf{C}\mathbf{C}^\dagger\mathbf{A}\mathbf{R}^\dagger\mathbf{R}\|_F^2 \leq (1 + \epsilon)\|\mathbf{K} - \mathbf{K}_k\|_F^2,
\]

where the expectation is taken w.r.t. the random column and row selection.

Theorem 10 and Theorem 11 together show that the \( 1 + \epsilon \) relative-error bound is guaranteed with high probability when \( \mathbf{C} \) and \( \mathbf{R} \) are formed by adaptive sampling and \( \mathbf{U} \) is computed by the efficient approach in (9).

Figure 2: The plot of \( \frac{s}{n} \) against the approximation error \( \|\mathbf{K} - \mathbf{C}\mathbf{U}\mathbf{C}^T\|_F^2/\|\mathbf{K}\|_F^2 \).
6. Experiments

In this section we conduct several sets of illustrative experiments to show the effect of the intersection matrix. We compare among the standard/modified/sketch Nyström methods with different settings of $c$ and $s$. We do not compare with other kernel approximation methods for the reasons stated in Paragraph 7 of Section 1.

6.1 Setup

Let $X = [x_1, \ldots, x_n]$ be the $d \times n$ data matrix, and $K$ be the RBF kernel matrix with each entry computed by $K_{ij} = \exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma^2}\right)$ where $\sigma$ is the scaling parameter.

When comparing the kernel approximation error $\|K - CUC^T\|_F^2$, we set the scaling parameter $\sigma$ in the following way. We let $k = \lceil n/100 \rceil$ and define

$$\eta = \frac{\|K_k\|_F^2}{\|K\|_F^2} = \frac{\sum_{i=1}^{k} \sigma_i^2(K)}{\sum_{i=1}^{n} \sigma_i^2(K)},$$

which indicate the importance of the top one percent singular values of $K$. In general $\eta$ grows with $\sigma$. We set $\sigma$ such that $\eta = 0.9$ or $0.99$.

Since the main focus of this work is the intersection matrix, we simply use uniform sampling to compute $C = KP$ without comparing with other sketching techniques. It is evident that the three methods compared in this paper can all benefit from better sketch matrix $C$. The uniform sampling algorithm is randomized, but we hope to rule out the randomness in our comparisons. Thus we first randomly permute the columns of $X$ before performing a kernel approximation method. In this way, we do not actually perform uniform sampling to form $C$; in fact, the first $c$ columns of $K$ consist a uniformly sampled subset of columns.

All methods are implemented in MATLAB and run on a laptop with Intel i5 2.5GHz CUP and 8GB RAM. To compare the running time, we set MATLAB in the single thread mode.

6.2 Kernel Approximation Accuracy

We conduct experiments on several datasets available at the LIBSVM site. The datasets are summarized in Table 3. In this set of experiments, we study the effect of the Sketch-Nyström method by fixing $c = \lceil n/100 \rceil$ and varying $s$ from $2c$ to $40c$. We use two kinds of sketching matrix $S$: uniform sampling and leverage score sampling. We plot $\frac{s}{n}$ against the approximation error $\|K - CUC^T\|_F^2/\|K\|_F^2$ in Figure 2. The standard and modified Nyström methods are included for comparisons.

Figure 2 shows that the Sketch-Nyström method is significantly better than the standard Nyström method when $s$ is slightly larger than $c$, e.g. $s = 2c$. Recall that the modified Nyström method is a special case of the Sketch-Nyström method where $s = n$. We can see that the Sketch-Nyström method is nearly as accurate as the modified Nyström method when $s$ is far smaller than $n$, e.g. $s = 0.2n$.

The results also show that using uniform sampling and leverage score sampling to generate $S$ do not have much difference. Thus in practice one can simply compute $S$ by uniform sampling.
Figure 3: The plot of (log-scale) elapsed time against the (log-scale) misalignment defined in (10).

Figure 4: The plot of $c$ against the (log-scale) misalignment defined in (10).

6.3 Approximate Kernel Principal Component Analysis

We apply the standard/modified/sketch Nyström methods to approximately compute kernel principal component analysis (KPCA), and contrast with the exact solution. Experiment setting follows Zhang and Kwok (2010). We fix $k = 3$ and vary $c$. As for our Sketch-Nyström method, we set $s = 2c, 4c, 8c$; considering that computing $S$ by uniform sampling or leverage score sampling yields the same empirical performance, here we use only uniform sampling. Let $CUC^T$ be the low-rank approximation formed by standard/modified/sketch Nyström methods. Let $VAV^T$ be the $k$-eigenvalue decomposition of $CUC^T$. 

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Table 4: A summary of the datasets for kernel approximation.

| Dataset    | Pendigit | UPS       | Mushrooms | Gisette | DNA       |
|------------|----------|-----------|-----------|---------|-----------|
| #Instance  | 10,992   | 9,298     | 8,124     | 7,000   | 2,000     |
| #Attribute | 16       | 256       | 112       | 3       | 180       |
| #Class     | 10       | 10        | 2         | 2       | 3         |
| Scaling Parameter $\sigma$ | 0.7 | 15 | 3 | 50 | 4 |

6.3.1 Quality of the Approximate Eigenvectors

In the first set of experiments, we measure the distance between the true eigenvectors $U_{K,k}$ and the approximate eigenvectors $\tilde{V}$ by

$$\text{Misalignment} = \frac{1}{k} \| U_{K,k} - \tilde{V}\tilde{V}^T U_{K,k} \|^2_F, \in [0, 1].$$ (10)

Small misalignment indicates high approximation quality.

We conduct experiments on the datasets summarized in Table 3. We record the elapsed time of the entire procedure—computing (part of) the kernel matrix, computing $C$ and $U$ by the kernel approximation methods, computing the $k$-eigenvalue decomposition of $CUC^T$. We plot the elapsed time against misalignment defined in Figure 3. Results on the Letters dataset are not reported because the exact $k$-eigenvalue decomposition on MATLAB ran out of memory, making it impossible to calculate the misalignment.

At the end of Section 3.2 we mentioned the importance of space cost of the kernel approximation methods and that all three methods being compared cost $O(nc + nd)$ memory. Since $n$ and $d$ are constants, we plot $c$ against misalignment in Figure 4 to show the memory efficiency.

The results shows that using the same amount of time or memory, the misalignment incurred by the standard Nyström method is usually tens of times higher than our Sketch-Nyström method. Experiments also shows that with fixed $c$, the Sketch-Nyström method is nearly as accuracy as the modified Nyström method when $s = 8c \ll n$.

6.3.2 Quality of the Generalization

In the second set of experiments, we test the generalization performance of the kernel approximation methods on classification tasks. The classification datasets are described in Table 4. For each dataset, we randomly sample $n_1 = 50\%n$ data points for training and the rest 50% for test.

We denote $K \in \mathbb{R}^{n_1 \times n_1}$ be the RBF kernel matrix of the training data and $k(x) \in \mathbb{R}^{n_1}$ be defined by $[k(x)]_i = \exp\left(-\frac{\|x-x_i\|^2}{2\sigma^2}\right)$, where $x_i$ is the $i$-th training datum. In the training step, we approximately compute the top 3 eigenvalues and eigenvectors, denote $\Lambda \in \mathbb{R}^{3 \times 3}$ and $\mathbf{V} \in \mathbb{R}^{n_1 \times 3}$. The feature vector (extracted by KPCA) of the $i$-th training datum is the $i$-th column of $\Lambda^{0.5} \mathbf{V}^T$. In the test step, the feature vector of test data $x$ is $\hat{\Lambda}^{-0.5} \hat{\mathbf{V}}^T k(x)$. The we put the training labels and feature vectors of training and test data into the MATLAB $k$-nearest-neighbor classifier $\text{knnclassify}$ to classify the test data. We fix the number of nearest neighbors to be 10. The scaling parameter of the RBF kernel $\sigma$ is chosen to minimize the classification error without kernel approximation; the scaling
Figure 5: The plot of $c$ against the classification error.

Figure 6: The plot of elapsed time against the classification error.
parameters of each dataset is listed in Table 4. Since the kernel approximation methods are randomized, we repeat the training and test procedure 20 times and record the average elapsed time and average classification error.

We plot $c$ against the classification error in Figure 5 and the elapsed time (excluding the time cost of KNN) against the classification error in Figure 6. Using the same amount of memory, the Sketch-Nyström method is significantly better than the standard Nyström method, especially when $c$ is small. Using the same amount of time, the Sketch-Nyström method is marginally better than the standard Nyström method. This set of experiments also indicates that the Sketch-Nyström method with $s = 4c$ or $8c$ yields the best empirical performance.

![Graphs showing NMI against $c$ for different datasets](image)

Figure 7: The plot of $c$ against NMI.

6.4 Approximate Spectral Clustering

We evaluate the performance of the kernel approximation methods on the spectral clustering task following the work of Fowlkes et al. (2004). We conduct experiments on the datasets summarized in Table 4 and use RBF kernel with the same setting of $\sigma$.

We describe the approximate spectral clustering in the following. Suppose we want to cluster $n$ data points to $k$ classes. We use the RBF kernel matrix $K$ as the adjacency matrix and let $CUC^T \approx K$ be the low-rank approximation. The degree matrix $D = \text{diag}(d)$ is a diagonal matrix with $d = CUC^T1_n$, and the normalized graph Laplacian is $L = I_n - D^{-1/2}(CUC^T)D^{-1/2}$. The bottom $k$ eigenvectors of $L$ is the top $k$ eigenvectors
which can be efficiently computed according to Appendix A. We denote the top $k$ eigenvectors by $\tilde{V} \in \mathbb{R}^{n \times k}$, and normalize the rows of $\tilde{V}$. Finally we take normalized rows of $\tilde{V}$ as input of $k$-means clustering. Since the Nyström methods are randomized, we repeat this procedure 20 times and record the average elapsed time and the average normalized mutual information (NMI) of clustering.

We plot $c$ against NMI in Figure 7 and the elapsed time (excluding the time cost of $k$-means) against NMI in Figure 8. Figure 7 shows that using the same amount of memory, the performance of Sketch-Nyström method is better than the standard Nyström method. However, using the same amount of time, the Sketch-Nyström method and the standard Nyström method achieves nearly the same performance.

### 7. Conclusion and Future Work

In this paper we have studied the Sketch-Nyström method for approximating large-scale symmetric matrices and provided theoretical analysis. We have shown that the Sketch-Nyström method potentially costs time linear in $n$, while it is nearly as accurate as the best possible sketching method. The Sketch-Nyström method is theoretically better than the standard/modified Nyström methods because the standard/modified Nyström methods
cost time quadratic in \( n \) to attain the same accuracy. Experiments show that our Sketch-Nyström is nearly as accurate as the modified Nyström method and nearly as efficient as the standard Nyström method.

The technique of Sketch-Nyström can be straightforwardly applied to speed up the CUR matrix decomposition, and theoretical analysis shows that the accuracy is almost unaffected. In this way, for an \( m \times n \) large-scale matrix, the time cost of computing the intersection matrix drops from \( O(mn) \) to \( O(\min\{m, n\}) \).

We have also established a lower error bound of the Sketch-Nyström method. The analysis of the main theorem does not require \( \mathcal{P} \subset \mathcal{S} \) (defined in Section 4.1), which may be the reason why there is a big gap between the upper error bound and the lower error bound. There is strong empirical evidence that enforcing \( \mathcal{P} \subset \mathcal{S} \) invariably and significantly improves the accuracy. It is possible that using \( \mathcal{P} \subset \mathcal{S} \) in the analysis will much improve the error bound of Sketch-Nyström.

Appendix A. Approximately Solving the Eigenvalue Decomposition and Linear System

In this section we show how to use the standard/modified/sketch Nyström methods to speed up eigenvalue decomposition and linear system. The two lemmas are well known results. We show them here for the sake of self-containing.

**Lemma 12 (Approximate Eigenvalue Decomposition)** Given \( C \in \mathbb{R}^{n \times c} \) and \( U \in \mathbb{R}^{c \times c} \). Then the eigenvalue decomposition of \( \tilde{K} = CUC^T \) can be computed in time \( O(nc^2) \).

**Remark 13** From the proof below we can see that the SVD of \( C \) must be computed in order to compute the eigenvalue decomposition of \( CUC^T \). Thus computing the SVD of \( C \) in Algorithm 2 does not cost additional time.

**Proof** It cost \( O(nc^2) \) time to compute the SVD

\[
C = U_C \Sigma_C V_C^T
\]

and \( O(c^3) \) time to compute \( Z = (\Sigma_C V_C^T)U(\Sigma_C V_C^T)^T \in \mathbb{R}^{c \times c} \). It costs \( O(c^3) \) time to compute the eigenvalue decomposition \( Z = V_Z \Lambda_Z V_Z^T \). Combining the results above, we obtain

\[
CUC^T = (U_C \Sigma_C V_C^T)U(\Sigma_C V_C^T)^T = U_C Z U_C^T = (U_C V_Z) \Lambda_Z (U_C V_Z)^T.
\]

It then cost time \( O(nc^2) \) to compute the matrix product \( U_C V_Z \). Since \( U_C V_Z \) has orthonormal columns and \( \Lambda_Z \) is diagonal matrix, the eigenvalue decomposition of \( CUC^T \) is solved. The total time cost is \( O(nc^2) \) + \( O(c^3) \) = \( O(nc^2) \).
Lemma 14 (Approximately Solving Linear System) Given $C \in \mathbb{R}^{n \times c}$, SPDS matrix $U \in \mathbb{R}^{c \times c}$, vector $y \in \mathbb{R}^n$, and arbitrary positive real number $\alpha$. Then it costs time $O(nc^2)$ to solve the $n \times n$ linear system $(CUC^T + \alpha I_n)w = y$ to obtain $w \in \mathbb{R}^n$.

In addition, if the SVD of $C$ is given, then it takes only $O(c^3 + nc)$ time to solve the linear system.

Remark 15 The lemma shows that if the SVD of $C$ is computed, then the linear system can be solved much more efficiently. Therefore, computing the SVD of $C$ in Algorithm 2 is not a waste; the extra time cost by Algorithm 2 is compensated here.

Proof Since the matrix $(CUC^T + \alpha I_n)$ is nonsingular when $\alpha > 0$ and $U$ is SPDS, the solution is $w^* = (CUC^T + \alpha I_n)^{-1}y$. Instead of directly computing the matrix inversion, we can expand the matrix inversion by the Sherman-Morrison-Woodbury matrix identity and obtain

$$(CUC^T + \alpha I_n)^{-1} = \alpha^{-1}I_n - \alpha^{-1}C(U^{-1} + C^T C)^{-1}C^T.$$  

Thus the solution to the linear system is

$$w^* = \alpha^{-1}y - \alpha^{-1}C(U^{-1} + C^T C)^{-1}C^T y.$$  

Suppose we are only given $C$ and $U$. The matrix product $C^T C$ costs time $O(nc^2)$, the matrix inversions cost time $O(c^3)$, and multiplying matrix with vector costs time $O(nc)$. Thus the total time cost is $O(nc^2) + O(c^3) + O(nc) = O(nc^2)$.

Suppose we are given $U$ and the SVD $C = UC \Sigma V_C$. The matrix product

$$C^T C = V_C \Sigma U_C^T U_C \Sigma V_C = V_C \Sigma^2 V_C$$

can be computed in time $O(c^3)$. Thus the total time cost is merely $O(c^3 + nc)$. 

Appendix B. Proof of Theorem 1

The modified Nyström method trivially satisfies requirement R1 with $\epsilon = 0$. However, it violates requirement R2 because computing the intersection matrix by solving $\min_U \|K - CUC^T\|^2_F$ costs time $O(n^2c)$.

To show that the standard Nyström method cannot satisfy both requirements simultaneously, we provide such an adversarial case that assumptions A1 and A2 can both be satisfied and that requirements R1 and R2 cannot hold simultaneously. The adversarial case is the block diagonal matrix

$$K = \text{diag}(B, \ldots, B),$$

where

$$B = (1 - a)I_p + a1_p1_p^T, \quad a < 1, \quad \text{and } p = \frac{n}{k}.$$
and let \( a \to 1 \). The proof of Theorem 4 in (Wang et al., 2014a) showed that sampling certain \( c = 2k/\gamma \) columns of \( K \) to form \( C \) makes assumptions A1 and A2 in Question 1 be satisfied, where \( \text{Time}(C) = o(n) \). This indicates that \( C \) is a good sketch of \( K \). The problem is caused by the way the intersection matrix (denoted \( U^{\text{nys}} \)) is computed. Wang and Zhang (2013, Theorem 12) showed that to make requirement R1 in Question 1 satisfied, \( c \) must be greater than \( \Omega(\sqrt{nk/}(\epsilon + \gamma)) \). Thus it takes \( O(nc^2) \geq \Omega(n^2k/(\epsilon + \gamma)) \) to compute the rank-\( k \) eigenvalue decomposition of \( C U^{\text{nys}} C^T \) or the linear system \((C U^{\text{nys}} C^T + \alpha I_n)w = y \). Thus, requirement R2 is violated.

**Appendix C. Key Lemmas**

Section C.1 and Section C.2 respectively decomposes the error incurred by CUR and Sketch-Nyström deterministically using elementary matrix algebra and singular value inequalities. Section C.3 bounds the singular values \( \sigma_i(S^T U C) \) and the approximate matrix multiplications.

Here we additionally define some notation. Let \( C \) be an \( n \times c \) matrix and \( U_C \in \mathbb{R}^{n \times c} \) be the first \( c \) left singular vectors of \( C \). We defined \( U_C^\perp \) be an \( n \times (n - c) \) matrix with orthonormal columns satisfying \( U_C U_C^T + U_C^\perp (U_C^\perp)^T = I_n \) and \( U_C^T U_C^\perp = 0 \). In this way, the following equalities holds:

\[
U_C^\perp (U_C^\perp)^T K = K - U_C U_C^T K = K - C C^\dagger K.
\]

**C.1 Deterministic Bound of CUR Matrix Decomposition**

**Lemma 16** Let \( A, C, R \) be any given \( m \times n, m \times c, r \times n \) matrices with \( c \leq n \) and \( r \leq m \). Let \( S_C \) and \( S_R \) be any \( m \times s_c, n \times s_r \) matrices with \( s_c < m \) and \( s_r < n \). The intersection matrices \( U^* \) and \( \tilde{U} \) are respectively defined in (8) and (9). Define

\[
A^\perp = A - C U^* R = A - CC^\dagger AR^\dagger R.
\]

Then the following inequalities hold deterministically:

\[
\|A - CUR\|_F^2 \leq \|A^\perp\|_F^2 + \sigma^{-4}_{\min}(S_C U C) \sigma^{-4}_{\min}(V_R^T S_R) \cdot \|S_C^T U C A^\perp S_R (V_R^T S_R)^T\|_F^2
\]

and

\[
\|S_C^T U C A^\perp S_R (V_R^T S_R)^T\|_F \leq \|I_n S_R S_R^T V_R\|_2 \|T_C S_C S_C^\perp U_C^\perp (U_C^\perp)^T A\|_F + \sigma^2_{\max}(S_C U C) \|A V_R^\perp (V_R^\perp)^T S_R S_R^T V_R\|_F.
\]

**Proof** We let the SVD of \( C \) and \( R \) be \( C = U_C \Sigma_C V_C^T \) and \( R = U_R \Sigma_R V_R^T \). We define \( Z^* \) by

\[
C U^* R = U_C (\Sigma_C V_C^T U^* R \Sigma_R) V_R^T \triangleq U_C Z^* V_R^T,
\]

and similarly defined \( \tilde{Z} \) by

\[
C \tilde{U} R \triangleq U_C \tilde{Z} V_R^T.
\]

We defined \( Z \) by \( Z = \tilde{Z} - Z^* \) and obtain that

\[
U_C Z V_R^T = C (\tilde{U} - U^*) R.
\]
It follows from the definition of $\tilde{U}$ and $\tilde{Z}$ that

$$
\tilde{Z} = \Sigma C V_C^T \tilde{U} U_R \Sigma_R = \Sigma C V_C^T (S_C^T C)^\dagger (S_C^T A S_R) (R S_R)^\dagger U_R \Sigma_R = \Sigma C V_C^T (S_C^T U C \Sigma C V_C^T)^\dagger (S_C^T A S_R) (U_R \Sigma_R V_R^T S_R)^\dagger U_R \Sigma_R = (S_C^T U C)^\dagger (S_C^T A S_R) (V_R S_R)^\dagger = \arg\min_X \| S_C^T A S_R - (S_C^T U C) X (V_R^T S_R) \|^2_F.
$$

It follows that

$$
(S_C^T U C)^T (S_C^T U C) \tilde{Z} (V_R^T S_R) (V_R^T S_R)^T = (S_C^T U C)^T (S_C^T A S_R) (V_R^T S_R)^T = (S_C^T U C)^T S_C^\dagger \sum \sigma_i (S_C^T U C)^T V_R^T S_R (V_R^T S_R)^T,
$$

where $A^\perp$ is defined by

$$
A^\perp \triangleq A - C U^* R = A - U C Z^* V_R^T
= (I_m - C C^\dagger) A + (C C^\dagger) A (I_n - R^R R)
= U_C (U_C^\dagger)^T A + U_C U_C^T A V_R (V_R^T).
$$

Then we have

$$
(S_C^T U C)^T S_C^\dagger \sum \sigma_i (S_C^T U C)^T (V_R^T S_R) (V_R^T S_R)^T = (S_C^T U C)^T (S_C^T U C) (\tilde{Z} - Z^*) (V_R^T S_R) (V_R^T S_R)^T = (S_C^T U C)^T (S_C^T U C) Z (V_R^T S_R) (V_R^T S_R)^T.
$$

It follows that

$$
Z = [(S_C^T U C)^T (S_C^T U C)]^\dagger [(S_C^T U C)^T S_C^\dagger \sum \sigma_i (S_C^T U C)^T V_R^T S_R (V_R^T S_R)^T] [(V_R^T S_R) (V_R^T S_R)^T]^\dagger.
$$

Theorem 3.3.16 in (Horn and Johnson) shows that

$$
\sigma_i (W X Y) \leq \sigma_{\max} (W) \sigma_i (Y) \leq \sigma_{\max} (Y) \sigma_i (X),
$$

and thus we can bound the Frobenius norm of $Z$ by

$$
\|Z\|^2_F = \sum_i \sigma_i^2 (Z)
\leq \sum_i \sigma_{\max}^2 [(S_C^T U C)^T (S_C^T U C)]^\dagger \sum_i \sigma_i^2 [(V_R^T S_R) (V_R^T S_R)^T]^\dagger
\leq \sigma_{\max}^4 (S_C^T U C) \sigma_{\max}^2 (V_R^T S_R) \sum_i \sigma_i^2 [(S_C^T U C)^T S_C^\dagger \sum \sigma_i (S_C^T U C)^T V_R^T S_R (V_R^T S_R)^T].
$$

We obtain that

$$
\|Z\|_F \leq \sigma_{\min}^2 (S_C^T U C) \sigma_{\min}^2 (V_R^T S_R) \cdot \| (S_C^T U C)^T S_C^\dagger \sum \sigma_i (S_C^T U C)^T V_R^T S_R (V_R^T S_R)^T \|_F. (12)
$$
Expanding $A^\perp$ by (11), we obtain
\[
\| (S_C^T U_C)^T S_C^T A^\perp S_R (V_R^T S_R)^T \|_F \\
\leq \| (S_C^T U_C)^T S_C^T U_C^\perp (U_C^\perp)^T A S_R (V_R^T S_R)^T \|_F \\
+ \| (S_C^T U_C)^T S_C^T U_C^\perp A V_R^T (V_R^T S_R)^T \|_F \\
\leq \| U_C^T S_C^T S_C^T U_C^\perp (U_C^\perp)^T A \|_F \| I_n S_R S_R^T V_R \|_2 \\
+ \| (S_C^T U_C)^T S_C^T U_C^\perp A V_R^T (V_R^T S_R)^T S_R S_R^T V_R \|_F. \tag{13}
\]

In this way, the Frobenius norm of $Z$ is upper bounded.

Now we expand the error term $\| A - C U R \|_F^2$ by
\[
\| A - C U R \|_F^2 = \| A - C U^* R + C U^* R - C U R \|_F^2 \\
= \| A - C U^* R \|_F^2 + \| C U^* R - C U R \|_F^2 + 2 \text{tr} [(A - C U^* R)^T (C(U^* - U) R)]. \tag{14}
\]

We show the trace in equation equals to zero in the following. We expand the term $A - C U^* R$ by
\[
A - C U^* R = (I_m - C C^\dagger) A + (C C^\dagger) A (I_n - R R^\dagger).
\]

Since $(I_m - C C^\dagger)^T C = 0$ and $R (I_n - R R^\dagger)^T = 0$, the trace term in (14) equals to zero. We thus have
\[
\| A - C U R \|_F^2 = \| A - C U^* R \|_F^2 + \| C U^* R - C U R \|_F^2 \\
= \| A - C U^* R \|_F^2 + \| U_C Z V_R^T \|_F^2, \tag{15}
\]

where the latter equality follows from the definition of $Z$. The lemma follows directly from (12), (13), and (15).

\section{Deterministic Error Bound for the Nyström Approximation}

\begin{lemma}
Let $K$ be an $n \times n$ symmetric matrix, $S$ be any $n \times s$ matrix with $s \leq n$, and $U^{\text{mod}}$ and $U^{\text{m}}$ be defined in (4) and (5) respectively. Define
\[
K^\perp = K - C U^{\text{mod}} C = K - C C^\dagger K (C^\dagger)^T C^T
\]
and $U_C \in \mathbb{R}^{n \times c}$ be the left singular vectors of $C$. The following inequalities holds deterministically:
\[
\| K - C U^{\text{sr}} C^T \|_F^2 \leq \| K^\perp \|_F^2 + \sigma_{\min}^{-2}(S^T U_C) \| (S^T U_C)^T S^T K^\perp S (S^T U_C) \|_F^2,
\]
and
\[
\| (S^T U_C)^T S^T K^\perp S (S^T U_C) \|_F \leq \left( \| I_n S S^T U_C \|_2 + \sigma_{\max}^2(S U_C) \right) \cdot \| (S^T U_C)^T S^T U_C^\perp (U_C^\perp)^T K \|_F.
\]
\end{lemma}

\begin{proof}
The lemma follows from Lemma 16 by setting $R = C^T$.
\end{proof}
C.3 Leverage Score Sampling

Lemma 18 (Approximate Matrix Product, Theorem 7 in Drineas et al. (2008))
Suppose we are given a matrix $X \in \mathbb{R}^{d \times n}$ with orthogonal columns, an arbitrary matrix $Y \in \mathbb{R}^{n \times p}$, and an integer $s \leq n$. Let $S \in \mathbb{R}^{n \times s}$ be the leverage score sampling matrix corresponding to the leverage scores of $X$. Then

$$\mathbb{E}\|X^T Y - X^T S S^T Y\|_F \leq \frac{1}{\sqrt{s}} \|X\|_F \|Y\|_F.$$  

Applying the Markov’s inequality, the following respectively holds with probability $1 - \delta$:

$$\|X^T Y - X^T S S^T Y\|_F \leq \frac{1}{\delta \sqrt{s}} \|X\|_F \|Y\|_F.$$  

Lemma 19 (Theorem 17 in Woodruff (2014))
Let $C$ be an $n \times c$ matrix and $U_C$ be the $n \times c$ left singular vectors of $C$. Let $S \in \mathbb{R}^{n \times s}$ be the leverage score sampling matrix corresponding to the leverage scores of $C$. Then the singular values of $S^T U_C$ satisfy

$$\sigma_i^2(S^T U_C) = 1 \pm O(n^{-1/2} \epsilon \log c) = 1 + o(1),$$  

with probability at least $\delta$.

Appendix D. Proof of Theorem 3

We prove the theorem in the following. The proof relies on Lemmas 17, 18, and 19. We first bound the term $\|I_n S S^T U_C\|_2$ using Lemma 18:

$$\|I_n S S^T U_C\|_2 = \|I_n S S^T U_C - I_n U_C + I_n U_C\|_2 \leq \|I_n S S^T U_C - I_n U_C\|_2 + \|I_n U_C\|_2 \leq \|I_n S S^T U_C - I_n U_C\|_F + 1 \leq \frac{1}{\delta_1 \sqrt{s}} \|I_n\|_F \|U_C\|_F + 1 \quad (\text{w.p. } 1 - \delta_1)$$

$$= \frac{\sqrt{nc}}{\delta_1 \sqrt{s}} + 1 = \frac{\sqrt{nc}}{\delta_1 \sqrt{s}} \left(1 + o(1)\right).$$  

(16)

It follows from $U_C^T U_C = 0$ and Lemma 18 that

$$\|(S^T U_C)^T S^T U_C^\perp (U_C^\perp)^T K\|_F = \|(S^T U_C)^T S^T U_C^\perp (U_C^\perp)^T K - U_C^T U_C^\perp (U_C^\perp)^T K\|_F \leq \frac{1}{\delta_1 \sqrt{s}} \|U_C^\perp (U_C^\perp)^T K\|_F$$

$$\leq \frac{\sqrt{c}}{\delta_2 \sqrt{s}} \|U_C^\perp (U_C^\perp)^T K\|_F$$  

(17)

Letting $s = 2cn^{1/2} \epsilon^{-1/2} \delta_1^{-1} \delta_2^{-1/2}$, by Lemma 19 we have that

$$\sigma_i^2(S^T U_C) = 1 + O(n^{-1/2} \epsilon^{1/2} \log c) = 1 + o(1),$$  

(18)
which is very close to one with probability 0.9.

Setting $\delta_1 = \delta_2 = 0.1$ and $s = 400c n^{1/2} \epsilon^{-1/2}$, with probability at least 0.7, we have

$$\| (S^T U_C) S^T K^\perp S (S^T U_C) \|_F \leq \left( \| I_n S S^T U_C \|_2 + \sigma_{\max}^2 (S U_C) \right) \| (S^T U_C) S^T U_C (U_C^\perp)^T K \|_F,$$

$$\leq \frac{c \sqrt{n}}{\delta_1 \delta_2 s} \left( 1 + o(1) \right) \| U_C (U_C^\perp)^T K \|_F,$$

$$\leq 0.5 \sqrt{\epsilon} \| U_C (U_C^\perp)^T K \|_F.$$  

Here the first inequality follows from Lemma 17, and the second inequality follows from (16) and (17).

Finally, it follows from Lemma 17 and (18) that

$$\| K - C U^m C^T \|_F^2 \leq \| K \|_F^2 + \sigma_{\min}^2 (S^T U_C) \| (S^T U_C) S^T K^\perp S (S^T U_C) \|_F^2,$$

$$\leq \| K \|_F^2 + \epsilon \| U_C (U_C^\perp)^T K \|_F^2,$$

$$= \| K \|_F^2 + \epsilon \| K - C C^\dagger K \|_F^2.$$ 

Finally, the theorem follows from the inequality above and that $\| K - C C^\dagger K \|_F^2 \leq \| K - C C^\dagger K \|_F^2 + \| C C^\dagger K (I_n - C C^\dagger) \|_F^2 = \| K - C C^\dagger K (C^\dagger)^T C^T \|_F^2.$

Appendix E. Proof of Corollary 8

Let $p_i$ be the sampling probability defined in Line 3 of Algorithm 2. Let $\tilde{p}_i = 1$ if $i \in P$, and let $\tilde{p}_i = p_i$ otherwise. Apparently, modifying the sampling probabilities in this way is equivalent to enforcing $P \subset S$. The expected number of sampled indices is increased by

$$\sum_{i \in [n]} (\tilde{p}_i - p_i) = \sum_{i \in P} (1 - p_i) \leq c.$$ 

Since $\tilde{p}_i \geq p_i$, the sample probabilities satisfy

$$\tilde{p}_i \geq \frac{s}{c} \| e_i^T U_C \|_2^2,$$

and thus Lemma 18 and Lemma 19 both hold if we compute the column selection matrix $S$ using the new sampling probabilities. Hence the error bound in Theorem 3 still holds. The expected number of columns of $S$ is

$$\tilde{s} \leq s + c = O(\epsilon^{-1/2} n^{1/2} c) + c = O(\epsilon^{-1/2} n^{1/2} c).$$

Appendix F. Proof of Theorem 6

We prove the theorem in the following. The proof relies on Lemmas 17, 22 and Corollary 21. We let $s = O(\epsilon_0^{-1} \log n)$ and specify $\epsilon_0$ later.
We first bound the term \( \|I_nSS^TU_C\|_F^2 \):
\[
\|I_nSS^TU_C\|_F^2 = \|I_nSS^TU_C - I_nU_C + I_nU_C\|_F^2 \\
\leq \|I_nSS^TU_C - I_nU_C\|_F^2 + \|I_nU_C\|_F^2 \\
\leq \|\epsilon_0\|I_n\|F\|U_C\|_F + 1 \\
= \sqrt{\epsilon_0}\|I_n\|F\|U_C\|_F + 1 \quad \text{(w.p. } 1 - 1/n) \\
= \frac{\sqrt{\epsilon_0}}{\sqrt{\epsilon_0}n} + 1.
\]

Here the last inequality follows from Lemma 22.

By this setting of \( s \), Corollary 21 ensures that \( \sigma_{\max}^2(S^TU_C) \leq 1 + O(\sqrt{\epsilon_0} \log n) < 1.1 \) fails with exponentially low probability.

By the same setting of \( s \), it follows from Lemma 22 that
\[
\|(S^TU_C)^TS^TU_C(U_C^\perp)^TK\|_F = \|(S^TU_C)^TS^TU_C(U_C^\perp)^TK - U_C^\perp(U_C^\perp)^TK\|_F \\
\leq \sqrt{\epsilon_0}\|U_C\|_F\|U_C^\perp(U_C^\perp)^TK\|_F \\
= \sqrt{\epsilon_0}\|U_C^\perp(U_C^\perp)^TK\|_F.
\]

Applying Lemma 17, we have that
\[
\|(S^TU_C)^TS^TU_C(U_C^\perp)^TK\|_F \\
\leq \left(\|I_nSS^TU_C\|_F^2 + \sigma_{\max}^2(SU_C)\right)\|(S^TU_C)^TS^TU_C(U_C^\perp)^TK\|_F \\
\leq (\sqrt{\epsilon_0}n + 2.1)\sqrt{\epsilon_0}\|U_C^\perp(U_C^\perp)^TK\|_F.
\]

Letting \( \epsilon_0^{-1} = 2e^{-1/2}n^{1/2} + 4\epsilon^{-1}c \), we have
\[
\|(S^TU_C)^TS^TU_C(U_C^\perp)^TK\|_F \leq \sqrt{\epsilon}\|U_C^\perp(U_C^\perp)^TK\|_F.
\]

Thus we set
\[
s = O(\epsilon_0^{-1} \log n) = O((\epsilon^{-1/2} + n^{1/2})\epsilon^{-1/2}c \log n).
\]

Since \( 1 \ll c \ll s \), it follows from Corollary 21 that \( \sigma_{\min}^{-8}(S^TU_C) \) is a constant slightly larger than 1 with exponentially low failure probability. It finally follows from Lemma 17 that
\[
\|K - CU_C^\perp C^T\|_F^2 \leq \|K\|_F^2 + \sigma_{\min}^{-8}(S^TU_C)\|(S^TU_C)^TS^TK^\perp S(S^TU_C)\|_F^2 \\
\leq \|K\|_F^2 + \epsilon\|U_C^\perp(U_C^\perp)^TK\|_F^2,
\]
by which the theorem follows.

**F.1 Properties of Random Gaussian Matrix**

**Lemma 20 (Spectral of Gaussian Matrices (Vershynin, 2010))** Let \( G \) be an \( N \times n \) matrix \( (N > n) \) whose entries are independent standard Gaussian variables. Then for every \( t \geq 0 \), the following holds with probability at least \( 1 - 2e^{-t^2/2} \):
\[
\sqrt{N} - \sqrt{n} - t \leq \sigma_{\min}(G) \leq \sigma_{\max}(G) \leq \sqrt{N} + \sqrt{n} + t.
\]
If $G$ is a standard Gaussian matrix and $U$ has orthonormal columns, then $GU$ is also a standard Gaussian matrix, and thus the singular values of $GU$ are bounded by the lemma. The following corollary follows directly from the lemma and will be used in our proof.

**Corollary 21** Let $G$ be an $s \times n$ standard Gaussian matrix and $S = \frac{1}{\sqrt{s}}G$. Let $U$ be an $n \times c$ matrix with orthonormal columns. When $s = 4c/e^2$, the following holds with probability at least $1 - 2e^{-c/2}$

$$\sigma_i(SU) = 1 \pm \epsilon$$

**Lemma 22 (Approximate Matrix Product by Gaussian Projection)** Given two matrices $A \in \mathbb{R}^{m \times n_1}$ and $B \in \mathbb{R}^{m \times n_2}$. Let $G$ be an $s \times m$ standard Gaussian matrix and $S = \frac{1}{\sqrt{s}}G$. When $s \geq O(\epsilon^{-2}\log(n_1 + n_2))$, the following holds with probability at least $1 - \frac{1}{n_1+n_2}$:

$$\|A^T S^T SB - A^TB\|_F \leq \epsilon\|A\|_F\|B\|_F.$$  

**Proof** For two vectors $a, b \in \mathbb{R}^m$, we let $x = a/\|a\|_2$ and $y = b/\|b\|_2$. Then the approximate vector product is

$$\frac{\langle Sa, Sb \rangle}{\|a\|_2\|b\|_2} = \langle Sx, Sy \rangle = \frac{1}{2}\left[\|Sx\|_2^2 + \|Sy\|_2^2 - \|S(x - y)\|_2^2\right]$$

$$= \frac{1}{2}\left[(\|Sx\|_2^2 - \|x\|_2^2) + (\|Sy\|_2^2 - \|y\|_2^2) - (\|S(x - y)\|_2^2 - \|x - y\|_2^2)\right] + \langle x, y \rangle.$$ 

It follows that

$$\frac{\langle Sa, Sb \rangle - \langle a, b \rangle}{\|a\|_2\|b\|_2} = \frac{1}{2}\left[(\|Sx\|_2^2 - \|x\|_2^2) + (\|Sy\|_2^2 - \|y\|_2^2) - (\|S(x - y)\|_2^2 - \|x - y\|_2^2)\right].$$

For any vector $z \in \mathbb{R}^m$, the proof of Lemma 18 in (Woodruff, 2014) shows that $\|Sz\|_2^2$ is equal in distribution to $\frac{1}{s}\|z\|_2^2\xi$ where $\xi$ is a $\chi^2$ random variable with $s$ degree of freedom. Concentration bound in the proof of Lemma 18 in (Woodruff, 2014) shows that $\xi = (1 \pm \epsilon)s$ with probability at least $1 - 2e^{-s\epsilon^2/16}$.

To bound the error in the approximate matrix product, we need to bound $n_1 + n_2 + n_1n_2$ terms. Applying the union bound, we have for all $i \in [n_1]$ and $j \in [n_2]$

$$\|Sx_i\|_2^2 - \|x_i\|_2^2 \leq \epsilon,$$

$$\|Sy_j\|_2^2 - \|y_j\|_2^2 \leq \epsilon,$$

$$\|S(x_i - y_j)\|_2^2 - \|x_i - y_j\|_2^2 \leq 2\epsilon$$

hold with probability at least

$$1 - 2(n_1 + n_2 + n_1n_2)e^{-s\epsilon^2/16}.$$ 

Setting $s = O(\epsilon^{-2}\log(n_1 + n_2))$ yields that

$$\forall i \in [n_1] \text{ and } j \in [n_2], \quad \frac{\langle Sa_i, Sb_j \rangle - \langle a_i, b_j \rangle}{\|a_i\|_2\|b_j\|_2} \leq \epsilon.$$
with probability at least $1 - \frac{1}{n_1 + n_2}$. Notice that $\langle Sa_i, Sb_j \rangle$ is the $(i, j)$-th entry of $A^T S^T S B$, we thus obtain

$$\|A^T S^T S B - A^T B\|_F^2 = \sum_{i,j} \left( \langle Sa_i, Sb_j \rangle - \langle a_i, b_j \rangle \right)^2 \leq \epsilon^2 \sum_{i,j} \|a_i\|_2^2 \|b_j\|_2^2 = \epsilon^2 \|A\|_F^2 \|B\|_F^2.$$ 

\hspace{1cm} \blacksquare

Appendix G. Proof of Theorem 7

Without loss of generality, we assume that $K$ can be partitioned as in (1). Suppose that $\text{rank}(W) = \text{rank}(K)$. We have that $\text{rank}(W) = \text{rank}(C) = \text{rank}(K)$ because

$$\text{rank}(K) \geq \text{rank}(C) \geq \text{rank}(W). \tag{19}$$

Thus there exists a matrix $X$ such that

$$\begin{bmatrix} K_{21}^T \\ K_{22} \end{bmatrix} = CX^T = \begin{bmatrix} WX^T \\ K_{21}X^T \end{bmatrix},$$

and it follows that $K_{21} = XW$ and $K_{22} = K_{21}X^T = XWX^T$. Then we have that

$$C = \begin{bmatrix} I \\ X \end{bmatrix} W,$$

$$K = \begin{bmatrix} W \\ XW \\ XWX^T \end{bmatrix} = \begin{bmatrix} I \\ X \end{bmatrix} W \begin{bmatrix} I \\ X^T \end{bmatrix} = CW^\dagger C^T. \tag{20}$$

Thus $S^T KS = (S^T C) W^\dagger (C^T S)$. The Sketch-Nyström approximation is

$$\tilde{K}_{c,s}^{sn} = C (S^T C)^\dagger (S^T KS) (C^T S)^\dagger C^T$$

$$= C \underbrace{(S^T C)^\dagger (S^T C)}_{c \times s} \underbrace{W^\dagger}_{s \times c} \underbrace{(C^T S) (C^T S)^\dagger}_{s \times c} C^T$$

$$= CW^\dagger C^T$$

$$= K,$$

where the second equality and the last equality follows from (20), and the third equality follows from that $s \geq c$.

Conversely, when $K = C (S^T C)^\dagger (S^T KS) (C^T S)^\dagger C^T$, we have $\text{rank}(K) \leq \text{rank}(C)$. Thus there exists a matrix $X$ such that

$$\begin{bmatrix} K_{21}^T \\ K_{22} \end{bmatrix} = CX^T = \begin{bmatrix} WX^T \\ K_{21}X^T \end{bmatrix}, $$

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and therefore $K_{21} = XW$. Then we have that
\[
C = \begin{bmatrix} W \\ K_{21} \end{bmatrix} = \begin{bmatrix} I \\ X \end{bmatrix} W,
\]
so $\text{rank}(C) \leq \text{rank}(W)$. Apply (19) again we have $\text{rank}(K) = \text{rank}(W)$.

Appendix H. Proof of Theorem 10

The error incurred by the approximate CUR can be decomposed by Lemma 16, and thus we only need to bound the terms $\sigma_i(S_C^T U_C), \sigma_j(V_R^T S_R), \|I_n S_R S^T_R V_R\|_2, \|U_C^T S_C^T U_C^T (U_C^T)^T A\|_F,$ and $\|AV_R^\perp (V_R^\perp)^T S_R S^T_R V_R\|_F$. These terms can be bounded in exactly the same way as in the proof of Theorem 3. The following three inequalities respectively hold with probability at least 1 $− \delta_1, 1 − \delta_2, 1 − \delta_3$:
\[
\|I_n S_R S^T_R V_R\|_2 \leq 1 + \frac{\sqrt{nr}}{\delta_1 \sqrt{s_r}} = \frac{\sqrt{nr}}{1} (1 + o(1)),
\]
\[
\|U_C^T S_C^T U_C^T (U_C^T)^T A\|_F \leq \frac{\sqrt{c}}{\delta_2 \sqrt{s_c}} \|U_C^T (U_C^T)^T A\|_F,
\]
\[
\|AV_R^\perp (V_R^\perp)^T S_R S^T_R V_R\|_F \leq \frac{\sqrt{r}}{\delta_3 \sqrt{s_r}} \|AV_R^\perp (V_R^\perp)^T\|_F.
\]

Using the same technique as in the proof of Theorem 3, the singular values satisfy $\sigma_i^2(S_C^T U_C) = 1 \pm o(1)$ and $\sigma_j^2(V_R^T S_R) = 1 \pm o(1)$ for all $i \in [c]$ and $j \in [r]$ with probability 0.9.

Define
\[
A^\perp = A − CU^* R = A − CC^T AR^T R.
\]

It follows from Lemma 16 that
\[
\|S_C^T U_C^T S_C^T A^\perp S_R (V_R^T S_R)^T\|_F \\
\leq \|I_n S_R S^T_R V_R\|_2 \|U_C^T S_C^T U_C^T (U_C^T)^T A\|_F + \sigma_{\max}(S_C^T U_C) \|AV_R^\perp (V_R^\perp)^T S_R S^T_R V_R\|_F \\
\leq 2 \frac{\sqrt{nr}}{\delta_1 \sqrt{s_r s_c}} \|U_C^T (U_C^T)^T A\|_F + \frac{\sqrt{r}}{\delta_3 \sqrt{s_r}} \|AV_R^\perp (V_R^\perp)^T\|_F.
\]

Letting $\delta_1 = \delta_2 = \delta_3 = 0.1$ and $s_r = \mathcal{O}(\sqrt{nr} \epsilon^{-1/2})$ and $s_c = \mathcal{O}(\sqrt{nr} \epsilon^{-1/2})$, we obtain that
\[
\|S_C^T U_C^T S_C^T A^\perp S_R (V_R^T S_R)^T\|_F \\
\leq 0.25 \sqrt{\epsilon} \|U_C^T (U_C^T)^T A\|_F + 0.25 (\epsilon/n)^{1/4} \|AV_R^\perp (V_R^\perp)^T\|_F \\
\leq 0.5 \sqrt{\epsilon} \|A^\perp\|_F
\]
holds with probability at least 0.6. Here the last inequality follows from that $\epsilon^{-1} \ll n$ and that $\|A^\perp\|_F$ is greater than both of $\|U_C^T (U_C^T)^T A\|_F$ and $\|AV_R^\perp (V_R^\perp)^T\|_F$.

Finally, it follows from (21), Lemma 16, and the bound on the singular values that
\[
\|A − C\U R\|_F^2 \leq \|A^\perp\|_F^2 + \sigma_{\min}(S_C^T U_C)\sigma_{\min}(V_R^T S_R) \|(S_C^T U_C)^T S_C^T A^\perp S_R (V_R^T S_R)^T\|_F^2 \\
\leq (1 + \epsilon) \|A^\perp\|_F^2 = (1 + \epsilon) \|A − CC^T AR^T R\|_F^2,
\]

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by which the theorem follows.

Applying the same argument on the CUR decomposition $A^T \approx R^T U^T C^T$, the setting $s_r = O(\sqrt{mr}e^{-1/2})$ and $s_c = O(\sqrt{mc}e^{-1/2})$ yields the same bound. Thus $s_r = O(\sqrt{qr}e^{-1/2})$ and $s_c = O(\sqrt{qc}e^{-1/2})$ for $q = \min\{m, n\}$ suffices.

Appendix I. Proof of Theorem 11

We define the projection operation $P_{C,k}(A) = CX$ where $X$ is defined by

$$X = \underset{\text{rank}(X) \leq k}{\arg\min} \|A - CX\|_F^2.$$  

By sampling $c = 2k\epsilon^{-1}(1 + o(1))$ columns of $A$ by the near-optimal algorithm of Boutsidis et al. (2011) to form $C \in \mathbb{R}^{n \times c_1}$, we have that

$$E\|A - P_{C,k}(A)\|_F^2 \leq (1 + \epsilon)\|A - A_k\|_F^2.$$  

Applying Lemma 3.11 of Boutsidis and Woodruff (2014), there exists a much smaller matrix $Z \in \mathbb{R}^{m \times k}$ with orthogonal columns in the column space of $C$ such that

$$\|A - CC^T A\|_F^2 \leq \|A - ZZ^T A\|_F^2 \leq \|A - P_{C,k}(A)\|_F^2.$$  

Notice that the algorithm does not compute $Z$.

Let $R_1^T \in \mathbb{R}^{r \times r_1}$ be columns of $A^T$ selected by the dual-set sparsification algorithm of Boutsidis et al. (2011), $R_2^T \in \mathbb{R}^{r \times r_2}$ be columns of $A^T$ selected by adaptive sampling according to the residual $A^T - R_1^T (R_1^T)^+ A^T$, and $R^T = [R_1^T, R_2^T]$. Equivalently, $R^T$ contains $r = 2k\epsilon^{-1}(1 + o(1))$ columns of $A^T$ selected by the near-optimal column selection algorithm of Boutsidis et al. (2011). By the adaptive sampling theorem of Wang and Zhang (2013) we have

$$E\|A - ZZ^T A\|_F^2 \leq E\|A - ZZ^T A\|_F^2 + \frac{k}{r_2}E\|A - AR^T A^T R^T\|_F^2,$$

$$\leq (1 + \epsilon)\|K - K_k\|_F^2 + \epsilon\|K - K_k\|_F^2$$

$$\leq (1 + 2\epsilon)\|K - K_k\|_F^2. \quad (22)$$  

It remains to show $\|A - CC^T A R^T\|_F^2 \leq \|A - ZZ^T A R^T\|_F^2$. Since the columns of $Z$ are contained in the column space of $C$, for any matrix $Y$ the inequality $\|(I_m - CC^T)Y\|_F^2 \leq \|(I_m - ZZ^T)Y\|_F^2$ holds. Then we obtain

$$\|A - CC^T A R^T\|_F^2 = \|A - AR^T + AR^T R - CC^T A R^T\|_F^2$$

$$= \|A(I_n - R^T R)\|_F^2 + \|(I_m - CC^T)AR^T\|_F^2$$

$$\leq \|A(I_n - R^T R)\|_F^2 + \|(I_m - ZZ^T)AR^T\|_F^2$$

$$= \|A(I_n - R^T R) + (I_m - ZZ^T)AR^T\|_F^2$$

$$= \|A - ZZ^T A R^T\|_F^2. \quad (23)$$  

The theorem follows from (22) and (23).
Appendix J. Proof of Theorem 9

We prove Theorem 9 by constructing an adversarial case. Theorem 9 follows trivially from the following theorem.

**Theorem 23** Let \( A \) be an \( n \times n \) symmetric matrix defined in Lemma 25 with \( \alpha \to 1 \) and \( k \) be any positive integer less than \( n \). Let \( P \) be any subset of \([n]\) with cardinality \( c \) and \( C \in \mathbb{R}^{n \times c} \) contains \( c \) columns of \( A \) indexed by \( P \). Let \( S \) be any \( n \times s \) column selection matrix satisfying \( P \subset S \), where \( S \subset [n] \) is the index set formed by \( S \). Then the following inequality holds:

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

**Proof** Let \( A \) and \( B \) be defined in Lemma 25. We prove the theorem using Lemma 25 and Lemma 27. Let \( n = pk \) and \( C \) consists of \( c_i \) columns sampled from \( A \) and \( \hat{C}_i \) consists of the first \( c_i \) columns of \( B \). Let \( S = \text{diag}(S_1, \cdots, S_k) \) be an \( n \times s \) column selection matrix, where \( S_1 \) is an \( n \times s_i \) column selection matrix and \( s_1 + \cdots + s_k = s \). Without loss generality, we assume that \( S_i \) selects the first \( s_i \) columns. Then in Appendix J, the intersection matrix \( U \) is computed by

\[
U = (S^T C)^T (S^T A S)(C^T S)^T C^T, \\
= [\text{diag}(S_1^T C_1, \cdots, S_k^T C_k)] [\text{diag}(S_1^T B S_1, \cdots, S_k^T B S_k)] [\text{diag}(\hat{C}_1^T \hat{S}_1, \cdots, \hat{C}_k^T \hat{S}_k)]^T \nonumber \\
= \text{diag}\left((S_1^T C_1)^T (S_1^T B S_1)(C_1^T S_1)^T, \cdots, (S_k^T C_k)^T (S_k^T B S_k)(C_k^T S_k)^T\right). \nonumber
\]

The Sketch-Nystrom approximation of \( A \) is a block-diagonal matrix whose the \( i \)-th \((i \in [k])\) diagonal block is the \( p \times p \) matrix

\[
[A_{C,s}^{sn}]_{ii} = \hat{C}_i (S_i^T \hat{C}_i)^T (S_i^T B S_i) (\hat{C}_i^T S_i)^T \hat{C}_i^T.
\]

It follows from Lemma 27 that for any \( i \in [k] \)

\[
\lim_{\alpha \to 1} \frac{\|B - [A_{C,s}^{sn}]_{ii}\|_F^2}{(1 - \alpha)^2} = (p - c_i) \left( 1 + \frac{2}{c_i} \right) + \frac{(p - s_i)^2}{s_i^2},
\]

and thus

\[
\lim_{\alpha \to 1} \frac{\|A - \hat{A}_{C,s}^{sn}\|_F^2}{(1 - \alpha)^2} = \lim_{\alpha \to 1} \sum_{i=1}^k \frac{\|B - [A_{C,s}^{sn}]_{ii}\|_F^2}{(1 - \alpha)^2} \\
= \sum_{i=1}^k (p - c_i) \left( 1 + \frac{2}{c_i} \right) + \frac{(p - s_i)^2}{s_i^2} \\
= \left( \sum_{i=1}^k p - c_i - 2 \right) + \left( 2p \sum_{i=1}^k \frac{1}{c_i} \right) \left( p^2 \sum_{i=1}^k \frac{1}{s_i^2} \right) - \left( 2p \sum_{i=1}^k \frac{1}{s_i} \right) + k \\
\geq n - c - 2k + \frac{2nk}{c} + \frac{kn^2}{s^2} - \left( \frac{2nk}{c} - \frac{2nk}{s} \right) + k \\
= \left( n - c \right) \left( 1 + \frac{2k}{c} \right) + \frac{k(n - s)^2}{s^2}.
\]

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Here the inequality follows by minimizing over \(c_1, \ldots, c_k\) and \(s_1, \ldots, s_k\) with constraints \(\sum_i c_i = c\) and \(\sum_i s_i = s\). Finally, it follows from Lemma 25 that
\[
\lim_{\alpha \to 1} \frac{\|A - \tilde{A}_s\|_F^{2}}{\|A - A_k\|_F^{2}} \geq \frac{n - c}{n - k} \left(1 + \frac{2k}{c}\right) + \frac{n - s \cdot k(n - s)}{n - k - s^2}.
\]

\[\blacksquare\]

J.1 Key Lemmas

Lemma 24 provides a useful tool for expanding the Moore-Penrose inverse of partitioned matrices.

**Lemma 24 (Page 179 of Ben-Israel and Greville (2003))** Given a matrix \(X \in \mathbb{R}^{m \times n}\) of rank \(c\) which has a nonsingular \(c \times c\) submatrix \(X_{11}\). By rearrangement of columns and rows by permutation matrices \(P\) and \(Q\), the submatrix \(X_{11}\) can be bought to the top left corner of \(X\), that is,
\[
PXQ = \begin{bmatrix}
X_{11} & X_{12} \\
X_{21} & X_{22}
\end{bmatrix}.
\]

Then the Moore-Penrose inverse of \(X\) is
\[
X^\dagger = Q \left[ I_c \atop T^T \right] \left( I_c + TT^T \right)^{-1} X_{11}^{-1} \left( I_c + H^T H \right)^{-1} \begin{bmatrix} I_c & H^T \end{bmatrix} P,
\]
where \(T = X_{11}^{-1} X_{12}\) and \(H = X_{21} X_{11}^{-1}\).

Lemmas 25 and 27 will be used to prove Theorem 23.

**Lemma 25 (Lemma 19 of Wang and Zhang (2013))** Given \(n\) and \(k\), we let \(B\) be an \(\frac{n}{k} \times \frac{n}{k}\) matrix whose diagonal entries equal to one and off-diagonal entries equal to \(\alpha \in [0, 1)\). We let \(A\) be an \(n \times n\) block-diagonal matrix
\[
A = \text{diag}(B, \ldots, B).
\]

Let \(A_k\) be the best rank-\(k\) approximation to the matrix \(A\), then we have that
\[
\|A - A_k\|_F^2 = (1 - \alpha)^2(n - k).
\]

**Lemma 26** The following equality holds for any nonzero real number \(a\):\[
(aI_c + b1_c1_T^T)^{-1} = a^{-1}I_c - \frac{b}{a(a + bc)}1_c1^T_c.
\]

**Proof** We apply the Sherman-Morrison-Woodbury matrix identity
\[
(X + YZR)^{-1} = X^{-1} - X^{-1}Y(Z^{-1} + RX^{-1}Y)^{-1}RX^{-1}
\]
to expand the left-hand side and directly obtain the right-hand side. \[\blacksquare\]
Lemma 27 For an $n \times n$ matrix $B$ with diagonal entries equal to one and off-diagonal entries equal to $\alpha$, let $\tilde{B}$ be the Sketch-Nyström approximation of $B$. Let $R$ and $S$ be the index sets formed by $R$ and $S$, respectively. When $R \subset S$, the error incurred by the Sketch-Nyström method satisfies
\[
\lim_{\alpha \to 1} \frac{\|B - \tilde{B}\|_F^2}{(1 - \alpha)^2} \geq (n - c)(1 + \frac{2}{c}) + \frac{(n - s)^2}{s^2}.
\]

Proof We let $C = BR \in \mathbb{R}^{n \times c}$, $B_1 = S^TBS \in \mathbb{R}^{s \times s}$, and $C_1 = S^TC = S^TBR \in \mathbb{R}^{s \times c}$. Without loss of generality, we assume that $R$ selects the first $c$ columns and $S$ selects the first $s$ columns. We partition $B$ and $C$ by:
\[
B = \begin{bmatrix} B_1 & B_3 \\ B_3^T & B_2 \end{bmatrix} \quad \text{and} \quad C = \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = \begin{bmatrix} W \\ C_{12} \\ C_2 \end{bmatrix}.
\]
We further partition $B_1 \in \mathbb{R}^{s \times s}$ by
\[
B_1 = \begin{bmatrix} W & C_{12} \\ C_{12}^T & B_{12} \end{bmatrix},
\]
where
\[
C_{12} = \alpha \mathbf{1}_{s-c} \mathbf{1}_c^T \quad \text{and} \quad B_{12} = (1 - \alpha) \mathbf{1}_{s-c} + \alpha \mathbf{1}_{s-c} \mathbf{1}_c^T.
\]
The intersection matrix is computed by
\[
U = (S^TC)^\dagger(S^TBS)(C^TS)^\dagger = C_1^\dagger B_1 (C_1^\dagger)^T
\]
It is not hard to see that $C_1$ contains the first $c$ rows of $B_1$.
We expand the Moore-Penrose inverse of $C_1$ by Lemma 24 and obtain
\[
C_1^\dagger = W^{-1}(I_c + H^TH)^{-1} \begin{bmatrix} I_c & H^T \end{bmatrix},
\]
where
\[
W^{-1} = \left((1 - \alpha)I_c + \alpha \mathbf{1}_c \mathbf{1}_c^T\right)^{-1} = \frac{1}{1 - \alpha} I_c - \frac{\alpha}{(1 - \alpha)(1 - \alpha + c\alpha)} \mathbf{1}_c \mathbf{1}_c^T
\]
and
\[
H = C_{12} W^{-1} = \frac{\alpha}{1 - \alpha + c\alpha} \mathbf{1}_{s-c} \mathbf{1}_c^T.
\]
It is easily verified that $H^TH = \left(\frac{\alpha}{1 - \alpha + c\alpha}\right)^2 (s - c) \mathbf{1}_c \mathbf{1}_c^T$, and thus it follows from Lemma 26 that
\[
(I_c + H^TH)^{-1} = I_c - \frac{(s - c)\alpha^2}{c(s - c)\alpha^2 + (1 - \alpha + c\alpha)^2} \mathbf{1}_c \mathbf{1}_c^T.
\]
Then we obtain
\[
C_1^\dagger = W^{-1}(I_c + H^TH)^{-1} \begin{bmatrix} I_c & H^T \end{bmatrix} = \left(\frac{1}{1 - \alpha} I_c + \gamma \mathbf{1}_c \mathbf{1}_c^T\right) \begin{bmatrix} I_c & H^T \end{bmatrix},
\]
(25)
where
\[
\gamma_1 = c\gamma_2 \gamma_3 - \gamma_2 \frac{\gamma_3}{1 - \alpha},
\]
\[
\gamma_2 = (1 - \alpha)(1 - \alpha + \alpha^2),
\]
\[
\gamma_3 = \frac{(s - c)\alpha^2}{c(s - c)\alpha^2 + (1 - \alpha + \alpha^2)^2}.
\]

Then
\[
[I_c, H^T]B_1[I_c, H^T]^T = W + B_{13}^T H + H^T B_{13} + H^T B_{12} H
= (1 - \alpha)I_c + \gamma_4 1_c 1_c^T, \tag{26}
\]
where
\[
\gamma_4 = \alpha (3as - \alpha c - 2\alpha + \alpha^2 c - 3\alpha^2 s + \alpha^2 + \alpha^2 s^2 + 1)
/ (\alpha c - \alpha + 1)^2.
\]

It follows from (25) (26) that
\[
U = C_1^T B_1 (C_1^T) = \left( \frac{1}{1 - \alpha} I_c + \gamma_1 1_c 1_c^T \right) \left( (1 - \alpha)I_c + \gamma_4 1_c 1_c^T \right) \left( \frac{1}{1 - \alpha} I_c + \gamma_1 1_c 1_c^T \right)
= \frac{1}{1 - \alpha} I_c + \gamma_5 1_c 1_c^T,
\]
where
\[
\gamma_5 = \gamma_1 + \left( c\gamma_1 + \frac{1}{1 - \alpha} \right) \left( c\gamma_1 \gamma_4 + \gamma_1 (1 - \alpha) + \frac{\gamma_4}{1 - \alpha} \right).
\]

Then we have
\[
WU = I_c + \gamma_6 1_c 1_c^T,
\]
\[
\gamma_6 = (1 - \alpha + \alpha c)\gamma_5 + \frac{\alpha}{1 - \alpha}.
\]

We partition the Sketch-Nyström approximation by
\[
\tilde{B} = \begin{bmatrix}
\tilde{W} \\
\tilde{B}_{21} \\
\tilde{B}_{22}
\end{bmatrix},
\]
where
\[
\tilde{B}_{11} = WUW = (1 - \alpha)I_c + (\alpha + (1 - \alpha + \alpha c)\gamma_6)1_c 1_c^T,
\]
\[
\tilde{B}_{21} = WU(\alpha 1_c 1_{n-c}^T) = \alpha(1 + c\gamma_6)1_c 1_{n-c}^T,
\]
\[
\tilde{B}_{22} = (\alpha 1_{n-c} 1_c^T)U(\alpha 1_c 1_{n-c}^T) = \alpha^2 c \left( \frac{1}{1 - \alpha} + \gamma_5 c \right)1_c 1_{n-c}^T.
\]

The approximate error is
\[
\|B - \tilde{B}\|_F^2 = \|W - \tilde{W}\|_F^2 + 2\|B_{21} - \tilde{B}_{21}\|_F^2 + \|B_{22} - \tilde{B}_{22}\|_F^2.
\]
where

\[
\|W - \tilde{W}\|_F^2 = \|(1 - \alpha + \alpha c)\gamma_6 1_c 1_c^T\|_F^2 = c^2(1 - \alpha + \alpha c)^2 \gamma_6^2,
\]

\[
\|B_{21} - \tilde{B}_{21}\|_F^2 = \|\alpha c_6 1_c 1_{n-c}\|_F^2 = \alpha^2 c^3(n - c)\gamma_6^2,
\]

\[
\|B_{22} - \tilde{B}_{22}\|_F^2 = (n - c)(n - c - 1)\alpha^2\left(\frac{\alpha c}{1 - \alpha} + \alpha c^2\gamma_5 - 1\right)^2 + (n - c)\left(\frac{\alpha^2 c}{1 - \alpha} + \alpha^2 c^2\gamma_5 - 1\right)^2.
\]

We let

\[
\eta \triangleq \frac{\|B - \tilde{B}\|_F^2}{(1 - \alpha)^2},
\]

which is a symbolic expression of \(\alpha, n, s,\) and \(c.\) We then simplify the expression using MATLAB and substitute the \(\alpha\) in \(\eta\) by 1, and we obtain

\[
\lim_{\alpha \to 1} \eta = (n - c)(1 + 2/c) + (n - s)^2/s^2,
\]

by which the lemma follows.

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