REVISITING THE NYSTRÖM METHOD FOR IMPROVED LARGE-SCALE MACHINE LEARNING

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Abstract. We reconsider randomized algorithms for the low-rank approximation of symmetric positive semi-definite (SPSD) matrices such as Laplacian and kernel matrices that arise in data analysis and machine learning applications. Our main results consist of an empirical evaluation of the performance quality and running time of sampling and projection methods on a diverse suite of SPSD matrices. Our results highlight complementary aspects of sampling versus projection methods, and they point to differences between uniform and nonuniform sampling methods based on leverage scores. We complement our empirical results with a suite of worst-case theoretical bounds for both random sampling and random projection methods. These bounds are qualitatively superior to existing bounds—*e.g.*, improved additive-error bounds for spectral and Frobenius norm error and relative-error bounds for trace norm error.

1. Introduction

We reconsider randomized algorithms for the low-rank approximation of symmetric positive semi-definite (SPSD) matrices such as Laplacian and kernel matrices that arise in data analysis and machine learning applications. Our goal is to obtain an improved understanding, both empirically and theoretically, of the complementary strengths of sampling versus projection methods on realistic data. Our main results consist of an evaluation of the performance quality and running time of sampling and projection methods on a diverse suite of dense and sparse SPSD matrices drawn both from machine learning as well as more general data analysis applications. These results are not intended to be comprehensive but instead to be illustrative of how Nyström-based randomized algorithms for the low-rank approximation of SPSD matrices behave in a broad range of realistic machine learning and data analysis applications.

In addition to being of interest in their own right, our empirical results point to several directions that are not explained well by existing theory. (For example, that the results are much better than existing worst-case theory would suggest, and that sampling with respect to the statistical leverage scores leads to results that are complementary to those achieved by projection-based methods.) Thus, we complement our empirical results with a suite of worst-case theoretical bounds for both random sampling and random projection methods. These bounds are qualitatively superior to existing bounds—*e.g.*, improved additive-error bounds for spectral and Frobenius norm error and relative-error bounds for trace norm error. Importantly, by considering random sampling and random projection algorithms on an equal footing, we identify within our analysis deterministic structural properties of the input data and sampling/projection methods that are responsible for high-quality low-rank approximation.

In more detail, our main contributions are fourfold.

- First, we provide an empirical illustration of the complementary strengths and weaknesses of data-independent random projection methods and data-dependent random sampling methods when applied to SPSD matrices. We do so for a diverse class of SPSD matrices drawn from machine learning and more general data analysis applications, and we consider reconstruction error with respect to the spectral, Frobenius, as well as trace norms. Depending on the parameter settings, the matrix norm of interest, the data set under consideration, etc., one or the other method might be preferable. In addition, we illustrate how these empirical properties can often be understood in terms of the structural nonuniformities of the input data that are of independent interest.
- Second, we consider the running time of high-quality sampling and projection algorithms. For random sampling algorithms, the computational bottleneck is typically the exact or approximate

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computation of the importance sampling distribution with respect to which one samples; and for random projection methods, the computational bottleneck is often the implementation of the random projection. By exploiting and extending recent work on "fast" random projections and related recent work on "fast" approximation of the statistical leverage scores, we illustrate that high-quality leverage-based random sampling and high-quality random projection algorithms have comparable running times. Although both are slower than simple (and in general much lower-quality) uniform sampling, both can be implemented more quickly than a naïve computation of an orthogonal basis for the top part of the spectrum.

- Third, our main technical contribution is a set of deterministic structural results that hold for any "sketching matrix" applied to an SPSD matrix. (A precise statement of these results is given in Theorems 1, 2, and 3 in Section 4.1.) We call these "deterministic structural results" since there is no randomness involved in their statement or analysis and since they depend on structural properties of the input data matrix and the way the sketching matrix interacts with the input data. In particular, they highlight the importance of the so-called statistical leverage scores (and other related structural nonuniformities having to do with the subspace structure of the input matrix), which have proven important in other applications of random sampling and random projection algorithms.
- Fourth, our main algorithmic contribution is to show that when the low-rank sketching matrix represents certain random projection or random sampling operations, then we obtain worst-case quality-of-approximation bounds that hold with high probability. (A precise statement of these results is given in Lemmas 1, 2, 3, and 4 in Section 4.2.) These bounds are qualitatively better than existing bounds (when nontrivial prior bounds even exist); they hold for reconstruction error of the input data with respect to the spectral norm and trace norm as well as the Frobenius norm; and they illustrate how high-quality random sampling algorithms and high-quality random projection algorithms can be treated from a unified perspective.

A novel aspect of our work is that we adopt a unified approach to these low-rank approximation questions—unified in the sense that we consider both sampling and projection algorithms on an equal footing, and that we illustrate how the structural nonuniformities responsible for high-quality low-rank approximation in worst-case analysis also have important empirical consequances in a diverse class of SPSD matrices. By identifying deterministic structural conditions responsible for high-quality low-rank approximation of SPSD matrices, we highlight complementary aspects of sampling and projection methods; and by illustrating the empirical consequences of structural nonuniformities, we provide theory that is a much closer guide to practice than has been provided by prior work. More generally, we should note that, although it is beyond the scope of this paper, our deterministic structural results could be used to check, in an *a posteriori* manner, the quality of a sketching method for which one cannot establish an *a priori* bound.

Our analysis is timely for several reasons. First, in spite of the empirical successes of Nyström-based and other randomized low-rank methods, existing theory for the Nyström method is quite modest. For example, existing worst-case bounds such as those of [21] are very weak, especially compared with existing bounds for least-squares regression and general low-rank matrix approximation problems [22, 23, 45].[1] Moreover, many other worst-case bounds make strong assumptions about the coherence properties of the input data [38, 28]. Second, there have been conflicting views in the literature about the usefulness of uniform sampling versus nonuniform sampling based on the empirical statistical leverage scores of the data in realistic data analysis and machine learning applications. For example, some work has concluded that the statistical leverage scores of realistic data matrices are fairly uniform, meaning that the coherence is small and thus uniform sampling is appropriate [61, 38], while other work has demonstrated that leverage scores are often very nonuniform in ways that render uniform sampling inappropriate and that can be essential to highlight properties of downstream interest [53, 47]. Third, in recent years several high-quality numerical implementations of randomized matrix algorithms for least-squares and low-rank approximation problems have been developed [3, 49, 62, 54, 48]. These have been developed from a "scientific computing" perspective, where condition numbers, spectral norms, etc. are of greater interest [46], and where relatively strong homogeneity assumptions can be made about the input data. In many "data analytics" applications, the questions one asks are very different, and the input data are much less well-structured; and thus we expect that some of

[1] This statement may at first surprise the reader, since an SPSD matrix is an example of a general matrix, and one might suppose that the existing theory for general matrices could be applied to SPSD matrices. While this is true, these existing methods for general matrices do not in general respect the symmetry or positive semi-definiteness of the input.

our results will help guide the development of algorithms and implementations that are more appropriate for large-scale analytics applications.

In the next section, Section 2, we start by presenting some notation, preliminaries, and related prior work. Then, in Section 3 we present our main empirical results; and in Section 4 we present our main theoretical results. We conclude in Section 5 with a brief discussion of our results in a broader context.

2. Notation, Preliminaries, and Related Prior Work

In this section, we introduce the notation used throughout the paper, and we address several preliminary considerations, including reviewing related prior work.

2.1. Notation.

Let $\mathbf{A} \in \mathbb{R}^{n\times n}$ be an arbitrary SPSD matrix with eigenvalue decomposition $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{U}^T$, where we partition $\mathbf{U}$ and $\mathbf{\Sigma}$ as

$$\mathbf{U} = \begin{pmatrix} \mathbf{U}_1 & \mathbf{U}_2 \end{pmatrix} \text{ and } \mathbf{\Sigma} = \begin{pmatrix} \mathbf{\Sigma}_1 & \\ & \mathbf{\Sigma}_2 \end{pmatrix}. \tag{1}$$

Here, $\mathbf{U}_1$ has k columns and spans the top k-dimensional eigenspace of $\mathbf{A}$, and $\mathbf{\Sigma}_1 \in \mathbb{R}^{k\times k}$ is full-rank.[2] Given $\mathbf{A}$ and a rank parameter k, the *statistical leverage scores of* $\mathbf{A}$ *relative to the best rank-k approximation to* $\mathbf{A}$ equal the squared Euclidean norms of the rows of the $n \times k$ matrix $\mathbf{U}_1$:

$$\ell_j = \|(\mathbf{U}_1)_j\|^2. \tag{2}$$

The leverage scores provide a more refined notion of the structural nonuniformities of $\mathbf{A}$ than does the notion of *coherence*, $\mu = \frac{n}{k}\max_{i\in\{1,\dots,n\}} \ell_i$, which equals (up to scale) the largest leverage score; and they have been used historically in regression diagnostics to identify particularly influential or outlying data points. Less obviously, the statistical leverage scores play a crucial role in recent work on randomized matrix algorithms: they define the key structural nonuniformity that must be dealt with in order to obtain high-quality low-rank and least-squares approximation of general matrices via random sampling and random projection methods [45]. Although Equation (2) defines them with respect to a particular basis, the statistical leverage scores equal the diagonal elements of the projection matrix onto the span of that basis, and thus they can be computed from any basis spanning the same space. Moreover, they can be approximated more quickly than the time required to compute that basis with a truncated SVD or a QR decomposition [20].

We denote by $\mathbf{S}$ an arbitrary $n \times \ell$ "sketching" matrix that, when post-multiplying a matrix $\mathbf{A}$, maps points from $\mathbb{R}^n$ to $\mathbb{R}^\ell$. We are most interested in the case where $\mathbf{S}$ is a random matrix that represents a random sampling process or a random projection process, but we do not impose this as a restriction unless explicitly stated. In order to provide high-quality low-rank matrix approximations, we control the error of our approximation in terms of the interaction of the sketching matrix $\mathbf{S}$ with the eigenspaces of $\mathbf{A}$, and thus we let

$$\mathbf{\Omega}_1 = \mathbf{U}_1^T\mathbf{S} \quad \text{and } \mathbf{\Omega}_2 = \mathbf{U}_2^T\mathbf{S} \tag{3}$$

denote the projection of $\mathbf{S}$ onto the top and bottom eigenspaces of $\mathbf{A}$, respectively.

Recall that, by keeping just the top k singular vectors, the matrix $\mathbf{A}_k := \mathbf{U}_1\mathbf{\Sigma}_1\mathbf{U}_1^T$ is the best rank-k approximation to $\mathbf{A}$, when measured with respect to any unitarily-invariant matrix norm, *e.g.*, the spectral, Frobenius, or trace norm. For a vector $x \in \mathbb{R}^n$, let $\|\mathbf{x}\|_\xi$, for $\xi = 1, 2, \infty$, denote the 1-norm, the Euclidean norm, and the ∞-norm, respectively. Then, $\|\mathbf{A}\|_2 = \|\mathrm{Diag}(\mathbf{\Sigma})\|_\infty$ denotes the *spectral norm* of $\mathbf{A}$; $\|\mathbf{A}\|_\mathrm{F} = \|\mathrm{Diag}(\mathbf{\Sigma})\|_2$ denotes the *Frobenius norm* of $\mathbf{A}$; and $\|\mathbf{A}\|_\star = \|\mathrm{Diag}(\mathbf{\Sigma})\|_1$ denotes the *trace norm* (or nuclear norm) of $\mathbf{A}$. Clearly,

$$\|\mathbf{A}\|_2 \le \|\mathbf{A}\|_\mathrm{F} \le \|\mathbf{A}\|_\star \le \sqrt{n}\,\|\mathbf{A}\|_\mathrm{F} \le n\,\|\mathbf{A}\|_2\,.$$

We quantify the quality of our algorithms by the "additional error" (above and beyond that incurred by the best rank-k approximation to $\mathbf{A}$). In the theory of algorithms, bounds of the form provided by (15) and (16) below are known as *additive-error bounds*, the reason being that the additional error is an additive factor of the form ε times a size scale that is larger than the "base error" incurred by the best rank-k approximation. In this case, the goal is to minimize the "size scale" of the additional error. Bounds of this form are very different and in general weaker than when the additional error enters as a multiplicative factor, such as when the error bounds are of the form $\|\mathbf{A}-\tilde{\mathbf{A}}\| \le f(n,k,\eta)\|\mathbf{A}-\mathbf{A}_k\|$, where $f(\cdot)$ is some function and η represents

[2] Variants of our results hold trivially if the rank of $\mathbf{A}$ is k or less, and so we focus on this more general case here.

other parameters of the problem. These latter bounds are of greatest interest when $f = 1 + \epsilon$, for an error parameter ϵ, as in (17) and (18) below. These *relative-error bounds*, in which the size scale of the additional error equals that of the base error, provide a *much* stronger notion of approximation than additive-error bounds.

2.2. **Preliminaries.** In machine learning applications, one is often interested in symmetric positive semi-definite (SPSD) matrices, *e.g.*, kernel matrices and Laplacian matrices, where this low-rank approximation approach (in particular, the sampling-based approach) is often called the Nyström method [61, 21, 38]. The Nyström method—both randomized and deterministic variants—has proven useful in applications where the kernel matrices are reasonably well-approximated by low-rank matrices; and it has been applied to Gaussian process regression, spectral clustering and image segmentation, manifold learning, and a range of other common machine learning tasks [61, 60, 25, 56, 65, 38]. The simplest Nyström-based procedure selects actual columns from the original data set uniformly at random and then uses those columns to construct a low-rank SPSD approximation. Although this procedure can be effective in practice for certain input matrices, two extensions (both of which are more expensive) can substantially improve the performance, *e.g.*, lead to lower reconstruction error for a fixed number of column samples, both in theory and in practice. The first extension is to sample columns with a judiciously-chosen nonuniform importance sampling distribution; and the second extension is to randomly mix (or combine linearly) columns before sampling them. For the random sampling algorithms, an important question is what importance sampling distribution should be used to construct the sample; while for the random projection algorithms, an important question is how to implement the random projections. In either case, appropriate consideration should be paid to questions such as whether the data are sparse or dense, how the eigenvalue spectrum decays, the nonuniformity properties of eigenvectors, *e.g.*, as quantified by the statistical leverage scores, whether one is interested in reconstructing the matrix or performing a downstream machine learning task, and so on.

The following sketching model subsumes both of these classes of methods.

- *SPSD Sketching Model.* Let $\mathbf{A}$ be an $n \times n$ positive semi-definite matrix, and let $\mathbf{S}$ be a matrix of size $n \times \ell$, where $\ell \ll n$. Take

$$\mathbf{C} = \mathbf{A}\mathbf{S} \quad \text{and } \mathbf{W} = \mathbf{S}^T\mathbf{A}\mathbf{S}.$$

  Then $\mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T$ is a low-rank approximation to $\mathbf{A}$ with rank at most ℓ.

We should note that the SPSD Sketching Model, formulated in this way, is *not* guaranteed to be numerically stable: if $\mathbf{W}$ is ill-conditioned, then instabilities may arise in forming the product $\mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T$. Thus, we are also interested in $\mathbf{C}\mathbf{W}_k^\dagger\mathbf{C}^T$, where $\mathbf{W}_k$ is the best rank-k approximation to $\mathbf{W}$, and where k is a rank parameter. For example, one might specify k and then "oversample" by choosing $\ell > k$ but still be interested in an approximation that has rank no greater than k. Often, "filtering" a low-rank approximation in this way through a (lower) rank-k space has a regularization effect: for example, relative-error CUR matrix decompositions are implicitly regularized by letting the "middle matrix" have rank no greater than k [22, 47]; and [15] considers a regularization of the uniform column sampling Nyström extension where, before forming the extension, all singular values of $\mathbf{W}$ smaller than a threshold are truncated to zero. For our empirical evaluation, we consider both cases, which we refer to as "non-rank-restricted" and "rank-restricted," respectively. For our theoretical results, for simplicity of notation, we do *not* describe the generalization of our results to this rank-restricted model; but we note that our analysis could be extended to include this, *e.g.*, by letting the sketching matrix $\mathbf{S}$ be a combination of a sampling operation and an operation that projects to the best rank-k approximation.

The choice of distribution for the sketching matrix $\mathbf{S}$ leads to different classes of low-rank approximations. For example, if $\mathbf{S}$ represents the process of sampling, either uniformly or according to a nonuniform importance sampling distribution, then we refer to the resulting approximation as a Nyström extension; if $\mathbf{S}$ consists of random linear combinations of most or all of the columns of $\mathbf{A}$, then we refer to the resulting approximation as a projection-based SPSD approximation. In this paper, we focus on Nyström extensions and projection-based SPSD approximations that fit the above SPSD Sketching Model. In particular, we do not consider adaptive schemes, which iteratively select columns to progressively decrease the approximation error. While these methods often perform well in practice [10, 9, 24, 38], rigorous analyses of them are hard to come by—interested readers are referred to the discussion in [24, 38].

2.3. **Related Prior Work.** Motivated by large-scale data analysis and machine learning applications, recent theoretical and empirical work has focused on "sketching" methods such as random sampling and random projection algorithms; a large part of the recent body of this work on randomized matrix algorithms has been summarized in the recent monograph of Mahoney [45] and the recent review article of Halko, Martinsson, and Tropp [31]. Here, we note that, on the empirical side, both random projection methods (*e.g.*, [12, 26, 59] and [6]) and random sampling methods (*e.g.*, [53, 47]) have been used in applications for clustering and classification of general data matrices; and that some of this work has highlighted the importance of the statistical leverage scores that we use in this paper [53, 47, 45, 63]. In parallel, so-called Nyström-based methods have also been used in machine learning applications. Originally used by Williams and Seeger to solve regression and classification problems involving Gaussian processes when the SPSD matrix $\mathbf{A}$ is well-approximated by a low-rank matrix [61, 60], the Nyström extension has been used in a large body of subsequent work. For example, applications of the Nyström method to large-scale machine learning problems include [56, 36, 37, 43] and [66, 40, 65], and applications in statistics and signal processing include [52, 7, 11, 55, 8, 10, 9].

Much of this work has focused on new proposals for selecting columns (*e.g.*, [66, 64, 41, 1, 40]) and/or coupling the method with downstream applications (*e.g.*, [5, 17, 33, 32, 42, 4]). The most detailed results are provided by [38] (as well as the conference papers on which it is based [36, 35, 37]). Interestingly, they observe that uniform sampling performs quite well, suggesting that in the data they considered the leverage scores are quite uniform, which also motivated the related work [57, 50]. This is in contrast with applications in genetics [53], term-document analysis [47], and astronomy [63], where the statistical leverage scores were seen to be very nonuniform in ways of interest to the downstream scientist; we return to this issue in Section 3.

On the theoretical side, much of the work has followed that of Drineas and Mahoney [21], who provided the first rigorous bounds for the Nyström extension of a general SPSD matrix. They show that when $\Omega(k\varepsilon^{-4}\ln\delta^{-1})$ columns are sampled with an importance sampling distribution that is proportional to the square of the diagonal entries of $\mathbf{A}$, then

$$\|\mathbf{A}-\mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\|_\xi \leq \|\mathbf{A}-\mathbf{A}_k\|_\xi + \varepsilon \sum\nolimits_{k=1}^{n} (\mathbf{A})_{ii}^2 \tag{4}$$

holds with probability $1-\delta$, where $\xi = 2, F$ represents the Frobenius or spectral norm. (Actually, they prove a stronger result of the form given in Equation (4), except with $\mathbf{W}^\dagger$ replaced with $\mathbf{W}_k^\dagger$, where $\mathbf{W}_k$ represents the best rank-k approximation to $\mathbf{W}$ [21].) Subsequently, Kumar, Mohri, and Talwalkar show that if sufficiently many columns (meaning $\Omega(\tau k \ln(k/\delta))$ columns, where τ is a measure of the coherence of the range of $\mathbf{A}$) are sampled uniformly at random with replacement from an $\mathbf{A}$ that has *exactly* rank k, then one achieves exact recovery, *i.e.*, $\mathbf{A} = \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T$, with high probability [36]. Gittens extends this to the case where $\mathbf{A}$ is only approximately low-rank [28]. In particular, he shows that if $\Omega(\mu k \ln k)$ columns are sampled uniformly at random (either with or without replacement), then

$$\left\|\mathbf{A}-\mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_2 \leq \|\mathbf{A}-\mathbf{A}_k\|_2\left(1+\frac{2n}{\ell}\right) \tag{5}$$

with probability exceeding $1-\delta$ and

$$\left\|\mathbf{A}-\mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_2 \leq \|\mathbf{A}-\mathbf{A}_k\|_2 + \frac{2}{\delta}\cdot\|\mathbf{A}-\mathbf{A}_k\|_\star \tag{6}$$

with probability exceeding $1-2\delta$. We have described these prior theoretical bounds in detail to emphasize how strong, relative to the prior work, our new bounds are. For example, Equation (4) provides an additive-error approximation with a very large scale; the bounds of Kumar, Mohri, and Talwalkar require a sampling complexity that depends on the coherence of the input matrix [36], which means that unless the coherence is very low one needs to sample essentially all the rows and columns in order to reconstruct the matrix; Equation (5) provides a bound where the additive scale depends on n; and Equation (6) provides a spectral norm bound where the scale of the additional error is the (much larger) trace norm. Table 1 compares the bounds on the approximation errors of SPSD sketches derived in this work to those available in the literature.

Our bounds in Table 1 (established as Lemmas 1–4 in Section 4.2) exhibit a common structure: for the spectral and Frobenius norms, we see that the additional error is on a larger scale than the optimal error, and the trace norm bounds all guarantee relative error approximations. This follows from, as detailed in Section 4.1, the fact that the SPSD sketching procedure can be understood as forming column-sample/projection-based approximations to the *square root* of $\mathbf{A}$, then squaring this approximation to obtain

sketch type	ℓ	$\Vert\mathbf{A}-\mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\Vert_2$	$\Vert\mathbf{A}-\mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\Vert_F$	$\Vert\mathbf{A}-\mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\Vert_\star$
Prior works				
[21], Nyström	$\Omega(\varepsilon^{-4}k)$	$\mathrm{opt}_2 + \varepsilon\sum_{i=}^n A_{ii}^2$	$\mathrm{opt}_F + \varepsilon\sum_{i=1}^n A_{ii}^2$	–
[10], Nyström	$\Omega(1)$	–	–	$\mathrm{O}\left(\frac{n-\ell}{n}\right)\Vert\mathbf{A}\Vert_\star$
[57], Nyström	$\Omega(\tau r \ln r)$	0	0	0
[38], Nyström	$\Omega(1)$	$\mathrm{opt}_2 + \mathrm{O}(\frac{2n}{\sqrt{\ell}})\Vert\mathbf{A}\Vert_2$	$\mathrm{opt}_F + \mathrm{O}(n(\frac{k}{\ell})^{1/4})\Vert\mathbf{A}\Vert_2$	–
This work				
Nyström	$\Omega((1-\varepsilon)^{-1}\mu k \ln k)$	$\mathrm{opt}_2(1+\frac{n}{\varepsilon\ell})$	$\mathrm{opt}_F(1+\sqrt{\varepsilon^{-1}}) + \varepsilon^{-1}\mathrm{opt}_\star$	$\mathrm{opt}_\star(1+\varepsilon^{-1})$
leverage-based	$\Omega((\beta\varepsilon)^{-1}k\ln(k/\beta))$	$\mathrm{opt}_2 + \varepsilon\mathrm{opt}_\star$	$(1+\sqrt{\varepsilon})\mathrm{opt}_F + \varepsilon\mathrm{opt}_\star$	$(1+\varepsilon)\mathrm{opt}_\star$
Fourier-based	$\Omega(\varepsilon^{-1}k\ln n \ln k)$	$\frac{\varepsilon}{(1-\sqrt{\varepsilon})\ln k}\left(\mathrm{opt}_2 + \frac{1}{\ln n}\mathrm{opt}_\star\right)$	$(1+\sqrt{\varepsilon})\mathrm{opt}_F + \varepsilon\mathrm{opt}_\star$	$(1+\varepsilon)\mathrm{opt}_\star$
Gaussian-based	$\Omega(k\varepsilon^{-1})$	$\frac{\varepsilon\ln k}{k}\mathrm{opt}_2 + \frac{\varepsilon}{k}\mathrm{opt}_\star$	$(1+\sqrt{\varepsilon})\mathrm{opt}_F + \sqrt{\varepsilon}\mathrm{opt}_\star$	$(1+\varepsilon)\mathrm{opt}_\star$

TABLE 1. Comparison of our bounds on the approximation errors of several types of SPSD sketches with those provided in prior works. Here, opt_ξ is the smallest ξ-norm error possible when approximating $\mathbf{A}$ with a rank-k matrix, $r = \mathrm{rank}(\mathbf{A})$, ℓ is the number of column samples sufficient for the stated bounds to hold, and k is a target rank. With the exception of [21], which samples columns with probability proportional to their Euclidean norms, and our novel leverage-based Nyström bound, these bounds are for sampling columns or linear combinations of columns uniformly at random. All bounds hold with constant probability.

the resulting approximation to $\mathbf{A}$. The squaring process unavoidably results in potentially large additional errors in the case of the spectral and Frobenius norms— whether or not the additional errors are large in practice depends upon the properties of the matrix and the form of stochasticity used in the sampling process. For instance, from our bounds it is clear that Gaussian-based SPSD sketches are expected to have lower additional error in the spectral norm than any of the other sketches considered.

We also see, in the case of uniform Nyström extensions, a necessary dependence on the coherence of the input matrix since columns are sampled uniformly at random. However, we also see that the scales of the additional error of the Frobenius and trace norm bounds are substantially improved over those in prior results. The large additional error in the spectral norm error bound is necessary in the worse case [28]. Lemmas 1, 2 and 3 in Section 4.2—which respectively address leverage-based, Fourier-based, and Gaussian-based SPSD sketches—show that spectral norm additive-error bounds with additional error on a substantially smaller scale can be obtained if one first mixes the columns before sampling from $\mathbf{A}$ or one samples from a judicious nonuniform distribution over the columns.

Table 2 illustrates the gap between the theoretical results currently available in the literature and what is observed in practice: it depicts the ratio between the error bounds in Table 1 and the average errors observed over 10 runs of the SPSD approximation algorithms (the error bound from [57] is not considered in the table, as it does not apply at the number of samples ℓ used in the experiments). Several trends can be identified; among them, we note that the bounds provided in this paper for Gaussian-based sketches come quite close to capturing the errors seen in practice, and the Frobenius and trace norm error guarantees of the leverage-based and Fourier-based sketches tend to more closely reflect the empirical behavior than the error guarantees provided in prior work for Nyström sketches. Overall, the trace norm error bounds are quite accurate. On the other hand, prior bounds are sometimes more informative in the case of the spectral norm (with the notable exception of the Gaussian sketches). Several important points can be gleaned from these observations. First, the accuracy of the Gaussian error bounds suggests that the main theoretical contribution of this work, the deterministic structural results given as Theorems 1 through 3, captures the underlying behavior of the SPSD sketching process. This supports our belief that this work provides a foundation for truly informative error bounds. Given that this is the case, it is clear that the analysis of the stochastic elements of the SPSD sketching process is much sharper in the Gaussian case than in the leverage-score, Fourier, and Nyström cases. We expect that, at least in the case of leverage and Fourier-based sketches, the stochastic analysis can and will be sharpened to produce error guarantees almost as informative as the ones we have provided for Gaussian-based sketches.

source, sketch	pred./obs. spectral error	pred./obs. Frobenius error	pred./obs. trace error
Enron, $k = 60$			
[21], Nyström	3041	66.2	–
[10], Nyström	–	–	2.0
[38], Nyström	331.2	77.7	–
Lemma 1, leverage-based	12888	21	1.2
Lemma 2, Fourier-based	201.0	42.7	1.6
Lemma 3, Gaussian-based	10.1	5.6	1.2
Lemma 4, Nyström	9.4	385.2	5.4
Protein, $k = 10$			
[21], Nyström	119.2	18.6	–
[10], Nyström	–	–	3.6
[38], Nyström	33.4	20.5	–
Lemma 1, leverage-based	42.5	6.9	2.0
Lemma 2, Fourier-based	297.5	21.7	3.1
Lemma 3, Gaussian-based	3.8	3.3	1.8
Lemma 4, Nyström	86.3	91.3	8
AbaloneD, $\sigma = .15, k = 20$			
[21], Nyström	349.9	42.5	–
[10], Nyström	–	–	2.0
[38], Nyström	62.9	46.7	–
Lemma 1, leverage-based	235.3	14.6	1.3
Lemma 2, Fourier-based	139.4	36.9	1.7
Lemma 3, Gaussian-based	5.2	4.7	1.1
Lemma 4, Nyström	12.9	228.3	5.1
WineS, $\sigma = 1, k = 20$			
[21], Nyström	422.5	41.0	–
[10], Nyström	–	–	2.1
[38], Nyström	72.8	44.2	–
Lemma 1, leverage-based	244.9	13.4	1.2
Lemma 2, Fourier-based	186.7	36.8	1.7
Lemma 3, Gaussian-based	6.6	4.7	1.2
Lemma 4, Nyström	13.7	222.6	5.1

Table 2. Comparison of the empirically observed approximation errors to the guarantees provided in this and other works, for several datasets. Each approximation was formed using $\ell = 6k \ln k$ samples. To evaluate the error guarantees, $\delta = 1/2$ was taken and all constants present in the statements of the bounds were replaced with ones. The observed errors were taken to be the average errors over 10 runs of the approximation algorithms. The datasets, described in Section 3.1, are representative of several classes of matrices prevalent in machine learning applications.

3. Empirical Aspects of SPSD Low-rank Approximation

In this section, we present our main empirical results, which consist of evaluating sampling and projection algorithms applied to a diverse set of SPSD matrices. In addition to understanding the relative merits, in terms of both running time and solution quality, of different sampling/projection schemes, we would like to understand the effects of various data preprocessing decisions. The bulk of our empirical evaluation considers two random projection procedures and two random sampling procedures for the sketching matrix $\mathbf{S}$: for random projections, we consider using SRFTs (Subsampled Randomized Fourier Transforms) as well as uniformly sampling from Gaussian mixtures of the columns; and for random sampling, we consider sampling columns uniformly at random as well as sampling columns according to a nonuniform importance sampling distribution that depends on the empirical statistical leverage scores. In the latter case of leverage score-based sampling, we also consider the use of both the (naïve and expensive) exact algorithm as well as a (recently-developed fast) approximation algorithm. Section 3.1 starts with a brief description of the data sets we consider; and then Section 3.2 briefly describes the effect of various data preprocessing decisions. Then, in Section 3.3, we present our main results on reconstruction quality for the random sampling and random projection methods; and, in Section 3.4, we discuss running time issues, and we present our main results for running time and reconstruction quality for both exact and approximate versions of leverage-based sampling.

We emphasize that we don't intend these results to be "comprehensive" but instead to be "illustrative" case-studies—that are representative of a much wider range of applications than have been considered previously. In particular, we would like to illustrate the tradeoffs between these methods in different realistic applications in order, *e.g.*, to provide directions for future work. For instance, *prima facie*, algorithms based on leverage-based column sampling might be expected to be more expensive than those based on uniform column sampling or random projections, but (based on previous work for general matrices [22, 23, 45]) they might also be expected to deliver lower approximation errors. Similarly, using approximate leverage scores to construct the importance sampling distribution might be expected to perform worse than using exact leverage scores, but this might be acceptable given its computational advantages. In addition to clarifying some of these issues, our empirical evaluation also illustrates ways in which existing theory is insufficient to explain the success of sampling and projection methods. This motivates our improvements to existing theory that we describe in Section 4.

With respect to our computation environment, all of our computations were conducted using 64-bit MATLAB R2012a under Ubuntu on a 2.6–GHz quad-core Intel i7 machine with 6Gb of RAM. To allow for accurate timing comparisons, all computations were carried out in a single thread. When applied to an $n \times n$ SPSD matrix $\mathbf{A}$, our implementation of the SRFT requires $\mathrm{O}(n^2 \ln n)$ operations, as it applies MATLAB's `fft` to the entire matrix $\mathbf{A}$ and *then* it samples ℓ columns from the resulting matrix. We note that the SRFT computation can be made more competitive: a more rigorous implementation of the SRFT algorithm could reduce this running time to $\mathrm{O}(n^2 \ln \ell)$; but due to the complexities involved in optimizing pruned FFT codes, we did not pursue this avenue.

3.1. **Data Sets.** Table 3 provides summary statistics for the data sets used in our empirical evaluation. In order to illustrate the complementary strengths and weaknesses of different sampling versus projection methods in a wide range of realistic applications, we consider four classes of matrices which are commonly encountered in machine learning and data analysis applications: normalized Laplacians of very sparse graphs drawn from "informatics graph" applications; dense matrices corresponding to Linear Kernels from machine learning applications; dense matrices constructed from a Gaussian Radial Basis Function Kernel (RBFK); and sparse RBFK matrices constructed using Gaussian radial basis functions, truncated to be nonzero only for nearest neighbors. Although not exhaustive, this collection of data sets represents a wide range of data sets with very different (sparsity, spectral, leverage score, etc.) properties that have been of interest recently not only in machine learning but in data analysis more generally.

To understand better the Laplacian data, recall that, given a graph with weighted adjacency matrix $\mathbf{W}$, its normalized graph Laplacian is

$$\mathbf{A} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2},$$

where $\mathbf{D}$ is the diagonal matrix of weighted degrees of the nodes of the graph, *i.e.*, $D_{ii} = \sum_{j \neq i} W_{ij}$. This Laplacian is an SPSD matrix, but note that *not* all SPSD matrices can be written as the Laplacian of a graph. Similarly, to understand better the remaining data, recall that, given a set of data points $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$, the Linear Kernel matrix $\mathbf{A}$ corresponding to those points is given by

$$A_{ij} = \langle \mathbf{x}_i, \mathbf{x}_k \rangle.$$

Given the same set of data points, one can construct more general nonlinear kernels. For example, a Gaussian RBFK matrix $\mathbf{A}^\sigma$ is given by

$$A_{ij}^\sigma = \exp\left(\frac{-\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}{\sigma^2}\right),$$

where σ, a nonnegative number, defines the scale of the kernel. Informally, σ defines the "size scale" over which pairs of points $\mathbf{x}_i$ and $\mathbf{x}_j$ "see" each other. Typically σ is determined by a global cross-validation criterion, as $\mathbf{A}^\sigma$ is generated for some specific machine learning task; and, thus, one may have no *a priori* knowledge of the behavior of the spectrum or leverage scores of $\mathbf{A}^\sigma$ as σ is varied. Accordingly, we consider

Name	Description	n	d	%nnz
Laplacian Kernels				
HEP	arXiv High Energy Physics collaboration graph	9877	NA	0.06
GR	arXiv General Relativity collaboration graph	5242	NA	0.12
Enron	subgraph of the Enron email graph	10000	NA	0.22
Gnutella	Gnutella peer to peer network on Aug. 6, 2002	8717	NA	0.09
Linear Kernels				
Dexter	bag of words	2000	20000	83.8
Protein	derived feature matrix for S. cerevisiae	6621	357	99.7
SNPs	DNA microarray data from cancer patients	5520	43	100
Gisette	images of handwritten digits	6000	5000	100
Dense RBF Kernels				
AbaloneD	physical measurements of abalones	4177	8	100
WineD	chemical measurements of wine	4898	12	100
Sparse RBF Kernels				
AbaloneS	physical measurements of abalones	4177	8	82.9/48.1
WineS	chemical measurements of wine	4898	12	11.1/88.0

TABLE 3. The data sets used in our empirical evaluation ([39], [34], [30], [29], [51], [16], [2]). Here, n is the number of data points, and d is the number of features in the input space before kernelization. For Laplacian "kernels," n is the number of nodes in the graph (and thus there is no d since the graph is "given" rather than "constructed"). The %nnz for the Sparse RBF Kernels depends on the σ parameter; see Table 4.

Gaussian RBFK matrices with different values of σ. Finally, given the same data points, $\mathbf{x}_1, \ldots, \mathbf{x}_n$, one can construct sparse Gaussian RBFK matrices

$$A_{ij}^{(\sigma,\nu,C)} = \left[\left(1 - \frac{\|\mathbf{x}_i - \mathbf{x}_j\|_2}{C}\right)^{\nu}\right]^{+} \cdot \exp\left(\frac{-\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}{\sigma^2}\right),$$

where $[x]^+ = \max\{0, x\}$. When ν is larger than $(d+1)/2$, this matrix is positive semidefinite; and as the cutoff point C decreases this matrix becomes more sparse [27]. For simplicity, in our empirical evaluation, we fix $\nu = \lceil (d+1)/2 \rceil$ and $C = 3\sigma$, and we vary σ. As with the effect of varying σ, the effect of varying the sparsity parameter C is not obvious *a priori*— C is typically chosen according to a global criterion to ensure good performance at a specific machine learning task, without consideration for its effect on the spectrum or leverage scores of $A_{ij}^{(\sigma,\nu,C)}$.

To illustrate the diverse range of properties exhibited by these four classes of data sets, consider Table 4. Several observations are particularly relevant to our discussion below.

- All of the Laplacian Kernels drawn from informatics graph applications are extremely sparse in terms of number of nonzeros, and they all tend to have very slow spectral decay, as illustrated both by the quantity $\lceil \|\mathbf{A}\|_{\mathrm{F}}^2 / \|\mathbf{A}\|_2^2 \rceil$ (this is the *stable rank*, which is a numerically stable (under)estimate of the rank of $\mathbf{A}$) as well as by the relatively small fraction of the Frobenius norm that is captured by the best rank-k approximation to $\mathbf{A}$. For the Laplacian Kernels we considered two values of the rank parameter k that were chosen (somewhat) arbitrarily; many of the results we report continue to hold qualitatively if k is chosen to be (say) an order of magnitude larger.
- Both the Linear Kernels and the Dense RBF Kernels are much denser and are much more well-approximated by moderately to very low-rank matrices. In addition, both the Linear Kernels and the Dense RBF Kernels have statistical leverage scores that are much more uniform—there are several ways to illustrate this, none of them perfect, and here, we illustrate this by considering the k^{th} largest leverage score. For the Linear Kernels and the Dense RBF Kernels, this quantity is one to two orders of magnitude smaller than for the Laplacian Kernels.
- For the Dense RBF Kernels, we consider two values of the σ parameter, again chosen (somewhat) arbitrarily. For both AbaloneD and WineD, we see that decreasing σ from 1 to 0.15, *i.e.*, letting

Name	%nnz	$\left\lceil \frac{\|\mathbf{A}\|_{\mathrm{F}}^2}{\|\mathbf{A}\|_2^2} \right\rceil$	k	$\frac{\lambda_{k+1}}{\lambda_k}$	$100\frac{\|\mathbf{A}-\mathbf{A}_k\|_{\mathrm{F}}}{\|\mathbf{A}\|_{\mathrm{F}}}$	$100\frac{\|\mathbf{A}-\mathbf{A}_k\|_\star}{\|\mathbf{A}\|_\star}$	kth-largest leverage score
HEP	0.06	3078	20	0.998	7.8	0.4	0.261
HEP	0.06	3078	60	0.998	13.2	1.1	0.278
GR	0.12	1679	20	0.999	10.5	0.74	0.286
GR	0.12	1679	60	1	17.9	2.16	0.289
Enron	0.22	2588	20	0.997	7.77	0.352	0.492
Enron	0.22	2588	60	0.999	12.0	0.94	0.298
Gnutella	0.09	2757	20	1	8.1	0.41	0.381
Gnutella	0.09	2757	60	0.999	13.7	1.20	0.340
Dexter	83.8	176	8	0.963	14.5	.934	0.067
Protein	99.7	24	10	0.987	42.6	7.66	0.008
SNPs	100	3	5	0.928	85.5	37.6	0.002
Gisette	100	4	12	0.90	90.1	14.6	0.005
AbaloneD (dense, $\sigma = .15$)	100	41	20	0.992	42.1	3.21	0.087
AbaloneD (dense, $\sigma = 1$)	100	4	20	0.935	97.8	59	0.012
WineD (dense, $\sigma = 1$)	100	31	20	0.99	43.1	3.89	0.107
WineD (dense, $\sigma = 2.1$)	100	3	20	0.936	94.8	31.2	0.009
AbaloneS (sparse, $\sigma = .15$)	82.9	400	20	0.989	15.4	1.06	0.232
AbaloneS (sparse, $\sigma = 1$)	48.1	5	20	0.982	90.6	21.8	0.017
WineS (sparse, $\sigma = 1$)	11.1	116	20	0.995	29.5	2.29	0.2
WineS (sparse, $\sigma = 2.1$)	88.0	39	20	0.992	41.6	3.53	0.098

Table 4. Summary statistics for the data sets from Table 3 that we used in our empirical evaluation.

data points "see" fewer nearby points, has two important effects: first, it results in matrices that are much less well-approximated by low-rank matrices; and second, it results in matrices that have much more heterogeneous leverage scores. For example, for AbaloneD, the fraction of the Frobenius norm that is captured decreases from 97.8 to 42.1 and the k^{th} largest leverage score increases from 0.012 to 0.087.

- For the Sparse RBF Kernels, there are a range of sparsities, ranging from above the sparsity of the sparsest Linear Kernel, but all are denser than the Laplacian Kernels. Changing the σ parameter has the same effect (although it is even more pronounced) for Sparse RBF Kernels as it has for Dense RBF Kernels. In addition, "sparsifying" a Dense RBF Kernel also has the effect of making the matrix less well approximated by a low-rank matrix and of making the leverage scores more nonuniform. For example, for AbaloneD with $\sigma = 1$ (respectively, $\sigma = 0.15$), the fraction of the Frobenius norm that is captured decreases from 97.8 (respectively, 42.1) to 90.6 (respectively, 15.4), and the k^{th} largest leverage score increases from 0.012 (respectively, 0.087) to 0.017 (respectively, 0.232).

As we see below, when we consider the RBF Kernels as the width parameter and sparsity are varied, we observe a range of intermediate cases between the extremes of Linear Kernels and Laplacian Kernels.

3.2. **Effects of Data Analysis Preprocessing Decisions.** Before proceeding with our main empirical results, we pause to describe the effects of various machine learning and data analysis "design decisions" on the behavior of both Nyström-based algorithms in general as well as on the behavior of the statistical leverage scores in particular. We should emphasize that, for "worst case" matrices, very little can be said in this regard. Thus, these observations are based on our experiences with the diverse data sets from Section 3.1. While not completely general, these observations are likely to hold in modified form for many other realistic data, and they can potentially be useful as heuristic guides to practice. For example, if preprocessing does not significantly change the leverage score distribution, then one could compute the leverage scores on the raw data and use these to sample columns from the processed data or to certify that the data have low coherence. Likewise, the behavior of the leverage scores as the rank parameter k is varied or as the σ scale parameter of RBF kernels varies is of interest, as it is expensive to compute the leverage scores anew for each value of k or σ as part of a cross-validation computation.

One common preprocessing step is to "whiten" the data before applying a machine learning algorithm. If the data are given in the form of $\mathbf{X} \in \mathbb{R}^{n \times d}$ where the ith row of $\mathbf{X}$ is an observation of d covariates, then these covariates may have different means and characteristic size scales (*i.e.*, variances). In this case, it is often appropriate to transform the covariates so they all have zero mean and are on the same size scale. The whitening transform generates a new matrix $\hat{\mathbf{X}}$, corresponding to these transformed covariates, by removing the mean of each column and rescaling the columns so they all have unit norm. In our experience, whitening modifies the statistical leverage scores, often by making them somewhat more homogeneous, but for a fixed rank parameter k it does not change them too substantially, *e.g.*, to within no more than a multiplicative factor of 2. Given the sensitivity of matrix reconstruction algorithms to various structural properties of the input data that we describe below, however, the more important observation is that whitening tends to decrease the effective rank of the input data set, and at the same time it often tends to shrink the spectral gaps. As shown below, this has observable consequences on the reconstruction errors of all the Nyström methods considered, but in particular those involving approximate leverage score computations.

Another preprocessing decision has to do with the choice of rank k with which to describe the data. This is typically determined according to an exogeneously-specified "model selection" criterion that does not explicitly take into account the spectrum or leverage score structure of the input matrix. It enters our discussion since we consider sampling columns with probabilities proportional to their statistical leverage scores *relative to a rank-k space*, and thus the leverage scores depend on k. In our experience, increasing k tends to uniformize or homogeneize the leverage scores, often gradually, but sometimes quite substantially. (We should note, however, that there are exceptions to this, where one observes very strong localization on low-order eigenvectors of data matrices [18].)

Yet another preprocessing decision has to do with the choice of the σ scale parameter in Gaussian RBFK matrices. As with the rank parameter, the scale parameter σ in practice is determined according to an exogeneously-specified model selection criterion that does not explicitly take into account the spectrum or leverage score structure of the input matrix. In our experience, as σ increases, the leverage scores become more and more uniform; and they become more heterogeneous as σ decreases. Informally, as a data point "sees" more data points, any outlying effect is mitigated. Varying σ also has an effect on the spectrum. As a general rule, letting $\sigma \to 0$ tends to make the spectrum of $\mathbf{A}^\sigma$ flatter, *i.e.*, decay more slowly, and letting $\sigma \to \infty$ makes $\mathbf{A}^\sigma$ lower-rank. Recall that the diagonal entries of $\mathbf{A}^\sigma$ are identically one, and as $\sigma \to \infty$, $\mathbf{A}^\sigma$ tends to the matrix of all ones. That is, increasing σ corresponds to considering all the observations $\mathbf{x}_i$ as being equally dissimilar, so all columns are equally noninformative. On the other hand, as $\sigma \to 0$, $\mathbf{A}^\sigma$ approaches the identity, and very dissimilar observations (in the sense that $\|\mathbf{x}_i - \mathbf{x}_j\|_2$ is large) are penalized more heavily than similar observations, and thus there is some nonuniformity in the columns of $\mathbf{A}^\sigma$. In some cases, we observed that, as the scale σ decreases, the leverage scores stabilize, identifying the same columns as being important or influential over a range of scales.

3.3. Reconstruction Accuracy of Sampling and Projection Algorithms.

Here, we describe the performances of the various Nyström-based low-rank extensions—column sampling uniformly at random without replacement, column sampling according to the nonuniform leverage score probabilities, and sampling using Gaussian and SRFT mixtures of the columns—in terms of reconstruction accuracy for the data sets described in Section 3.1. We describe general observations we have made about each class of matrices in turn, and then we summarize our observations. We consider only the use of exact leverage scores here, and we postpone until Section 3.4 a discussion of running time issues and similar reconstruction results when approximate leverage scores are used for the importance sampling distribution. In each case, we present results for both the "non-rank-restricted" case as well as the "rank-restricted" case. Recall that by non-rank-restricted, we mean that the error

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_\xi / \left\|\mathbf{A} - \mathbf{A}_k\right\|_\xi \tag{7}$$

is plotted; while by rank-restricted, we mean that the error

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}_k^\dagger\mathbf{C}^T\right\|_\xi / \left\|\mathbf{A} - \mathbf{A}_k\right\|_\xi \tag{8}$$

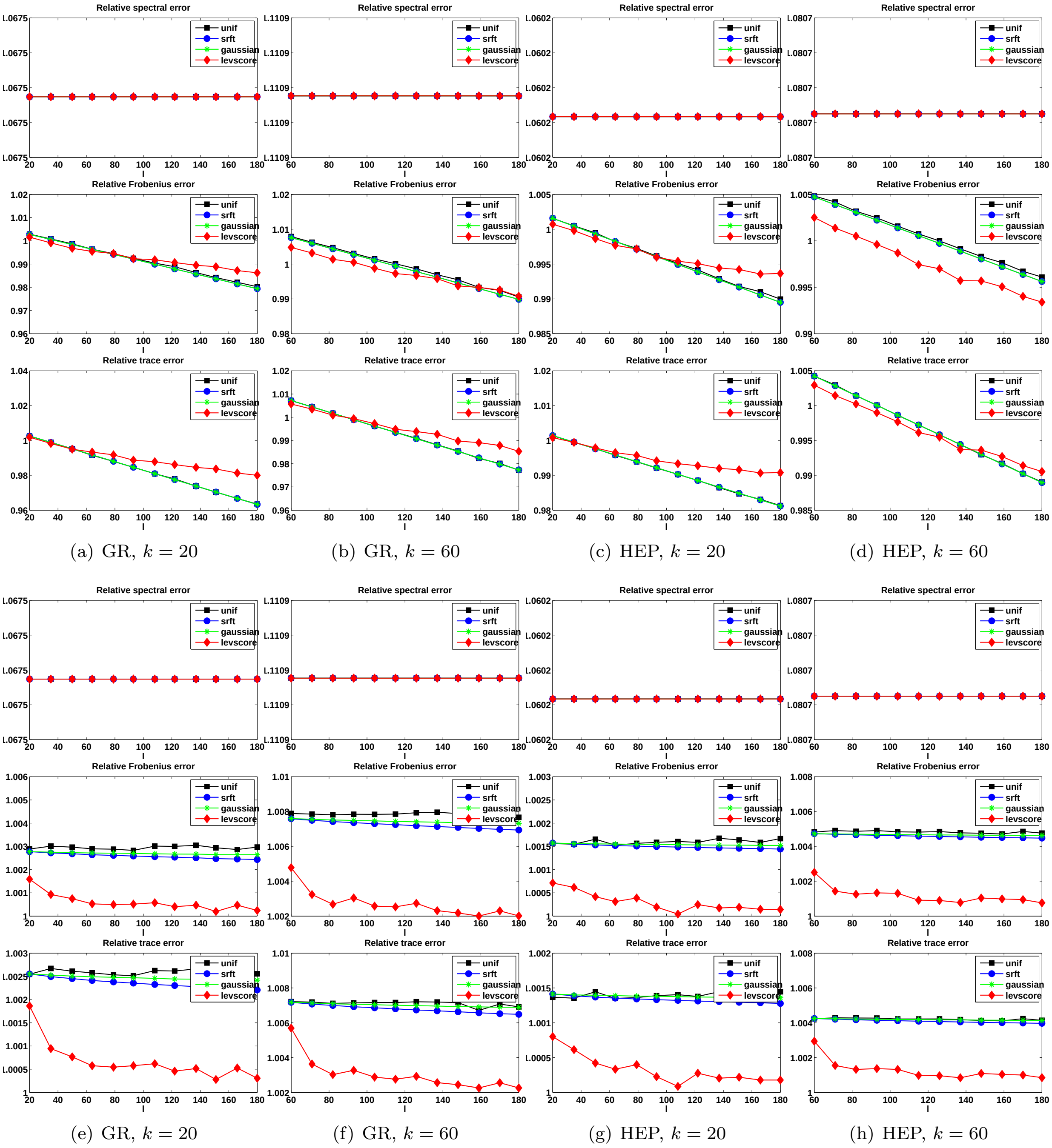
is plotted. Note that previous work has shown that relative-error guarantees can be obtained, *e.g.*, with CUR matrix decompositions, not only when one projects onto the span of judiciously-chosen columns, analogously to Eqn. (7) and as our worst-case guarantees in this paper are formulated, but also when one restricts the rank of the low-rank approximation to be no greater than k by projecting onto the best rank-k approximation to the original matrix [22]. We evaluate the "rank-restricted" case of the form of Eqn. (8), that depends on projecting onto the best rank-k approximation of the subsample (and not the original matrix) since it is more algorithmically tractable; but we note that similar but "smoother" results (*e.g.*, the error is much more monotonic as a function of the number of samples, when compared with the "rank-restricted" results we present below) are obtained empirically with this more expensive rank-restriction procedure.

Finally, we note that previous work has shown that the statistical leverage scores reflect an important nonuniformity structure in the columns of the general data matrices [47, 45]; that randomly sampling columns according to this distribution results in lower worst-case error (for problems such as least-squares approximation and low-rank approximation of general matrices) than sampling columns uniformly at random [22, 23, 45]; and that leverage scores have proven useful in a wide range of practical applications [53, 47, 45, 63]. In spite of this, ours is the first work to implement and evaluate leverage score sampling for low-rank approximation of SPSD matrices.

3.3.1. *Graph Laplacians.* Figure 1 and Figure 2 show the reconstruction error results for sampling and projection methods applied to several normalized graph Laplacians. The former shows GR and HEP, each for two values of the rank parameter, and the latter shows Enron and Gnutella, again each for two values of the rank parameter. Both figures show the spectral, Frobenius, and trace norm approximation errors, as a function of the number of column samples ℓ, relative to the error of the optimal rank-k approximation of $\mathbf{A}$. In both figures, the first four (*i.e.*, top) subfigures show the results for the non-rank-restricted case, and the last four (*i.e.*, bottom) subfigures show the results for the rank-restricted case. In particular, in the rank-restricted case, the low-rank approximation is "filtered" through a rank-k space, and thus the approximation ratio is always greater than unity.

These and subsequent figures contain a lot of information, some of which is peculiar to the given data sets and some of which is more general. In light of subsequent discussion, several observations are worth making about the results presented in these two figures.

- All of the Nyström extensions provide quite accurate approximations—relative to the best possible approximation factor for that norm, and relative to bounds provided by existing theory, as reviewed in Section 2.3—even with only k column samples (or in the case of the Gaussian and SRFT mixtures, with only k linear combinations of vectors). Upon examination, this is partly due to the extreme sparsity and extremely slow spectral decay of these data sets which means, as shown in Table 3, that only a small fraction of the (spectral or Frobenius or trace) mass is captured by the optimal rank 20 or 60 approximation. Thus although an SPSD sketch constructed from 20 or 60 vectors also only captures a small portion of the mass of the matrix, the relative error is small.
- The scale of the Y axes is different between different figures and subfigures. This is to highlight properties within a given plot, but it can hide several things. In particular, note that the scale for the spectral norm is generally larger than for the Frobenius norm, which is generally larger than for the trace norm, consistent with the size of those norms; and that the scale is larger for higher-rank approximations, *e.g.* compare GR $k = 20$ with GR $k = 60$, also consistent with the larger amount of mass captured by higher-rank approximations.
- Both the non-rank-restricted and rank-restricted results are the same for $\ell = k$. For $\ell > k$, the non-rank-restricted errors tend to decrease (or at least not increase, as for GR and HEP the spectral norm error is flat as a function of ℓ), which is intuitive. While the rank-restricted errors also tend to decrease for $\ell > k$, the decrease is much less (since the rank-restricted plots are bounded below by unity) and the behavior is much more complicated as a function of increasing ℓ.
- The X axes ranges from k to $9k$ for the $k = 20$ plots and to $3k$ for the $k = 60$ plots. As a practical matter, choosing ℓ between k and (say) $2k$ or $3k$ is probably of greatest interest. In this regime, there is an interesting tradeoff for the non-rank-restricted plots: for moderately large values of ℓ in this regime, the error for leverage-based sampling is moderately better than for uniform sampling or random projections, while if one chooses ℓ to be much larger then the improvements from leverage-based sampling saturate and the uniform sampling and random projection methods are better. This is most obvious in the Frobenius norm plots, although it is also seen in the trace norm plots, and it suggests that some combination of leverage-based sampling and uniform sampling might be best.



(a) GR, $k = 20$

(b) GR, $k = 60$

(c) HEP, $k = 20$

(d) HEP, $k = 60$

(e) GR, $k = 20$

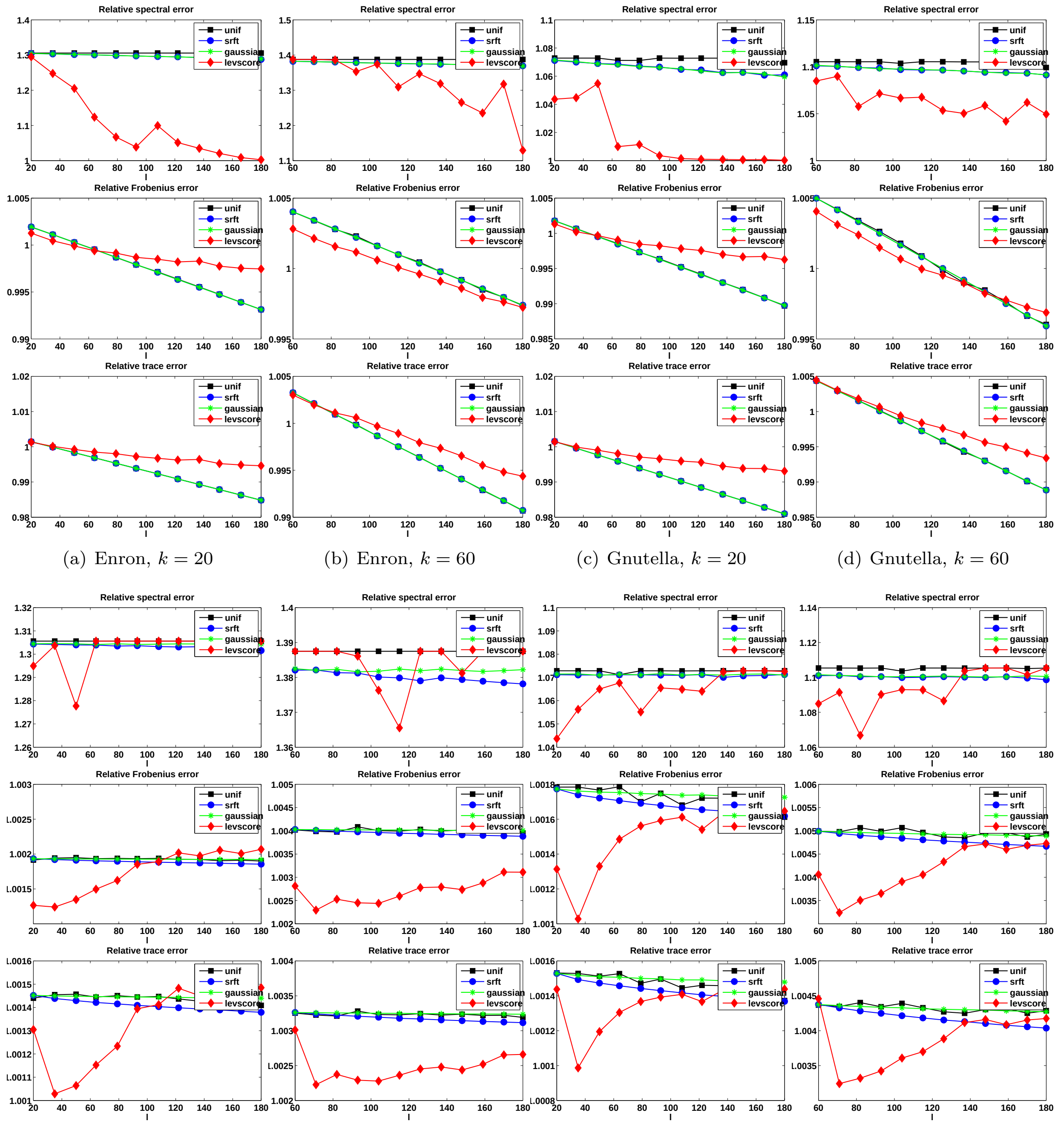
(f) GR, $k = 60$

(g) HEP, $k = 20$

(h) HEP, $k = 60$

FIGURE 1. The spectral, Frobenius, and trace norm errors (top to bottom, respectively, in each subfigure) of several (non-rank-restricted in top panels and rank-restricted in bottom panels) SPSD sketches, as a function of the number of columns samples ℓ, for the GR and HEP Laplacian data sets, with two choices of the rank parameter k.

- For the rank-restricted plots, in some cases, *e.g.*, with GR and HEP, the errors for leverage-based sampling are much better than for the other methods and quickly improve with increasing ℓ until they saturate; while in other cases, *e.g.*, with Enron and Gnutella, the errors for leverage-based sampling improve quickly and then degrade with increasing ℓ. Upon examination, the former phenomenon is similar to what was observed in the non-rank-restricted case and is due to the strong "bias" provided



(a) Enron, $k = 20$ (b) Enron, $k = 60$ (c) Gnutella, $k = 20$ (d) Gnutella, $k = 60$

(e) Enron, $k = 20$ (f) Enron, $k = 60$ (g) Gnutella, $k = 20$ (h) Gnutella, $k = 60$

FIGURE 2. The spectral, Frobenius, and trace norm errors (top to bottom, respectively, in each subfigure) of several (non-rank-restricted in top panels and rank-restricted in bottom panels) SPSD sketches, as a function of the number of columns samples ℓ, for the Enron and Gnutella Laplacian data sets, with two choices of the rank parameter k.

by the leverage score importance sampling distribution to the top part of the spectrum, allowing the sampling process to focus very quickly on the low-rank part of the input matrix. (In some cases, this is due to the fact that the heterogeneity of the leverage score importance sampling distribution means that one is likely to choose the same high leverage columns multiple times, rather than increasing the accuracy of the extension by adding new columns whose leverage scores are lower.) The latter phenomenon of degrading error quality as ℓ is increased is more complex and seems to be due to some sort or "overfitting" caused by this strong bias and by choosing many more than k columns.

- The behavior of the approximations with respect to the spectral norm is quite different from the behavior in the Frobenius and trace norms. In the latter, as the number of samples ℓ increases, the errors tend to decrease, although in an erratic manner for some of the rank-restricted plots; while for the former, the errors tend to be much flatter as a function of increasing ℓ for at least the Gaussian, SRFT, and uniformly sampled extensions.

All in all, there seems to be quite complicated behavior for low-rank extensions for these Laplacian data sets. Several of these observations can also be made for subsequent figures; but in some other cases the (very sparse and not very low rank) structural properties of the data are primarily responsible.

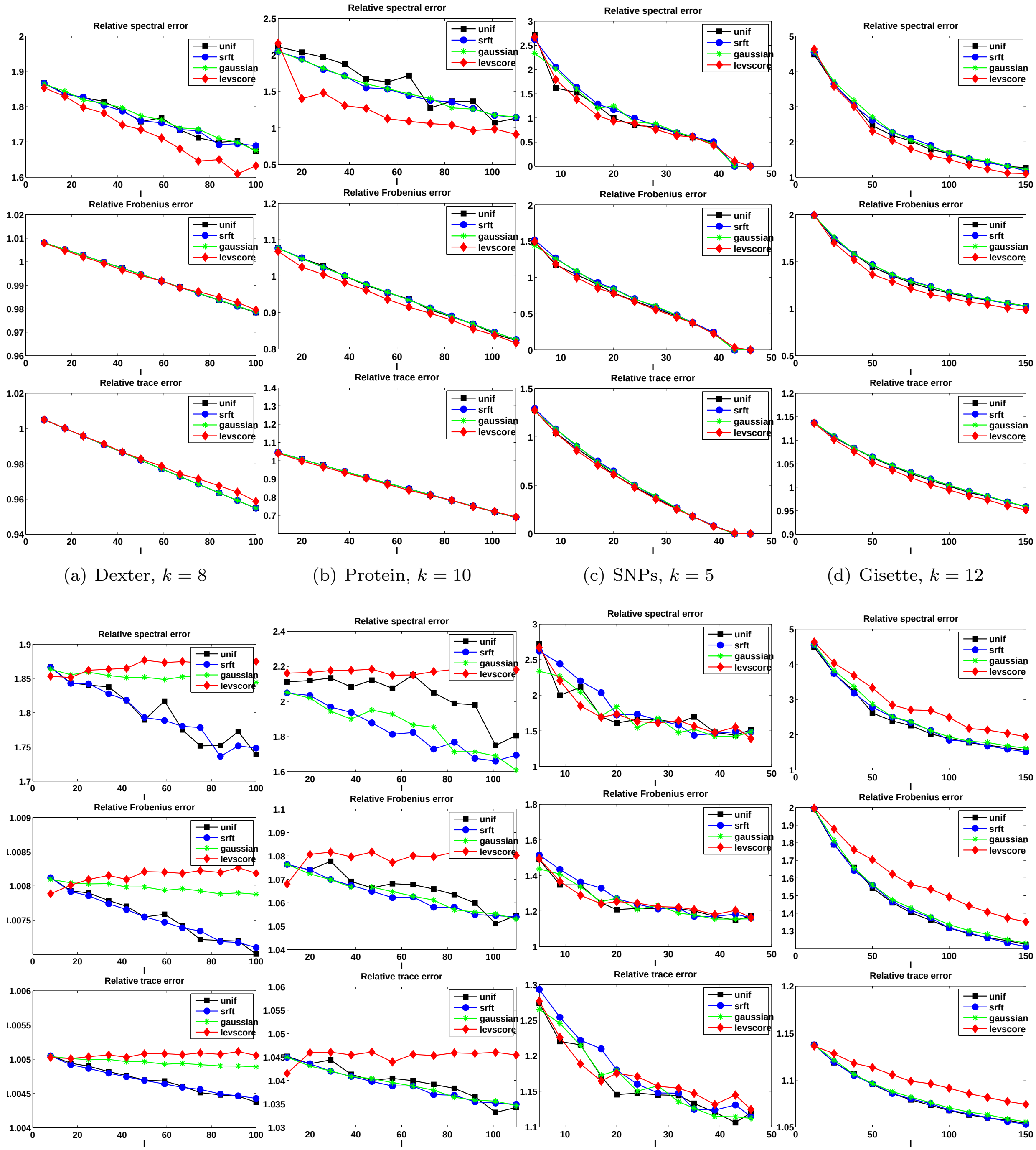
3.3.2. *Linear Kernels.* Figure 3 shows the reconstruction error results for sampling and projection methods applied to several Linear Kernels. The data sets (Dexter, Protein, SNPs, and Gisette) are all quite low-rank and have fairly uniform leverage scores. Several observations are worth making about the results presented in this figure.

- All of the methods perform quite similarly for the non-rank-restricted case: all have errors that decrease smoothly with increasing ℓ, and in this case there is little advantage to using methods other than uniform sampling (since they perform similarly and are more expensive). Also, since the ranks are so low and the leverage scores are so uniform, the leverage score extension is no longer significantly distinguished by its tendency to saturate quickly.
- The scale of the Y axes is much larger than for the Laplacian data sets, mostly since the matrices are much more well-approximated by low-rank matrices, although the scale decreases as one goes from spectral to Frobenius to trace reconstruction error, as before.
- For SNPs and Gisette, the rank-restricted reconstruction results are very similar for all four methods, with a smooth decrease in error as ℓ is increased, although interestingly using leverage scores is slightly worse for Gisette. For Dexter and Protein, the situation is more complicated: using the SRFT always leads to smooth decrease as ℓ is increased, and uniform sampling generally behaves the same way also; Gaussian projections behave this way for Protein, but for Dexter Gaussian projections are noticably worse than SRFT and uniform sampling; and, except for very small values of ℓ, leverage-based sampling is worse still and gets noticably worse as ℓ is increased. Even this poor behavior of leverage score sampling on the Linear Kernels is notably worse than for the rank-restricted Laplacians, where there was a range of moderately small ℓ where leverage score sampling was much superior to other methods.

These linear kernels (and also to some extent the dense RBF kernels below that have larger σ parameter) are examples of relatively "nice" machine learning data sets that are similar to matrices where uniform sampling has been shown to perform well previously [56, 36, 37, 38]; and for these matrices our empirical results agree with these prior works.

3.3.3. *Dense and Sparse RBF Kernels.* Figure 4 and Figure 5 present the reconstruction error results for sampling and projection methods applied to several dense RBF and sparse RBF kernels. Several observations are worth making about the results presented in these figures.

- For the non-rank-restricted results, all of the methods have errors that decrease with increasing ℓ. In particular, for larger values of σ and for denser data, the decrease is somewhat more regular, and the four methods tend to perform similarly. For larger values of σ and sparser data, leverage score sampling is somewhat better. This parallels what we observed with the Linear Kernels, except that here the leverage score sampling is somewhat better for all values of ℓ.
- For the non-rank-restricted results for the smaller values of σ, leverage score sampling tends to be much better than uniform sampling and projection-based methods. For the sparse data, however, this effect saturates; and we again observe (especially when σ is smaller in AbaloneS and WineS) the tradeoff we observed previously with the Laplacian data—leverage score sampling is better when ℓ is moderately larger than k, while uniform sampling and random projections are better when ℓ is much larger than k.
- For the rank-restricted results, we see that when σ is large, all of the results tend to perform similarly. (The exception to this is WineS, for which leverage score sampling starts out much better than other

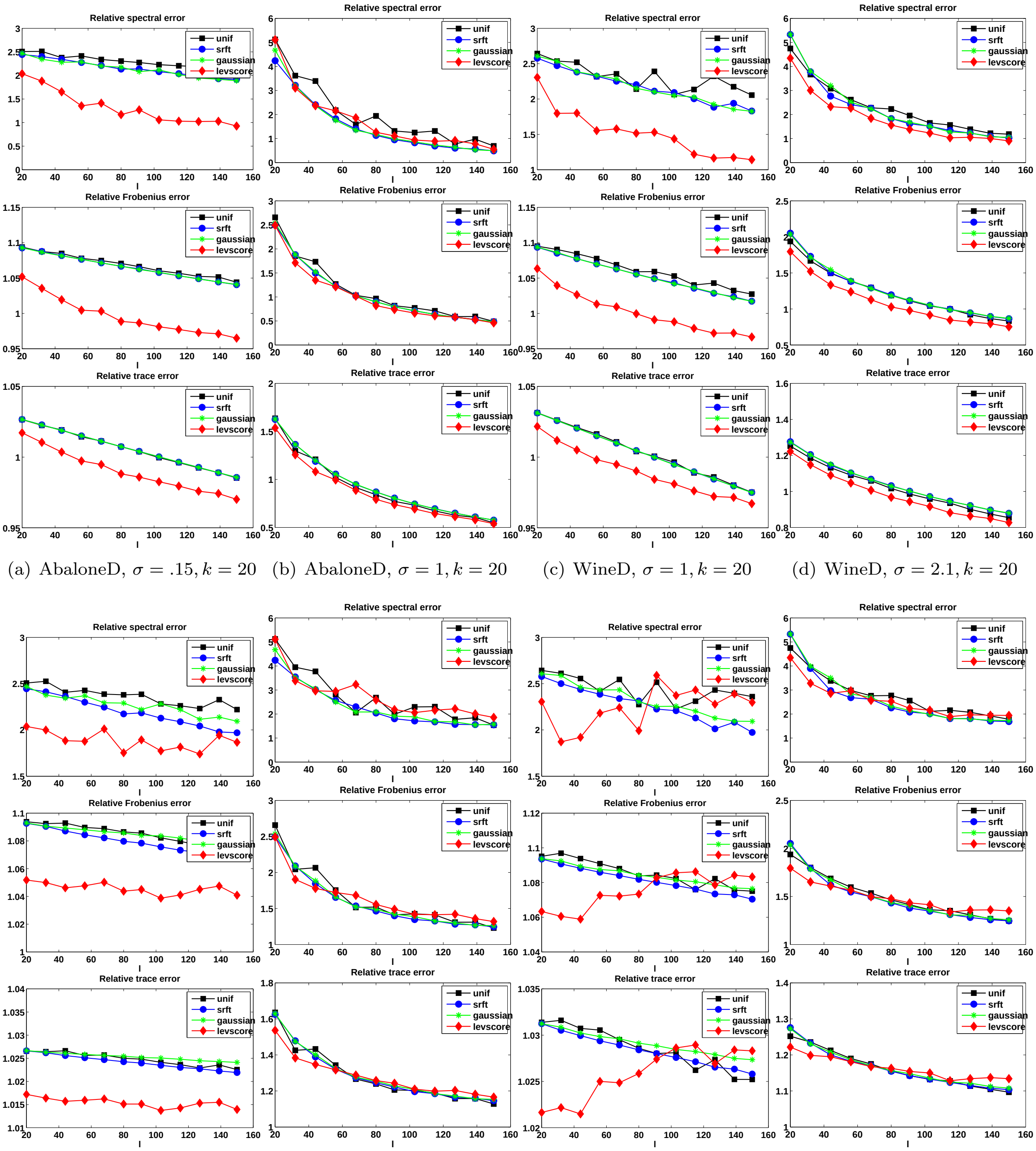


(a) Dexter, $k = 8$ (b) Protein, $k = 10$ (c) SNPs, $k = 5$ (d) Gisette, $k = 12$

(e) Dexter, $k = 8$ (f) Protein, $k = 10$ (g) SNPs, $k = 5$ (h) Gisette, $k = 12$

FIGURE 3. The spectral, Frobenius, and trace norm errors (top to bottom, respectively, in each subfigure) of several (non-rank-restricted in top panels and rank-restricted in bottom panels) SPSD sketches, as a function of the number of columns samples ℓ, for the Linear Kernel data sets.

methods and then gets worse as ℓ is increased.) On the other hand, when σ is small, the results are more complex. Leverage score sampling is typically much better than other methods, although the results are quite choppy as a function of ℓ, and in some cases the effect diminished as ℓ is increased.

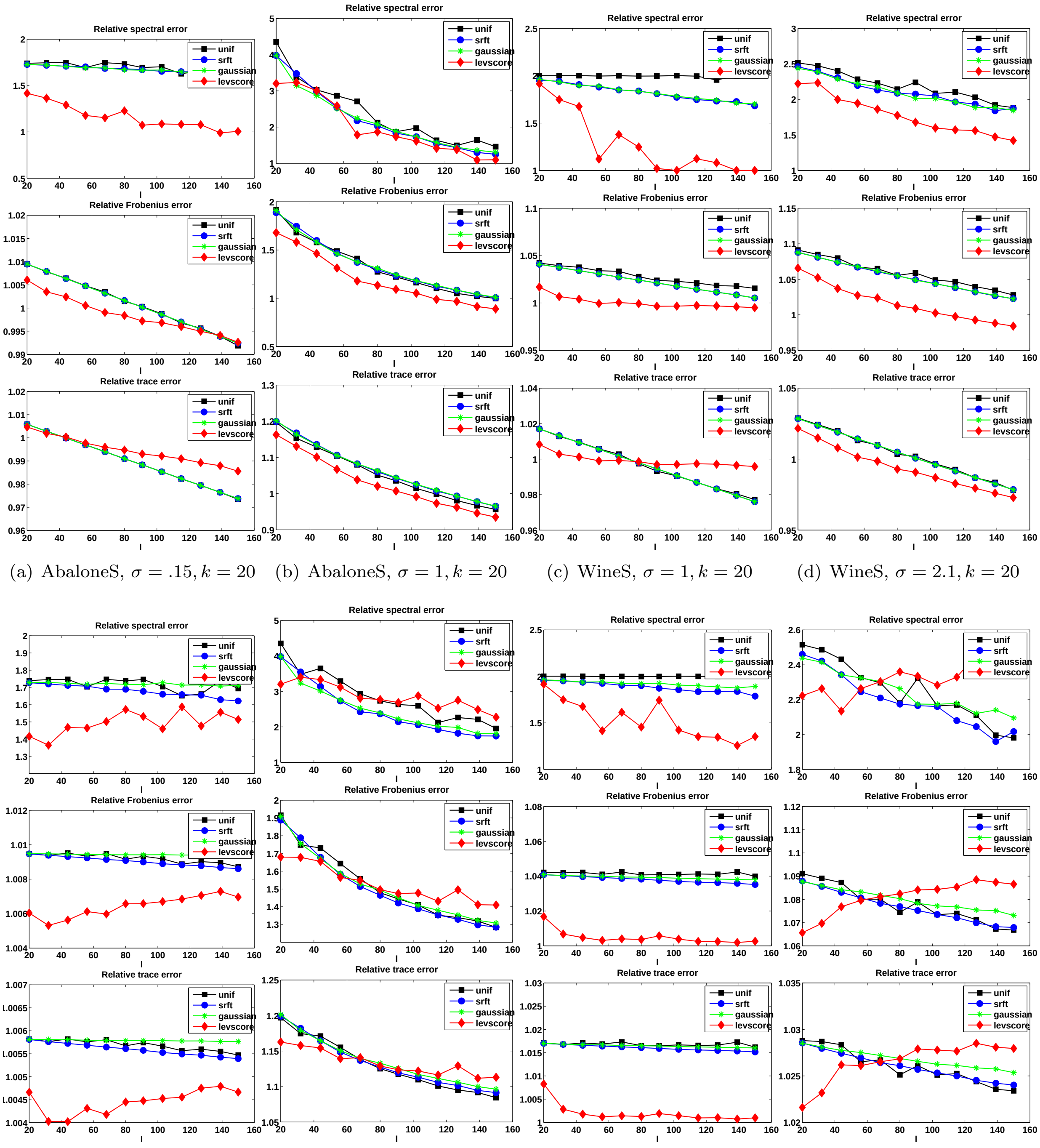


(a) AbaloneD, $\sigma = .15, k = 20$ (b) AbaloneD, $\sigma = 1, k = 20$ (c) WineD, $\sigma = 1, k = 20$ (d) WineD, $\sigma = 2.1, k = 20$

(e) AbaloneD, $\sigma = .15, k = 20$ (f) AbaloneD, $\sigma = 1, k = 20$ (g) WineD, $\sigma = 1, k = 20$ (h) WineD, $\sigma = 2.1, k = 20$

FIGURE 4. The spectral, Frobenius, and trace norm errors (top to bottom, respectively, in each subfigure) of several (non-rank-restricted in top panels and rank-restricted in bottom panels) SPSD sketches, as a function of the number of columns samples ℓ, for several dense RBF data sets.

Recall from Table 4 that for smaller values of σ and for sparser kernels, the SPSD matrices are less well-approximated by low-rank matrices, and they have more heterogeneous leverage scores. Thus, they are more similar to the Laplacian data than the Linear Kernel data; and this suggests (as we have observed) that



(a) AbaloneS, $\sigma = .15, k = 20$ (b) AbaloneS, $\sigma = 1, k = 20$ (c) WineS, $\sigma = 1, k = 20$ (d) WineS, $\sigma = 2.1, k = 20$

(e) AbaloneS, $\sigma = .15, k = 20$ (f) AbaloneS, $\sigma = 1, k = 20$ (g) WineS, $\sigma = 1, k = 20$ (h) WineS, $\sigma = 2.1, k = 20$

Figure 5. The spectral, Frobenius, and trace norm errors (top to bottom, respectively, in each subfigure) of several (non-rank-restricted in top panels and rank-restricted in bottom panels) SPSD sketches, as a function of the number of columns samples ℓ, for several sparse RBF data sets.

leverage score sampling should perform relatively better than uniform column sampling and projection-based schemes when in these two cases. In particular, nowhere do we see that leverage score sampling performs much worse than other methods, as we saw with the rank-restricted Linear Kernel results.

3.3.4. *Summary of Comparison of Sampling and Projection Algorithms.* Before proceeding, there are several summary observations that we can make about sampling versus projection methods for the data sets we have considered.

- Linear Kernels and to a lesser extent Dense RBF Kernels with larger σ parameter have relatively low-rank and relatively uniform leverage scores, and in these cases uniform sampling does quite well. These data sets correspond most closely with those that have been studied previously in the machine learning literature, and for these data sets our results are in agreement with that prior work.
- Sparsifying RBF Kernels and/or choosing a smaller σ parameter tends to make these kernels less well-approximated by low-rank matrices and to have more heterogeneous leverage scores. In general, these two properties need not be directly related—the spectrum is a property of eigenvalues, while the leverage scores are determined by the eigenvectors—but for the data we examined they are related, in that matrices with more slowly decaying spectra also often have more heterogeneous leverage scores.
- For Dense RBF Kernels with smaller σ and Sparse RBF Kernels, leverage score sampling tends to do much better than other methods. Interestingly, the Sparse RBF Kernels have many properties of very sparse Laplacian Kernels corresponding to relatively-unstructured informatics graphs, an observation which should be of interest for researchers who construct sparse graphs from data using, *e.g.*, "locally linear" methods, to try to reconstruct hypothesized low-dimensional manifolds.
- Reconstruction quality under leverage score sampling saturates, as a function of choosing more samples ℓ; this is seen both for non-rank-restricted and rank-restricted situations. As a consequence, there can be a tradeoff between leverage score sampling or other methods being better, depending on the values of ℓ that are chosen.
- Although they are potentially ill-conditioned, non-rank-restricted approximations behave better in terms of reconstruction quality. Rank-constrained approximations tend to have much more complicated behavior as a function of increasing the numbe of samples ℓ, including choppier and non-monotonic behavior. This is particularly severe for leverage score sampling, but it occurs with other methods; and it suggests that other forms of regularization (other than what is essentially a Tikhonov form of regularization for the rank-restricted cases) might be appropriate.

In general, *all* of the sampling and projection methods we considered perform *much* better on the SPSD matrices we considered than previous worst-case bounds (*e.g.*, [21, 38, 28]) would suggest. (That is, even the worst results correspond to single-digit approximation factors in relative scale.) This observation is intriguing, because the motivation of leverage score sampling (and, recall, that in this context random projections should be viewed as performing uniform random sampling in a randomly-rotated basis where the leverage scores have been approximately uniformized [45]) is very much tied to the Frobenius norm, and so there is no *a priori* reason to expect its good performance to extend to the spectral or trace norms. Motivated by this, we revisit the question of proving improved worst-case theoretical bounds in Section 4.

Before describing these improved theoretical results, however, we address in Section 3.4 running time questions. After all, a naïve implementation of sampling with exact leverage scores is slower than other methods (and much slower than uniform sampling). As shown below, by using the recently developed algorithm of [20], not only does this approximation algorithm run in time comparable with random projections (for certain parameter settings), but it leads to approximations that soften the strong bias that the exact leverage scores provide toward the best rank-k approximation to the matrix, thereby leading to improved reconstruction results in many cases.

3.4. **Reconstruction Accuracy of Leverage Score Approximation Algorithms.** A naïve view might assume that computing probabilities that permit leverage-based sampling requires an $O(n^3)$ computation of the full SVD, or at least the full computation of a partial SVD, and thus that it would be much more expensive than recently-developed random projection methods. Indeed, an "exact" computation of the leverage scores with a QR decomposition or truncated SVD takes roughly $\mathrm{O}(n^2k)$ time (and the running time results of Section 3.3 actually used this naïve procedure). Recent work, however, has shown that relative-error approximations to all the statistical leverage scores can be computed more quickly than this exact algorithm [20]. Here, we implement and evaluate a version of this algorithm, and we evaluate it both in terms of running time and in terms of reconstruction quality on the diverse suite of real data matrices we considered above. We note that ours is the first work to provide an empirical evaluation of an implementation

```
Input: $\mathbf{A} \in \mathbb{R}^{n \times d}$ (with SVD $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$), error parameter $\epsilon \in (0, 1/2]$.
Output: $\tilde{\ell}_i, i = 1, \ldots, n$, approximations to the leverage scores of $\mathbf{A}$.
    (1) Let $\mathbf{\Pi}_1 \in \mathbb{R}^{r_1 \times n}$ be an SRFT with
            $r_1 = \Omega(\epsilon^{-2}(\sqrt{d} + \sqrt{\ln n})^2 \ln d)$
    (2) Compute $\mathbf{\Pi}_1\mathbf{A} \in \mathbb{R}^{r_1 \times d}$ and its QR factorization $\mathbf{\Pi}_1\mathbf{A} = \mathbf{Q}\mathbf{R}$.
    (3) Let $\mathbf{\Pi}_2 \in \mathbb{R}^{d \times r_2}$ be a matrix of i.i.d. standard Gaussian random variables, where
            $r_2 = \Omega\left(\epsilon^{-2} \ln n\right).$
    (4) Construct the product $\mathbf{\Omega} = \mathbf{A}\mathbf{R}^{-1}\mathbf{\Pi}_2$.
    (5) For $i = 1, \ldots, n$ compute $\tilde{\ell}_i = \left\|\Omega_{(i)}\right\|_2^2$.
```

Algorithm 1: Algorithm (originally Algorithm 1 in [20]) for approximating the leverage scores ℓ_i of an $n \times d$ matrix $\mathbf{A}$, where $n \gg d$, to within a multiplicative factor of $1 \pm \epsilon$. The running time of the algorithm is $\mathrm{O}(nd \ln(\sqrt{d} + \sqrt{\ln n}) + nd\epsilon^{-2} \ln n + d^2\epsilon^{-2}(\sqrt{d} + \sqrt{\ln n})^2 \ln d)$.

```
Input: $\mathbf{A} \in \mathbb{R}^{n \times d}$, a rank parameter $k$, and an error parameter $\epsilon \in (0, 1/2]$.
Output: $\hat{\ell}_i, i = 1, \ldots, n$, approximations to the leverage scores of $\mathbf{A}$ filtered through its dominant dimension-$k$ subspace.
    (1) Construct $\mathbf{\Pi} \in \mathbb{R}^{d \times 2k}$ with i.i.d. standard Gaussian entries.
    (2) Compute $\mathbf{B} = \left(\mathbf{A}\mathbf{A}^T\right)^q \mathbf{A}\mathbf{\Pi} \in \mathbb{R}^{n \times 2k}$ with
            $q \geq \left\lceil \frac{\ln\left(1 + \sqrt{\frac{k}{k-1}} + \mathrm{e}\sqrt{\frac{2}{k}}\sqrt{\min\{n, d\} - k}\right)}{2\ln(1 + \epsilon/10) - 1/2} \right\rceil,$
    (3) Approximate the leverage scores of $\mathbf{B}$ by calling Algorithm 1 with inputs $\mathbf{B}$ and $\epsilon$; let $\hat{\ell}_i$
        for $i = 1, \ldots, n$ be the outputs of Algorithm 1.
```

Algorithm 2: Algorithm (originally Algorithm 4 in [20]) for approximating the leverage scores (relative to the best rank-k approximation to $\mathbf{A}$) of a general $n \times d$ matrix $\mathbf{A}$ with those of a matrix that is close by in the spectral norm. This algorithm runs in time $\mathrm{O}(ndkq) + T_1$, where T_1 is the running time of Algorithm 1.

of the leverage score approximation algorithms of [20], illustrating empirically the tradeoffs between cost and efficiency in a practical setting.

3.4.1. *Description of the Approximation Algorithm.* Algorithm 1 (which originally appeared as Algorithm 1 in [20]) takes as input an arbitrary $n \times d$ matrix $\mathbf{A}$, where $n \gg d$, and it returns as output a $1 \pm \epsilon$ approximation to *all* of the statistical leverage scores of the input matrix. The original algorithm of [20] uses a subsampled Hadamard transform and requires r_1 to be somewhat larger. That an SRFT with a smaller value of r_1 can be used instead is a consequence of the fact that Lemma 3 in [20] is also satisfied by an SRFT matrix with the given r_1; this is established in [58, 13].

The running time of this algorithm, given in the caption of the algorithm, is roughly $O(nd \ln d)$ when $d = \Omega(\ln n)$. Thus Algorithm 1 generates relative-error approximations to the leverage scores of a tall and skinny matrix $\mathbf{A}$ in time $o(nd^2)$, rather than the $\mathrm{O}(nd^2)$ time that would be required to compute a QR decomposition or a thin SVD of the $n \times d$ matrix $\mathbf{A}$. The basic idea behind how Algorithm 1 works is as follows. If we had a QR decomposition of $\mathbf{A}$, then we could postmultiply $\mathbf{A}$ by the inverse of the "R" matrix to obtain an orthogonal matrix spanning the column space of $\mathbf{A}$; and from this $n \times d$ orthogonal matrix, we could read off the leverage scores from the Euclidean norms of the rows. Of course, computing the QR decomposition would require $O(nd^2)$ time. To get around this, Algorithm 1 premultiplies $\mathbf{A}$ by a structured random projection $\mathbf{\Pi}_1$, computes a QR decomposition of $\mathbf{\Pi}_1\mathbf{A}$, and postmultiplies $\mathbf{A}$ by $\mathbf{R}^{-1}$. Since $\mathbf{\Pi}_1$ is an

```
Input: $\mathbf{A} \in \mathbb{R}^{n \times d}$, a rank parameter $k$, and an iteration parameter $q$.
Output: $\hat{\ell}_i, i \in= 1, \dots, n$, approximations to the leverage scores of $\mathbf{A}$ filtered through its dominant dimension-$k$ subspace.
    (1) Construct an SRHT matrix $\mathbf{\Pi} \in \mathbb{R}^{d \times r}$, where
            $r \geq \left\lceil 36\epsilon^{-2}[\sqrt{k} + \sqrt{8\ln(kd)}]^2 \ln(k) \right\rceil.$
    (2) Compute $\mathbf{B} = \left(\mathbf{A}\mathbf{A}^T\right)^q \mathbf{A}\mathbf{\Pi} \in \mathbb{R}^{n \times r}$, where $q \geq 0$ is an integer.
    (3) Return the leverage scores of $\mathbf{B}$.
```

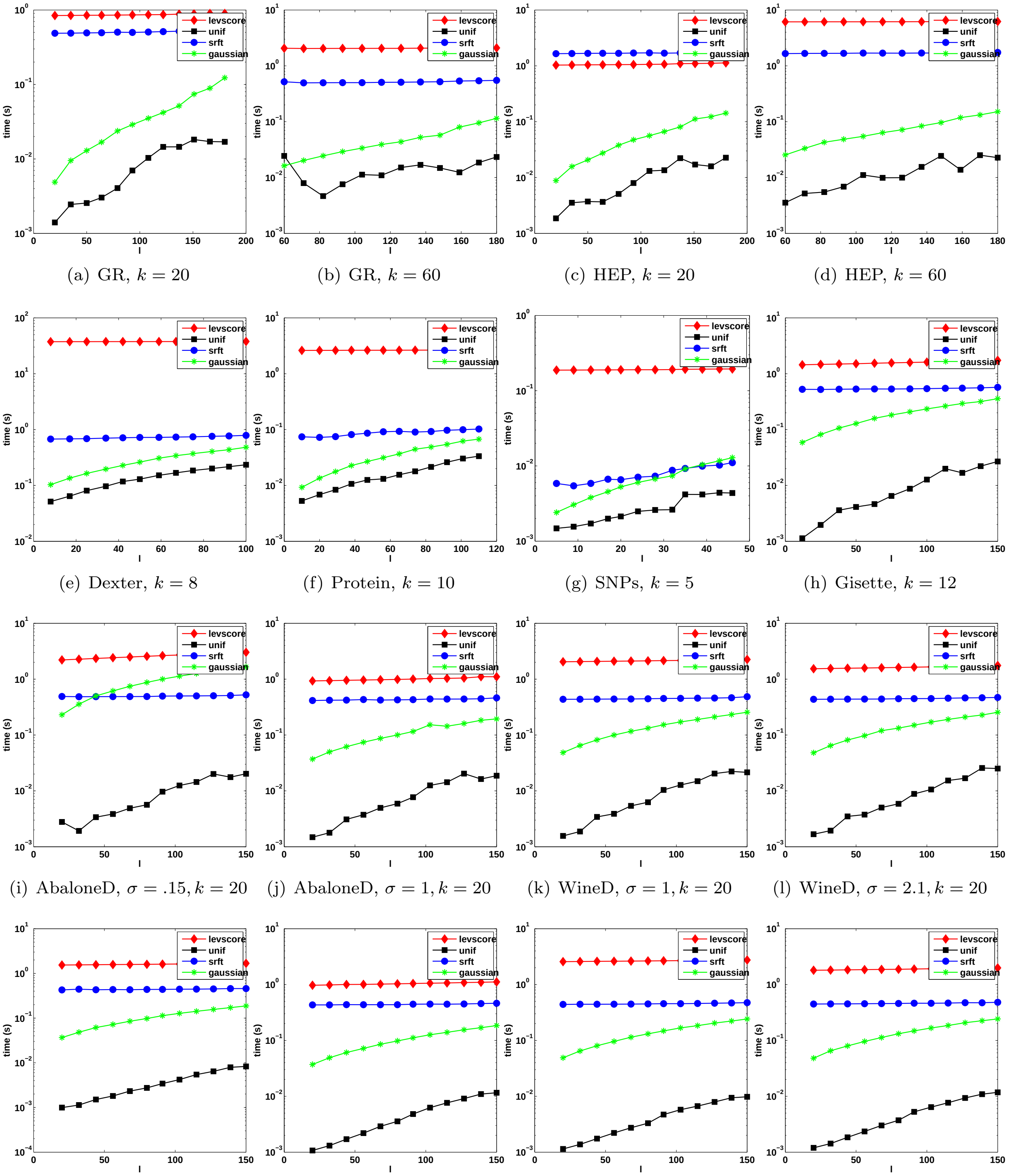
Algorithm 3: Algorithm for approximating the leverage scores (relative to the best rank-k approximation to $\mathbf{A}$) of a general $n \times d$ matrix $\mathbf{A}$ with those of a matrix that is close by in the spectral norm. This is a modified version of Algorithm 2, in which the random projection is implemented with an SRFT rather than a Gaussian random matrix, and where the number of "iterations" q is prespecified. This algorithm runs in time $\mathrm{O}(nd \ln r + ndrq + nr^2)$ since $\mathbf{A}\mathbf{\Pi}$ can be computed in time $\mathrm{O}(nd \ln r)$.

SRFT, premultiplying by it takes roughly $O(nd \ln d)$ time, and $\mathbf{\Pi}_1\mathbf{A}$ needs to be post multiplied by a second random projection in order to compute all of the leverage scores in the allotted time; see [20] for details. This algorithm is simpler than the algorithm in which we are primarily interested that is applicable to square SPSD matrices, but we start with it since it illustrates the basic ideas of how our main algorithm works and since our main algorithm calls it as a subroutine. We note, however, that this algorithm is directly useful for approximating the leverage scores of Linear Kernel matrices $\mathbf{A} = \mathbf{X}\mathbf{X}^T$, when $\mathbf{X}$ is a tall and skinny matrix.

Consider, next, Algorithm 2 (which originally appeared as Algorithm 4 in [20]), which takes as input an *arbitrary* $n \times d$ matrix $\mathbf{A}$ and a rank parameter k, and returns as output a $1 \pm \epsilon$ approximation to *all* of the statistical leverage scores (relative to the best rank-k approximation) of the input. An important technical point is that the problem of computing the leverage scores of a matrix relative to a low-dimensional space is ill-posed, essentially because the spectral gap between the k^{th} and the $(k+1)^{st}$ eigenvalues can be small, and thus Algorithm 2 actually computes approximations to the leverage scores of a matrix that is near to $\mathbf{A}$ in the spectral norm (or the Frobenius norm if $q = 0$). See [20] for details. Basically, this algorithm uses Gaussian sampling to find a matrix close by to $\mathbf{A}$ in the Frobenius norm or spectral norm and then approximates the leverage scores of this matrix by using Algorithm 1 on the smaller, very rectangular matrix $\mathbf{B}$. When $\mathbf{A}$ is square, as in our applications, Algorithm 2 is typically more costly than direct computation of the leverage scores, at least for dense matrices (but it does have the advantage that the number of iterations is bounded, independent of properties of the matrix, which is not true for typical iterative methods to compute low-rank approximations).

Of greater practical interest is Algorithm 3, which is a modification of Algorithm 2 in which the Gaussian random projection is replaced with an SRFT. That is, Algorithm 3 uses an SRFT projection to find a matrix close by to $\mathbf{A}$ in the Frobenius norm or spectral norm (depending on the value of q), and then exactly computes the leverage scores of this matrix. This improves the running time to $\mathrm{O}(n^2 \ln(\sqrt{k} + \sqrt{\ln n}) + n^2(\sqrt{k} + \sqrt{\ln n})^2 \ln(k)q + n(\sqrt{k} + \sqrt{\ln n})^4 \ln^2(k))$, which is $o(n^2 k)$ when $q = 0$. Thus an important point for Algorithm 3 (as well as for Algorithm 2) is the parameter q which describes the number of iterations. For $q = 0$ iterations, we get an inexpensive Frobenius norm approximation; while for higher q, we get better spectral norm approximations that are more expensive. This flexibility is of interest, as one may want to approximate the leverage scores accurately or simply find crude approximations useful for obtaining SPSD sketches with low reconstruction error.

Finally, note that although choosing the number of iterations q as we did in Algorithm 2 is convenient for worst-case analysis, as a practical implementational matter it is easier either to choose q based on spectral gap information revealed during the running of the algorithm or to prespecify q to be small integer, *e.g.*, 2 or 3, before the algorithm runs. Both of these have an interpretation of accelerating the rate of decay of the spectrum with a power iteration, but they behave somewhat differently due to the different stopping conditions. Below, we consider both variants.



(a) GR, $k = 20$ (b) GR, $k = 60$ (c) HEP, $k = 20$ (d) HEP, $k = 60$

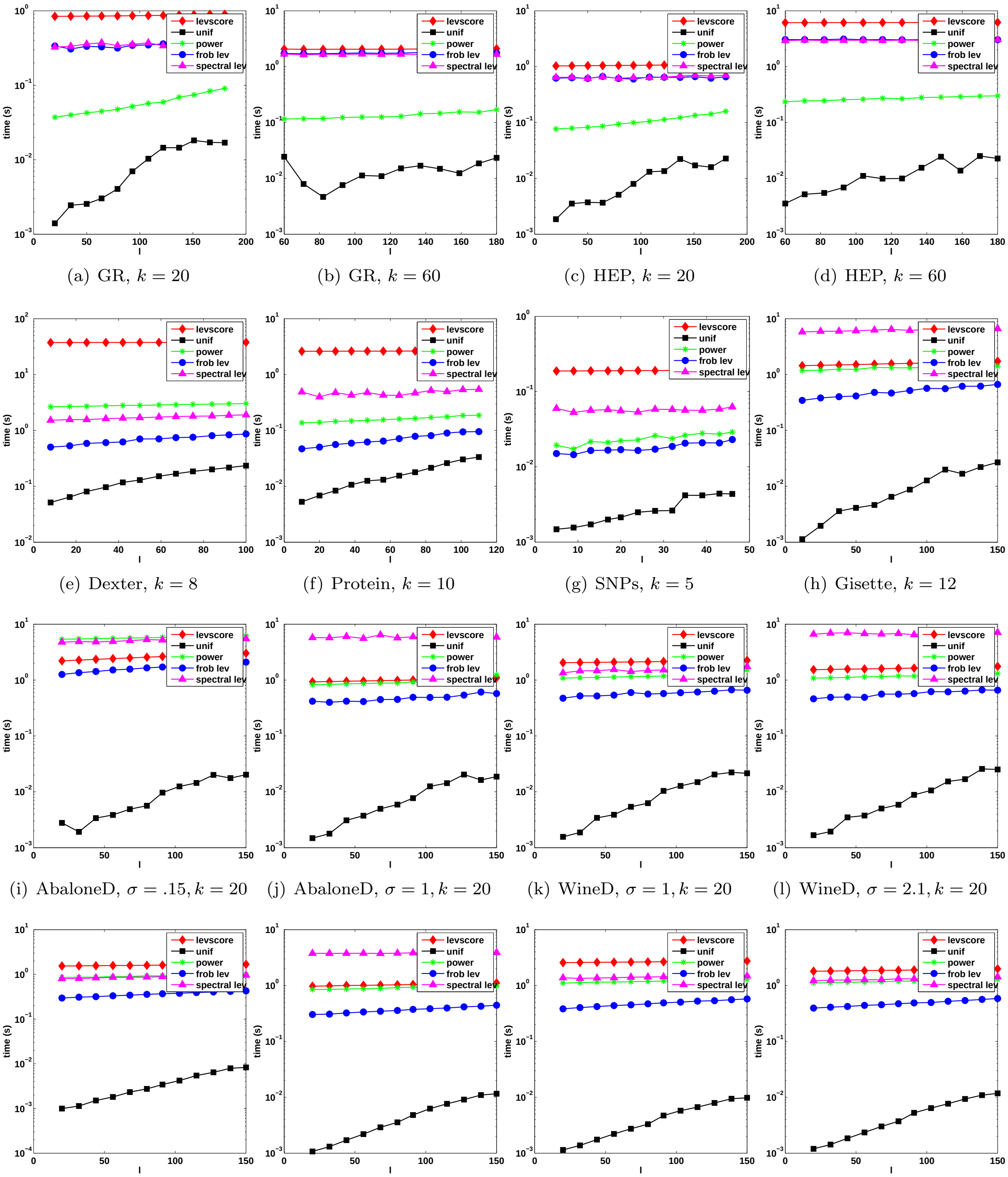
(e) Dexter, $k = 8$ (f) Protein, $k = 10$ (g) SNPs, $k = 5$ (h) Gisette, $k = 12$

(i) AbaloneD, $\sigma = .15, k = 20$ (j) AbaloneD, $\sigma = 1, k = 20$ (k) WineD, $\sigma = 1, k = 20$ (l) WineD, $\sigma = 2.1, k = 20$

(m) AbaloneS, $\sigma = .15, k = 20$ (n) AbaloneS, $\sigma = 1, k = 20$ (o) WineS, $\sigma = 1, k = 20$ (p) WineS, $\sigma = 2.1, k = 20$

FIGURE 6. The times required to compute the (non-rank-restricted) SPSD sketches, as a function of the number of columns samples ℓ for several data sets and two choices of the rank parameter k.

3.4.2. *Running Time Comparisons.* Here, we describe the performances of the various random sampling and random projection low-rank extensions considered in Section 3.3 in terms of their running time, where



(a) GR, $k = 20$ (b) GR, $k = 60$ (c) HEP, $k = 20$ (d) HEP, $k = 60$

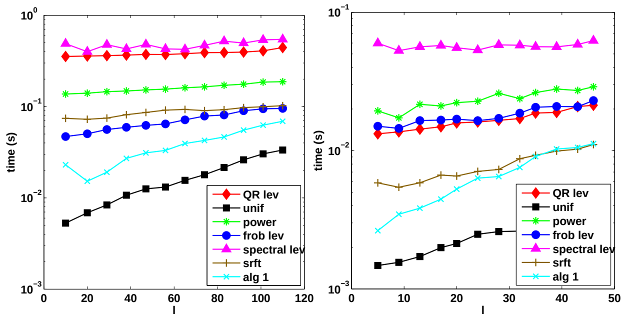
(e) Dexter, $k = 8$ (f) Protein, $k = 10$ (g) SNPs, $k = 5$ (h) Gisette, $k = 12$

(i) AbaloneD, $\sigma = .15, k = 20$ (j) AbaloneD, $\sigma = 1, k = 20$ (k) WineD, $\sigma = 1, k = 20$ (l) WineD, $\sigma = 2.1, k = 20$

(m) AbaloneS, $\sigma = .15, k = 20$ (n) AbaloneS, $\sigma = 1, k = 20$ (o) WineS, $\sigma = 1, k = 20$ (p) WineS, $\sigma = 2.1, k = 20$

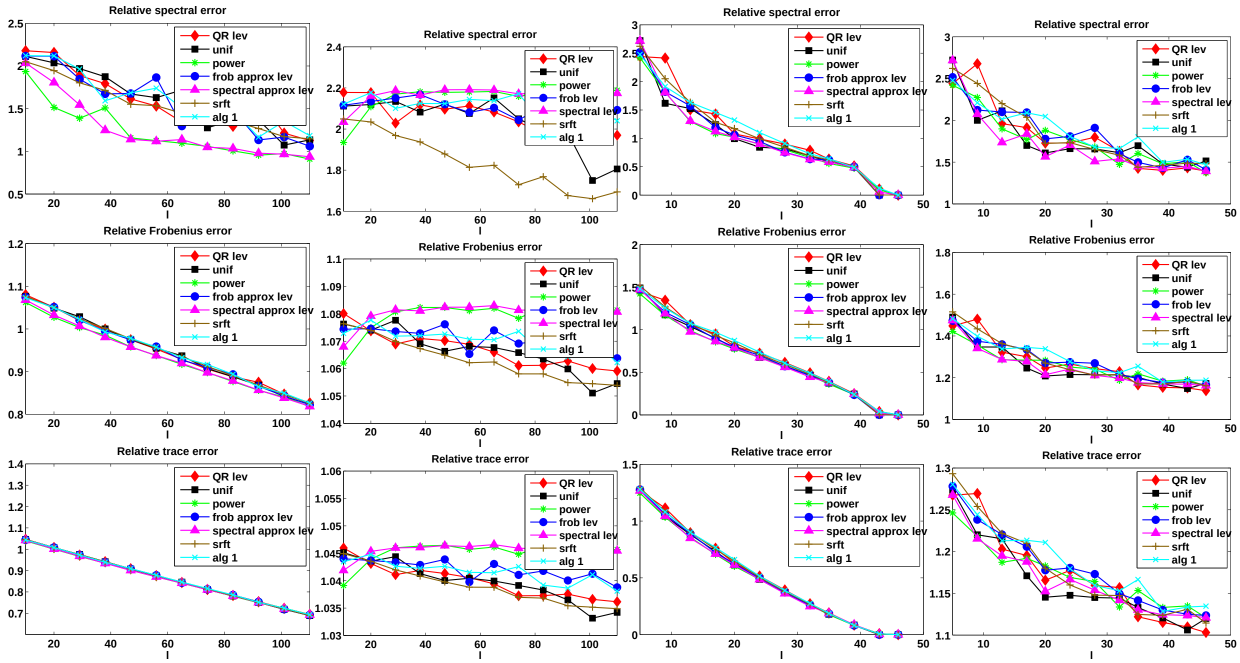
FIGURE 7. The times required to compute the (non-rank-restricted) approximate leverage score-based Nyström extensions, as a function of the number of columns samples ℓ for several data sets.

the method that involves using the leverage scores to construct the importance sampling distribution is implemented both by computing the leverage scores "exactly" by calling a truncated SVD, as a black box,



(a) Protein, $k = 10$ (b) SNPs, $k = 5$

FIGURE 8. The running time of (non-rank-restricted) Nyström extensions computed using Algorithm 1 compared with that of other approximate leverage score-based Nyström extensions, as a function of the number of column samples ℓ for two Linear Kernel datasets. The parameters in Algorithm 1 were taken to be $r_1 = \epsilon^{-2}\ln(d\delta^{-1})(\sqrt{d} + \sqrt{\ln(n\delta^{-1})})^2$ and $r_2 = \epsilon^{-2}(\ln n + \ln \delta^{-1})$ with $\epsilon = 1$ and $\delta = 1/10$.



(a) Protein, $k = 10$, non-rank-restricted (b) Protein, $k = 10$, rank-restricted (c) SNPs, $k = 5$, non-rank-restricted (d) SNPs, $k = 5$, rank-restricted

FIGURE 9. The spectral, Frobenius, and trace norm errors (top to bottom, respectively, in each subfigure) of Nyström extensions computed using Algorithm 1 compared with those of other approximate leverage score-based Nyström schemes, as a function of the number of columns samples ℓ, for two Linear Kernel data sets. The parameters in Algorithm 1 were taken to be $r_1 = \epsilon^{-2}\ln(d\delta^{-1})(\sqrt{d}+\sqrt{\ln(n\delta^{-1})})^2$ and $r_2 = \epsilon^{-2}(\ln n + \ln \delta^{-1})$ with $\epsilon = 1$ and $\delta = 1/10$.

as well as computing them approximately by using one of several versions of Algorithm 3. Our running time results are presented in Figure 6 and Figure 7.

We start with the results described in Figure 6, which shows the running times, as a function of ℓ, for the low-rank approximations described in Section 3.3: *i.e.*, for column sampling uniformly at random without replacement; for column sampling according to the exact nonuniform leverage score probabilities; and for sampling using Gaussian and SRFT mixtures of the columns. Several observations are worth making about the results presented in this figure.

- Uniform sampling is always less expensive and typically much less expensive than the other methods, while (with one minor exception) sampling according to the *exact* leverage scores is always the most expensive method.
- For most matrices, using the SRFT is nearly as expensive as exact leverage score sampling. This is most true for the very sparse graph Laplacian Kernels, largely since the SRFT does not respect sparsity. The main exception to this is for the dense and relatively well-behaved Linear Kernels, where especially for large values of ℓ the SRFT is quite fast and usually not too much more expensive than uniform sampling.
- The "fast Fourier" methods underlying the SRFT can take advantage of the structure of the Linear Kernels to yield algorithms that are similar to Gaussian projections and much better than exact leverage score computation. Note that the reason that SRFT is worse than Gaussians here is that the matrices we are considering are not extremely large, and we are not interested in very large values of the rank parameter. Extending in both those directions leads to Gaussian projections being slower than SRFT, as the trends in the figures clearly indicate.
- Gaussian projections are not too much slower than uniform sampling for the extremely sparse Laplacian Kernels—this is due to the sparsity of the Laplacian Kernels, since Gaussian projections can take advantage of the fast matrix-vector multiply, while the SRFT-based scheme cannot—but this advantage is lost for the (denser) Sparse RBF Kernels, to the extent that there is little running time improvement relative to the Dense RBF Kernels. In addition, Gaussian projections are relatively slower, when compared to the SRFT and uniform sampling, for the Dense RBF Kernels than for the Linear Kernels, although both of those data sets are maximally dense.

We next turn to the results described in Figure 7, which shows the running times, as a function of ℓ, for several variants of approximate leverage-based sampling. For ease of comparison, the timings for uniform sampling ("unif") and exact leverage score sampling ("levscore") are depicted in Figure 7 using the same colors (black and red, respectively) as used in Figure 6. In addition to these two baselines, Figure 7 shows running time results for the following three variants of approximate leverage score sampling: "frob lev" (which is Algorithm 3 with $q = 0$ and $r = 2k$); "spectral lev" (Algorithm 3 with $q = 4$ and $r = 2k$); and "power". The "power" scheme is a version of Algorithm 3 where $r = k$ and q is determined by monitoring the convergence of the leverage scores of $\mathbf{A}^{2q+1}\mathbf{\Pi}$ and terminating when the change in the leverage scores between iterations, as measured in the infinity norm, is smaller than 10^{-2}. This is simply a version of subspace iteration with a convergence criterion appropriate for the task at hand. Since "frob lev" requires one application of an SRFT, its timing results are depicted using the same color (blue) as the SRFT timing results in Figure 6. (There are no other correspondences between the colors in the two figures.) Several observations are worth making about the results presented in this figure.

- These approximate leverage score-based algorithms can be orders of magnitude faster than exact leverage score computation; but, especially for "spectral lev" when q is not prespecified to be 2 or 3, they can even be somewhat slower. Exactly which is the case depends upon the properties of the matrix and the parameters used in the approximation algorithm, including especially the number of power iterations.
- The "frob lev" approximation method has running time comparable to the running time of the SRFT, which is expected, given that this computation is the theoretical bottleneck for its running time. In particular, for larger values of ℓ for Linear Kernels, the running time or "frob lev" is not too much worse than that of uniform sampling.
- The "spectral lev" and "power" approximations with $q > 0$ are more expensive than the $q = 0$ "frob lev" approximation, which is a result of the relatively-expensive matrix-matrix multiplication. For the Linear Kernels, both are much better than the exact leverage score computation, and for most other data at least "power" is somewhat less expensive than the exact leverage score computation. For example, this is particularly true for the Laplacian Kernels.

Recall that the cost associated with these SPSD sketches is two-fold: first, the cost to construct the sample by sampling columns uniformly at random, by computing a nonuniform importance sampling distribution, or by performing a random projection to uniformize the leverage scores; and second, the cost to construct the low-rank approximation from the sample. For uniform sampling, the latter step dominates the cost, while for more sophisticated methods the former step typically dominates the cost. In particular, note that the approximate leverage score sampling methods are still sufficiently expensive that the cost to compute the importance sampling probabilities still dominates the cost to construct the low-rank approximation.

Finally, Algorithm 1 can be used to approximate quickly the leverage scores of matrices of the form $\mathbf{A} = \mathbf{X}\mathbf{X}^T$, when $\mathbf{X} \in \mathbb{R}^{n \times d}$ is a rectangular matrix of sufficent aspect ratio, and in such cases it is faster than Algorithm 3. Specifically, for the first dimensional reduction step in Algorithm 1 to be beneficial (*i.e.*, to ensure $r_1 < n$), the condition $n = \Omega(d \ln d)$ is necessary; for the second dimensional reduction step to be beneficial (*i.e.*, to ensure $r_2 < d$), the condition $d = \Omega(\ln n)$ must be satisfied. Figure 8 illustrates, using the Linear Kernel datasets Protein and SNPs (which satisfy these constraints), two points.

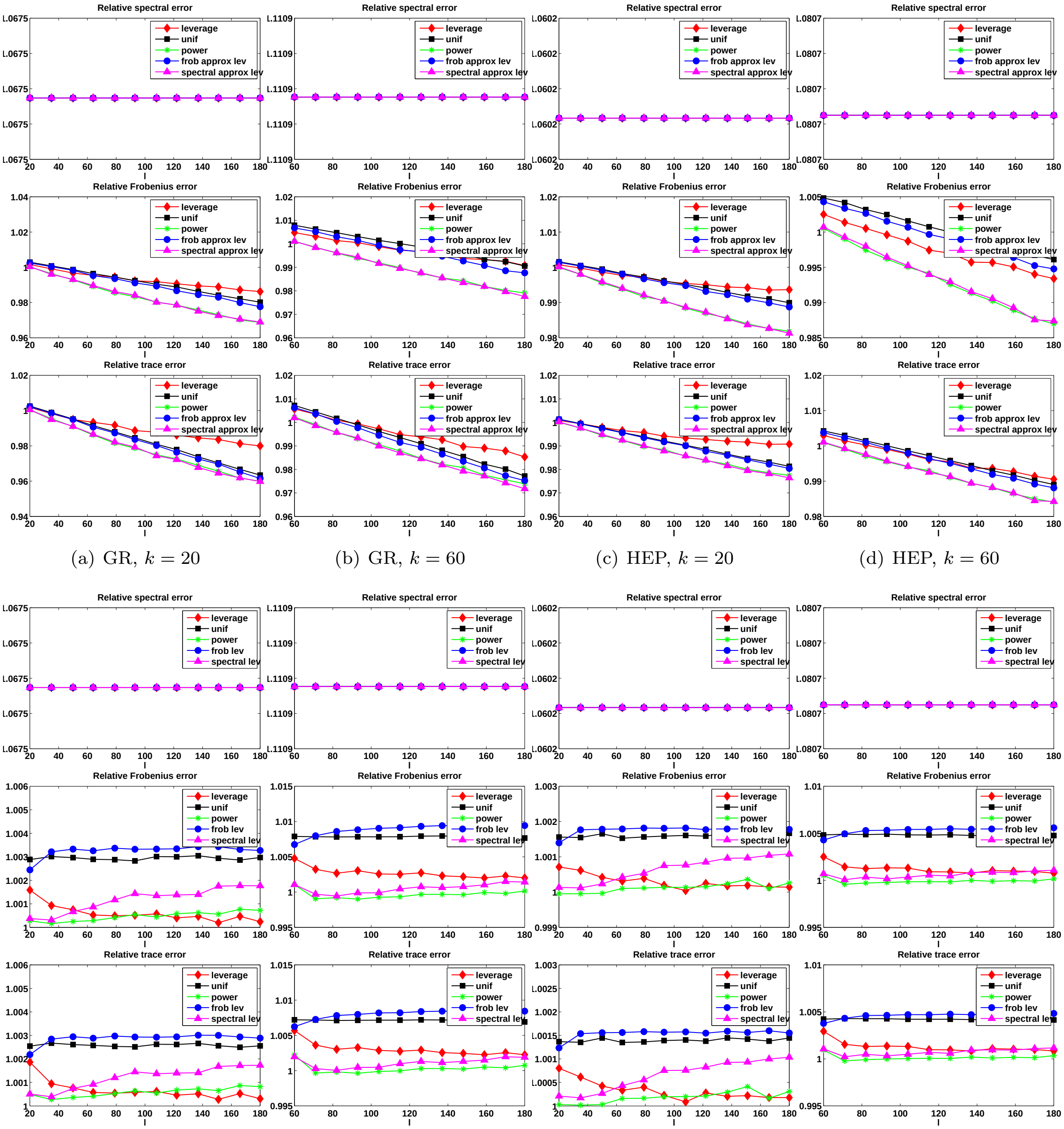
- Most importantly, the running time of Algorithm 1 on these rectangular matrices is faster than performing a QR decomposition on $\mathbf{A}$ and is comparable to applying a SRFT to $\mathbf{A}$.
- In addition, the running time of Algorithm 1 is significantly faster than the other approximate leverage score algorithms.

Figure 9 shows that these improved running time gains can come at the cost of a slight loss in the accuracy (relative to the exact computation of the leverage scores) of the low-rank approximations; the accuracy of the other approximate leverage score algorithms is discussed in the following subsection.

3.4.3. *Reconstruction Accuracy Results.* Here, we describe the performances of the various Nyström-based low-rank approximations that use approximate leverage scores in terms of reconstruction accuracy for the data sets described in Section 3.1. The results are presented in Figure 10 through Figure 14. The setup for these results parallels that for the Nyström-based low-rank approximation results described in Section 3.3, and these figures parallel Figure 1 through Figure 5. To provide a baseline for the comparison, we also plot the previous reconstruction errors for sampling with the exact leverage scores as well as the uniform column sampling extension (using the same red and black colors, respectively). Several observations are worth making about the results presented in these figures.

- For Laplacian Kernels, for the non-rank-restricted results, "frob lev" is only slightly better than uniform sampling (although subsequent figures show that this is peculiar to the Laplacian Kernels), while "power" and "spect lev" are substantially better than uniform sampling. Interestingly, all of those methods also lead to better reconstruction results even than using the more expensive exact leverage scores. This is true, both in terms of reconstruction quality for a given ℓ, and also in that using the approximate leverage scores does not lead to the saturation effect that we see when using the exact leverage scores.
- For Laplacian Kernels, for the rank-restricted results, the "frob lev" results are similar to the exact leverage score results for $\ell = k$, but the quality degrades considerably as ℓ increases. On the other hand, "power" and "spectral lev" are much better than using the exact leverage scores when $\ell = k$, and are slightly better or only slightly worse as ℓ increases.
- For the Linear Kernels, all the methods perform similarly in the non-rank-restricted case; while in the rank-restricted case, the methods that use approximate leverage scores tend to parallel the exact leverage score results, both when those get better and when those get worse with increasing ℓ.
- For both the dense and sparse RBF data sets, for the non-rank-restricted case, the approximate leverage score algorithms tend to parallel the exact leverage score algorithm, and they are not substantially better. In particular, both "power" and "spectral lev" tend to saturate when the exact method saturates, but in those cases "frob lev" tends not to saturate.
- For both the dense and sparse RBF data sets, for the rank-restricted case, the results depend on the value of the σ width parameter. When σ is larger and the matrices are more homogeneous, all the methods tend to parallel each other (although WineS is an exception). When σ is smaller, "frob lev" is generally better than uniform sampling but worse than the other methods for $\ell = k$, but it degrades with increasing ℓ; while both "power" and "spectral lev" tend to parallel the results for the exact leverage scores.

Note that the difference between different approximate leverage score algorithms often corresponds to a difference in the spectral gaps of the corresponding matrices. From Table 4, if we fix k and use the approximate leverage scores filtered through rank k to form a Nyström approximation to $\mathbf{A}$, the accuracy of

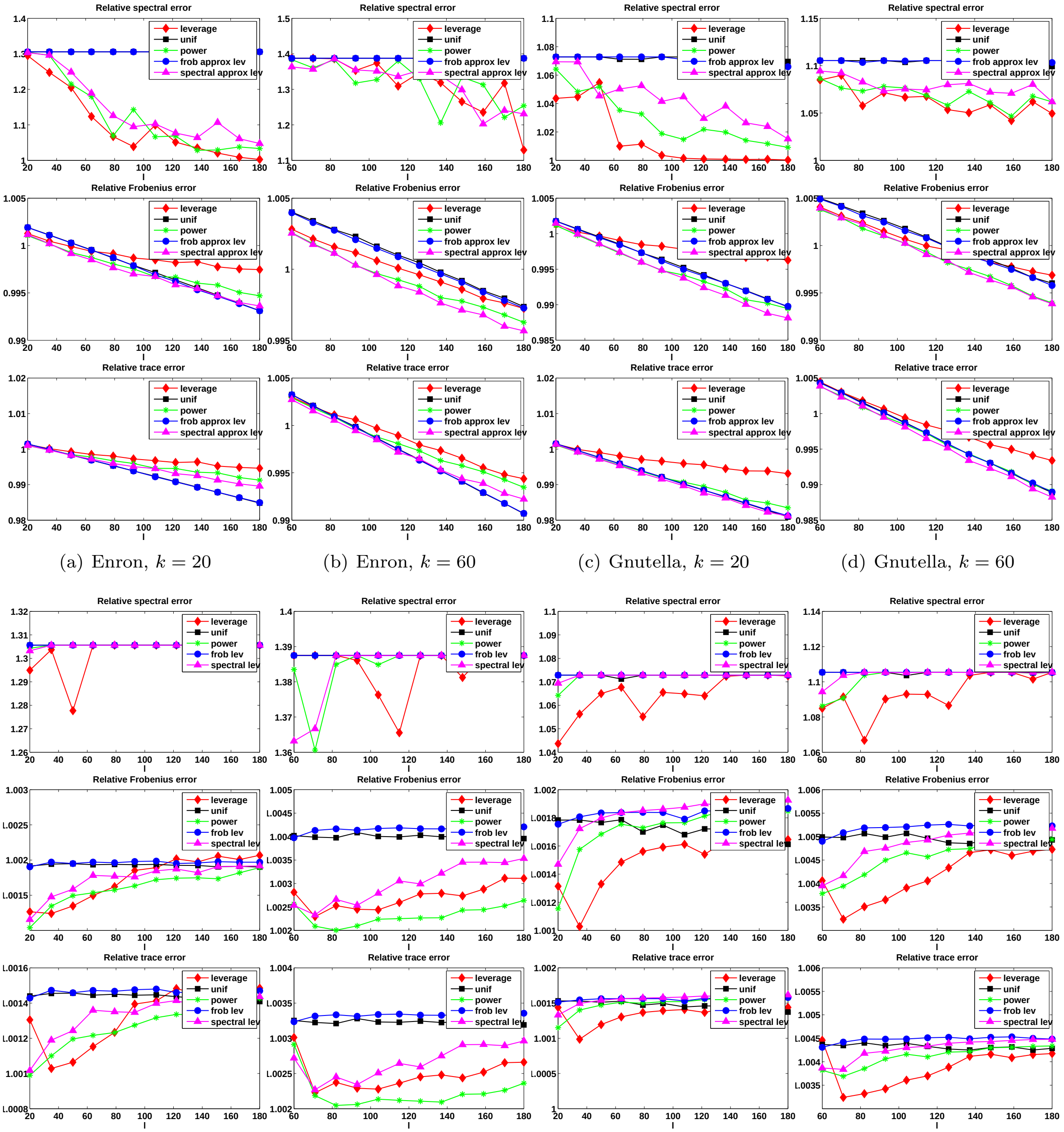


(a) GR, $k = 20$ (b) GR, $k = 60$ (c) HEP, $k = 20$ (d) HEP, $k = 60$

(e) GR, $k = 20$ (f) GR, $k = 60$ (g) HEP, $k = 20$ (h) HEP, $k = 60$

Figure 10. The spectral, Frobenius, and trace norm errors (top to bottom, respectively, in each subfigure) of several (non-rank-restricted in top panels and rank-restricted in bottom panels) approximate leverage score-based Nyström schemes, as a function of the number of columns samples ℓ, for the GR and HEP Laplacian data sets, with two choices of the rank parameter k.

that approximation has a strong dependence on the spectral gap of $\mathbf{A}$ at rank k, as measured by $\frac{\sigma_k}{\sigma_{k+1}}$. In general, the larger the spectral gap, the more accurate the approximation. This phenomena can also be understood in terms of the convergence of the approximate leverage scores: the approximation algorithms are essentially truncated versions of the subspace iteration method for computing the top k eigenvectors of

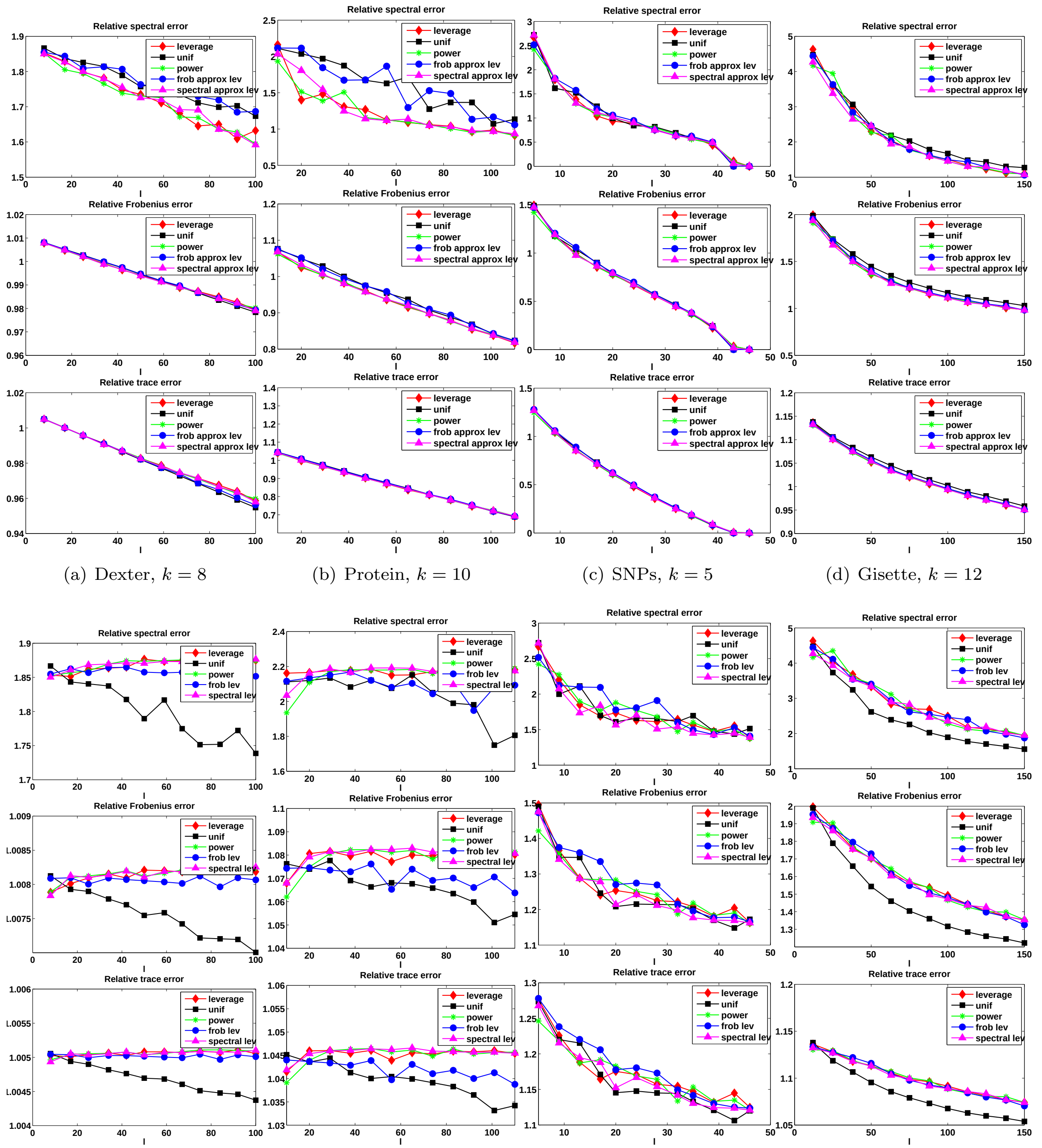


(a) Enron, $k = 20$ (b) Enron, $k = 60$ (c) Gnutella, $k = 20$ (d) Gnutella, $k = 60$

(e) Enron, $k = 20$ (f) Enron, $k = 60$ (g) Gnutella, $k = 20$ (h) Gnutella, $k = 60$

FIGURE 11. The spectral, Frobenius, and trace norm errors (top to bottom, respectively, in each subfigure) of several (non-rank-restricted in top panels and rank-restricted in bottom panels) approximate leverage score-based Nyström schemes, as a function of the number of columns samples ℓ, for the Enron and Gnutella Laplacian data sets, with two choices of the rank parameter k.

A. It is a classical result that the spectral gap determines the rate of convergence of the subspace iteration process to the desired eigenvectors: the larger it is, the fewer iterations of the process are required to get accurate approximations of the top eigenvectors. It follows immediately that the larger the spectral gap, the more accurate the approximate leverage scores generated by these approximation algorithms are. Our

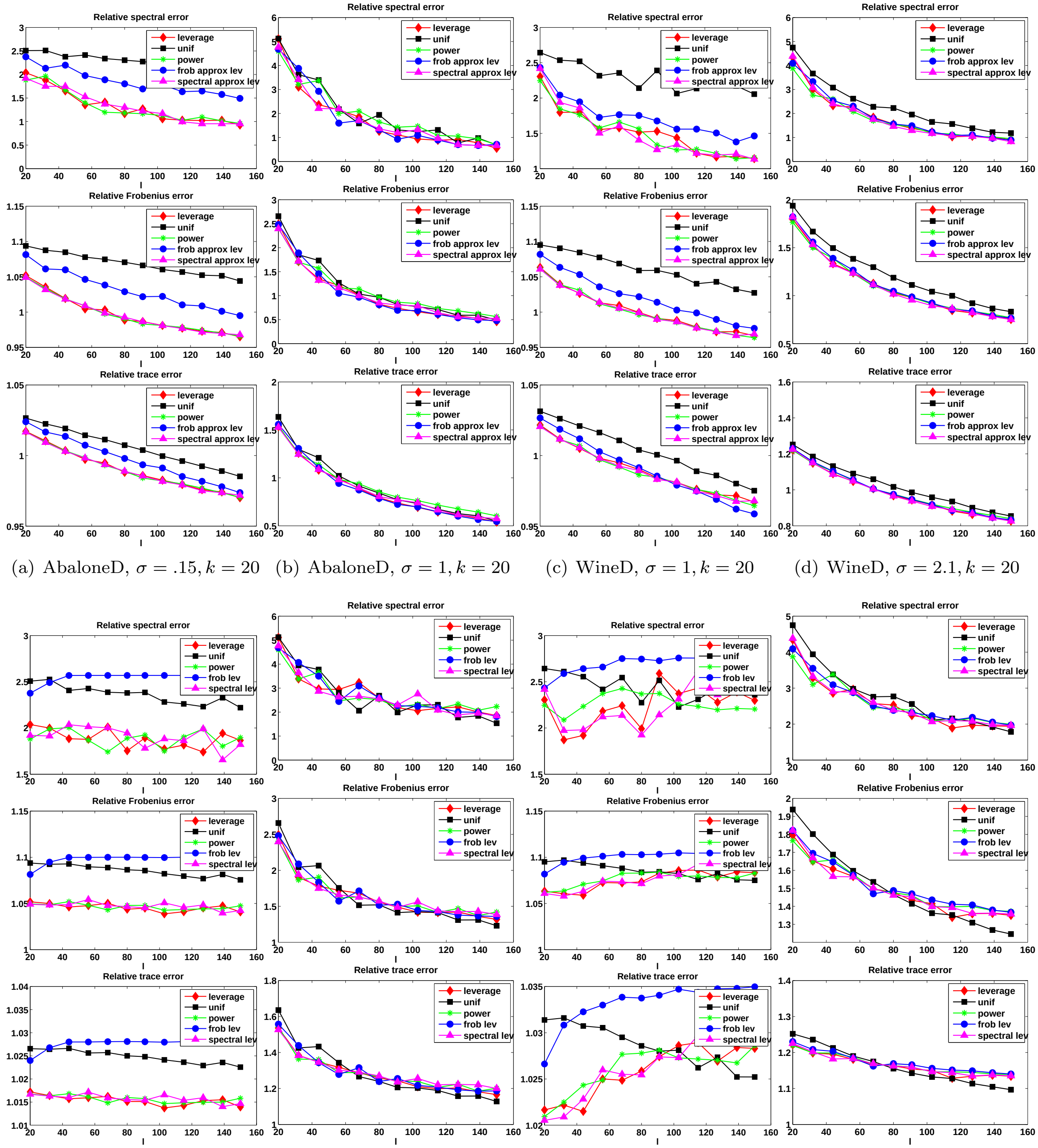


(a) Dexter, $k = 8$ (b) Protein, $k = 10$ (c) SNPs, $k = 5$ (d) Gisette, $k = 12$

(e) Dexter, $k = 8$ (f) Protein, $k = 10$ (g) SNPs, $k = 5$ (h) Gisette, $k = 12$

FIGURE 12. The spectral, Frobenius, and trace norm errors (top to bottom, respectively, in each subfigure) of several (non-rank-restricted in top panels and rank-restricted in bottom panels) approximate leverage score-based Nyström schemes, as a function of the number of columns samples ℓ, for the Linear Kernel data sets

empirical results illustrate the complexities and subtle consequences of these properties in realistic machine learning applications.

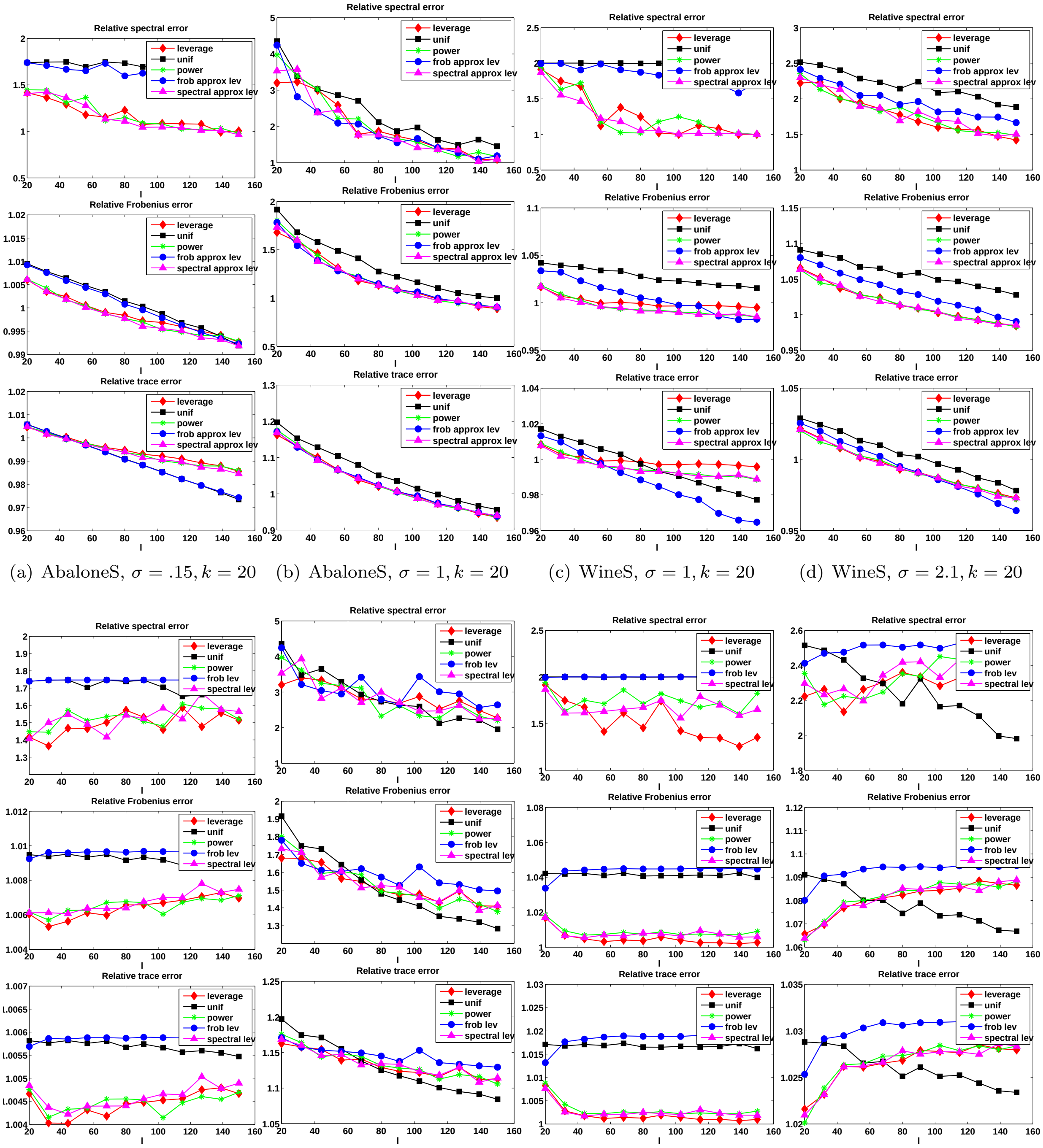


(a) AbaloneD, $\sigma = .15, k = 20$ (b) AbaloneD, $\sigma = 1, k = 20$ (c) WineD, $\sigma = 1, k = 20$ (d) WineD, $\sigma = 2.1, k = 20$

(e) AbaloneD, $\sigma = .15, k = 20$ (f) AbaloneD, $\sigma = 1, k = 20$ (g) WineD, $\sigma = 1, k = 20$ (h) WineD, $\sigma = 2.1, k = 20$

FIGURE 13. The spectral, Frobenius, and trace norm errors (top to bottom, respectively, in each subfigure) of several (non-rank-restricted in top panels and rank-restricted in bottom panels) approximate leverage score-based Nyström schemes, as a function of the number of columns samples ℓ, for several dense RBF data sets.

3.4.4. *Summary of Leverage Score Approximation Algorithms.* Before proceeding, there are several summary observations that we can make about the running time and reconstruction quality of approximate leverage score sampling algorithms for the data sets we have considered.



(a) AbaloneS, $\sigma = .15, k = 20$ (b) AbaloneS, $\sigma = 1, k = 20$ (c) WineS, $\sigma = 1, k = 20$ (d) WineS, $\sigma = 2.1, k = 20$

(e) AbaloneS, $\sigma = .15, k = 20$ (f) AbaloneS, $\sigma = 1, k = 20$ (g) WineS, $\sigma = 1, k = 20$ (h) WineS, $\sigma = 2.1, k = 20$

FIGURE 14. The spectral, Frobenius, and trace norm errors (top to bottom, respectively, in each subfigure) of several (non-rank-restricted in top panels and rank-restricted in bottom panels) approximate leverage score-based Nyström schemes, as a function of the number of columns samples ℓ, for several sparse RBF data sets.

- The running time of computing the exact leverage scores is generally much worse than that of uniform sampling and both SRFT-based and Gaussian-based random projection methods.

- The running time of computing approximations to the leverage scores can, with appropriate choice of parameters, be much faster than the exact computation of the leverage scores; and, especially for "frob lev," can be comparable to the running time of the random projection (SRFT or Gaussian) used in the leverage score approximation algorithm. For the methods that involve $q > 0$ iterations to compute stronger approximations to the leverage scores, the running time can vary considerably depending on details of the stopping condition.
- The leverage scores computed by the "frob lev" procedure are typically very different than the "exact" leverage scores, but they are leverage scores for a low-rank space that is near the best rank-k approximation to the matrix. This is often sufficient for good low-rank approximation, although the reconstruction accuracy can degrade in the rank-restricted cases as ℓ is increased.
- The approximate leverage scores computed from "power" and "spectral lev" approach those of the exact leverage scores, as q is increased; and they obtain reconstruction accuracy that is no worse, and in many cases is better, than than obtained by the exact leverage scores. This suggests that, by not fitting exactly to the empirical statistical leverage scores, we are observing a form of regularization.
- The running time of Algorithm 1, when applied to "tall" matrices for which $n \gg d$, is faster than the running time of performing a QR decomposition of the matrix $\mathbf{A}$; and it is comparable to the running time of applying a random projection to $\mathbf{A}$ (which is the computational bottleneck of applying Algorithm 1). Thus, one could use this algorithm to compute approximations to the leverage scores to obtain relative-error approximations to a least-squares problem involving $\mathbf{A}$ [22, 23, 45], or one could use the sketch thereby obtained as a preconditioner to an iterative method to solve the least-squares problem, in a manner analogous to how Blendenpik or LSRN does so with a random projection [3, 49].

Previous work has showed that one can implement random projection algorithms to provide low-rank approximations with error comparable to that of the SVD in less time than state-of-the art Krylov solvers and other "exact" numerical methods. Our empirical results show that these random projection algorithms can be used in two complementary ways to approximate SPSD matrices of interest in machine learning: first, they can be used directly to compute projection-based low-rank approximation; and second, they can be used to compute approximations to the leverage scores, which can be used to compute sampling-based low-rank approximation. With the right choice of parameters, the two complementary approaches have roughly comparable running times, and neither one dominates the other in terms of reconstruction accuracy.

4. Theoretical Aspects of SPSD Low-rank Approximation

In this section, we present our main theoretical results, which consist of a suite of bounds on the quality of low-rank approximation under several different sketching methods. As mentioned above, these were motivated by our empirical observation that *all* of the sampling and projection methods we considered perform *much* better on the SPSD matrices we considered than previous worst-case bounds (*e.g.*, [21, 38, 28]) would suggest. We start in Section 4.1 with deterministic structural conditions for the spectral, Frobenius, and trace norms; and then in Section 4.2 we use these results to provide our bounds for several random sampling and random projection procedures.

4.1. Deterministic Error Bounds for Low-rank SPSD Approximation.

In this section, we present three theorems that provide error bounds for the spectral, Frobenius, and trace norm approximation errors under the SPSD Sketching Model of Section 2.2. These are provided in Sections 4.1.1, 4.1.2, and 4.1.3, respectively, and they are followed by several more general remarks in Section 4.1.4. Note that these bounds hold for *any*, *e.g.*, deterministic or randomized, sketching matrix $\mathbf{S}$. Thus, *e.g.*, one could use them to check, in an *a posteriori* manner, the quality of a sketching method for which one cannot establish an *a priori* bound. Rather than doing this, we use these results (in Section 4.2 below) to derive *a priori* bounds for when the sketching operation consists of common random sampling and random projection algorithms.

4.1.1. *Spectral Norm Bounds.* We start with a bound on the spectral norm of the residual error. Although this result is trivial to prove, given prior work, it highlights several properties that we use in the analysis of our subsequent results.

Theorem 1. *Let* $\mathbf{A}$ *be an* $n \times n$ *SPSD matrix with eigenvalue decomposition partitioned as in Equation* (1), $\mathbf{S}$ *be a sampling matrix of size* $n \times \ell$, *and* $\mathbf{\Omega}_1$ *and* $\mathbf{\Omega}_2$ *be as defined in Equation* (3). *Then when* $\mathbf{C} = \mathbf{AS}$

and $\mathbf{W} = \mathbf{S}^T\mathbf{A}\mathbf{S}$*, the corresponding low-rank SPSD approximation satisfies*

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_2 \le \|\mathbf{\Sigma}_2\|_2 + \left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_2^2,$$

assuming $\mathbf{\Omega}_1$ *has full row rank.*

Proof. In [28], it is shown that

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_2 = \left\|\mathbf{A}^{1/2} - \mathbf{P}_{\mathbf{A}^{1/2}\mathbf{S}}\mathbf{A}^{1/2}\right\|_2^2. \tag{9}$$

Next, recall that $\mathbf{\Omega}_i = \mathbf{U}_i^T\mathbf{S}$, and assume that $\mathbf{\Omega}_1$ has full row rank. It can be shown that

$$\|\mathbf{X} - \mathbf{P}_{\mathbf{X}\mathbf{S}}\mathbf{X}\|_2^2 \le \|\mathbf{\Sigma}_2\|_2^2 + \left\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_2^2, \tag{10}$$

for any arbitrary matrix $\mathbf{X}$ [14, 31]. The theorem follows by combining these results. □

Remark. The proof of Theorem 1 proceeds in two steps. The first step relates low-rank approximation of an SPSD matrix $\mathbf{A}$ under the SPSD Sketching Model of Section 2.2 to column sketching (*e.g.*, sampling or projecting) from the square-root of $\mathbf{A}$. A much weaker form of this was used in [21], but the stronger form that we use here in Equation (9) was first proved in [28]. The second step is to use a deterministic structural result that holds for sampling/projecting from an arbitrary matrix. A bound of the form of Equation (10) was originally proven in [14] for solving the Column Subset Selection Problem, and it was improved in [31], where it was applied to a random projection algorithm. Although the analyses of our next two results are more complicated, they follow the same high-level two-step approach.

4.1.2. *Frobenius Norm Bounds.* Next, we state and prove the following bound on the Frobenius norm of the residual error. The proof parallels that for the spectral norm bound, in that we divide it into two analogous parts, but the analysis is somewhat more complex.

Theorem 2. *Let* $\mathbf{A}$ *be an* $n \times n$ *SPSD matrix with eigenvalue decomposition partitioned as in Equation* (1)*,* $\mathbf{S}$ *be a sampling matrix of size* $n \times \ell$*, and* $\mathbf{\Omega}_1$ *and* $\mathbf{\Omega}_2$ *be as defined in Equation* (3)*. Then when* $\mathbf{C} = \mathbf{A}\mathbf{S}$ *and* $\mathbf{W} = \mathbf{S}^T\mathbf{A}\mathbf{S}$*, the corresponding low-rank SPSD approximation satisfies*

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_\mathrm{F} \le \|\mathbf{\Sigma}_2\|_\mathrm{F} + \sqrt{2}\left\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_\mathrm{F} + \left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_\mathrm{F}^2,$$

assuming $\mathbf{\Omega}_1$ *has full row rank.*

Proof. In [28], it is shown that $\mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T = \mathbf{A}^{1/2}\mathbf{P}_{\mathbf{A}^{1/2}\mathbf{S}}\mathbf{A}^{1/2}$, and from this it follows that

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_\mathrm{F} = \left\|\mathbf{A}^{1/2}(\mathbf{I} - \mathbf{P}_{\mathbf{A}^{1/2}\mathbf{S}})\mathbf{A}^{1/2}\right\|_\mathrm{F}.$$

To bound this, we first use the unitary invariance of the Frobenius norm and the fact that $\mathbf{P}_{\mathbf{A}^{1/2}\mathbf{S}} = \mathbf{U}\mathbf{P}_{\mathbf{\Sigma}^{1/2}\mathbf{U}^T\mathbf{S}}\mathbf{U}^T$ to obtain

$$E := \left\|\mathbf{A}^{1/2}(\mathbf{I} - \mathbf{P}_{\mathbf{A}^{1/2}\mathbf{S}})\mathbf{A}^{1/2}\right\|_\mathrm{F}^2 = \left\|\mathbf{\Sigma}^{1/2}(\mathbf{I} - \mathbf{P}_{\mathbf{\Sigma}^{1/2}\mathbf{U}^T\mathbf{S}})\mathbf{\Sigma}^{1/2}\right\|_\mathrm{F}^2.$$

Then we take

$$\mathbf{Z} = \mathbf{\Sigma}^{1/2}\mathbf{U}^T\mathbf{S}\mathbf{\Omega}_1^\dagger\mathbf{\Sigma}_1^{-1/2} = \begin{pmatrix}\mathbf{I}\\ \mathbf{F}\end{pmatrix}, \tag{11}$$

where $\mathbf{I} \in \mathbb{R}^{k\times k}$ and $\mathbf{F} \in \mathbb{R}^{n-k\times k}$ is given by $\mathbf{F} = \mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\mathbf{\Sigma}_1^{-1/2}$. The latter equality holds because of our assumption that $\mathbf{\Omega}_1$ has full row rank. Since the range of $\mathbf{Z}$ is contained in the range of $\mathbf{\Sigma}^{1/2}\mathbf{U}^T\mathbf{S}$,

$$E \le \left\|\mathbf{\Sigma}^{1/2}(\mathbf{I} - \mathbf{P}_\mathbf{Z})\mathbf{\Sigma}^{1/2}\right\|_\mathrm{F}^2.$$

In [31], it is shown that

$$\mathbf{P}_\mathbf{Z} \preceq \begin{pmatrix}\mathbf{I} - (\mathbf{I} + \mathbf{F}^T\mathbf{F})^{-1} & -(\mathbf{I} + \mathbf{F}^T\mathbf{F})^{-1}\mathbf{F}^T\\ -\mathbf{F}(\mathbf{I} + \mathbf{F}^T\mathbf{F})^{-1} & \mathbf{I} - \mathbf{F}(\mathbf{I} + \mathbf{F}^T\mathbf{F})^{-1}\mathbf{F}^T\end{pmatrix}. \tag{12}$$

This implies that

$$\begin{aligned}
E &\leq \left\|\boldsymbol{\Sigma}^{1/2}\begin{pmatrix}\mathbf{I}-(\mathbf{I}+\mathbf{F}^T\mathbf{F})^{-1} & -(\mathbf{I}+\mathbf{F}^T\mathbf{F})^{-1}\mathbf{F}^T\\ -\mathbf{F}(\mathbf{I}+\mathbf{F}^T\mathbf{F})^{-1} & \mathbf{I}-\mathbf{F}(\mathbf{I}+\mathbf{F}^T\mathbf{F})^{-1}\mathbf{F}^T\end{pmatrix}\boldsymbol{\Sigma}^{1/2}\right\|_{\mathrm{F}}^2\\
&= \left\|\boldsymbol{\Sigma}_1^{1/2}\big(\mathbf{I}-(\mathbf{I}+\mathbf{F}^T\mathbf{F})^{-1}\big)\boldsymbol{\Sigma}_1^{1/2}\right\|_{\mathrm{F}}^2 + 2\left\|\boldsymbol{\Sigma}_1^{1/2}(\mathbf{I}+\mathbf{F}^T\mathbf{F})^{-1}\mathbf{F}^T\boldsymbol{\Sigma}_2^{1/2}\right\|_{\mathrm{F}}^2 \qquad (13)\\
&\quad + \left\|\boldsymbol{\Sigma}_2^{1/2}\big(\mathbf{I}-\mathbf{F}(\mathbf{I}+\mathbf{F}^T\mathbf{F})^{-1}\mathbf{F}^T\big)\boldsymbol{\Sigma}_2^{1/2}\right\|_{\mathrm{F}}^2\\
&:= T_1 + T_2 + T_3.
\end{aligned}$$

Next, we provide bounds for T_1, T_2, and T_3. Using the fact that $\mathbf{0} \preceq \mathbf{I}-\mathbf{F}(\mathbf{I}+\mathbf{F}^T\mathbf{F})^{-1}\mathbf{F}^T \preceq \mathbf{I}$, we can bound T_3 with

$$T_3 \leq \|\boldsymbol{\Sigma}_2\|_{\mathrm{F}}^2.$$

Likewise, the fact that $\mathbf{I}-(\mathbf{I}+\mathbf{F}^T\mathbf{F})^{-1} \preceq \mathbf{F}^T\mathbf{F}$ (which is shown in [31]) implies that we can bound T_1 as

$$T_1 \leq \left\|\boldsymbol{\Sigma}_1^{1/2}\mathbf{F}^T\mathbf{F}\boldsymbol{\Sigma}_1^{1/2}\right\|_{\mathrm{F}}^2 = \left\|\big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)^T\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\right\|_{\mathrm{F}}^2 \leq \left\|\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\right\|_{\mathrm{F}}^4.$$

To bound T_2, we first expand in terms of the trace:

$$\begin{aligned}
T_2 &= 2\operatorname{Tr}\left(\boldsymbol{\Sigma}_2^{1/2}\mathbf{F}(\mathbf{I}+\mathbf{F}^T\mathbf{F})^{-1}\boldsymbol{\Sigma}_1(\mathbf{I}+\mathbf{F}^T\mathbf{F})^{-1}\mathbf{F}^T\boldsymbol{\Sigma}_2^{1/2}\right)\\
&= 2\operatorname{Tr}\left(\boldsymbol{\Sigma}_2^{1/2}\mathbf{F}\mathbf{M}^T\mathbf{M}\mathbf{F}^T\boldsymbol{\Sigma}_2^{1/2}\right), \qquad (14)
\end{aligned}$$

where

$$\begin{aligned}
\mathbf{M} &:= \boldsymbol{\Sigma}_1^{1/2}(\mathbf{I}+\mathbf{F}^T\mathbf{F})^{-1}\\
&= \boldsymbol{\Sigma}_1^{1/2}\big[\boldsymbol{\Sigma}_1^{-1/2}\boldsymbol{\Sigma}_1\boldsymbol{\Sigma}_1^{-1/2} + \boldsymbol{\Sigma}_1^{-1/2}\big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)^T\big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)\boldsymbol{\Sigma}_1^{-1/2}\big]^{-1}\\
&= \boldsymbol{\Sigma}_1\big[\boldsymbol{\Sigma}_1 + \big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)^T\big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)\big]^{-1}\boldsymbol{\Sigma}_1^{1/2}.
\end{aligned}$$

We observe that

$$\boldsymbol{\Sigma}_1 + \big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)^T\big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big) \succeq \boldsymbol{\Sigma}_1,$$

so

$$\big[\boldsymbol{\Sigma}_1 + \big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)^T\big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)\big]^{-1} \preceq \boldsymbol{\Sigma}_1^{-1},$$

which in turn implies that

$$\boldsymbol{\Sigma}_1^{1/2}\big[\boldsymbol{\Sigma}_1 + \big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)^T\big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)\big]^{-1}\boldsymbol{\Sigma}_1^{1/2} \preceq \mathbf{I}.$$

Since $\|\mathbf{A}\mathbf{B}\|_2 = \|\mathbf{B}\mathbf{A}\|_2$ for any nonsingular matrices $\mathbf{A}$ and $\mathbf{B}$, we see that

$$\left\|\big[\boldsymbol{\Sigma}_1 + \big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)^T\big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)\big]^{-1}\boldsymbol{\Sigma}_1\right\|_2 \leq 1.$$

Thus we deduce that

$$\big[\boldsymbol{\Sigma}_1 + \big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)^T\big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)\big]^{-1}\boldsymbol{\Sigma}_1^2\big[\boldsymbol{\Sigma}_1 + \big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)^T\big(\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)\big]^{-1} \preceq \mathbf{I}.$$

In turn, this implies that

$$\mathbf{M}^T\mathbf{M} \preceq \boldsymbol{\Sigma}_1.$$

Using this estimate in Equation (14), we find that

$$\begin{aligned}
T_2 &\leq 2\operatorname{Tr}\left(\boldsymbol{\Sigma}_2^{1/2}\mathbf{F}\boldsymbol{\Sigma}_1\mathbf{F}^T\boldsymbol{\Sigma}_2^{1/2}\right) = 2\operatorname{Tr}\left(\boldsymbol{\Sigma}_2\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big(\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\big)^T\boldsymbol{\Sigma}_2\right)\\
&= 2\left\|\boldsymbol{\Sigma}_2\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\right\|_{\mathrm{F}}^2.
\end{aligned}$$

Combining our estimates for T_1, T_2, and T_3 with Equation (13) gives

$$E = \left\|\mathbf{A}^{1/2}(\mathbf{I}-\mathbf{P}_{\mathbf{A}^{1/2}\mathbf{S}})\mathbf{A}^{1/2}\right\|_{\mathrm{F}}^2 \leq \|\boldsymbol{\Sigma}_2\|_{\mathrm{F}}^2 + 2\left\|\boldsymbol{\Sigma}_2\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\right\|_{\mathrm{F}}^2 + \left\|\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\right\|_{\mathrm{F}}^4.$$

The claimed bound follows by applying the subadditivity of the square-root function:

$$\left\|\mathbf{A}^{1/2}(\mathbf{I}-\mathbf{P}_{\mathbf{A}^{1/2}\mathbf{S}})\mathbf{A}^{1/2}\right\|_{\mathrm{F}} \leq \|\boldsymbol{\Sigma}_2\|_{\mathrm{F}} + \sqrt{2}\left\|\boldsymbol{\Sigma}_2\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\right\|_{\mathrm{F}} + \left\|\boldsymbol{\Sigma}_2^{1/2}\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^\dagger\right\|_{\mathrm{F}}^2.$$

□

Remark. The quality of approximation guarantee provided by Theorem 2 depends on two quantities, $\left\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_{\mathrm{F}}$ and $\left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_{\mathrm{F}}^2$, that depend in two slightly different ways on how the singular value structure of $\mathbf{A}$ interacts with the sampled version of the subspace structure. As we see in Section 4.2, the extent to which we can bound each of these for different sketching procedures is slightly different.

4.1.3. *Trace Norm Bounds.* Finally, we state and prove the following bound on the trace norm of the residual error. The proof method is analogous to that for the spectral and Frobenius norm bounds.

Theorem 3. *Let $\mathbf{A}$ be an $n \times n$ SPSD matrix with eigenvalue decomposition partitioned as in Equation* (1), *$\mathbf{S}$ be a sampling matrix of size $n \times \ell$, and $\mathbf{\Omega}_1$ and $\mathbf{\Omega}_2$ be as defined in Equation* (3). *Then when $\mathbf{C} = \mathbf{AS}$ and $\mathbf{W} = \mathbf{S}^T\mathbf{AS}$, the corresponding low-rank SPSD approximation satisfies*

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_\star \leq \mathrm{Tr}\left(\mathbf{\Sigma}_2\right) + \left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_{\mathrm{F}}^2,$$

assuming $\mathbf{\Omega}_1$ has full row rank.

Proof. Since $\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T = \mathbf{A}^{1/2}(\mathbf{I} - \mathbf{P}_{\mathbf{A}^{1/2}\mathbf{S}})\mathbf{A}^{1/2} \succeq 0$, its trace norm simplifies to its trace. Thus

$$\begin{aligned}\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_\star &= \mathrm{Tr}\left(\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right) = \mathrm{Tr}\left(\mathbf{\Sigma}^{1/2}(\mathbf{I} - \mathbf{P}_{\mathbf{\Sigma}^{1/2}\mathbf{S}})\mathbf{\Sigma}^{1/2}\right)\\ &\leq \mathrm{Tr}\left(\mathbf{\Sigma}^{1/2}(\mathbf{I} - \mathbf{P}_{\mathbf{Z}})\mathbf{\Sigma}^{1/2}\right),\end{aligned}$$

where $\mathbf{Z} = \begin{pmatrix}\mathbf{I}\\ \mathbf{F}\end{pmatrix}$ is defined in Equation (11). The semidefinite upper bound on $\mathbf{P}_{\mathbf{Z}}$ supplied in Equation (12) implies that

$$\mathrm{Tr}\left(\mathbf{\Sigma}^{1/2}(\mathbf{I} - \mathbf{P}_{\mathbf{Z}})\mathbf{\Sigma}^{1/2}\right) \leq \mathrm{Tr}\left(\mathbf{\Sigma}_1^{1/2}(\mathbf{I} - (\mathbf{I} + \mathbf{F}^T\mathbf{F})^{-1})\mathbf{\Sigma}_1^{1/2}\right) + \mathrm{Tr}\left(\mathbf{\Sigma}_2^{1/2}(\mathbf{I} - \mathbf{F}(\mathbf{I} + \mathbf{F}^T\mathbf{F})^{-1}\mathbf{F}^T)\mathbf{\Sigma}_2^{1/2}\right).$$

Recall the estimate $\mathbf{I} - (\mathbf{I} + \mathbf{F}^T\mathbf{F})^{-1} \preceq \mathbf{F}^T\mathbf{F}$ (shown in [31]) and the basic estimate $\mathbf{I} - \mathbf{F}(\mathbf{I} + \mathbf{F}^T\mathbf{F})^{-1}\mathbf{F}^T \preceq \mathbf{I}$. Together these imply that

$$\begin{aligned}\mathrm{Tr}\left(\mathbf{\Sigma}^{1/2}(\mathbf{I} - \mathbf{P}_{\mathbf{Z}})\mathbf{\Sigma}^{1/2}\right) &\leq \mathrm{Tr}\left(\mathbf{\Sigma}_1^{1/2}\mathbf{F}^T\mathbf{F}\mathbf{\Sigma}_1^{1/2}\right) + \mathrm{Tr}\left(\mathbf{\Sigma}_2\right)\\ &= \mathrm{Tr}\left(\mathbf{\Sigma}_2\right) + \left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_{\mathrm{F}}^2.\end{aligned}$$

The final equality follows from substituting the definition of $\mathbf{F}$ and identifying the squared Frobenius norm. We have established the claimed bound.

□

Remark. Since the identity $\left\|\mathbf{X}\right\|_{\mathrm{F}}^2 = \left\|\mathbf{X}\mathbf{X}^T\right\|_\star$ holds for any matrix $\mathbf{X}$, the squared Frobenius norm terms present in the deterministic error bounds for the Frobenius and trace norm errors are on the scale of $\left\|\mathbf{\Sigma}_2\right\|_\star$ when $\left\|\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_2$ is O(1).

4.1.4. *Additional Remarks on Our Deterministic Structural Results.* Before applying these deterministic structural results in particular randomized algorithmic settings, we pause to make several additional remarks about these three theorems.

Remark. We emphasize that these theorems are deterministic structural results that bound the excess error (beyond that of the optimal rank-k approximation) of low-rank approximations which follow our SPSD sketching model. That is, there is no randomness in their statement or analysis. In particular, these bounds hold for deterministic as well as randomized sketching matrices $\mathbf{S}$. In the latter case, the randomness enters only through $\mathbf{S}$, and one needs to show that the condition that $\mathbf{\Omega}_1$ has full row rank is satisfied with high probability; conditioned on this, the quality of the bound is determined by terms that depend on how the sketching matrix interacts with the subspace structure of the matrix $\mathbf{A}$.

Remark. In particular, we remind the reader that (although it is beyond the scope of this paper to explore this point in detail) these deterministic structural results could be used to check, in an *a posteriori* manner, the quality of a sketching method for which one cannot establish an *a priori* bound.

Remark. We also emphasize that the assumption that $\mathbf{\Omega}_1$ has full row rank is very non-trivial; and that it is false, in worst-case at least and for non-trivial parameter values, for common sketching methods such as uniform sampling. To see that some version of leverage-based sampling is needed to ensure this condition, recall that $\mathbf{U}_1^T\mathbf{U}_1 = \mathbf{I}$ and thus that $\mathbf{\Omega}_1\mathbf{\Omega}_1^T = \mathbf{U}_1^T\mathbf{S}\mathbf{S}^T\mathbf{U}_1$ can be viewed as approximating $\mathbf{I}$ with a small number of rank-1 components of $\mathbf{U}_1^T\mathbf{U}_1$. The condition that $\mathbf{\Omega}_1$ has full row rank is equivalent to $\left\|\mathbf{U}_1^T\mathbf{U}_1 - \mathbf{U}_1^T\mathbf{S}\mathbf{S}^T\mathbf{U}_1\right\|_2 < 1$. Work on approximating the product of matrices by random sampling shows that to obtain non-trivial bounds one must sample with respect to the norm of the rank-1 components [19], which here (since we are approximating the product of two orthogonal matrices) equal the statistical leverage scores. From this perspective, random projections satisfy this condition since (informally) they rotate to a random basis where the leverage scores of the rotated matrix are approximately uniform and thus where uniform sampling is appropriate [23, 45].

Remark. As observed recently [4], methods that use knowledge of a matrix square root Φ (*i.e.*, a Φ such that $\mathbf{A} = \Phi\Phi^T$) typically lead to $\Omega(n^2)$ complexity. An important feature of our approach is that we only use the matrix square root implicitly—that is, inside the analysis, and not in the statement of the algorithm—and thus we do *not* incur any such cost.

Remark. For some randomized sampling schemes, it may be difficult to obtain a sharp bound on $\left\|\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_\xi$ for $\xi = 2, F$. In these situations, the bounds on the excess error supplied by Theorems 1, 2, and 3 may be quite pessimistic. On the other hand, since $\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T = \mathbf{A}^{1/2}(\mathbf{I} - \mathbf{P}_{\mathbf{A}^{1/2}\mathbf{S}})\mathbf{A}^{1/2}$, it follows that $0 \preceq \mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T \preceq \mathbf{A}$. This implies that the errors of *any* Nyström extension, deterministic or randomized, satisfy at least the crude bound $\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_\xi \leq \|\mathbf{A}\|_\xi$.

4.2. **Stochastic Error Bounds for Low-rank SPSD Approximation.** In this section, we apply the three theorems from Section 4.1 to bound the reconstruction errors for several random sampling and random projection methods that conform to our SPSD Sketching Model. In particular, we consider two variants of random sampling and two variants of random projections: sampling columns according to an importance sampling distribution that depends on the statistical leverage scores (in Section 4.2.1); randomly projecting by using subsampled randomized Fourier transformations (in Section 4.2.2); randomly projecting by uniformly sampling from Gaussian mixtures of the columns (in Section 4.2.3); and, finally, sampling columns uniformly at random (in Section 4.2.4).

Before establishing these results, we pause here to provide a brief review of running time issues, some of which were addressed empirically in Section 3. The computational bottleneck for random sampling algorithms (except for uniform sampling that we address in Section 4.2.4, which is trivial to implement) is often the exact or approximate computation of the importance sampling distribution with respect to which one samples; and the computational bottleneck for random projection methods is often the implementation of the random projection. For example, if the sketching matrix $\mathbf{S}$ is a random projection constructed as an $n \times \ell$ matrix of i.i.d. Gaussian random variables, as we use in Section 4.2.3, then the running time of dense data in RAM is not substantially faster than computing $\mathbf{U}_1$, while the running time can be much faster for certain sparse matrices or for computation in parallel or distributed environments. Alternately, if the sketching matrix $\mathbf{S}$ is a Fourier-based projection, as we use in Section 4.2.2, then the running time for data stored in RAM is typically $O(n^2 \ln k)$, as opposed to the $O(n^2 k)$ time that would be needed to compute $\mathbf{U}_1$. These running times depend sensitively on the size of the data and the model of data access; see [45, 31] for detailed discussions of these issues.

In particular, for random sampling algorithms that use a leverage-based importance sampling distribution, as we use in Section 4.2.1, it is often said that the running time is no faster than that of computing $\mathbf{U}_1$. (This $O(n^2k)$ running time claim is simply the running time of the naïve algorithm that computes $\mathbf{U}_1$ "exactly," *e.g.*, with a variant of the QR decomposition, and then reads off the Euclidean norms of the rows.) However, the randomized algorithm of [20] that computes relative-error approximations to *all* of the statistical leverage in a time that is qualitatively faster—in worst-case theory and, by using existing high-quality randomized numerical code [3, 49, 31], in practice—gets around this bottleneck, as was shown in Section 3. The computational bottleneck for the algorithms of [20] is that of applying a random projection, and thus the running time for leverage-based Nyström extension is that of applying a ("fast" Fourier-based or "slow" Gaussian-based, as appropriate) random projection to $\mathbf{A}$ [20]. See Section 3 or [3, 49, 31] for additional details.

4.2.1. *Sampling with Leverage-based Importance Sampling Probabilities.* Here, the columns of $\mathbf{A}$ are sampled with replacement according to a nonuniform probability distribution determined by the (exact or approximate) statistical leverage scores of $\mathbf{A}$ relative to the best rank-k approximation to $\mathbf{A}$, which in turn depend on nonuniformity properties of the top k-dimensional eigenspace of $\mathbf{A}$. To add flexibility (*e.g.*, in case the scores are computed only approximately with the fast algorithm of [20]), we formulate the following lemma in terms of any probability distribution that is β-close to the leverage score distribution. In particular, consider any probability distribution satisfying

$$p_j \geq \frac{\beta}{k} \left\|(\mathbf{U}_1)_j\right\|_2^2 \quad \text{and} \quad \sum\nolimits_{j=1}^n p_j = 1,$$

where $\beta \in (0,1]$. Given these (β-approximate) leverage-based probabilities, the sampling matrix is $\mathbf{S} = \mathbf{RD}$ where $\mathbf{R} \in \mathbb{R}^{n \times \ell}$ is a column selection matrix that samples columns of $\mathbf{A}$ from the given distribution—*i.e.*, $\mathbf{R}_{ij} = 1$ iff the ith column of $\mathbf{A}$ is the jth column selected—and $\mathbf{D}$ is a diagonal rescaling matrix satisfying $\mathbf{D}_{jj} = \frac{1}{\sqrt{\ell p_i}}$ iff $\mathbf{R}_{ij} = 1$. For this case, we can prove the following.

Lemma 1. *Let $\mathbf{A}$ be an $n \times n$ SPSD matrix and $\mathbf{S}$ be a sampling matrix of size $n \times \ell$ corresponding to a leverage-based probability distribution derived from the top k-dimensional eigenspace of $\mathbf{A}$, satisfying*

$$p_j \geq \frac{\beta}{k} \left\|(\mathbf{U}_1)_j\right\|_2^2 \quad \textit{and} \quad \sum\nolimits_{j=1}^n p_j = 1,$$

for some $\beta \in (0,1]$. Fix a failure probability $\delta \in (0,1]$ and approximation factor $\varepsilon \in (0,1]$.

If $\ell \geq 3200(\beta\varepsilon^2)^{-1} k \ln(4k/(\beta\delta))$, then the corresponding low-rank SPSD approximation satisfies

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_2 \leq \left\|\mathbf{A} - \mathbf{A}_k\right\|_2 + \varepsilon^2 \left\|\mathbf{A} - \mathbf{A}_k\right\|_\star, \tag{15}$$

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_\mathrm{F} \leq (1 + \sqrt{2}\varepsilon) \left\|\mathbf{A} - \mathbf{A}_k\right\|_\mathrm{F} + \varepsilon^2 \left\|\mathbf{A} - \mathbf{A}_k\right\|_\star, \quad \textit{and} \tag{16}$$

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_\star \leq (1 + \varepsilon^2) \left\|\mathbf{A} - \mathbf{A}_k\right\|_\star, \tag{17}$$

each with probability at least $1 - 4\delta - 0.4$.

Proof. In [44, proof of Proposition 22] it is shown that if ℓ satisfies the given bound and the samples are drawn from an approximate subspace probability distribution, then

$$\left\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_\mathrm{F} \leq \varepsilon \left\|\mathbf{\Sigma}_2\right\|_\mathrm{F}$$

with probability at least $1 - 2\delta - 0.2$. It follows that similarly

$$\left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_\mathrm{F}^2 \leq \varepsilon^2 \left\|\mathbf{\Sigma}_2^{1/2}\right\|_\mathrm{F}^2 = \varepsilon^2 \left\|\mathbf{\Sigma}_2\right\|_\star$$

with probability at least $1-2\delta-0.2$. These estimates used in Theorems 2 and 3 yield the stated bounds for the Frobenius and trace norms. The spectral norm error follows from Theorem 1, the bound on $\left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_\mathrm{F}^2$, and the fact that the spectral norm of a matrix is smaller than its Frobenius norm.

□

Remark. The additive scale factors for the spectral and Frobenius norm bounds are much improved relative to the prior results of [21]. At root, this is since the leverage score importance sampling probabilities highlight structural properties of the data (*e.g.*, how to satisfy the condition in Theorems 1, 2, and 3 that $\mathbf{\Omega}_1$ has full row rank) in a more refined way than the importance sampling probabilities of [21].

Remark. These improvements come at additional computational expense, but we remind the reader that leverage-based sampling probabilities of the form used by Lemma 1 can be computed faster than the time needed to compute the basis $\mathbf{U}_1$ [20]. The computational bottleneck of the algorithm of [20] is the time required to perform a random projection on the input matrix.

Remark. Not surprisingly, constant factors such as 3200 (as well as other similarly large factors below) and a failure probability bounded away from zero are artifacts of the analysis; the empirical behavior of this sampling method is much better. This has been observed previously [22, 47].

4.2.2. *Random Projections with Subsampled Randomized Fourier Transforms.* Here, the columns of $\mathbf{A}$ are randomly mixed using a unitary matrix before the columns are sampled. In particular, $\mathbf{S} = \sqrt{\frac{n}{\ell}}\mathbf{DTR}$, where $\mathbf{D}$ is a diagonal matrix of Rademacher random variables, $\mathbf{T}$ is a highly incoherent unitary matrix, and $\mathbf{R}$ restricts to ℓ columns. For concreteness, and because it has an associated fast transform, we consider the case where $\mathbf{T}$ is the normalized Fourier transform of size $n \times n$. For this case, we can prove the following.

Lemma 2. *Let $\mathbf{A}$ be an $n \times n$ SPSD matrix and $\mathbf{S} = \sqrt{\frac{n}{\ell}}\mathbf{DFR}$ be a sampling matrix of size $n \times \ell$, where $\mathbf{D}$ is a diagonal matrix of Rademacher random variables, $\mathbf{F}$ is a normalized Fourier matrix of size $n \times n$, and $\mathbf{R}$ restricts to ℓ columns. Fix a failure probability $\delta \in (0,1)$, approximation factor $\varepsilon \in (0,1)$, and assume that $k \geq 4$.*

If $\ell \geq 24\varepsilon^{-1}[\sqrt{k} + \sqrt{8\ln(8n/\delta)}]^2 \ln(8k/\delta)$, then the corresponding low-rank SPSD approximation satisfies

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_2 \leq \left(1 + \frac{1}{1-\sqrt{\varepsilon}} \cdot \left(5 + \frac{16\ln(n/\delta)^2}{\ell}\right)\right) \left\|\mathbf{A} - \mathbf{A}_k\right\|_2 + \frac{2\ln(n/\delta)}{(1-\sqrt{\varepsilon})\ell} \left\|\mathbf{A} - \mathbf{A}_k\right\|_\star,$$

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_\mathrm{F} \leq (1 + \sqrt{44\varepsilon}) \left\|\mathbf{A} - \mathbf{A}_k\right\|_\mathrm{F} + 22\varepsilon \left\|\mathbf{A} - \mathbf{A}_k\right\|_\star, \text{ and}$$

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_\star \leq (1 + 22\varepsilon) \left\|\mathbf{A} - \mathbf{A}_k\right\|_\star, \tag{18}$$

each with probability at least $1 - \delta$.

Proof. In [13, proof of Theorem 4], it is shown that for this choice of $\mathbf{S}$ and number of samples ℓ,

$$\begin{aligned}\left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_2^2 &\leq \frac{1}{1-\sqrt{\varepsilon}} \cdot \left(5\left\|\mathbf{\Sigma}_2^{1/2}\right\|_2^2 + \frac{\ln(n/\delta)}{\ell}\left(\left\|\mathbf{\Sigma}_2^{1/2}\right\|_\mathrm{F} + \sqrt{8\ln(n/\delta)}\left\|\mathbf{\Sigma}_2^{1/2}\right\|_2\right)^2\right) \\ &= \frac{1}{1-\sqrt{\varepsilon}} \cdot \left(5\left\|\mathbf{\Sigma}\right\|_2 + \frac{\ln(n/\delta)}{\ell}\left(\left\|\mathbf{\Sigma}_2\right\|_\star^{1/2} + \sqrt{8\ln(n/\delta)}\left\|\mathbf{\Sigma}_2\right\|_2^{1/2}\right)^2\right) \\ &\leq \frac{1}{1-\sqrt{\varepsilon}} \cdot \left(\left(5 + \frac{16\ln(n/\delta)^2}{\ell}\right)\left\|\mathbf{\Sigma}_2\right\|_2 + \frac{2\ln(n/\delta)}{\ell}\left\|\mathbf{\Sigma}_2\right\|_\star\right)\end{aligned}$$

and

$$\left\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_\mathrm{F} \leq \sqrt{22\varepsilon}\left\|\mathbf{\Sigma}_2\right\|_\mathrm{F}$$

with probability at least $1 - \delta$. Likewise, with the same probability

$$\left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_\mathrm{F}^2 \leq 22\varepsilon\left\|\mathbf{\Sigma}_2^{1/2}\right\|_\mathrm{F}^2 = 22\varepsilon\left\|\mathbf{\Sigma}_2\right\|_\star.$$

These estimates used in Theorems 1, 2, and 3 yield the stated bounds. □

Remark. Suppressing the dependence on δ and ε, the spectral norm bound ensures that when $k = \Omega(\ln n)$ and $\ell = \Omega(k \ln k)$, then

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_2 = \mathrm{O}\left(\frac{\ln n}{\ln k}\left\|\mathbf{A} - \mathbf{A}_k\right\|_2 + \frac{1}{\ln k}\left\|\mathbf{A} - \mathbf{A}_k\right\|_\star\right).$$

This should be compared to the guarantee established in Lemma 3 below for Gaussian-based SPSD sketches constructed using the same number of measurements:

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_2 = \mathrm{O}\left(\left\|\mathbf{A} - \mathbf{A}_k\right\|_2 + \frac{1}{k\ln k}\left\|\mathbf{A} - \mathbf{A}_k\right\|_\star\right).$$

Lemma 2 guarantees that errors on this order can be achieved if one increases the number of samples by a logarithm factor in the dimension: specifically, such a bound is achieved when $k = \Omega(\ln n)$ and $\ell = \Omega(k \ln k \ln n)$. The difference between the number of samples necessary for Fourier-based sketches and Gaussian-based sketches is reflective of the differing natures of the random projections: the geometry of any k-dimensional subspace is preserved under projection onto the span of $\ell = \mathrm{O}(k)$ Gaussian random vectors [31], but the sharpest analysis available suggests that to preserve the geometry of such a subspace under projection onto the span of ℓ SRFT vectors, ℓ must satisfy $\ell = \Omega(\max\{k, \ln n\} \ln k)$ [58]. We note, however, that in practice the Fourier-based and Gaussian-based SPSD sketches have similar reconstruction errors.

Remark. The structure of the Frobenius and trace norm bounds for the Fourier-based projection are identical to the structure of the corresponding bounds from Lemma 1 for leverage-based sampling (and the bounds could be made identical with appropriate choice of parameters). This is not surprising since (informally) Fourier-based (and other) random projections rotate to a random basis where the leverage scores are approximately uniform and thus where uniform sampling is appropriate [45]. The disparity of the spectral norm bounds suggests that leverage-based SPSD sketches should be expected to be more accurate in the spectral norm than Fourier-based sketches; the empirical results of Section 3.3 support this interpretation. The running times of the Fourier-based and the leverage-based algorithms are the same, to leading order, if the algorithm of [20] (which uses the same transform $\mathbf{S} = \sqrt{\frac{n}{\ell}}\mathbf{DHR}$) is used to approximate the leverage scores.

4.2.3. *Random Projections with I.I.D. Gaussian Random Matrices.* Here, the columns of $\mathbf{A}$ are randomly mixed using Gaussian random variables before sampling. Thus, the entries of the sampling matrix $\mathbf{S} \in \mathbb{R}^{n\times\ell}$ are i.i.d. standard Gaussian random variables. We consider two cases: first, when the number of samples is comparable to and only slightly larger than the desired rank, *i.e.*, $\ell = k + p$ for some parameter p; and second, when the number of samples is logarithmically larger than the desired rank $\ell = \Omega(k \ln k)$. The former case has proven to be a useful parameterization for certain numerical implementations [45, 31]; we already see that the guarantees here are as good as those for the leverage-based sampling algorithm with $\Omega(k \ln k)$ samples, and better than those for Fourier-based sampling. The latter case is more expensive, but we see that the bounds are considerably sharper, suggesting that in situations where one desires high accuracy, one can use SPSD sketches based on $\Omega(k \ln k)$ Gaussian-based samples. For these two cases, we prove the following.

Lemma 3. *Let $\mathbf{A}$ be an $n\times n$ SPSD matrix and $\mathbf{S} \in \mathbb{R}^{n\times\ell}$ be a matrix of i.i.d standard Gaussians. If $\ell = k+p$ where $p = k\varepsilon^{-2}$ for some $\varepsilon \in (0,1]$ and $k > 4$, then the corresponding low-rank SPSD approximation satisfies*

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_2 \leq \left(1 + 89\varepsilon^2 + 874\varepsilon^2\frac{\ln k}{k}\right) \cdot \|\mathbf{A} - \mathbf{A}_k\|_2 + 219\frac{\varepsilon^2}{k} \cdot \|\mathbf{A} - \mathbf{A}_k\|_\star\,,$$

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_{\mathrm{F}} \leq (1 + 7\varepsilon) \cdot \|\mathbf{A} - \mathbf{A}_k\|_{\mathrm{F}} + 45\varepsilon^2 \cdot \|\mathbf{A} - \mathbf{A}_k\|_\star + \left(30\varepsilon\sqrt{\frac{\ln k}{k}} + 874\varepsilon^2\frac{\ln k}{k}\right) \cdot \|\mathbf{A} - \mathbf{A}_k\|_2\,,$$

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_\star \leq (1 + 45\varepsilon^2) \cdot \|\mathbf{A} - \mathbf{A}_k\|_\star + 874\varepsilon^2\frac{\ln k}{k} \cdot \|\mathbf{A} - \mathbf{A}_k\|_2$$

each with probability at least $1 - 2k^{-1} - 4\mathrm{e}^{-k/\varepsilon^2}$.

If additionally $\ell \geq 2\varepsilon^{-2}k\ln k$, *then*

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_2 \leq \left(1 + 89\varepsilon^2\frac{1}{\ln k} + 874\varepsilon^2\frac{1}{k}\right) \cdot \|\mathbf{A} - \mathbf{A}_k\|_2 + 219\frac{\varepsilon}{k\ln k} \cdot \|\mathbf{A} - \mathbf{A}_k\|_\star\,,$$

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_{\mathrm{F}} \leq \left(1 + \frac{7}{\sqrt{\ln k}}\varepsilon\right) \cdot \|\mathbf{A} - \mathbf{A}_k\|_{\mathrm{F}} + \frac{45}{\ln k}\varepsilon^2 \cdot \|\mathbf{A} - \mathbf{A}_k\|_\star + \left(\frac{15}{\sqrt{k}}\varepsilon + \frac{437}{k}\varepsilon^2\right) \cdot \|\mathbf{A} - \mathbf{A}_k\|_2$$

$$\left\|\mathbf{A} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_\star \leq \left(1 + \frac{45}{\ln k}\varepsilon^2\right) \cdot \|\mathbf{A} - \mathbf{A}_k\|_\star + \frac{437}{k}\varepsilon^2 \cdot \|\mathbf{A} - \mathbf{A}_k\|_2$$

each with probability at least $1 - 2k^{-1} - 4k^{-k/\varepsilon^2}$.

As before, this result is established by bounding the quantities involved in Theorems 1, 2, and 3. The following deviation bounds, established in [31, Section 10], are useful in that regard: if $\mathbf{D}$ is a diagonal matrix, $\ell = k + p$ with $p > 4$ and $u, t \geq 1$, then

$$\mathbb{P}\left\{\left\|\mathbf{D}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_2 > \|\mathbf{D}\|_2\left(\sqrt{\frac{3k}{p+1}} \cdot t + \frac{\mathrm{e}\sqrt{\ell}}{p+1} \cdot tu\right) + \|\mathbf{D}\|_{\mathrm{F}}\frac{\mathrm{e}\sqrt{\ell}}{p+1} \cdot t\right\} \leq 2t^{-p} + \mathrm{e}^{-u^2/2}, \text{ and}$$

$$\mathbb{P}\left\{\left\|\mathbf{D}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_{\mathrm{F}} > \|\mathbf{D}\|_{\mathrm{F}}\sqrt{\frac{3k}{p+1}} \cdot t + \|\mathbf{D}\|_2\frac{\mathrm{e}\sqrt{\ell}}{p+1} \cdot tu\right\} \leq 2t^{-p} + \mathrm{e}^{-u^2/2}. \tag{19}$$

Proof. First consider the case where $p = k\varepsilon^{-2}$. Estimate the terms in (19) with

$$\begin{aligned}\sqrt{\frac{3k}{p+1}} &\leq \sqrt{\frac{3k}{p}} = \sqrt{3}\varepsilon \\ \frac{\sqrt{\ell}}{p+1} &\leq \frac{\varepsilon^2\sqrt{k(1+1/\varepsilon^2)}}{k} \leq \varepsilon\sqrt{\frac{2}{k}}\end{aligned}$$

and take $t = \mathrm{e}$ and $u = \sqrt{2\ln k}$ in (19) to obtain that

$$\begin{aligned}\left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_2^2 &\leq \left[\left(\sqrt{3}\mathrm{e} + 2\mathrm{e}^2\sqrt{\frac{\ln k}{k}}\right)\varepsilon \cdot \left\|\mathbf{\Sigma}_2^{1/2}\right\|_2 + \frac{2\mathrm{e}^2\varepsilon}{\sqrt{k}} \cdot \left\|\mathbf{\Sigma}_2^{1/2}\right\|_\mathrm{F}\right]^2 \\ &\leq 2\left(\sqrt{3}\mathrm{e} + 2\mathrm{e}^2\sqrt{\frac{\ln k}{k}}\right)^2 \varepsilon^2 \cdot \|\mathbf{\Sigma}_2\|_2 + \frac{4\mathrm{e}^4\varepsilon^2}{k} \cdot \|\mathbf{\Sigma}_2\|_\star \\ &\leq \left(12\mathrm{e}^2 + 16\mathrm{e}^4\frac{\ln k}{k}\right)\varepsilon^2 \cdot \|\mathbf{\Sigma}_2\|_2 + \frac{4\mathrm{e}^4\varepsilon^2}{k} \cdot \|\mathbf{\Sigma}_2\|_\star\end{aligned}$$

with probability at least $1 - k^{-1} - 2\mathrm{e}^{-k/\varepsilon^2}$ and

$$\left\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_\mathrm{F} \leq \sqrt{3}\varepsilon\mathrm{e} \cdot \|\mathbf{\Sigma}_2\|_\mathrm{F} + \mathrm{e}^2\varepsilon\sqrt{\frac{8\ln k}{k}} \cdot \|\mathbf{\Sigma}_2\|_2$$

with the same probability. Likewise,

$$\begin{aligned}\left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_\mathrm{F}^2 &\leq \left(\sqrt{3}\varepsilon\mathrm{e} \cdot \left\|\mathbf{\Sigma}_2^{1/2}\right\|_\mathrm{F} + \mathrm{e}^2\varepsilon\sqrt{\frac{8\ln k}{k}} \cdot \left\|\mathbf{\Sigma}_2^{1/2}\right\|_2\right)^2 \\ &\leq 6\varepsilon^2\mathrm{e}^2 \cdot \left\|\mathbf{\Sigma}_2^{1/2}\right\|_\mathrm{F}^2 + 16\mathrm{e}^4\varepsilon^2\frac{\ln k}{k} \cdot \|\mathbf{\Sigma}_2\|_2 \\ &= 6\varepsilon^2\mathrm{e}^2 \cdot \|\mathbf{\Sigma}_2\|_\star + 16\mathrm{e}^4\varepsilon^2\frac{\ln k}{k} \cdot \|\mathbf{\Sigma}_2\|_2\end{aligned}$$

with the same probability. These estimates used in Theorems 1, 2, and 3 yield the stated bounds for the case where $\ell = k(1 + \varepsilon^{-2})$.

Now consider the case that $\ell \geq 2\varepsilon^{-2}k\ln k$. This implies $p \geq \varepsilon^{-2}k\ln k$, so we have the estimates

$$\begin{aligned}\sqrt{\frac{3k}{p+1}} &\leq \sqrt{\frac{3k}{p}} \leq \sqrt{\frac{3}{\ln k}}\varepsilon \\ \frac{\sqrt{\ell}}{p+1} &\leq \frac{\sqrt{k+p}}{p} \leq \sqrt{\frac{\varepsilon^4}{k\ln^2 k} + \frac{\varepsilon^2}{k\ln k}} < \sqrt{\frac{2}{k\ln k}}\varepsilon.\end{aligned}$$

As before, take $t = \mathrm{e}$ and $u = \sqrt{2\ln k}$ in (19) to obtain that

$$\begin{aligned}\left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_2^2 &\leq \left[\varepsilon\left(\mathrm{e}\sqrt{\frac{3}{\ln k}} + 2\mathrm{e}^2\sqrt{\frac{1}{k}}\right) \cdot \left\|\mathbf{\Sigma}_2^{1/2}\right\|_2 + \varepsilon\mathrm{e}^2\sqrt{\frac{2}{k\ln k}} \cdot \left\|\mathbf{\Sigma}_2^{1/2}\right\|_\mathrm{F}\right]^2 \\ &\leq 2\varepsilon^2\left(\mathrm{e}\sqrt{\frac{3}{\ln k}} + 2\mathrm{e}^2\sqrt{\frac{1}{k}}\right)^2 \cdot \|\mathbf{\Sigma}_2\|_2 + \frac{4\varepsilon^2\mathrm{e}^4}{k\ln k} \cdot \left\|\mathbf{\Sigma}_2^{1/2}\right\|_\mathrm{F}^2 \\ &\leq \left(\frac{12\mathrm{e}^2}{\ln k} + \frac{16\mathrm{e}^4}{k}\right)\varepsilon^2 \cdot \|\mathbf{\Sigma}_2\|_2 + \frac{4\varepsilon^2\mathrm{e}^4}{k\ln k} \cdot \|\mathbf{\Sigma}_2\|_\star\end{aligned}$$

with probability at least $1 - k^{-1} - 2k^{-k/\varepsilon^2}$ and

$$\left\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_\mathrm{F} \leq \sqrt{\frac{3}{\ln k}}\varepsilon\mathrm{e} \cdot \|\mathbf{\Sigma}_2\|_\mathrm{F} + \frac{2\mathrm{e}^2}{\sqrt{k}}\varepsilon \cdot \|\mathbf{\Sigma}_2\|_2$$

with the same probability. Likewise,

$$\begin{aligned}\left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_{\mathrm{F}}^2 &\leq \left(\sqrt{\frac{3}{\ln k}}\varepsilon \mathrm{e}\cdot\left\|\mathbf{\Sigma}_2^{1/2}\right\|_{\mathrm{F}} + \frac{2\mathrm{e}^2}{\sqrt{k}}\varepsilon\cdot\left\|\mathbf{\Sigma}_2^{1/2}\right\|_2\right)^2 \\ &\leq \frac{6}{\ln k}\varepsilon^2\mathrm{e}^2\cdot\left\|\mathbf{\Sigma}_2\right\|_\star + \frac{8\mathrm{e}^4}{k}\varepsilon^2\cdot\left\|\mathbf{\Sigma}_2\right\|_2\end{aligned}$$

with the same probability. These estimates used in Theorems 1, 2, and 3 yield the stated bounds for the case where ℓ is logarithmically larger than k. □

Remark. The way we have parameterized these bounds for Gaussian-based projections makes explicit the dependence on various parameters, but hides the structural simplicity of these bounds. In particular, since $\|\cdot\|_2 \leq \|\cdot\|_{\mathrm{F}} \leq \|\cdot\|_\star$, note that the Frobenius norm bounds are upper bounded by a term that depends on the Frobenius norm of the error and a term that depends on the trace norm of the error; and that, similarly, the trace norm bounds are upper bounded by a multiplicative factor that can be set to $1+\epsilon$ with an appropriate choice of parameters.

4.2.4. *Sampling Columns Uniformly at Random.* Here, the columns of $\mathbf{A}$ are sampled uniformly at random (with or without replacement). Such uniformly-at-random column sampling only makes sense when the leverage scores of the top k-dimensional invariant subspace of the matrix are sufficiently uniform that no column is significantly more informative than the others. For this case, we can prove the following.

Lemma 4. *Let $\mathbf{A}$ be an $n \times n$ SPSD matrix and $\mathbf{S}$ be a sampling matrix of size $n \times \ell$ corresponding to sampling the columns of $\mathbf{A}$ uniformly at random (with or without replacement). Let μ denote the coherence of the top k-dimensional eigenspace of $\mathbf{A}$ and fix a failure probability $\delta \in (0,1)$ and accuracy factor $\varepsilon \in (0,1)$. If*

$$\ell \geq 2\mu\varepsilon^{-2}k\ln\left(\frac{k}{\delta}\right),$$

then the corresponding low-rank SPSD approximation satisfies

$$\begin{aligned}\left\|\mathbf{A}-\mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_2 &\leq \left(1+\frac{n}{(1-\varepsilon)\ell}\right)\left\|\mathbf{A}-\mathbf{A}_k\right\|_2, \\ \left\|\mathbf{A}-\mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_{\mathrm{F}} &\leq \left(1+\frac{1}{\delta}\sqrt{\frac{2}{1-\varepsilon}}\right)\left\|\mathbf{A}-\mathbf{A}_k\right\|_{\mathrm{F}} + \frac{1}{\delta(1-\varepsilon)}\left\|\mathbf{A}-\mathbf{A}_k\right\|_\star, \text{ and} \\ \left\|\mathbf{A}-\mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\right\|_\star &\leq \left(1+\frac{1}{\delta(1-\varepsilon)}\right)\left\|\mathbf{A}-\mathbf{A}_k\right\|_\star,\end{aligned}$$

each with probability at least $1-4\delta$.

Proof. In [28], it is shown that

$$\left\|\mathbf{\Omega}_1^\dagger\right\|_2^2 \leq \frac{n}{(1-\varepsilon)\ell}$$

with probability at least $1-\delta$ when ℓ satisfies the stated bound. Observe that $\|\mathbf{\Omega}_2\|_2 \leq \|\mathbf{U}_2\|_2\|\mathbf{S}\|_2 \leq 1$, so

$$\left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_2^2 \leq \left\|\mathbf{\Sigma}_2^{1/2}\right\|_2^2\left\|\mathbf{\Omega}_1^\dagger\right\|_2^2 \leq \|\mathbf{\Sigma}_2\|_2\frac{n}{(1-\varepsilon)\ell}$$

with probability at least $1-\delta$. Also,

$$\left\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_{\mathrm{F}} \leq \sqrt{\frac{n}{(1-\varepsilon)\ell}}\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\|_{\mathrm{F}} \tag{20}$$

with at least the same probability. Observe that since $\mathbf{S}$ selects ℓ columns uniformly at random,

$$\mathbb{E}\left\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\right\|_{\mathrm{F}}^2 = \mathbb{E}\left\|\mathbf{\Sigma}_2\mathbf{U}_2^T\mathbf{S}\right\|_{\mathrm{F}}^2 = \sum_{i=1}^{\ell}\mathbb{E}\|\mathbf{x}_i\|^2,$$

where the summands $\mathbf{x}_i$ are distributed uniformly at random over the columns of $\mathbf{\Sigma}_2\mathbf{U}_2^T$. Regardless of whether $\mathbf{S}$ selects the columns with replacement or without replacement, the summands all have the same expectation:

$$\mathbb{E}\|\mathbf{x}_i\|^2 = \frac{1}{n}\sum_{j=1}^n \|(\mathbf{\Sigma}_2\mathbf{U}_2^T)^j)\|^2 = \frac{1}{n}\|\mathbf{\Sigma}_2\mathbf{U}_2\|_{\mathrm{F}}^2 = \frac{1}{n}\|\mathbf{\Sigma}_2\|_{\mathrm{F}}^2 .$$

Consequently,

$$\mathbb{E}\,\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\|_{\mathrm{F}}^2 = \frac{\ell}{n}\|\mathbf{\Sigma}_2\|_{\mathrm{F}}^2 ,$$

so by Jensen's inequality

$$\mathbb{E}\,\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\|_{\mathrm{F}} \leq \left(\mathbb{E}\,\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\|_{\mathrm{F}}^2\right)^{1/2} = \sqrt{\frac{\ell}{n}}\,\|\mathbf{\Sigma}_2\|_{\mathrm{F}} .$$

Now applying Markov's inequality to (20), we see that

$$\left\|\mathbf{\Sigma}_2\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_{\mathrm{F}} \leq \frac{1}{\delta}\sqrt{\frac{1}{(1-\varepsilon)}}\,\|\mathbf{\Sigma}_2\|_{\mathrm{F}}$$

with probability at least $1-2\delta$. Using similar reasoning, we can conclude that

$$\left\|\mathbf{\Sigma}_2^{1/2}\mathbf{\Omega}_2\mathbf{\Omega}_1^\dagger\right\|_{\mathrm{F}}^2 \leq \frac{1}{(1-\varepsilon)\delta}\left\|\mathbf{\Sigma}_2^{1/2}\right\|_{\mathrm{F}}^2 = \frac{1}{(1-\varepsilon)\delta}\|\mathbf{\Sigma}_2\|_\star$$

also with probability at least $1-2\delta$. These estimates used in Theorems 1, 2, and 3 yield the stated bounds. □

Remark. As with previous bounds for uniform sampling, *e.g.*, [38, 28], these results for uniform sampling are much weaker than our bounds from the previous subsections, since the sampling complexity depends on the coherence of the input matrix. When the matrix has small coherence, however, these bounds are similar to the bounds derived from the leverage-based sampling probabilities. Recall that, by the algorithm of [20], the coherence of an arbitrary input matrix can be computed in roughly the time it takes to perform a random projection on the input matrix.

5. Discussion and Conclusion

We have presented a unified approach to the Nyström-based low-rank approximation of Laplacian and kernel matrices that arise in machine learning and data analysis applications; and in doing so we have provided qualitatively-improved worst-case theory and clarified the performance of these algorithms in practical settings. Our theoretical and empirical results suggest several obvious directions for future work.

In general, our empirical evaluation demonstrates that, to obtain moderately high-quality low-rank approximations, as measured by minimizing the reconstruction error, depends in complicated ways on the spectral decay, the leverage score structure, the eigenvalue gaps in relevant parts of the spectrum, etc. (Ironically, our empirical evaluation also demonstrates that *all* the Nyström extensions are reasonably-effective at approximating both sparse and dense, and both low-rank and high-rank matrices which arise in practice. That is, with only roughly $\mathrm{O}(k)$ measurements, the spectral, Frobenius, and trace approximation errors stay within a small multiplicative factor of around 3 of the optimal rank-k approximation errors. The reason for this is that matrices for which uniform sampling is least appropriate tend to be those which are least well-approximated by low-rank matrices, meaning that the residual error is much larger.) Thus, *e.g.*, depending on whether one is interested in ℓ being slightly larger or much larger than k, leverage-based sampling or a random projection might be most appropriate; and, more generally, an ensemble-based method that draws complementary strengths from each of these methods might be best.

In addition, we should note that, in situations where one is concerned with the quality of approximation of the actual eigenspaces, one desires both a small spectral norm error (because by the Davis–Kahan sinΘ theorem and similar perturbation results, this would imply that the range space of the Nyström approximation effectively captures the top k-dimensional eigenspace of $\mathbf{A}$) as well as to use as few samples as possible (because one prefers to approximate the top k-dimension eigenspace of $\mathbf{A}$ with as close to a k-dimensional subspace as possible). Our results suggest that the leverage score probabilities supply the best sampling scheme for balancing these two competing objectives.

More generally, although our empirical evaluation consists of *random* sampling and *random* projection algorithms, our theoretical analysis clearly decouples the randomness in the algorithm from the structural heterogenities in the Euclidean vector space that are responsible for the poor performance of uniform sampling algorithms. Thus, if those structural conditions can be satisfied with a deterministic algorithm, then one can certify (after running the algorithm) that good approximation guarantees hold for particular input matrices in less time than is required for general matrices. Moreover, this structural decomposition suggests greedy heuristics—*e.g.*, greedily keep some number of columns according to approximate statistical leverage scores and "residualize." In our experience, a procedure of this form often performs quite well in practice, although theoretical guarantees tend to be much weaker; and thus we expect that, when coupled with our results, such procedures will perform quite well in practice in many large-scale machine learning applications.

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