On the Nyström Method for Approximating a Gram Matrix for Improved Kernel-Based Learning *

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Abstract

A problem for many kernel-based methods is that the amount of computation required to find the solution scales as $O(n^3)$, where n is the number of training examples. We develop and analyze an algorithm to compute an easily-interpretable low-rank approximation to an $n \times n$ Gram matrix G such that computations of interest may be performed more rapidly. The approximation is of the form $\tilde{G}_k = CW_k^+C^T$, where C is a matrix consisting of a small number c of columns of G and W_k is the best rank-k approximation to W, the matrix formed by the intersection between those c columns of G and the corresponding c rows of G. An important aspect of the algorithm is the probability distribution used to randomly sample the columns; we will use a judiciously-chosen and data-dependent nonuniform probability distribution. Let $\|\cdot\|_2$ and $\|\cdot\|_F$ denote the spectral norm and the Frobenius norm, respectively, of a matrix, and let G_k be the best rank-k approximation to G. We prove that by choosing $O(k/\epsilon^4)$ columns

$$\left\|G - CW_k^+C^T\right\|_\xi \leq \|G - G_k\|_\xi + \epsilon \sum_{i=1}^{n} G_{ii}^2,$$

both in expectation and with high probability, for both $\xi = 2, F$, and for all $k : 0 \leq k \leq \mathrm{rank}(W)$. This approximation can be computed using $O(n)$ additional space and time, after making two passes over the data from external storage. The relationships between this algorithm, other related matrix decompositions, and the Nyström method from integral equation theory are discussed.

1 Introduction

1.1 Background

Given a collection $\mathcal{X}$ of data points, which are often but not necessarily elements of $\mathbb{R}^m$, techniques such as linear Support Vector Machines (SVMs), Gaussian Processes (GPs), Principle Component Analysis (PCA), and the related Singular Value Decomposition (SVD), identify and extract structure from $\mathcal{X}$ by computing linear functions, i.e., functions in the form of dot products, of the data. For example, in PCA the subspace spanned by the first k eigenvectors is used to give a k dimensional model of the data with minimal residual; thus, it provides a low-dimensional representation of the data. Such spectral analysis has a rich theoretical foundation and has numerous practical applications.

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In many cases, however, there is nonlinear structure in the data (or the data, e.g. text, may not support the basic linear operations of addition and scalar multiplication). In these cases, kernel-based learning methods have proved to be quite useful [9, 33]. Kernel-based learning methods are a class of statistical learning algorithms, the best known examples of which are SVMs [9]. In this approach, data items are mapped into high-dimensional spaces, where information about their mutual positions (in the form of inner products) is used for constructing classification, regression, or clustering rules. Kernel-based algorithms exploit the information encoded in the inner product between all pairs of data items and are successful in part because there is often an efficient method to compute inner products between very complex or even infinite dimensional vectors. Thus, kernel-based algorithms provide a way to deal with nonlinear structure by reducing nonlinear algorithms to algorithms that are linear in some feature space $\mathcal{F}$ that is nonlinearly related to the original input space.

More precisely, assume that the data consists of vectors $X^{(1)}, \ldots, X^{(n)} \in \mathcal{X} \subset \mathbb{R}^m$ and let $X \in \mathbb{R}^{m \times n}$ be the matrix whose i-th column is $X^{(i)}$. In kernel-based methods, a set of features is chosen that define a space $\mathcal{F}$, where it is hoped relevant structure will be revealed, the data $\mathcal{X}$ are then mapped to the feature space $\mathcal{F}$ using a mapping $\Phi : \mathcal{X} \to \mathcal{F}$, and then classification, regression, or clustering is performed in $\mathcal{F}$ using traditional methods such as linear SVMs, GPs, or PCA. If $\mathcal{F}$ is chosen to be a dot product space and if one defines the kernel matrix, also known as the Gram matrix, $G \in \mathbb{R}^{n \times n}$ as $G_{ij} = k(x_i, x_j) = (\Phi(x_i), \Phi(x_j))$, then any algorithm whose operations can be expressed in the input space in terms of dot products can be generalized to an algorithm which operates in the feature space by substituting a kernel function for the inner product. In practice, this means presenting the Gram matrix G in place of the input covariance matrix $X^T X$. Relatedly, using the kernel k instead of a dot product in the input space corresponds to mapping the data set into a (usually) high-dimensional dot product space $\mathcal{F}$ by a (usually nonlinear) mapping $\Phi : \mathbb{R}^m \to \mathcal{F}$, and taking dot products there, i.e., $k(x_i, x_j) = (\Phi(x_i), \Phi(x_j))$. Note that for the commonly-used Mercer kernels, G is a symmetric positive semidefinite (SPSD) matrix.

The generality of this framework should be emphasized. For example, there has been much work recently on dimensionality reduction for nonlinear manifolds in high-dimensional spaces. See, e.g., Isomap, local linear embedding, and graph Laplacian eigenmap [36, 32, 4] as well as Hessian eigenmaps and semidefinite embedding [11, 37]. These methods first induce a local neighborhood structure on the data and then use this local structure to find a global embedding of the manifold in a lower dimensional space. The manner in which these different algorithms use the local information to construct the global embedding is quite different, but in [26] they are interpreted as kernel PCA applied to specially constructed Gram matrices.

This "kernel trick" has been quite successful for extracting nonlinear structure in large data sets when the features are chosen such that the structure in the data is more manifest in the feature space than in the original space. Although in many cases the features are chosen such that the Gram matrix is sparse, in which case sparse matrix computation methods may be used, in other applications the Gram matrix is dense, but is well approximated by a low-rank matrix. In this case, calculations of interest (such as the matrix inversion needed in GP prediction, the quadratic programming problem for SVMs, and the computation of the eigendecomposition of the Gram matrix) will still generally take space which is $O(n^2)$ and time which is $O(n^3)$. This is prohibitive if n, the number of data points, is large. Recent work in the learning theory community has focused on taking advantage of this low-rank structure in order to perform learning tasks of interest more efficiently. For example, in [2], several randomized methods are used in order to speed up kernel PCA. These methods have provable guarantees on the quality of their approximation and may be viewed as replacing the kernel function k by a "randomized kernel" which behaves like k in expectation. Relatedly, in [40], uniform sampling without replacement is used to choose a small

set of basis training points, from which an approximation to the Gram matrix is constructed. Although this algorithm does not come with provable performance guarantees, it may be viewed as a special case of our main algorithm, and it was shown empirically to perform well on two data sets for approximate GP classification and regression. It was also interpreted in terms of the Nyström method from integral equation theory; this method has also been applied recently in the learning theory community to approximate the solution of spectral partitioning for image and video segmentation [21] and to extend the eigenfunctions of a data-dependent kernel to new data points [6, 28]. Related work taking advantage of low-rank structure includes [34, 20, 39, 8, 30, 38, 3].

1.2 Summary of Main Result

In this paper, we develop and analyze an algorithm to compute an easily-interpretable low-rank approximation to an $n \times n$ Gram matrix G. Our main result, the MAIN APPROXIMATION algorithm of Section 4.2, is an algorithm that, when given as input a SPSD matrix $G \in \mathbb{R}^{n \times n}$, computes a low-rank approximation to G of the form $\tilde{G}_k = CW_k^+C^T$, where $C \in \mathbb{R}^{n \times c}$ is a matrix formed by randomly choosing a small number c of columns (and thus rows) of G and $W_k \in \mathbb{R}^{c \times c}$ is the best rank-k approximation to W, the matrix formed by the intersection between those c columns of G and the corresponding c rows of G. The columns are chosen in c independent random trials (and thus with replacement) according to a judiciously-chosen and data-dependent nonuniform probability distribution. The nonuniform probability distribution will be carefully chosen and will be important for the provable bounds we obtain. Let $\|\cdot\|_2$ and $\|\cdot\|_F$ denote the spectral norm and the Frobenius norm, respectively, and let G_k be the best rank-k approximation to G. Our main result, presented in a more precise form in Theorem 3, is that under appropriate assumptions:

$$\left\|G - CW_k^+C^T\right\|_\xi \leq \|G - G_k\|_\xi + \epsilon \sum_{i=1}^{n} G_{ii}^2, \tag{1}$$

in both expectation and with high probability, for both $\xi = 2, F$, for all $k : 0 \leq k \leq \text{rank}(W)$. This approximation can be computed in $O(n)$ space and time after two passes over the data from external storage.

In addition to developing and analyzing an algorithm which provides a provably good decomposition of a Gram matrix, which may then be used to speed up kernel-based learning methods, this paper makes several contributions. First, it extends related work of Williams and Seeger [40] involving uniform sampling to a more natural general case and provides a discussion of when that is necessary. Second, it provides rigorous proofs of sufficient conditions for the methods to be applicable for any data set and discusses when other conditions may be more appropriate. Third, it clarifies several potential misconceptions that have appeared in the literature regarding the relationship between recent work on Nyström-based kernel methods [40, 38, 21] and the low-rank approximation algorithm of Frieze, Kannan, and Vempala [22, 16]. Finally, it extends random sampling methodology of the authors to a new application domain and it extends the ability of those methods from simply extracting linear structure of the data to extracting linear structure while respecting nonlinear structures such as the SPSD property.

1.3 Outline of the Paper

After this introduction, in Section 2 we provide a review of relevant linear algebra. Then, in Section 3 we review several aspects of our random sampling methodology of [15, 16, 17] that will be useful for the proofs in this paper; see also [18, 19]. In Section 4 we present our main algorithm and our main theorem, providing a brief discussion of the algorithm and a proof of the theorem.

Then, in Section 5 we discuss in detail several aspects of the algorithm and its relationship to previous work, with a particular emphasis on the relationships between our main algorithm, the Nyström method of [40, 38, 21], and our previous randomized SVD and CUR algorithms [16, 17]. Finally, in Section 6 we provide a brief conclusion.

2 Review of Relevant Linear Algebra

This section contains a review of linear algebra that will be useful throughout the paper. For more details about general linear algebra, see [23, 27, 7]; for more details about matrix perturbation theory, see [35]; and for more details about generalized inverses, see [29, 5].

For a vector $x \in \mathbb{R}^n$ we let $|x| = \left(\sum_{i=1}^n |x_i|^2\right)^{1/2}$ denote its Euclidean length. For a matrix $A \in \mathbb{R}^{m \times n}$ we let $A^{(j)}$, $j = 1, \ldots, n$, denote the j-th column of A as a column vector and $A_{(i)}$, $i = 1, \ldots, m$, denote the i-th row of A as a row vector. We denote matrix norms by $\|A\|_\xi$, using subscripts to distinguish between various norms. Of particular interest will be the Frobenius norm, the square of which is $\|A\|_F^2 = \sum_{i=1}^m \sum_{j=1}^n A_{ij}^2$, and the spectral norm, which is defined by $\|A\|_2 = \sup_{x \in \mathbb{R}^n,\ x \neq 0} \frac{|Ax|}{|x|}$. These norms are related to each other as: $\|A\|_2 \leq \|A\|_F \leq \sqrt{n}\,\|A\|_2$. If $A \in \mathbb{R}^{m \times n}$, then there exist orthogonal matrices $U = [u^1 u^2 \ldots u^m] \in \mathbb{R}^{m \times m}$ and $V = [v^1 v^2 \ldots v^n] \in \mathbb{R}^{n \times n}$ where $\left\{u^t\right\}_{t=1}^m \in \mathbb{R}^m$ and $\left\{v^t\right\}_{t=1}^n \in \mathbb{R}^n$ are such that

$$U^T A V = \Sigma = \mathbf{diag}(\sigma_1, \ldots, \sigma_\rho),$$

where $\Sigma \in \mathbb{R}^{m \times n}$, $\rho = \min\{m, n\}$ and $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_\rho \geq 0$. Equivalently, $A = U \Sigma V^T$. The three matrices U, V, and Σ constitute the Singular Value Decomposition (SVD) of A. If $k \leq r = \mathrm{rank}(A)$ and we define $A_k = U_k \Sigma_k V_k^T = \sum_{t=1}^k \sigma_t u^t v^{tT}$ then the distance (as measured by both $\|\cdot\|_2$ and $\|\cdot\|_F$) between A and any rank k approximation to A is minimized by A_k. An $n \times n$ matrix A is a symmetric positive semidefinite (SPSD) matrix if A is symmetric and $x^T A x \geq 0$ for all nonzero vectors x. If A is a SPSD matrix, then its SVD may be written $A = U \Sigma U^T$.

From the perturbation theory of matrices it is known that the size of the difference between two matrices can be used to bound the difference between the singular value spectrum of the two matrices [35, 7]. In particular, if $A, E \in \mathbb{R}^{m \times n}, m \geq n$, then:

$$\max_{t:1 \leq t \leq n} |\sigma_t(A + E) - \sigma_t(A)| \leq \|E\|_2 \tag{2}$$

and

$$\sum_{k=1}^n (\sigma_k(A + E) - \sigma_k(A))^2 \leq \|E\|_F^2 . \tag{3}$$

The latter inequality is known as the Hoffman-Wielandt inequality.

Let $A \in \mathbb{R}^{m \times n}$, let $W \in \mathbb{R}^{m \times m}$ and $Q \in \mathbb{R}^{n \times n}$ be symmetric positive definite matrices, and consider the following generalization of the four Moore-Penrose conditions:

$$\begin{aligned} AXA &= A & (4)\\ XAX &= X & (5)\\ (WAX)^T &= WAX & (6)\\ (QXA)^T &= QXA & (7) \end{aligned}$$

The unique X that satisfies these four conditions is denoted $X = A_{(W,Q)}^{(1,2)} = A_{(W,Q)}^+$ and is the $\{W, Q\}$-weighted-$\{1, 2\}$-generalized inverse of A. It can be expressed in terms of the unweighted

generalized inverse of A as: $A^+_{(W,Q)} = Q^{-1/2} \left(W^{1/2} A Q^{-1/2}\right)^+ W^{1/2}$. Note that if $W = I_m$ and $Q = I_n$ then the unique $X \in \mathbb{R}^{n \times n}$ satisfying these four conditions is the Moore-Penrose generalized inverse A^+. If $r = \mathrm{rank}(A)$, then in terms of the SVD the generalized inverse takes the following form: $A^+ = V \Sigma^{-1} U^T = \sum_{t=1}^{r} \sigma_t^{-1} v^t u^{tT}$.

3 Review of Our Random Sampling Methodology

Recent work in the theory of randomized algorithms has focused on matrix problems [22, 12, 1, 2, 13, 14, 15, 16, 17, 18, 19, 31]. In particular, our previous work has applied random sampling methods to the approximation of several common matrix computations such as matrix multiplication [15], the computation of low-rank approximations to a matrix [16], the computation of the CUR matrix decomposition [17], and approximating the feasibility of linear programs [18, 19]. In this section, we review two results that will be used in this paper.

3.1 Review of Approximate Matrix Multiplication

The BasicMatrixMultiplication algorithm to approximate the product of two matrices is presented and analyzed in [15]. When this algorithm is given as input a matrix, $A \in \mathbb{R}^{m \times n}$, a probability distribution $\{p_i\}_{i=1}^n$, and a number $c \leq n$, it returns as output a matrix $C \in \mathbb{R}^{m \times c}$ (such that $CC^T \approx AA^T$) whose columns are c randomly-chosen and suitably-rescaled columns of A. An important aspect of this algorithm is the probability distribution $\{p_i\}_{i=1}^n$ used to choose columns of A. Although one could always use a uniform distribution to choose the columns to form the matrix C, superior results are obtained if the probabilities are chosen judiciously. Sampling probabilities of the form (8), that depend on the lengths squared of the columns of A, are the *optimal sampling probabilities* for approximating AA^T by CC^T, in a sense made precise in [15]. Note that if these probabilities are relaxed such that $p_k \geq \beta \left|A^{(k)}\right|^2 / \|A\|_F^2$ for some positive $\beta \leq 1$, then bounds similar to those in the following theorem will be obtained, with a small β-dependent loss in accuracy. Note also that although we studied random sampling with replacement for ease of analysis, it is not known how to compute efficiently optimal nonuniform sampling probabilities when the sampling is performed without replacement. In [15] we prove a more general version of the following theorem.

Theorem 1 *Suppose $A \in \mathbb{R}^{m \times n}$, $c \in \mathbb{Z}^+$ such that $1 \leq c \leq n$, and $\{p_i\}_{i=1}^n$ are such that*

$$p_k = \frac{\left|A^{(k)}\right|^2}{\|A\|_F^2}. \tag{8}$$

Construct C with the BasicMatrixMultiplication *algorithm of [15], and let CC^T be an approximation to AA^T. Then,*

$$\mathbf{E}\left[\left\|AA^T - CC^T\right\|_F\right] \leq \frac{1}{\sqrt{c}} \|A\|_F^2 . \tag{9}$$

Furthermore, let $\delta \in (0,1)$ and $\eta = 1 + \sqrt{8 \log(1/\delta)}$. Then, with probability at least $1 - \delta$,

$$\left\|AA^T - CC^T\right\|_F \leq \frac{\eta}{\sqrt{c}} \|A\|_F^2 . \tag{10}$$

3.2 Review of Approximate Singular Value Decomposition

The LINEARTIMESVD algorithm is presented in [16]. It is an algorithm which, when given a matrix $A \in \mathbb{R}^{m \times n}$, uses $O(m+n)$ additional space and time to compute an approximation to the top k singular values and the corresponding left singular vectors of A. It does so by randomly choosing c columns of A and rescaling each appropriately to construct a matrix $C \in \mathbb{R}^{m \times c}$, computing the top k singular values and corresponding right singular vectors of C by performing an eigendecomposition of $C^T C$, and using this information to construct a matrix $H_k \in \mathbb{R}^{m \times k}$ consisting of approximations to the top k left singular vectors of A. A minor modification of the result from [16] yields the following theorem in which the additional error is stated with respect to the best rank k approximation for any $k \leq \text{rank}(C)$. This theorem holds for any set of sampling probabilities, but the best bounds are obtained when probabilities of the form (8) are used, in which case Theorem 2 may be combined with Theorem 1.

Theorem 2 *Suppose $A \in \mathbb{R}^{m \times n}$ and let H_k be the $m \times k$ matrix whose columns consist of the top k singular vectors of the $m \times c$ matrix C, as constructed from the* LINEARTIMESVD *algorithm of [16]. Then, for every $k : 0 \leq k \leq rank(C)$,*

$$\left\|A - H_k H_k^T A\right\|_F^2 \leq \|A - A_k\|_F^2 + 2\sqrt{k}\left\|AA^T - CC^T\right\|_F \tag{11}$$

$$\left\|A - H_k H_k^T A\right\|_2^2 \leq \|A - A_k\|_2^2 + 2\left\|AA^T - CC^T\right\|_2. \tag{12}$$

In addition, if $k = r = rank(C)$ then,

$$\left\|A - H_r H_r^T A\right\|_2^2 \leq \left\|AA^T - CC^T\right\|_2. \tag{13}$$

4 Approximating a Gram Matrix

Consider a set of n points in $\mathbb{R}^m$, denoted by $X^{(1)}, \ldots, X^{(n)}$, and let X be the $m \times n$ matrix whose i-th column is $X^{(i)}$. These points may be either the original data or the data after they have been mapped into the feature space. Then, define the $n \times n$ Gram matrix G as $G = X^T X$. Thus, G is a SPSD matrix and $G_{ij} = (X^{(i)}, X^{(j)})$ is the dot product between the data vectors $X^{(i)}$ and $X^{(j)}$. If G is dense but has good linear structure, i.e., is well-approximated by a low-rank matrix, then a computation of a easily-computable and easily-interpretable low-rank approximation to G, with provable error bounds, is of interest.

In this section, two algorithms are presented that compute such an approximation to a Gram matrix G. In Section 4.1, a preliminary algorithm is presented; it is a modification of an algorithm in the literature and is a special case of our main algorithm. Then, in Section 4.2, our main algorithm and our main theorem are presented. Finally, in Section 4.3, the proof of our main theorem is presented.

4.1 A Preliminary Nyström-Based Algorithm

In [40], a method to approximate G was proposed that, in our notation, chooses c columns from G uniformly at random and without replacement, and constructs an approximation of the form $\tilde{G} = CW^{-1}C^T$, where the $n \times c$ matrix C consists of the c chosen columns and W is a matrix consisting of the intersection of those c columns with the corresponding c rows. Analysis of this algorithm and issues such as the existence of the inverse were not addressed in [40], but computational experiments were performed and the procedure was shown to work well empirically on two data sets [40]. This method has been referred to as the Nyström method [40, 38, 21] since

it has an interpretation in terms of the Nyström technique for solving linear integral equations [10]. See Section 5 for a full discussion.

In Algorithm 1, the PRELIMINARY APPROXIMATION algorithm is presented. It is an algorithm that takes as input an $n \times n$ Gram matrix G and returns as output an approximate decomposition of the form $\tilde{G} = CW^+C^T$, where C and W are as in [40], and where W^+ is the Moore-Penrose generalized inverse of W. The c columns are chosen uniformly at random and with replacement. Thus, the PRELIMINARY APPROXIMATION algorithm is quite similar to the algorithm of [40], except that we sample with replacement and that we do not assume the existence of W^{-1}. Rather than analyzing this algorithm (which could be done by combining the analysis of Section 4.3 with the uniform sampling bounds of [15]), we present and analyze a more general form of it, for which we can obtain improved bounds, in Section 4.2. Note, however, that if the uniform sampling probabilities are nearly optimal, in the sense that $1/n \geq \beta G_{ii}^2 / \sum_{i=1}^n G_{ii}^2$ for some positive $\beta \leq 1$ and for every $i = 1, \ldots, n$, then bounds similar to those in Theorem 3 will be obtained for this algorithm, with a small β-dependent loss in accuracy.

Data : $n \times n$ Gram matrix G and $c \leq n$.
Result : $n \times n$ matrix $\tilde{G}$.
• Pick c columns of G in i.i.d. trials, uniformly at random with replacement; let $\mathcal{I}$ be the set of indices of the sampled columns.
• Let C be the $n \times c$ matrix containing the sampled columns.
• Let W be the $c \times c$ submatrix of G whose entries are $G_{ij}, i \in \mathcal{I}, j \in \mathcal{I}$.
• Return $\tilde{G} = CW^+C^T$.

Algorithm 1: The PRELIMINARY APPROXIMATION algorithm.

4.2 The Main Algorithm and the Main Theorem

In [15, 16, 17, 18, 19], we showed the importance of sampling columns and/or rows of a matrix with carefully chosen nonuniform probability distributions in order to obtain provable error bounds for a variety of common matrix operations. In Algorithm 2, the MAIN APPROXIMATION algorithm is presented. It is a generalization of the PRELIMINARY APPROXIMATION algorithm that allows the column sample to be formed using arbitrary sampling probabilities. The MAIN APPROXIMATION algorithm takes as input an $n \times n$ Gram matrix G, a probability distribution $\{p_i\}_{i=1}^n$, a number $c \leq n$ of columns to choose, and a rank parameter $k \leq c$. It returns as output an approximate decomposition of the form $\tilde{G}_k = CW_k^+C^T$, where C is an $n \times c$ matrix consisting of the chosen columns of G, each rescaled in an appropriate manner, and where W_k is a $c \times c$ matrix that is the best rank-k approximation to the matrix W, which is a matrix whose elements consist of those elements in G in the intersection of the chosen columns and the corresponding rows, each rescaled in an appropriate manner.

To implement this algorithm, two passes over the Gram matrix G from external storage and $O(n)$, i.e. sublinear in $O(n^2)$, additional space and time are sufficient (assuming that the sampling probabilities of the form, e.g., $p_i = G_{ii}^2 / \sum_{i=1}^n G_{ii}^2$ or $p_i = \left|G^{(i)}\right|^2 / \|G\|_F^2$ or $p_i = 1/n$ are used). Thus, this algorithm is efficient within the framework of the Pass-Efficient model; see [15] for more details. Note that if the sampling probabilities of the form $p_i = G_{ii}^2 / \sum_{i=1}^n G_{ii}^2$ are used, as in Theorem 3 below, then one may store the $m \times n$ data matrix X in external storage, in which case only those elements of G that are used in the approximation need to be computed.

In the simplest application of this algorithm, one could choose $k = c$, in which case $W_k = W$,

Data : $n \times n$ Gram matrix G, $\{p_i\}_{i=1}^n$ such that $\sum_{i=1}^n p_i = 1$, $c \leq n$, and $k \leq c$.

Result : $n \times n$ matrix $\tilde{G}$.

- Pick c columns of G in i.i.d. trials, with replacement and with respect to the probabilities $\{p_i\}_{i=1}^n$; let $\mathcal{I}$ be the set of indices of the sampled columns.
- Scale each sampled column (whose index is $i \in \mathcal{I}$) by dividing its elements by $\sqrt{cp_i}$; let C be the $n \times c$ matrix containing the sampled columns rescaled in this manner.
- Let W be the $c \times c$ submatrix of G whose entries are $G_{ij}/(c\sqrt{p_i p_j}), i \in \mathcal{I}, j \in \mathcal{I}$.
- Compute W_k, the best rank-k approximation to W.
- Return $\tilde{G}_k = CW_k^+ C^T$.

Algorithm 2: The MAIN APPROXIMATION algorithm.

and the decomposition is of the form $\tilde{G} = CW^+C^T$, where W^+ is the exact Moore-Penrose generalized inverse of the matrix W. In certain cases, however, computing the generalized inverse may be problematic since, e.g., it may amplify noise present in the low singular values. Note that, as a function of increasing k, the Frobenius norm bound (11) of Theorem 2 is not necessarily optimal for $k = \text{rank}(C)$. Also, although the bounds of Theorem 3 for the spectral norm for $k \leq \text{rank}(W)$ are in general worse than those for $k = \text{rank}(W)$, the former are of interest since our algorithms hold for any input Gram matrix and we make no assumptions about a model for the noise in the data.

The sampling matrix formalism of [15] is used in the proofs of Theorem 3 in Section 4.3, and thus we introduce it here. Let us define the sampling matrix $S \in \mathbb{R}^{n \times c}$ to be the zero-one matrix where $S_{ij} = 1$ if the i-th column of A is chosen in the j-th independent random trial and $S_{ij} = 0$ otherwise. Similarly, define the rescaling matrix $D \in \mathbb{R}^{c \times c}$ to be the diagonal matrix with $D_{tt} = 1/\sqrt{cp_{i_t}}$. Then, the $n \times c$ matrix

$$C = GSD$$

consists of the chosen columns of G, each of which has been rescaled by $1/\sqrt{cp_{i_t}}$, where i_t is the label of the column chosen in the t-th independent trial. Similarly, the $c \times c$ matrix

$$W = (SD)^T GSD = DS^T GSD$$

consists of the intersection between the chosen columns and the corresponding rows, each element of which has been rescaled by with $1/c\sqrt{p_{i_t} p_{j_t}}$. (This can also be viewed as forming W by sampling a number c of rows of C and rescaling. Note, however, that in this case the columns of A and the rows of C are sampled using the same probabilities.) In Algorithm 3, the MAIN APPROXIMATION is restated using this sampling matrix formalism. It should be clear that Algorithm 3 and Algorithm 2 yield identical results.

Before stating our main theorem, we wish to emphasize the structural simplicity of our main result. If, e.g., we choose $k = c$, then our main algorithm provides a decomposition of the form $\tilde{G} = CW^+C^T$:

$$\begin{pmatrix} \quad G \quad \end{pmatrix} \approx \begin{pmatrix} \quad \tilde{G} \quad \end{pmatrix} = \begin{pmatrix} \quad C \quad \end{pmatrix} \begin{pmatrix} \quad W \quad \end{pmatrix}^+ \begin{pmatrix} \quad C^T \quad \end{pmatrix}. \tag{14}$$

Up to rescaling, the MAIN APPROXIMATION algorithm returns an approximation $\tilde{G}$ which is created from two submatrices of G, namely C and W. In the uniform sampling case, $p_i = 1/n$, the

Data : $n \times n$ Gram matrix G, $\{p_i\}_{i=1}^n$ such that $\sum_{i=1}^n p_i = 1$, $c \leq n$, and $k \leq c$.

Result : $n \times n$ matrix $\tilde{G}$.

- Define the $(n \times c)$ matrix $S = \mathbf{0}_{n \times c}$;
- Define the $(c \times c)$ matrix $D = \mathbf{0}_{c \times c}$;
- **for** $t = 1, \ldots, c$ **do**
  - Pick $i_t \in [n]$, where $\mathbf{Pr}(i_t = i) = p_i$;
  - $D_{tt} = (cp_{i_t})^{-1/2}$;
  - $S_{i_t t} = 1$;

end

- Let $C = GSD$ and $W = DS^T GSD$.
- Compute W_k, the best rank-k approximation to W.
- Return $\tilde{G}_k = CW_k^+ C^T$.

Algorithm 3: The MAIN APPROXIMATION algorithm, restated.

diagonal elements of the rescaling matrix D are all n/c, and these all cancel out of the expression. In the nonuniform sampling case, C is a rescaled version of the columns of G and W is a rescaled version of the intersection of those columns with the corresponding rows. Alternatively, one can view C as consisting of the actual columns of G, without rescaling, and W as consisting of the intersection of those columns with the corresponding rows, again without rescaling, in the following manner. Let $\hat{C} = GS$, let $\hat{W} = S^T GS$, and let

$$\hat{W}^+ = \hat{W}^+_{D^2, D^{-2}} = D \left(D\hat{W}D \right)^+ D \tag{15}$$

be the $\{D^2, D^{-2}\}$-weighted-$\{1,2\}$-generalized inverse of $\hat{W}$. Then, $G \approx \tilde{G} = \hat{C}\hat{W}^+\hat{C}^T$.

The following theorem states our main result regarding the MAIN APPROXIMATION algorithm. Its proof may be found in Section 4.3.

Theorem 3 *Suppose G is an $n \times n$ SPSD matrix, let $k \leq c$ be a rank parameter, and let $\tilde{G}_k = CW_k^+ C^T$ be constructed from the* MAIN APPROXIMATION *algorithm of Algorithm 2 by sampling c columns of G with probabilities $\{p_i\}_{i=1}^n$ such that*

$$p_i = G_{ii}^2 / \sum_{i=1}^n G_{ii}^2. \tag{16}$$

Let $r = rank(W)$ and let G_k be the best rank-k approximation to G. In addition, let $\epsilon > 0$ and $\eta = 1 + \sqrt{8 \log(1/\delta)}$. If $c \geq 64k/\epsilon^4$, then

$$\mathbf{E}\left[\left\| G - \tilde{G}_k \right\|_F \right] \leq \|G - G_k\|_F + \epsilon \sum_{i=1}^n G_{ii}^2 \tag{17}$$

and if $c \geq 64k\eta^2/\epsilon^4$ then with probability at least $1 - \delta$

$$\left\| G - \tilde{G}_k \right\|_F \leq \|G - G_k\|_F + \epsilon \sum_{i=1}^n G_{ii}^2. \tag{18}$$

In addition, if $c \geq 4/\epsilon^2$ *then*

$$\mathbf{E}\left[\left\|G - \tilde{G}_k\right\|_2\right] \leq \|G - G_k\|_2 + \epsilon \sum_{i=1}^{n} G_{ii}^2 \tag{19}$$

and if $c \geq 4\eta^2/\epsilon^2$ *then with probability at least* $1 - \delta$

$$\left\|G - \tilde{G}_k\right\|_2 \leq \|G - G_k\|_2 + \epsilon \sum_{i=1}^{n} G_{ii}^2. \tag{20}$$

Several things should be noted about this result. First, if $k \geq r = \mathrm{rank}(W)$ then $W_k = W$, and an application of (13) of Theorem 2 leads to bounds of the form $\left\|G - \tilde{G}_r\right\|_2 \leq \epsilon \sum_{i=1}^{n} G_{ii}^2$, in expectation and with high probability. Second, the sampling probabilities used in Thoerem 3 may be written as $p_i = \left|X^{(i)}\right|^2 / \|X\|_F^2$, which only depend on dot products from the data matrix X. This is useful if X consists of the data after it has been mapped to the feature space $\mathcal{F}$. Finally, if the sampling probabilities were of the form $p_i = \left|G^{(i)}\right|^2 / \|G\|_F^2$ then they would preferentially choose data points that are more informative (in the sense of being longer) and/or more representative of the data (in the sense that they tend to be more well correlated with more data points). Instead the probabilities (16) ignore the correlations. As discussed in Sections 5 and 6, this leads to somewhat worse error bounds. To the best of our knowledge, it is not known how to sample with respect to correlations while respecting the SPSD property and obtaining provably good bounds with improved error bounds. This is of interest since in many applications it is likely that the data are approximately normalized by the way the data are generated, and it is the correlations that are of interest. Intuitively, this difficulty arises since it is difficult to identify structure in a matrix to ensure the SPSD property, unless, e.g., the matrix is diagonally dominant or given in the form $X^T X$. As will be seen in Section 4.3, the proof of Theorem 3 depends crucially on the decomposition of G as $G = X^T X$.

4.3 Proof of Theorem 3

Since $G = X^T X$ it follows that both the left and the right singular vectors of G are equal to the right singular vectors of X and that the singular values of G are the squares of the singular values of X. More formally, let the SVD of X be $X = U\Sigma V^T$. Then,

$$G = V\Sigma^2 V^T = XUU^T X^T. \tag{21}$$

Now, let us consider $C_X = XSD \in \mathbb{R}^{m \times c}$, i.e., the column sampled and rescaled version of X, and let the SVD of C_X be $C_X = \hat{U}\hat{\Sigma}\hat{V}^T$. Thus, in particular, $\hat{U}$ contains the left singular vectors of C_X. We do not specify the dimensions of $\hat{U}$ (and in particular how many columns $\hat{U}$ has) since we do not know the rank of C_X. Let $\hat{U}_k$ be the $m \times k$ matrix whose columns consist of the singular vectors of C_X corresponding to the top k singular values. Instead of exactly computing the left singular vectors U of X, we can approximate them by $\hat{U}_k$, computed from a column sample of X, and use this to compute an approximation $\tilde{G}$ to G.

We first establish the following lemma, which provides a bound on $\left\|G - \tilde{G}_k\right\|_\xi$ for $\xi = 2, F$.

Lemma 1 *If* $\tilde{G}_k = CW_k^+ C^T$ *then*

$$\left\|G - \tilde{G}_k\right\|_F = \left\|X^T X - X^T \hat{U}_k \hat{U}_k X\right\|_F \tag{22}$$

$$\left\|G - \tilde{G}_k\right\|_2 = \left\|X - \hat{U}_k \hat{U}_k^T X\right\|_2^2. \tag{23}$$

Proof: Recall that $C = GSD$ and $W = (SD)^T GSD = C_X^T C_X$. Thus, $W = \hat{V}\hat{\Sigma}^2\hat{V}$ and $W_k = \hat{V}\hat{\Sigma}_k^2\hat{V}^T$, where $\hat{\Sigma}_k$ is the diagonal matrix with the top k singular values of C_X on the diagonal and the remainder set to 0. Then since $C_X = XSD = \hat{U}\hat{\Sigma}\hat{V}^T$ and $W_k^+ = \hat{V}\hat{\Sigma}_k^{-2}\hat{V}^T$

$$\begin{aligned}
\tilde{G}_k &= GSD\,(W_k)^+\,(GSD)^T && (24)\\
&= X^T\hat{U}\hat{\Sigma}\hat{V}^T\left(\hat{V}\hat{\Sigma}_k^2\hat{V}^T\right)^+\hat{V}\hat{\Sigma}\hat{U}^T X && (25)\\
&= X^T\hat{U}_k\hat{U}_k^T X, && (26)
\end{aligned}$$

where $\hat{U}_k\hat{U}_k^T$ is a projection onto the space spanned by the top k singular vectors of W. (22) then follows immediately, and (23) follows since

$$X^TX - X^T\hat{U}_k\hat{U}_k^TX = \left(X - \hat{U}_k\hat{U}_k^TX\right)^T\left(X - \hat{U}_k\hat{U}_k^TX\right)$$

and since $\|\Omega\|_2^2 = \left\|\Omega^T\Omega\right\|_2$ for any matrix Ω.

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By combining (23) with Theorem 2, we see that

$$\begin{aligned}
\left\|G - \tilde{G}_k\right\|_2 &\leq \|X - X_k\|_2^2 + 2\left\|XX^T - C_XC_X^T\right\|_2\\
&\leq \|G - G_k\|_2 + 2\left\|XX^T - C_XC_X^T\right\|_2.
\end{aligned}$$

Since the sampling probabilities (16) are of the form $p_i = \left|X^{(i)}\right|^2 / \|X\|_F^2$, this may be combined with Theorem 1, from which, by choosing c appropriately, the spectral norm bounds (19) and (20) of Theorem 3 follow.

To establish the Frobenius norm bounds, define $E = XX^TXX^T - C_XC_X^TC_XC_X^T$. Then, we have that:

$$\begin{aligned}
\left\|G - \tilde{G}_k\right\|_F^2 &= \left\|X^TX\right\|_F^2 - 2\left\|XX^T\hat{U}_k\right\|_F^2 + \left\|\hat{U}_k^TXX^T\hat{U}_k\right\|_F^2 && (27)\\
&\leq \left\|X^TX\right\|_F^2 - 2\left(\sum_{t=1}^k \sigma_t^4(C_X) - \sqrt{k}\,\|E\|_F\right) + \sum_{t=1}^k \sigma_t^4(C_X) + \sqrt{k}\,\|E\|_F && (28)\\
&= \left\|X^TX\right\|_F^2 - \sum_{t=1}^k \sigma_t^4(C_X) + 3\sqrt{k}\,\|E\|_F && (29)\\
&\leq \left\|X^TX\right\|_F^2 - \sum_{t=1}^k \sigma_t^2(X^TX) + 4\sqrt{k}\,\|E\|_F, && (30)
\end{aligned}$$

where (27) follows by Lemmas 1 and 2, (28) follows by Lemmas 3 and 4, and (30) follows by Lemma 5. Since

$$\left\|X^TX\right\|_F^2 - \sum_{t=1}^k \sigma_t^2(X^TX) = \|G\|_F^2 - \sum_{t=1}^k \sigma_t^2(G) = \|G - G_k\|_F^2,$$

it follows that

$$\left\|G - \tilde{G}_k\right\|_F^2 \leq \|G - G_k\|_F^2 + 4\sqrt{k}\left\|XX^TXX^T - C_XC_X^TC_XC_X^T\right\|_F. \quad (31)$$

Since the sampling probabilities (16) are of the form $p_i = \left|X^{(i)}\right|^2 / \|X\|_F^2$, this may be combined with Lemma 6 and Theorem 1. Since $(\alpha^2+\beta^2)^{1/2} \leq \alpha+\beta$ for $\alpha, \beta \geq 0$, by using Jensen's inequality, and by choosing c appropriately, the Frobenius norm bounds (17) and (18) of Theorem 3 follow.

The next four lemmas are used to bound the right hand side of (22).

Lemma 2 *For every $k : 0 \leq k \leq rank(W)$ we have that:*

$$\left\| X^T X - X^T \hat{U}_k \hat{U}_k^T X \right\|_F^2 = \left\| X^T X \right\|_F^2 - 2 \left\| X X^T \hat{U}_k \right\|_F^2 + \left\| \hat{U}_k^T X X^T \hat{U}_k \right\|_F^2$$

Proof: Define $Y = X - \hat{U}_k \hat{U}_k^T X$. Then,

$$\begin{aligned} \left\| X^T X - X^T \hat{U}_k \hat{U}_k^T X \right\|_F^2 &= \left\| Y^T Y \right\|_F^2 \\ &= \mathbf{Tr}\left(Y^T Y Y^T Y \right) \\ &= \left\| X^T X \right\|_F^2 - 2\mathbf{Tr}\left(X X^T \hat{U}_k \hat{U}_k^T X X^T \right) + \mathbf{Tr}\left(\hat{U}_k^T X X^T \hat{U}_k \hat{U}_k^T X X^T \hat{U}_k \right), \end{aligned}$$

where the last line follows by multiplying out terms and since the trace is symmetric under cyclic permutations. The lemma follows since $\|\Omega\|_F^2 = \mathbf{Tr}\left(\Omega\Omega^T\right)$ for any matrix Ω.

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Lemma 3 *For every $k : 0 \leq k \leq rank(W)$ we have that:*

$$\left| \left\| X X^T \hat{U}_k \right\|_F^2 - \sum_{t=1}^{k} \sigma_t^4(C_X) \right| \leq \sqrt{k} \left\| X X^T X X^T - C_X C_X^T C_X C_X^T \right\|_F$$

Proof: Since $\sigma_t(C_X C_X^T) = \sigma_t^2(C_X)$ and since $\hat{U}$ is a matrix consisting of the singular vectors of $C_X = XSD$, we have that

$$\begin{aligned} \left| \left\| X X^T \hat{U}_k \right\|_F^2 - \sum_{t=1}^{k} \sigma_t^4(C_X) \right| &= \left| \sum_{t=1}^{k} \left| X X^T \hat{U}^{(t)} \right|^2 - \sum_{t=1}^{k} \left| C_X C_X^T \hat{U}^{(t)} \right|^2 \right| \\ &= \left| \sum_{t=1}^{k} \hat{U}^{(t)^T} \left(X X^T X X^T - C_X C_X^T C_X C_X^T \right) \hat{U}^{(t)} \right| \\ &\leq \sqrt{k} \left(\sum_{t=1}^{k} \left(\hat{U}^{(t)^T} \left(X X^T X X^T - C_X C_X^T C_X C_X^T \right) \hat{U}^{(t)} \right)^2 \right)^{1/2}, \end{aligned}$$

where the last line follows from the Cauchy-Schwartz inequality. The lemma then follows.

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Lemma 4 *For every $k : 0 \leq k \leq rank(W)$ we have that:*

$$\left\| \hat{U}_k^T X X^T \hat{U}_k \right\|_F^2 - \sum_{t=1}^{k} \sigma_t^4(C_X) \leq \sqrt{k} \left\| X X^T X X^T - C_X C_X^T C_X C_X^T \right\|_F$$

Proof: Recall that if a matrix U has orthonormal columns then $\left\| U^T \Omega \right\|_F \leq \|\Omega\|_F$ for any matrix Ω. Thus, we have that

$$\begin{aligned} \left\| \hat{U}_k^T X X^T \hat{U}_k \right\|_F^2 - \sum_{t=1}^{k} \sigma_t^4(C_X) &\leq \left\| X X^T \hat{U}_k \right\|_F^2 - \sum_{t=1}^{k} \sigma_t^4(C_X) \\ &\leq \left| \left\| X X^T \hat{U}_k \right\|_F^2 - \sum_{t=1}^{k} \sigma_t^4(C_X) \right| \end{aligned}$$

The remainder of the proof follows that of Lemma 3.

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Lemma 5 *For every $k : 0 \leq k \leq rank(W)$ we have that:*

$$\left| \sum_{t=1}^{k} \sigma_t^4(C_X) - \sigma_t^2(X^T X) \right| \leq \sqrt{k} \left\| XX^T XX^T - C_X C_X^T C_X C_X^T \right\|_F$$

Proof:

$$\begin{aligned} \left| \sum_{t=1}^{k} \sigma_t^4(C_X) - \sigma_t^2(X^T X) \right| &\leq \sqrt{k} \left(\sum_{t=1}^{k} \left(\sigma_t^4(C_X) - \sigma_t^2(X^T X) \right)^2 \right)^{1/2} \\ &= \sqrt{k} \left(\sum_{t=1}^{k} \left(\sigma_t(C_X C_X^T C_X C_X^T) - \sigma_t(XX^T XX^T) \right)^2 \right)^{1/2} \\ &\leq \sqrt{k} \left\| XX^T XX^T - C_X C_X^T C_X C_X^T \right\|_F, \end{aligned}$$

where the first inequality follows from the Cauchy-Schwartz inequality and the second inequality follows from the matrix perturbation result (3).

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The following is a result of the BasicMatrixMultiplication algorithm that is not found in [15], but that will be useful for bounding the additional error in (31). We state this result for a general $m \times n$ matrix A.

Lemma 6 *Suppose $A \in \mathbb{R}^{m \times n}$, $c \in \mathbb{Z}^+$ such that $1 \leq c \leq n$, and $\{p_i\}_{i=1}^n$ are such that $p_k = \left| A^{(k)} \right|^2 / \|A\|_F^2$. Construct C with the* BasicMatrixMultiplication *algorithm of [15]. Then,*

$$\mathbf{E}\left[\left\| AA^T AA^T - CC^T CC^T \right\|_F \right] \leq \frac{2}{\sqrt{c}} \|A\|_F^4. \tag{32}$$

Furthermore, let $\delta \in (0,1)$ and $\eta = 1 + \sqrt{8 \log(1/\delta)}$. Then, with probability at least $1 - \delta$,

$$\left\| AA^T AA^T - CC^T CC^T \right\|_F \leq \frac{2\eta}{\sqrt{c}} \|A\|_F^4. \tag{33}$$

Proof: First note that:

$$\begin{aligned} AA^T AA^T - CC^T CC^T &= AA^T AA^T - AA^T CC^T + AA^T CC^T - CC^T CC^T \\ &= AA^T \left(AA^T - CC^T \right) + \left(AA^T - CC^T \right) CC^T. \end{aligned}$$

Thus, by submultiplicitivity and subadditivity we have that for $\xi = 2, F$:

$$\left\| AA^T AA^T - CC^T CC^T \right\|_F \leq \|A\|_F^2 \left\| AA^T - CC^T \right\|_F + \left\| AA^T - CC^T \right\|_F \|C\|_F^2.$$

The lemma follows since $\|C\|_F^2 = \|A\|_F^2$ when $p_k = \left| A^{(k)} \right|^2 / \|A\|_F^2$, and by applying Theorem 1.

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5 Discussion Section

One motivation for the present work was to provide a firm theoretical basis for the Nyström-based algorithm of [40]. A second motivation was to clarify the relationships between our randomized SVD algorithms [16], our randomized CUR algorithms [17], and the Nyström-based methods of [40, 38, 21]. A third motivation was to extend our random sampling methodology to extract linear structure from matrices while preserving important nonlinear structure. In this section, we discuss these issues. Note that our ConstantTimeSVD algorithm of [16] is the algorithm originally analyzed by Frieze, Kannan, and Vempala [22], and thus a discussion of it corresponds also to a discussion of their algorithm of [22].

5.1 Summary of the Nyström Method

The Nyström method was originally introduced to handle approximations based on the numerical integration of the integral operator in integral equations, and it is well known for its simplicity and accuracy [10]. To illustrate the Nyström method, consider the eigenfunction problem:

$$\int_D K(t,s)\Phi(s)ds = \lambda\Phi(t) \;\; t \in D. \tag{34}$$

The resulting solution is first found at the set of quadrature node points, and then it is extended to all points in D by means of a special interpolation formula (see (39) below). This method requires the use of a quadrature rule. Assume that $D = [a,b] \subset \mathbb{R}$ and that the quadrature rule is the following:

$$\int_a^b y(s)ds = \sum_{j=1}^{n} w_j y(s_j), \tag{35}$$

where $\{w_j\}$ are the weights and $\{s_j\}$ are the quadrature points that are determined by the particular quadrature rule. If this rule is used to compute the integral occurring in (34), we have:

$$\int_a^b K(x,s)\Phi(s)ds \approx \sum_{j=1}^{n} w_j k(x,s_j)\tilde{\phi}(s_j), \tag{36}$$

and the integral equation (34) leads to an eigenvalue problem of the form:

$$\sum_{j=1}^{n} w_j k(x,s_j)\tilde{\phi}(s_j) = \tilde{\lambda}\tilde{\phi}(x). \tag{37}$$

Solving (37) leads to an approximate eigenvalue $\tilde{\lambda}$ and an approximate eigenfunction $\tilde{\phi}(x)$ and may be done via the Nyström method as follows. First, set $x = x_i$, $i = 1,\ldots,n$ in (37). This leads to an system of n algebraic equations:

$$\sum_{j=1}^{n} w_j k(x_i,s_j)\tilde{\phi}(s_j) = \tilde{\lambda}\tilde{\phi}(x_i), \tag{38}$$

that depend on the set $\{x_i\}$ of Nyström points. Although it is by no means necessary that the set of Nyström points is coincident with the set of quadrature points, they are often chosen to be so since in that case if the kernel $K(\cdot,\cdot)$ is symmetric then the matrix $k(\cdot,\cdot)$ in (38) is symmetric. Then, if $\tilde{\lambda}_m \neq 0$ the exact eigenvectors $\tilde{\phi}_m$ on the Nyström points can be extended to a function $\bar{\phi}_m(x)$ on the full domain by substituting it into (37):

$$\bar{\phi}_m(x) = \frac{1}{\tilde{\lambda}_m}\sum_{j=1}^{n} w_j k(x,s_j)\tilde{\phi}_m(s_j). \tag{39}$$

The function $\bar{\phi}_m(x)$ is the *Nyström extension* of the eigenvector $\tilde{\phi}_m$, and in the present context may be thought of as being an approximation to the exact eigenfunction Φ_m computed by extending a function computed on a (small) number n of points to the full (large) domain D.

In the applications we are considering, the data points are vectors in $\mathbb{R}^n$. Thus, consider an $m \times n$ matrix A consisting of m such vectors. Let c columns and r rows be chosen (without replacement) in some manner, and let A be partitioned as:

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \tag{40}$$

where $A_{11} \in \mathbb{R}^{c \times r}$ represents the subblock of matrix elements common to the sampled columns and the sampled rows, A_{21} and A_{12} are rectangular matrices consisting of elements with a sampled column label (exclusive) or sampled row label, respectively, and $A_{22} \in \mathbb{R}^{(m-c)\times(n-r)}$ consists of the remaining elements. If $c, r = O(1)$ then A_{11} is small and A_{22} is large. To be consistent with the notation of [16, 17], we let $C = [A_{11}^T A_{21}^T]^T$ and $R = [A_{11} A_{12}]$. Let the SVD of A_{11} be $A_{11} = \tilde{U}\tilde{\Sigma}\tilde{V}^T$, and let the rank of A_{11} be k.

Assume, for the moment, that A is a SPSD matrix and that the chosen rows are the same as the chosen columns. Then, A_{11} is also a SPSD matrix; in addition, $\tilde{V} = \tilde{U}$ are the eigenvalues of A_{11} and $\tilde{\Sigma}$ consists of the eigenvectors of A_{11}. In this case, the Nyström extension of $\tilde{U}$ gives the following approximation for the eigenvectors of the full matrix A:

$$\bar{U} = C\tilde{U}\Sigma^{-1} = \begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix} \tilde{U}\tilde{\Sigma}^{-1} = \begin{bmatrix} \tilde{U} \\ A_{21}\tilde{U}\tilde{\Sigma}^{-1} \end{bmatrix}. \tag{41}$$

Note that this Nyström extension of the restricted solution to the full set of data points is of the same form as (39).

More generally, if A is an arbitrary $m \times n$ matrix, then the Nyström extension of $\tilde{U}$ and $\tilde{V}$ gives the following approximation for the singular vectors of the full matrix A:

$$\bar{U} = \begin{bmatrix} \tilde{U} \\ A_{21}\tilde{V}\tilde{\Sigma}^{-1} \end{bmatrix}, \text{ and} \tag{42}$$

$$\bar{V} = \begin{bmatrix} \tilde{V} \\ A_{12}^T\tilde{U}\tilde{\Sigma}^{-1} \end{bmatrix}. \tag{43}$$

If both $\bar{U}$ and $\bar{V}$ have been computed then the Nyström extensions (42)–(43) also have an interpretation in terms of matrix completion. To see this, set $\tilde{A} = \bar{U}\tilde{\Sigma}\bar{V}^T$; then we have:

$$\tilde{A} = \begin{bmatrix} \tilde{U} \\ A_{21}\tilde{V}\tilde{\Sigma}^{-1} \end{bmatrix} \tilde{\Sigma} \begin{bmatrix} \tilde{V}^T & \tilde{\Sigma}^{-1}\tilde{U}^T A_{12} \end{bmatrix} \tag{44}$$

$$= \begin{bmatrix} A_{11} & \tilde{U}\tilde{U}^T A_{12} \\ A_{21}\tilde{V}\tilde{V}^T & A_{21}A_{11}^+ A_{12} \end{bmatrix} \tag{45}$$

$$= \begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix} A_{11}^+ \begin{bmatrix} A_{11} & A_{12} \end{bmatrix}. \tag{46}$$

Note that if A_{11} is nonsingular, then (45) becomes:

$$\tilde{A} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{21}A_{11}^{-1}A_{12} \end{bmatrix}. \tag{47}$$

In this case, the Nyström extension implicitly approximates A_{22} using $A_{21}A_{11}^{-1}A_{12}$, and the quality of the approximation of A by $\tilde{A}$ can be quantified by the norm of the Schur complement $\left\|A_{22} - A_{21}A_{11}^{-1}A_{12}\right\|_\xi$, $\xi = 2, F$. The size of this error norm is governed, e.g., by the extent to which the columns of A_{21} provide a good basis for the columns of A_{22}. If A_{11} is rectangular or square and singular then other terms in the matrix $\tilde{A}$ also contribute to the error. Note that (46) is of the form $A \approx \tilde{A} = CA_{11}^+R$. If A is a SPSD matrix and the chosen rows are the same as the chosen columns then (45) is modified appropriately and (46) is of the form $A \approx \tilde{A} = CW^+C^T$, which is the form of our main decomposition for a Gram matrix G. Note, however, that neither $\tilde{U}$ nor $\bar{U}$ are actually computed by our main approximation algorithm. In Sections 5.2 and 5.3, we discuss these issues further.

5.2 Relationship to the Randomized SVD Decompositions

Recall that the LINEARTIMESVD of [16] computes exactly the low-dimensional singular vectors of C. Let the SVD of C be $C = H\Sigma Z^T$. Then, the high-dimensional singular vectors of C are computed by extending the low-dimensional singular vectors as:

$$H = CZ\Sigma^{-1}, \tag{48}$$

and it is these that are taken as approximations of the left singular vectors of the original matrix A, in the sense that under appropriate assumptions:

$$\left\|A - HH^T A\right\|_\xi \leq \|A - A_k\|_\xi + \epsilon \|A\|_F , \tag{49}$$

in expectation and with high probability, for both $\xi = 2, F$. This is not a Nyström extension in the sense of Section 5.1 since although sampling is used to construct the matrix C a second level of sampling is never performed to construct A_{11}.

On the other hand, the CONSTANTTIMESVD algorithm of [16] (and thus the algorithm of Frieze, Kannan, and Vempala [22]) is similar except that it *approximates* the low-dimensional singular vectors of C. It does this by randomly sampling w rows of C and rescaling each appropriately to form a $w \times c$ matrix A_{11} (this matrix is called W in [16, 17], but it is constructed with different sampling probabilities than the W defined in this paper) and computing the eigenvectors of $A_{11}^T A_{11}$. These eigenvectors are then Nyström-extended via (42) to vectors $\bar{U}$ (denoted by $\tilde{H}$ in [16]) that approximate the left singular vectors of A. In this case, the projection $HH^T = C(C^TC)^+C^T$ of the LINEARTIMESVD algorithm is replaced by an approximate projection onto the column space of C of the form $\bar{U}\bar{U} = C(A_{11}^T A_{11})^+ C^T$. From this perspective, since $C^TC \approx A_{11}^T A_{11}$ we may view the LINEARTIMESVD of [16] as performing a Nyström-based extension of approximations of the eigenvectors of $A_{11}^T A_{11}$.

We emphasize these points since we would like to clarify several potential misunderstandings in the literature regarding the relationship between the Nyström-based algorithm of [40] and the approximate SVD algorithm of Frieze, Kannan, and Vempala [22]. For example, in [40, 38, 21] it is claimed that their Nyström-based methods are a special case of [22] and thus of the CONSTANTTIMESVD algorithm of [16]. Although the SVD algorithms of [16, 22] do represent a Nyström-based extension in the sense just described, several things should be noted. First, in order to obtain provable performance guarantees, the CONSTANTTIMESVD algorithm used in [16, 22] approximates the left (or right, but not both) singular vectors in a single Nyström-like extension of the form (42) (or (43) for the right singular vectors). This algorithm makes no assumptions about the symmetry or positive definiteness of the input matrix, and it does not take advantage of this structure if it exists. Second, and relatedly, in this algorithm there are two levels of sampling, and only the first depends directly on the elements of the matrix A; the second depends on the lengths of the rows of C. Thus, in general, the matrix A_{11} does not consist of the same rows as columns, even if A is a SPSD matrix. If A is a SPSD matrix, then one could approximate A as $\tilde{A} = \bar{U}\tilde{\Sigma}\bar{U}^T$, but the error associated with this is not the error that the theorems of [16, 22] bound. Third, the structure of the approximation obtained by [16, 22] is quite different from that of the approximation of [40] and (14). In the latter case it is of the form CW^+C^T, while in the former case it is of the form $P_C A$, where P_C is an exact or approximate projection onto the column space of C.

5.3 Relationship to the Randomized CUR Decompositions

To shed further light on the relationship between the CONSTANTTIMESVD algorithm used in [16, 22] and the Nyström-based methods of [40, 38, 21], it is worth considering the CUR decompositions of [17], which are structurally a generalization of our main matrix decomposition. A

CUR decomposition is a low-rank matrix decomposition of the form $A \approx CUR$, where C is a matrix consisting of a small number of columns of A, R is a matrix consisting of a small number of rows of A, and U is an appropriately-defined low-dimensional matrix. Examples may be found in [17], and also in [25, 24]. In particular, the LINEARTIMECUR and CONSTANTTIMECUR algorithms of [17] (so named due to their relationship with the correspondingly-named SVD algorithms of [16]) compute an approximation to a matrix $A \in \mathbb{R}^{m \times n}$ by sampling c columns and r rows of the matrix A to form matrices $C \in \mathbb{R}^{m \times c}$ and $R \in \mathbb{R}^{r \times n}$, respectively. The matrices C and R are constructed with carefully-chosen and data-dependent nonuniform probability distributions, and from C and R a matrix $U \in \mathbb{R}^{c \times r}$ is constructed such that under appropriate assumptions:

$$\|A - CUR\|_\xi \leq \|A - A_k\|_\xi + \epsilon \|A\|_F , \tag{50}$$

with high probability, for both $\xi = 2, F$. Although these algorithms apply to any matrix, and thus to a SPSD matrix, the computed approximation CUR (with the provable error bounds of the form (50)) is neither symmetric nor positive semidefinite in the latter case. The SPSD property is an important property in many applications, and thus it is desirable to obtain a low-rank approximation that respects this property. The analysis of the MAIN APPROXIMATION algorithm shows that if G is a SPSD matrix then we can choose $R = C^T$ and $U = A_{11}^+$ and obtain a SPSD approximation of the form $G \approx \tilde{G}_k = CW_k^+C^T$ with provable error bounds of the form (1). Note that this bound is worse than that of (50) since the scale of the additional error is larger. Although it may not be surprising that the bound is somewhat worse since we are requiring that the approximation is not just low rank but that in addition it respects the nonlinear SPSD property, the worse bound is likely due simply to the sampling probabilities that were used to obtain provable performance guarantees.

Since the CUR algorithms of [17] rely for their proofs of correctness on the corresponding SVD algorithms of [16], the Nyström discussion about the SVD algorithms is relevant to them. In addition, to understand the CUR algorithm in terms of matrix completion, consider an $m \times n$ matrix A with c columns and r rows chosen in some manner which is partitioned as in (40). Let $U \in \mathbb{R}^{c \times r}$ be an appropriately defined matrix as in [17], and let us decompose the original matrix A of (40) as $A \approx CUR$:

$$CUR = \begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix} U \begin{bmatrix} A_{11} & A_{12} \end{bmatrix} \tag{51}$$

$$= \begin{bmatrix} A_{11}UA_{11} & A_{11}UA_{12} \\ A_{21}UA_{11} & A_{21}UA_{12} \end{bmatrix}. \tag{52}$$

In [17] $U \neq A_{11}$, but we provide a definition for U such that $U \approx A_{11}^+$, in which case the structural similarity between (51) and (46) should be clear, as should the similarity between (52) and (45). For general matrices A, the CUR decomposition approximates A_{22} by $A_{22} = A_{21}UA_{12}$, but it also approximates A_{21} by $A_{21}UA_{11}$, A_{12} by $A_{11}UA_{12}$, and A_{11} by $A_{11}UA_{11}$. Thus, the quality of the approximation of the full matrix can not be quantified simply by the norm of the Schur complement $\left\|A_{22} - A_{21}A_{11}^+A_{12}\right\|_\xi$, and in [17] we bound $\|A - CUR\|_\xi$ directly. Relatedly, the quality of the approximation is determined, e.g., by how well a basis the chosen columns of C are for the remaining columns of A.

6 Conclusion

We have presented and analyzed an algorithm that provides an approximate decomposition of an $n \times n$ Gram matrix G which is of the form $G \approx \tilde{G}_k = CW_k^+C^T$ and which has provable error

bounds of the form (1). A crucial feature of this algorithm is the probability distribution used to randomly sample columns. We conclude with two open problems related to the choice of this distribution.

First, it would be desirable to choose the probabilities in Theorem 3 to be $p_i = \left|G^{(i)}\right|^2 / \|G\|_F^2$ and to establish bounds of the form (1) in which the scale of the additional error was $\|G\|_F = \left\|X^T X\right\|_F$ rather than $\sum_{i=1}^n G_{ii}^2 = \|X\|_F^2$. This would entail extracting linear structure while simultaneously respecting the SPSD property and obtaining improved scale of error. This would likely be a corollary of a CUR decomposition for a general $m \times n$ matrix A with error bounds of the form (50) in which $U = W_k^+$, where W is now the matrix consisting of the intersection of the chosen columns and (in general different) rows. This would simplify considerably the form of U found in [17] and would lead to improved interpretability. Second, we should also note that if capturing coarse statistics over the data is not of interest, but instead one is interested in other properties of the data, e.g., identifying outliers, then probabilities that depend on the data in some other manner, e.g., inversely with respect to their lengths squared, may be appropriate. We do not have provable bounds in this case.

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References

[1] D. Achlioptas and F. McSherry. Fast computation of low rank matrix approximations. In *Proceedings of the 33rd Annual ACM Symposium on Theory of Computing*, pages 611–618, 2001.

[2] D. Achlioptas, F. McSherry, and B. Schölkopf. Sampling techniques for kernel methods. In *Annual Advances in Neural Information Processing Systems 14: Proceedings of the 2001 Conference*, pages 335–342, 2002.

[3] Y. Azar, A. Fiat, A.R. Karlin, F. McSherry, and J. Saia. Spectral analysis of data. In *Proceedings of the 33rd Annual ACM Symposium on Theory of Computing*, pages 619–626, 2001.

[4] M. Belkin and P. Niyogi. Laplacian eigenmaps for dimensionality reduction and data representation. *Neural Computation*, 15(6):1373–1396, 2003.

[5] A. Ben-Israel and T.N.E. Greville. *Generalized Inverses: Theory and Applications*. Springer-Verlag, New York, 2003.

[6] Y. Bengio, J.F. Paiement, P. Vincent, O. Delalleau, N. Le Roux, and M. Ouimet. Out-of-sample extensions for LLE, Isomap, MDS, eigenmaps, and spectral clustering. In *Annual Advances in Neural Information Processing Systems 16: Proceedings of the 2003 Conference*, pages 177–184, 2004.

[7] R. Bhatia. *Matrix Analysis*. Springer-Verlag, New York, 1997.

[8] C.J.C. Burges. Simplified support vector decision rules. In *Proceedings of the 13th International Conference on Machine Learning*, pages 71–77, 1996.

[9] N. Cristianini and J. Shawe-Taylor. *An Introduction to Support Vector Machines and Other Kernel-based Learning Methods*. Cambridge University Press, Cambridge, 2000.

[10] L.M. Delves and J.L. Mohamed. *Computational Methods for Integral Equations.* Cambridge University Press, Cambridge, 1985.

[11] D.L. Donoho and C. Grimes. Hessian eigenmaps: Locally linear embedding techniques for high-dimensional data. *Proc. Natl. Acad. Sci. USA*, 100(10):5591–5596, 2003.

[12] P. Drineas, A. Frieze, R. Kannan, S. Vempala, and V. Vinay. Clustering in large graphs and matrices. In *Proceedings of the 10th Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 291–299, 1999.

[13] P. Drineas and R. Kannan. Fast Monte-Carlo algorithms for approximate matrix multiplication. In *Proceedings of the 42nd Annual IEEE Symposium on Foundations of Computer Science*, pages 452–459, 2001.

[14] P. Drineas and R. Kannan. Pass efficient algorithms for approximating large matrices. In *Proceedings of the 14th Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 223–232, 2003.

[15] P. Drineas, R. Kannan, and M.W. Mahoney. Fast Monte Carlo algorithms for matrices I: Approximating matrix multiplication. Technical Report YALEU/DCS/TR-1269, Yale University Department of Computer Science, New Haven, CT, February 2004.

[16] P. Drineas, R. Kannan, and M.W. Mahoney. Fast Monte Carlo algorithms for matrices II: Computing a low-rank approximation to a matrix. Technical Report YALEU/DCS/TR-1270, Yale University Department of Computer Science, New Haven, CT, February 2004.

[17] P. Drineas, R. Kannan, and M.W. Mahoney. Fast Monte Carlo algorithms for matrices III: Computing a compressed approximate matrix decomposition. Technical Report YALEU/DCS/TR-1271, Yale University Department of Computer Science, New Haven, CT, February 2004.

[18] P. Drineas, R. Kannan, and M.W. Mahoney. Sampling sub-problems of heterogeneous Max-Cut problems and approximation algorithms. Technical Report YALEU/DCS/TR-1283, Yale University Department of Computer Science, New Haven, CT, April 2004.

[19] P. Drineas, R. Kannan, and M.W. Mahoney. Sampling sub-problems of heterogeneous Max-Cut problems and approximation algorithms. In *Proceedings of the 22nd Annual International Symposium on Theoretical Aspects of Computer Science*, pages 57–68, 2005.

[20] S. Fine and K. Scheinberg. Efficient SVM training using low-rank kernel representations. *Journal of Machine Learning Research*, 2:243–264, 2001.

[21] C. Fowlkes, S. Belongie, F. Chung, and J. Malik. Spectral grouping using the Nyström method. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 26(2):214–225, 2004.

[22] A. Frieze, R. Kannan, and S. Vempala. Fast Monte-Carlo algorithms for finding low-rank approximations. In *Proceedings of the 39th Annual IEEE Symposium on Foundations of Computer Science*, pages 370–378, 1998.

[23] G.H. Golub and C.F. Van Loan. *Matrix Computations.* Johns Hopkins University Press, Baltimore, 1989.

[24] S.A. Goreinov and E.E. Tyrtyshnikov. The maximum-volume concept in approximation by low-rank matrices. *Contemporary Mathematics*, 280:47–51, 2001.

[25] S.A. Goreinov, E.E. Tyrtyshnikov, and N.L. Zamarashkin. A theory of pseudoskeleton approximations. *Linear Algebra and Its Applications*, 261:1–21, 1997.

[26] J. Ham, D.D. Lee, S. Mika, and B. Schölkopf. A kernel view of the dimensionality reduction of manifolds. Technical Report TR-110, Max Planck Institute for Biological Cybernetics, July 2003.

[27] R.A. Horn and C.R. Johnson. *Matrix Analysis*. Cambridge University Press, New York, 1985.

[28] S. Lafon. *Diffusion Maps and Geometric Harmonics*. PhD thesis, Yale University, 2004.

[29] M.Z. Nashed, editor. *Generalized Inverses and Applications*. Academic Press, New York, 1976.

[30] E. Osuna, R. Freund, and F. Girosi. An improved training algorithm for support vector machines. In *Proceedings of the 1997 IEEE Workshop on Neural Networks for Signal Processing VII*, pages 276–285, 1997.

[31] L. Rademacher, S. Vempala, and G. Wang. Matrix approximation and projective clustering via iterative sampling. *manuscript*.

[32] S.T. Roweis and L.K. Saul. Nonlinear dimensionality reduction by local linear embedding. *Science*, 290:2323–2326, 2000.

[33] B. Schölkopf, A. Smola, and K.-R. Müller. Nonlinear component analysis as a kernel eigenvalue problem. *Neural Computation*, 10:1299–1319, 1998.

[34] A.J. Smola and B. Schölkopf. Sparse greedy matrix approximation for machine learning. In *Proceedings of the 17th International Conference on Machine Learning*, pages 911–918, 2000.

[35] G.W. Stewart and J.G. Sun. *Matrix Perturbation Theory*. Academic Press, New York, 1990.

[36] J.B. Tenenbaum, V. de Silva, and J.C. Langford. A global geometric framework for nonlinear dimensionality reduction. *Science*, 290:2319–2323, 2000.

[37] K.Q. Weinberger, F. Sha, and L.K. Saul. Learning a kernel matrix for nonlinear dimensionality reduction. In *Proceedings of the 21st International Conference on Machine Learning*, pages 839–846, 2004.

[38] C.K.I. Williams, C.E. Rasmussen, A. Schwaighofer, and V. Tresp. Observations on the Nyström method for Gaussian process prediction. Technical report, University of Edinburgh, 2002.

[39] C.K.I. Williams and M. Seeger. The effect of the input density distribution on kernel-based classifiers. In *Proceedings of the 17th International Conference on Machine Learning*, pages 1159–1166, 2000.

[40] C.K.I. Williams and M. Seeger. Using the Nyström method to speed up kernel machines. In *Annual Advances in Neural Information Processing Systems 13: Proceedings of the 2000 Conference*, pages 682–688, 2001.