Abstract

Kernel methods offer the flexibility to learn complex relationships in modern, large data sets while enjoying strong theoretical guarantees on quality. Unfortunately, these methods typically require cubic running time in the data set size, a prohibitive cost in the large-data setting. Random feature maps (RFMs) and the Nyström method both consider low-rank approximations to the kernel matrix as a potential solution. But, in order to achieve desirable theoretical guarantees, the former may require a prohibitively large number of features $J$, and the latter may be prohibitively expensive for high-dimensional problems. We propose to combine the simplicity and generality of RFMs with a data-dependent feature selection scheme to achieve desirable theoretical approximation properties of Nyström with just $O(\log J)$ features. Our key insight is to begin with a large set of random features, then reduce them to a small number of weighted features in a data-dependent, computationally efficient way, while preserving the statistical guarantees of using the original large set of features. We demonstrate the efficacy of our method with theory and experiments—including on a data set with over 50 million observations. In particular, we show that our method achieves small kernel matrix approximation error and better test set accuracy with provably fewer random features than state-of-the-art methods.

1 Introduction

Kernel methods are essential to the machine learning and statistics toolkit because of their modeling flexibility, ease-of-use, and widespread applicability to problems including regression, classification, clustering, dimensionality reduction, and one and two-sample testing [10, 16, 19, 40]. In addition to good empirical performance, kernel-based methods come equipped with strong statistical and learning-theoretic guarantees [3, 4, 30, 44, 48, 49]. Because kernel methods are nonparametric, they are particularly attractive for large-scale problems, where they make it possible to learn complex, highly non-linear structure from data. Unfortunately, they exhibit poor scaling with data size. Given $N$ observations, $O(N^2)$ space is required to store the kernel matrix $K$ and typically $O(N^3)$ time is required to use it for learning, as this often entails inverting $K$ or computing its singular value decomposition.

To overcome poor scaling in $N$, various approximations to exact kernel methods have been devised. A widely-applicable and commonly used tactic is to replace $K$ with a rank-$J$ approximation, which reduces storage requirements to $O(NJ)$ and computational complexity of inversion or singular value decomposition.
while computing the solution where with a large set of random features, then reduce them to a small number of weighted features in a $k$-dependent nature of Nyström methods can provide statistical guarantees even when $J \ll N$, but these results either apply only to kernel ridge regression [14,36,52] or require burdensome recursive sampling schemes [28,31]. Random features, on the other hand, are simple to implement and use $J$ random features that are data-independent. For problems with both large $N$ and number of covariates $p$, an extension of random features called Fast Food RFM has been successfully applied at a fraction of the computational time required by Nyström-type approximations, which are exponentially more costly in terms of $p$ [25]. The price for this simplicity and data-independence is that a large number of random features is often needed to approximate the kernel matrix well [20,22,25,33,51].

The question naturally arises, then, as to whether we can combine the simplicity of random features and the ability to scale to large $p$ problems with the appealing approximation and statistical properties of Nyström-type approaches. We provide one possible solution by making random features data-dependent, and we show promising theoretical and empirical results. Our key insight is to begin with a large set of random features, then reduce them to a small number of weighted features in a data-dependent, computationally efficient way, while preserving the statistical guarantees of using the original large set of features. We frame the task of finding this small set of features as an optimization problem, which we solve using ideas from the coreset literature [5,6]. Using greedy optimization schemes such as the Frank–Wolfe algorithm, we show that a large set of $J_+$ random features can be compressed to an exponentially smaller set of just $O(\log J_+)$ features while still achieving the same statistical guarantees as using all $J_+$ features. We demonstrate that our method achieves superior performance to existing approaches on a range of real datasets—including one with over 50 million observations—in terms of kernel matrix approximation and classification accuracy.

2 Preliminaries and related work

Suppose we observe data \( \{(x_n,y_n)\}_{n=1}^{N} \) with predictors \( x_n \in \mathbb{R}^p \) and responses \( y_n \in \mathbb{R} \). In a supervised learning task, we aim to find a model \( f: \mathbb{R}^p \to \mathbb{R} \) among a set of candidates \( F \) that predicts the response well for new predictors. Modern data sets of interest often reach \( N \) in the tens of millions or higher, allowing analysts to learn particularly complex relationships in data. Nonparametric kernel methods [40] offer a flexible option in this setting; by taking \( F \) to be a reproducing kernel Hilbert space with positive-definite kernel \( k: \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R} \), they enable learning more nuanced details of the model \( f \) as more data are obtained. As a result, kernel methods are widespread not just in regression and classification but also in dimensionality reduction, conditional independence testing, one and two-sample testing, and more [10,15,16,41,54].

The problem, however, is that kernel methods become computationally intractable for large \( N \). We consider kernel ridge regression as a prototypical example [39]. Let \( K \in \mathbb{R}^{N \times N} \) be the kernel matrix consisting of entries \( K_{nm} := k(x_n,x_m) \). Collect the responses into the vector \( y \in \mathbb{R}^N \). Then kernel ridge regression requires solving

\[
\min_{\alpha \in \mathbb{R}^N} -\frac{1}{2}\alpha^T (K + \lambda I)\alpha + \alpha^T y,
\]

where \( \lambda > 0 \) is a regularization parameter. Computing and storing \( K \) alone has \( O(N^2) \) complexity, while computing the solution \( \alpha^* = (K + \lambda I)^{-1}y \) further requires solving a linear system, with cost \( O(N^3) \). Many other kernel methods have \( O(N^3) \) dependence as well; see Table[1].

To make kernel methods tractable on large datasets, a common practice is to replace the kernel matrix \( K \) with an approximate low-rank factorization \( \hat{K} := ZZ^T \approx K \), where \( Z \in \mathbb{R}^{N \times J} \) and \( J \ll N \). This factorization can be viewed as replacing the kernel function \( k \) with a finite-dimensional inner product \( k(x_n,x_m) \approx z(x_n)^T z(x_m) \) between features generated by a feature map \( z : \mathbb{R}^p \to \mathbb{R}^J \). Using this type of approximation significantly reduces downstream training time, as shown in the second column of Table[1]. Previous results show that as long as \( ZZ^T \) is close to \( K \) in the Frobenius norm, the optimal model \( f \) using \( \hat{K} \) is uniformly close to the one using \( K \) [11]; see the last column of Table[1].
Table 1: A comparison of training time for PCA, SVM, and ridge regression using the exact kernel matrix $K$ versus a low-rank approximation $\hat{K} = ZZ^T$, where $Z$ has $J$ columns. Exact training requires either inverting or computing the SVD of the true kernel matrix $K$ at a cost of $O(N^3)$ time, as shown in the first column. The second column refers to training the methods using a low-rank factorization $Z$. For ridge regression and PCA, the low-rank training cost reflects the time to compute and invert the feature covariance matrix $Z^TZ$. For SVM, the time refers to fitting a linear SVM on $Z$ using dual-coordinate decent with optimization tolerance $\rho$ [21]. The third column quantifies the uniform error between the function fit using $K$ and the function fit using $Z$. For specific details of how the bounds were derived, see Appendix D.

| Method              | Exact Training Cost | Low-Rank Training Cost | Approximation Error |
|---------------------|---------------------|------------------------|---------------------|
| PCA                 | $O(N^3)$            | $\Theta(NJ^2)$         | $O\left((1 - \frac{\rho}{N})\|\hat{K} - K\|_F\right)$ |
| SVM                 | $O(N^3)$            | $\Theta(NJ\log\frac{1}{\rho})$ | $O\left(\|\hat{K} - K\|_F^2\right)$ |
| Ridge Regression    | $O(N^3)$            | $\Theta(NJ^2)$         | $O\left(\frac{1}{\sqrt{N}}\|\hat{K} - K\|_F\right)$ |

However, finding a good feature map is a nontrivial task. One popular method, known as random Fourier features (RFF) [33], is based on Bochner’s Theorem:

**Theorem 2.1** (37 p. 19). A continuous, stationary kernel $k(x, y) = \phi(x - y)$ for $x, y \in \mathbb{R}^p$ is positive definite with $\phi(0) = 1$ if and only if there exists a probability measure $Q$ such that

$$\phi(x - y) = \int_{\mathbb{R}^p} e^{i\omega^T (x - y)}dQ(\omega)$$

$$= E_Q[\psi_\omega(x)\psi_\omega(y)^*], \quad \psi_\omega(x) := e^{i\omega^T x}. \tag{1}$$

**Theorem 2.1** implies that $z_{\text{complex}}(x) := (1/\sqrt{\mathcal{J}})[\psi_{\omega_1}(x), \cdots, \psi_{\omega_J}(x)]^T$, where $\omega_j \text{i.i.d.} Q$, provides a Monte–Carlo approximation of the true kernel function. As noted in [34], the real-valued feature map $z(x) := (1/\sqrt{\mathcal{J}})[\cos(\omega_1^T x + b_1), \cdots, \cos(\omega_J^T x + b_J)]^T$, $b_j \text{ unif. } [0, 2\pi]$ is also an unbiased estimator of the kernel function, and is the feature map assumed throughout unless otherwise stated. The resulting $N \times J$ feature matrix $Z$ yields estimates of the true kernel function with standard Monte-Carlo error rates of $O(1/\sqrt{\mathcal{J}})$ uniformly on compact sets [34] [45]. The RFF methodology also applies quite broadly. There are well-known techniques for obtaining samples from $Q$ for a variety of popular kernels such as the squared exponential, Laplace, and Cauchy [33], as well as extensions to more general random feature maps (RFMs), which apply to many types of non-stationary kernels [12] [25] [32].

The major drawback of RFMs is the $O(NJp)$ time and $O(NJ)$ memory costs associated with generating the feature matrix $Z$ [1]. Although these are linear in $N$ as desired, recent empirical evidence [22] suggests that $J$ needs to be quite large to provide competitive performance with other data analysis techniques. Recent work addressing this drawback has broadly involved two approaches: variance reduction and feature compression. Variance reduction techniques involve modifying the standard Monte–Carlo estimate of $k$, e.g. control variates, quasi-Monte–Carlo techniques, and importance sampling [1] [2] [8] [42] [53]. These either depend poorly on the data dimension $p$, or, for a fixed approximation error, reduce the number of features $J$ compared to RFM only by a constant. Feature compression techniques, on the other hand, involve two steps: (1) “up-projection,” in which the basic RFM methodology generates a large number $J_+ \text{ of features}$—followed by (2) “compression,” in which those features are used to find a smaller number $J$ while ideally retaining the kernel approximation error of the original $J_+$ features. Compact random feature maps [18] represent an instance of this technique in which compression is achieved using the Johnson–Lindenstrauss (JL) algorithm [23]. However, not only is the generation and storage of $J_+$ features prohibitively expensive for large datasets, JL compression is data-independent and leads to only a constant reduction in $J_+$ as we show in Appendix C (see summary in Table 2).
3 Random feature compression via coresets

In this section, we present an algorithm for approximating a kernel matrix $K \in \mathbb{R}^{N \times N}$ with a low-rank approximation $K \approx \hat{K} = ZZ^T$ obtained using a novel feature compression technique. In the up-projection step we generate $J_+$ random features, but only compute their values for a small, randomly-selected subset of $S \ll N^2$ datapoint pairs. In the compression step, we select a sparse, weighted subset of $J$ of the original $J_+$ features in a sequential greedy fashion. We use the feature values on the size-$S$ subset of all possible data pairs to decide, at each step, which feature to include and its weight. Once this process is complete, we compute the resulting weighted subset of $J$ features on the whole dataset. We use this low-rank approximation of the kernel in our original learning problem. Since we use a sparse weighted feature subset for compression—as opposed to past work, where $J = O(J_+)$ was required—while maintaining the same kernel approximation error as provided by RFM with $J_+$ features. These results are summarized in Table 2 and discussed in detail in Section 3.2.

3.1 Algorithm derivation

Let $Z_+ \in \mathbb{R}^{N \times J_+}$, $J_+ > J$, be a fixed up-projection feature matrix generated by RFM. Our goal is to use $Z_+$ to find a compressed low-rank approximation $K \approx \hat{K} = ZZ^T$, $Z \in \mathbb{R}^{N \times J}$. Motivated by the fact that spectral 0-norm bounds on $K - \hat{K}$ provide uniform bounds on the difference between learned models using $K$ and $\hat{K}$, as well as the fact that the Frobenius norm bounds the 2-norm, we aim to find such a $Z$ that minimizes the Frobenius norm error $\|K - ZZ^T\|_F$. By the triangle inequality,

$$\|K - ZZ^T\|_F \leq \|K - Z_+ Z_+^T\|_F + \|Z_+ Z_+^T - ZZ^T\|_F,$$

so constructing a good feature compression down to $J$ features amounts to picking $Z$ such that $Z_+ Z_+^T \approx ZZ^T$ in Frobenius norm. Let $Z_{+j} \in \mathbb{R}^N$ denote the $j$th column of $Z_+$. Then we would ideally like to solve the optimization

$$\arg\min_{w \in \mathbb{R}^{J_+}} \frac{1}{N^2} \|Z_+ Z_+^T - Z(w) Z(w)^T\|_F^2$$

s.t. $Z(w) := \left[ \sqrt{w_1}Z_{+1} \ldots \sqrt{w_J}Z_{+J} \right]$ \quad \text{(4)}$

$\|w\|_0 \leq J$. \quad \text{(5)}$

This optimization is intractable to solve exactly for two main reasons. First, computing the objective function requires computing $Z_+$, which itself takes $O(NJ_+p)$ time. But it is not uncommon for all three of $N$, $J_+$, and $p$ to be large, making this computation expensive. Second, the cardinality, or “0-norm,” constraint on $w$ yields a difficult combinatorial optimization. In order to address these issues, first note that

$$\frac{1}{N^2} \|Z_+ Z_+^T - Z(w) Z(w)^T\|_F^2 =$$

$$\mathbb{E}_{i,j \sim \pi} \left[ (z_{+i}^T z_{+j} - z_i(w)^T z_j(w))^2 \right],$$

where $\pi$ is the uniform distribution on the integers $\{1, \ldots, N\}$, and $z_{+i}$, $z_i(w)$ are the $i$th rows of $Z_+$, $Z(w)$, respectively. Therefore, we can generate a Monte Carlo estimate of the optimization objective by sampling $S$ pairs $i_\ell, j_\ell \overset{i.i.d.}{\sim} \pi$:

$$\frac{S}{N^2} \|Z_+ Z_+^T - Z(w) Z(w)^T\|_F^2 \approx \sum_{\ell=1}^S (z_{+i_\ell}^T z_{+j_\ell} - z_{i_\ell}(w)^T z_{j_\ell}(w))^2$$

$$= (1 - w)^T R R^T (1 - w) \text{ s.t.}$$

$$\text{(6)}$$
Theorem 3.2 and Corollary 3.3 provide a remarkable resolution to this issue: roughly, if we fix $J_+$ such that the basic random features method provides kernel approximation error $\epsilon > 0$ with high probability, then choosing $S = \Omega(J_+^2 (\log J_+)^2)$ and $J = \Omega(\log J_+)$ suffices to guarantee that the compressed feature kernel approximation error is also $O(\epsilon)$ with high probability. In contrast, previous feature compression methods required $J = \Omega(J_+)$ to achieve the same result; see Table 1.

3.2 Theoretical results

In order to employ Algorithm 1, we must choose the number $S$ of data pairs, the up-projected feature dimension $J_+$, and compressed feature dimension $J$. Selecting these three quantities involves a tradeoff between the computational cost of using Algorithm 1 and the resulting low-rank kernel approximation Frobenius error, but it is not immediately clear how to perform that tradeoff. Theorem 3.2 and Corollary 3.3 provide a remarkable resolution to this issue: roughly, if we fix $J_+$ such that the basic random features method provides kernel approximation error $\epsilon > 0$ with high probability, then choosing $S = \Omega(J_+^2 (\log J_+)^2)$ and $J = \Omega(\log J_+)$ suffices to guarantee that the compressed feature kernel approximation error is also $O(\epsilon)$ with high probability. In contrast, previous feature compression methods required $J = \Omega(J_+)$ to achieve the same result; see Table 1.
Furthermore, the compression coefficient is asymptotically bounded away from 1. That is, we obtain the exponential compression in Theorem 3.2 for the following reason: Frank–Wolfe and Assumption 3.1(a) is sufficient to guarantee that the compression coefficient \( \nu \) is given in Appendix B and depends on the following assumptions.

**Assumption 3.1.**

(a) There does not exist an \( i < j \) and \( \hat{i} < \hat{j} \), \((i, j) \neq (\hat{i}, \hat{j}), 1 \leq i, \hat{i} \leq N - 1 \) such that at least one of vectors \( x_i - x_j, x_i + x_j, x_i - x_j, x_i + x_j \) are equal, where \( x_i \in \mathbb{R}^p \) are the datapoints.

(b) \( Q(\omega), \omega \in \mathbb{R}^p \) has positive density on all of \( \mathbb{R}^p \), where \( Q \) is the measure induced by the kernel \( k \); see Theorem 2.1.

Assumption 3.1(a) is sufficient to guarantee that the compression coefficient \( \nu_{J_+} \) provided in Theorem 3.2 does not go to 1. If \( \nu_{J_+} \to 1 \) as \( J_+ \to \infty \), the amount of compression could go to zero asymptotically. When the \( x_i \)'s contain continuous (noisy) measurements, Assumption 3.1(a) is very mild since the difference or sum between two datapoints is unlikely to equal the difference or sum between two other datapoints. Assumption 3.1(b) is satisfied by most kernels used in practice (e.g. radial basis function, Laplace kernel, etc.).

We obtain the exponential compression in Theorem 3.2 for the following reason: Frank–Wolfe and GIGA converge linearly when the minimizer (in our case \( r \)) belongs to the relative interior of the feasible set of solutions [29]. With linear convergence, we need to run only a logarithmic number of iterations (which upper bounds the sparsity of \( r(\omega) \)) to approximate \( r \) sufficiently well. For fixed \( J_+ \), Lemma A.5 from [5] immediately implies that \( r \) belongs to the relative interior. As \( J_+ \to \infty \) (that is as we represent the kernel function exactly), we show that \( r \) asymptotically belongs to the relative interior, and we provide a lower bound on the distance of \( r^* \) to the boundary of the feasible set. This distance lower bound is key to the asymptotic bound on the compression coefficient given in Theorem 3.2 and Theorem 3.4.

**Theorem 3.2.** Fix \( \epsilon > 0, \delta \in (0, 1), \) and \( J_+ \in \mathbb{N} \). Then there is a constant \( \nu_{J_+} \in (0, 1) \) and \( 0 \leq c_3 \in [0, 1) \) such that if

\[
J = \Omega \left( -\frac{\log J_+}{\log \nu_{J_+}} \right) \quad \text{and} \quad S = \Omega \left( c_3^4 \left[ \frac{\log \frac{1}{\delta}}{\log \nu_{J_+}} \right]^4 \log J_+ \right),
\]

then with probability at least \( 1 - \delta \), the output \( Z \) of Algorithm 1 satisfies

\[
\frac{1}{N^2} \| Z_+ Z_+^T - Z Z^T \|_F^2 \leq \epsilon.
\]

Furthermore, the compression coefficient is asymptotically bounded away from 1. That is,

\[
0 < \limsup_{J_+ \to \infty} \nu_{J_+} < 1.
\]

**Corollary 3.3.** In the setting of Theorem 3.2, if we let \( J_+ = \Omega(1/\epsilon \log 1/\epsilon) \), then

\[
\frac{1}{N^2} \| K - Z Z^T \|_F^2 = O(\epsilon).
\]

**Proof.** Claim 1 of [33] implies that \( \frac{1}{N^2} \| K - Z_+ Z_+^T \|_F^2 = O(\epsilon) \) if we set \( J_+ = \Omega(1/\epsilon \log 1/\epsilon) \). The result follows by combining Theorem 3.2 and Eq. (2). \( \square \)

Table 2 uses the results of Theorem 3.2 and Corollary 3.3 to illustrate the benefit of using the proposed feature compression technique in the setting of kernel PCA and ridge regression. Since random features and random features with JL compression both have \( J = \Omega(J_+) \), the \( O(NJ_+^2) \) cost of computing the feature covariance matrix \( Z^T Z \) when training principal components analysis (PCA) or ridge regression dominates. In contrast, the dominant cost of random features with the proposed algorithm is the compression step: each iteration of FW has cost \( O(J_+ S) \), and we run it for \( O(\log J_+) \) iterations.
Table 2: A comparison of the computational cost of basic random feature maps (RFM), RFM with JL compression (RFM-JL), and RFM with our proposed compression using FW (RFM-FW) for fixed number of datapoints \(N\) and up-projection features \(J_+ = \frac{1}{\epsilon} \log \frac{1}{\epsilon}\). The first column specifies the number of compressed features \(J\) needed to retain the \(O(\epsilon)\) high probability kernel approximation error guarantee of RFM. The second and third columns list the complexity for computing the compressed features and using them for PCA / ridge regression, respectively. See Appendix C for derivations.

| Method       | Compressed Features \(J\) | Cost of Computing \(Z\) | PCA/Ridge Reg. Cost |
|--------------|---------------------------|-------------------------|---------------------|
| RFM          | \(O(J_+)\)               | \(O(NJ_+)\)            | \(O(NJ_+^2)\)       |
| RFM-JL       | \(O(J_+)\)               | \(O(NJ_+ \log J_+)\)   | \(O(NJ_+^2)\)       |
| RFM-FW       | \(O(\log J_+)\)          | \(O(SJ_+ + N \log J_+)\) | \(O(N(\log J_+)^2)\) |

While Corollary 3.3 says how large \(S\) must be for a given \(J_+\), it does not say how to pick \(J_+\), or equivalently how to choose the level of precision \(\epsilon\). As one would expect, the amount of precision needed depends on the downstream application. For example, recent theoretical work suggests that both kernel principal components analysis and kernel ridge regression require \(J_+\) to scale only sublinearly with the number of datapoints \(N\) to achieve the same statistical guarantees as an exact kernel machine trained on all \(N\) datapoints [2] [35] [43]. For kernel support vector machines (SVMs), on the other hand, [45] suggests that \(J_+\) needs to be larger than \(N\). Such a choice of \(J_+\) would make random features slower than training an exact kernel SVM. However, since [45] does not provide a lower bound, it is still an open theoretical question how \(J_+\) must scale with \(N\) for kernel SVM.

For \(J_+\) even moderately large, setting \(S = \Omega(J_+^2 (\log J_+)^2)\) to satisfy Theorem 3.2 will be prohibitively expensive. Fortunately, in practice, we find \(S \ll J_+^2\) suffices to provide significant practical computational gains without adversely affecting approximation error; see the results in Section 4. We conjecture that we see this behavior since we expect even a small number of data pairs \(S\) to be enough to guide feature compression in a data-dependent manner. We empirically verify this intuition in Fig. 4 of Section 4.

Finally, we provide an asymptotic upper bound for the compression coefficient \(\nu_{J_+}\). Note that we achieve greater compression of \(J_+\) when \(\nu_{J_+} \downarrow 0\). Hence, the upper bound below shows the asymptotic worst-case rate of compression.

**Theorem 3.4.** Suppose all \(\{(i, j) : i < j, 2 \leq j \leq N\}\) are sampled in Algorithm 1. Then,

\[
0 < \limsup_{J_+ \to \infty} \nu_{J_+} < 1 - \left(1 - \frac{\|K\|_F}{c_Q}\right)^2 < 1, \tag{9}
\]

where \(K\) is the true kernel matrix and

\[
c_Q := \frac{1}{N} \mathbf{E}_{\omega \sim Q} \|u(\omega, b)\|_2,
\]

\[
u(\omega, b) := (\cos(w^T x_i + b) \cos(w^T x_j + b))_1 \leq [N]. \tag{10}
\]

Recall that \(\|K\|_F^2 = \sum_{i=1}^N \lambda_i\), where the \(\lambda_i\) are the eigenvalues of \(K\). Theorem 3.4 says that the asymptotic worst-case rate of compression improves if the eigenvalues of \(K\) are small, which is what one would expect. Since we subsample only \(S\) of all possible pairs in Theorem 3.2, the upper bound in Theorem 3.4 does not necessarily apply. Nevertheless, for \(S\) moderately large, this upper bound roughly characterizes the worst-case rate of compression for Algorithm 1.

**4 Experiments**

In this section we provide an empirical comparison of basic random feature maps (RFM) [33], RFM with Johnson-Lindenstrauss compression (RFM-JL) [18], and the proposed algorithm with compression via greedy iterative geodesic ascent [6] (RFM-GIGA). We compare the performance of these methods applied to kernel SVM classification [49] on five real, large-scale datasets, summarized in Table 3. In particular, we assess their performance via two quality metrics—Frobenius error of
Table 3: Description of datasets

| Dataset                  | # of samples | Dimension | # of Classes |
|--------------------------|--------------|-----------|--------------|
| Adult                    | 48,842       | 123       | 2            |
| Human Activity Recognition| 10,299       | 561       | 6            |
| MNIST                    | 70,000       | 780       | 10           |
| Sensorless               | 58,000       | 9         | 11           |
| Criteo                   | 51,882,752   | 1,000,000 | 2            |

Figure 1: Kernel matrix approximation errors. Lower is better. Each point denotes the average over 20 simulations and the error bars represent one standard deviation.

The kernel approximation and test set classification error—as well as overall computation time for random feature projection and SVM training. We use the radial basis kernel $k(x, y) = e^{-\gamma \|x-y\|^2}$, and pick both $\gamma$ and the SVM regularization strength for each dataset by randomly sampling 10,000 datapoints, training an exact kernel SVM on those datapoints, and using 5-fold cross-validation. For both RFM-JL and RFM-GIGA we set $J_+ = 5000$, and for RFM-GIGA we set $S = 20,000$.

Figs. 1 and 2 show the relative kernel matrix approximation error $\frac{\|ZZ^T - K\|_F}{\|K\|_F}$ and test classification accuracy, respectively, as a function of the number of compressed features $J$. Note that since we cannot actually compute $K$ we approximate the relative Frobenius norm error by randomly sampling $10^4$ datapoints. We ran each experiment 20 times; the results in Figs. 1 and 2 show the mean across these trials with one standard deviation denoted with error bars. RFM-GIGA outperforms RFM and RFM-JL across all the datasets, on both metrics, for the full range of number of compressed features that we tested. This empirical result corroborates the theoretical results presented earlier in Section 3.2—in practice, RFM-GIGA requires approximately an order of magnitude fewer features than both RFM and RFM-JL.

To demonstrate the computational scalability of RFM-GIGA, we also plotted the relative kernel matrix approximation error versus computation time for the Criteo dataset, which consists of over 50 million data points. Before random feature projection and training, we used sparse random projections [27] to reduce the input dimensionality to 250 dimensions (due to memory constraints). We set $J_+ = 5000$ and $S = 2 \times 10^4$ as before, and let $J$ vary between $10^2$ and $10^3$. The results of this experiment in Fig. 3 suggest that RFM-GIGA provides a significant improvement in performance over both RFM and RFM-JL. Note that RFM-JL is very expensive in this setting—the up-projection step requires
Figure 2: Classification accuracy. Higher is better. Each point denotes the average over 20 simulations and the error bars represent one standard deviation.

Figure 3: Log clock time in seconds versus kernel matrix approximation quality on the Criteo dataset. Lower is better.
computing a $5 \times 10^8$ by $5 \times 10^3$ feature matrix—explaining its large computation time relative to RFM and RFM-GIGA. For test set classification, all the methods performed the same for all choices of $J$ (accuracy of $0.74 \pm 0.001$), so we do not provide the runtime vs. classification accuracy plot. This result is likely due to our compressing the $10^9$-dimensional feature space to 250 dimensions, making it hard for the SVM classifier to properly learn.

Given the empirical advantage of our proposed method, we next focus on understanding (1) if $S$ can be set much smaller than $\Omega(J_+^2 (\log J_+)^2))$ in practice and (2) if we can get an exponential compression of $J_+$ in practice as Theorem 3.2 and Theorem 3.4 guarantee.

To test the impact of $S$ on performance, we fixed $J_+ = 5,000$, and we let $S$ vary between $10^2$ and $10^6$. Figure 4 shows what the results in Fig. 1 would have looked like had we chosen a different $S$. We clearly see that after around only $S = 10,000$ there is a phase transition such that increasing $S$ does not further improve performance.

To better understand if we actually see an exponential compression in $J_+$ in practice, as our theory suggests, we set $J_+ = 10^5$ (i.e. very large) and fixed $S = 20,000$ as before. We examined the HIGGS dataset consisting of $1.1 \times 10^7$ samples, and let $J$ (the number of compressed features) vary between $500$ and $10^4$. Since GIGA can select the same random feature at different iterations (i.e. give it higher weight), $J$ reached 8,600 after $10^4$ GIGA iterations in Fig. 5. Fig. 5 shows that for $J \approx 2 \times 10^3$, increasing $J$ further has negligible impact on kernel approximation performance—only 0.001 difference in relative error. Fig. 5 shows that we are able to compress $J_+$ by around two orders of magnitude.

Finally, since our proofs of Theorem 3.2 and Theorem 3.4 assume Step 8 of Algorithm 1 is run using Frank-Wolfe instead of GIGA, we compare in Fig. 6 how the results in Fig. 1 change by using Frank-Wolfe instead. Fig. 6 shows that for $J$ small, GIGA has better approximation quality than FW but for larger $J$, the two perform nearly the same. This behavior agrees with the theory and empirical results of [6], where GIGA is motivated specifically for the case of high compression.

![Figure 4: We plot the relative Frobenius norm error against $S$ for $J_+$ fixed at 5,000. The solid black line corresponds to the results found in Fig. 1](image)

## 5 Conclusion

This work presents a new algorithm for scalable kernel matrix approximation. Our method involves first generating a low-rank approximation of the matrix, and then finding a sparse, weighted subset of the columns of the low-rank factor that minimizes the Frobenius norm error with the original low-rank approximation. Theoretical and empirical results suggest that the proposed method provides a significant improvement in scalability and approximation quality over past techniques. Potential directions for future work involve investigating the effects of variance reduction techniques for the up-projection step, using a similar compression technique on features generated by the Nyström method [50], and transfer learning of feature weights for multiple related datasets.
Figure 5: Let $S = 20,000$, $J_+ = 10^5$. We plot the relative Frobenius norm error against $J$ which varies between $500$ and $10^4$.

Figure 6: The performance of GIGA versus Frank-Wolfe for the experiment described in Fig. 5. Solid lines correspond to Frank-Wolfe and dashed with GIGA.

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A Proof of Theorem 3.4

The proofs of Theorem 3.2 and Theorem 3.4 rely on the main error bound for the Hilbert coreset construction problem (see Eq. (11) in [5]), which we restate in Lemma A.1. This bound depends on several key quantities given below.

- \( c_s := \frac{1}{\sqrt{\pi}} \cos(\omega^T x_{i_s} + b_i) \cos(\omega^T x_{j_s} + b_i) \), such that \( 1 \leq s \leq S \) and \( 1 \leq l \leq J_+ \).
- \( \hat{\sigma}_l^2 := \frac{1}{S} \sum_{s=1}^S c_{ls}^2 = \frac{1}{S} \| r_l \|_2^2 \)
- \( \hat{\sigma}^2 := \left( \sum_{l=1}^{J_+} \hat{\sigma}_l \right)^2 \)

The Hilbert construction problem solves

\[
\arg\min_{w \in \mathbb{R}^{J_+}} \frac{1}{S} \| r - r(w) \|_2^2 \text{ s.t. } \sum_{i=1}^{J_+} w_i \hat{\sigma}_i = \hat{\sigma}.
\] (11)

**Lemma A.1.** ([5] Theorem 4.4) Solving Eq. (11) with \( J \) iterations of Frank-Wolfe satisfies

\[
\frac{1}{S} \| r - r(w) \|_2^2 \leq \frac{\hat{\sigma}^2 \eta^2 \nu^2}{\nu^2 J - 2} + \frac{\eta^2 (J - 1)}{2}
\] (12)

where \( 0 \leq \nu < 1 \). Furthermore, \( \nu^2 = 1 - \frac{d^2}{\sigma^2} \) where \( d \) is the distance from \( r \) to the nearest boundary of the convex hull of \( \{ \hat{v}_i \}_{i=1}^J \) and \( \eta^2 := \frac{1}{S} \max_{i,j \in [J_+]} \left\| \frac{r_i}{\hat{\sigma}_i} - \frac{r_j}{\hat{\sigma}_j} \right\|^2 \), \( 0 \leq \eta \leq 2 \).

We will prove Theorem 3.4 first since the main idea of the exponential compression is captured in this proof. The proof of Theorem 3.2 is more involved since we use a number of concentration bounds to justify subsampling only \( S \) datapairs instead of all \( \frac{N(N-1)}{2} \) pairs above the diagonal. Both proofs will also depend on the following constants.

- \( \sigma_i^2 := \frac{1}{\sqrt{\pi}} \sum_{s=1}^{V^*} c_{is}^2 = \frac{1}{\sqrt{\pi}} \| r_i \|_2^2 \)
- \( \sigma^2 := \left( \sum_{l=1}^{J_+} \sigma_l \right)^2 \)

Here, \( V^* = \frac{N(N-1)}{2} \), i.e. when all pairs above the diagonal are taken.

While Lemma A.1 guarantees \( 0 < \nu_{J_+} < 1 \), it does not guarantee that \( \nu_{J_+} \to 1 \). The following Lemma is critical in showing \( \nu_{J_+} \) does not go to 1.

**Lemma A.2.** Let \( \{ x_i \}_{i=1}^K \) be a point set in \( \mathbb{R}^p \) that satisfies Assumption 3.1(a). Consider the vector \( v_{\omega,b} = (\cos(\omega^T x_i + b) \cos(\omega^T x_j + b))_{i,j \in [K-1]} \in \mathbb{R}^{K(K-1)/2} \). Let the unit vector \( u_{\omega,b} := \frac{v_{\omega,b}}{\| v_{\omega,b} \|} \).

If \( \omega_i \overset{i.i.d.}{\sim} F \) and \( b_i \overset{i.i.d.}{\sim} G \), where \( F \) has positive density on all of \( \mathbb{R}^p \) and \( G \) has positive density on \([0, 2\pi]\), then

\[
d \left( \text{ConvexHull}\{u_{\omega_i,b_i}\}_{i=1}^J, S^{K(K-1)/2-1} \right) \to 0 \quad \text{s.t.} \quad d(A, B) = \max_{a \in A, b \in B} \| a - b \|_2.
\] (13)

Here, \( S^{K(K-1)/2-1} \) denotes the surface of the unit sphere in \( \mathbb{R}^{K(K-1)/2} \).

**Proof.** By construction, each unit vector \( u_i := u_{\omega_i,b_i} \) hits some point on \( S^{K(K-1)/2-1} \), and hence, \( F,G \) induce a distribution on \( S^{K(K-1)/2-1} \). It suffices to show \( S^{K(K-1)/2-1} \) has positive density everywhere since, as \( J \to \infty \), any arbitrarily small neighborhood around a collection of points that cover \( S^{K(K-1)/2-1} \) will be hit by some \( u_i \) with probability 1. By standard convexity arguments, the convex...
hull of the $u_i$ will arbitrarily approach $S_{\frac{K(K-1)}{2}}^{-1}$ by taking the radius of the neighborhoods to zero. We now show $S_{\frac{K(K-1)}{2}}^{-1}$ has positive density everywhere. Since $u_i$ is just the normalized vector of $v_i := v_{\omega_i,b}$ and each component of $v_i$ is between $-1$ and 1, it suffices to show, by the continuity of the cosine function, that for any $\alpha \in \{-1,1\}$ there exist some $\omega_i, b_i$ such that $	ext{sign}(v_i) := (\text{sign}(v_i(l)))_{l \in \frac{K(K-1)}{2}}$ equals $\alpha$. Recall that 

$$\cos(a) \cos(b) = \frac{1}{2}(\cos(a + b) + \cos(a - b)).$$

Take $b_i = 0$. Then, Equation (14) implies $v_i(l) = \frac{1}{2}(\cos(\omega_i^T(x_i + x_j) + \cos(\omega_i^T(x_i - x_j)))$.

Consider the vector $\tilde{v}_i = (\cos(\omega_i^T(x_i + x_j), \cos(\omega_i^T(x_i - x_j)))_{l \in \frac{K(K-1)}{2}} \in \mathbb{R}^{K(K-1)}$. It suffices to show that for any $\tilde{a} \in \{-1,1\}^{K(K-1)}$, there exists an $\omega_i$ such that $\text{sign}(\tilde{v}_i) = \tilde{a}$. Recall that the cosine function has infinite VC dimension, namely that for any labeling $y_1, \ldots, y_M \in \{-1,1\}$ of distinct points $x_1, \ldots, x_M \in \mathbb{R}^p$, there exists an $\omega$ such that $\text{sign}(\cos((\omega^T x_m)) = y_m$. Take $M = K(K-1), y_m = 0, x_m = x_i + x_j$, and $x_{m+1} = x_i - x_j$. Since all the $x_m$ are distinct by Assumption 3.1(a), we can find an $\omega_i$ such that $\text{sign}(\tilde{v}_i) = \tilde{a}$ as desired.

We now prove Theorem 3.4.

**Proof.** Each $r_i \in \mathbb{R}^{\frac{N(N-1)}{2}}$ and the $r_i$’s are i.i.d. since $\omega_j, b_i$ are i.i.d. Now, $\tilde{r}_i := \frac{r_i}{\sigma_i}$ is a unit vector. By Lemma A.2,

$$d \left( \text{ConvexHull}\{r_i\}_{i=1}^{J_+}, S_{\frac{N(N-1)}{2}}^{\frac{K(K-1)}{2}} \right) \rightarrow 0$$

Define $\tilde{r} := \sum_{i=1}^{J_+} \tilde{r}_i$ and notice that $\tilde{r} = \frac{\tilde{r}}{\sigma}$. The distance $d_{J_+}$ between $\tilde{r}$ and the ConvexHull$\{r_i\}_{i=1}^{J_+}$ approaches $1 - ||\tilde{r}||$ since the ConvexHull$\{r_i\}_{i=1}^{J_+}$ approaches $S_{\frac{N(N-1)}{2}}^{\frac{K(K-1)}{2}}$. Hence,

$$\lim_{J_+ \rightarrow \infty} d_{J_+} = \lim_{J_+ \rightarrow \infty} ||\tilde{r}|| = \lim_{J_+ \rightarrow \infty} \frac{||r||}{\sigma}.$$  

Notice

$$r_s = \frac{1}{J_+} \sum_{t=1}^{J_+} \sum_{t=1}^{J_+} k(x_i, x_j).$$

Hence,

$$||r|| \rightarrow \frac{2}{N(N-1)} \sum_{i<j}(k(x_i, x_j))^2.$$  

Notice,

$$\sigma = \frac{1}{\sigma} \|\sigma\| = \frac{2}{N(N-1)} \mathbb{E}_{w,b}[(\cos(w^T x_i + b) \cos(w^T x_j + b))_{i<j}].$$

If $x \neq y$, then

$$k(x, y) = \mathbb{E}_{w,b}[(\cos(w^T x + b) \cos(w^T y + b)] < \mathbb{E}_{w,b}[(\cos(w^T x + b) \cos(w^T y + b)].$$

Hence, by Assumption 3.1(a)

$$\lim_{J_+ \rightarrow \infty} ||r|| \leq \frac{\|K\|_F}{\mathbb{E}_{w,b}[(\cos(w, b)])} < 1.$$  

Notice that,

$$\lim_{J_+ \rightarrow \infty} ||r|| \leq \frac{\|K\|_F}{\mathbb{E}_{w,b}[(\cos(w, b)])},$$

where $u(w, b)$ is defined in Theorem 3.4 Lemma A.1 says that $\nu_{J_+} = 1 - \frac{d^2}{\sigma^2}$, where $d$ is the distance from $r$ to the nearest boundary of the convex hull of $\{\frac{\tilde{r}_i}{\sigma_i}\}_{i=1}^{J_+}$. Hence, $d = \sigma d_{J_+}$ and Eq. (20) implies,

$$\lim inf_{J_+ \rightarrow \infty} d_{J_+} \leq 1 - \frac{\|K\|_F}{\mathbb{E}_{w,b}[(\cos(w, b)])}.$$  

13
Therefore, since $\eta^2 \leq 2$,
\[
\limsup_{J_+ \to \infty} J_+ = \limsup_{J_+ \to \infty} \frac{d^2_{J_+}}{2} = 1 - \liminf_{J_+ \to \infty} \frac{d^2_{J_+}}{2} \leq 1 - \frac{\left(1 - \frac{\|K\|_{F}}{\|x_{b}\|_{\infty}(z_{b})}\right)^2}{2}.
\] (22)

\section{Proof of Theorem 3.2}

The following technical lemma is needed to derive the probability bound in Theorem 3.2.

\textbf{Lemma B.1.} Suppose $\frac{\sigma^2}{J^2_{+}\sigma_i^2} \leq M$ for some $1 \leq M < \infty$ for all $i \in [J_+]$. For $S \geq 8 \frac{M^2}{\sigma^4} \log \left(\frac{2J_+}{M}\right)$
\[
P\left(\frac{\hat{\sigma}^2}{J^2_{+}\sigma_i^2} \geq 5M\right) \leq \delta
\] (23)
for all $i \in [J_+]$.

\textit{Proof.} Notice that
\[
E_{i_s,j_s} \hat{\sigma}_i^2 = \frac{1}{S} \sum_{s=1}^{S} E_{i_s,j_s} c^2_{is}
\]
\[
= \frac{1}{N^2} \sum_{s=1}^{N^2} c^2_{is}
\]
\[
= \sigma^2.
\]
Hence, $\hat{\sigma}_i^2$ is an unbiased estimator of $\sigma_i^2$. Each $c^2_{is} \leq \frac{1}{\sqrt{s}}$ is a bounded random variable, and the collection of random variables $\{c^2_{is}\}_{s=1}^{S}$ are i.i.d. since $i_s, j_s \sim \pi$. Hence, by Hoeffding’s inequality,
\[
P\left(|\hat{\sigma}^2 - \sigma_i^2| \geq t\right) \leq 2 \exp\left(-2S \frac{J_+ t^2}{M}\right).
\] (24)

Define the event $A_t := \bigcup_{i=1}^{J_+} \{||\hat{\sigma}_i^2 - \sigma_i^2| < t\}$ and pick $t$ such that $t \leq \min_{i \in [J_+]} \sigma_i^2$. Since $\sigma_i^2 \geq \frac{\sigma^2}{M}$ by assumption, it suffices to pick $0 < t \leq \frac{\sigma^2}{M}$. Conditioned on $A_t$, $\hat{\sigma}_i \leq \sqrt{\sigma_i^2 + t} \leq \sigma_i + \sqrt{t}$, which implies $\hat{\sigma}^2 \leq (\sigma + J_+ \sqrt{t})^2$. Therefore,
\[
P\left(\frac{\hat{\sigma}^2}{J^2_{+}\sigma_i^2} \geq cM\right) = P\left(A_t^c \cup \left\{\frac{\hat{\sigma}^2}{J^2_{+}\sigma_i^2} \geq cM\right\}\right) + P\left(A_t \cup \left\{\frac{\hat{\sigma}^2}{J^2_{+}\sigma_i^2} \geq cM\right\}\right)
\]
\[
\leq P\left(A_t^c\right) + P\left(A_t \cup \left\{\frac{\hat{\sigma}^2}{J^2_{+}\sigma_i^2} \geq cM\right\}\right)
\]
\[
\leq P\left(A_t^c\right) + P\left(A_t \cup \left\{\frac{\hat{\sigma}^2}{J^2_{+}\sigma_i^2} \geq cM \mid A_t\right\}\right)
\]
\[
\leq P\left(A_t^c\right) + P\left(\frac{(\sigma + \sqrt{t}J_+)^2}{J^2_{+}(\sigma_i^2 - t)} \geq cM \mid A_t\right).\] (25)
Notice that \( P\left( \frac{(\sigma + \sqrt{t} J_+)^2}{\sigma_i^2 - t} \geq cM^2 \mid A_i \right) \) is either 0 or 1 since \( \sigma_i \) and \( \sigma \) are constants. We pick \( t \) so that this probability is 0. To pick \( t \), notice that,

\[
\frac{(\sigma + \sqrt{t} J_+)^2}{J_+^2 (\sigma_i^2 - t)} = \frac{\left( \frac{\sigma}{\sigma_i} + \frac{\sqrt{t} J_+}{\sigma_i} \right)^2}{J_+^2 (1 - \frac{t}{\sigma_i^2})} \leq \frac{\left( J_+ \sqrt{M} + \frac{J_+ \sqrt{cM J_+}}{\sigma} \right)^2}{J_+^2 (1 - \frac{t}{\sigma_i^2})} \leq \frac{M \left( 1 + \frac{\sqrt{t} J_+}{\sigma} \right)^2}{1 - \frac{M J_+^2}{\sigma^2 t}},
\]

where the last inequality holds as long as \( 0 < t < \frac{\sigma^2}{M J_+^2} \) and follows by noting that \( \frac{1}{\sigma_i^2} \leq \frac{M J_+^2}{\sigma^2 t} \) by assumption. Pick \( t = \frac{\sigma^2}{4 J_+^2 M} \). Since \( 0 \leq \sigma \leq 1 \), this choice of \( t \) implies \( \frac{M \left( 1 + \frac{\sqrt{t} J_+}{\sigma} \right)^2}{1 - \frac{M J_+^2}{\sigma^2 t}} \leq 5M \).

Hence, for \( c = 5 \) and this choice of \( t \), \( P\left( \frac{(\sigma + \sqrt{t} J_+)^2}{\sigma_i^2 - t} \geq 5M \mid A_i \right) = 0 \). Combining Eq. 25 and Eq. (24), we have by a union bound that,

\[
P\left( \frac{\sigma^2}{J_+^2 \sigma_i^2} \geq 5M \right) \leq 2J_+ \exp \left( \frac{1}{8} S \frac{\sigma^4}{M^2} \right),
\]

for all \( i \in [J_+] \). Solving for \( S \) by setting the right hand side above to \( \delta \) yields the claim. \( \square \)

We have all the pieces to prove Theorem 3.2. We follow the proof strategy in [5, Theorem 5.2].

**Proof.** Let \( R^* = \left[z_{+1}^T \circ z_{+1}^T \cdots z_{+N_{-1}}^T \circ z_{+N_{-1}}^T \circ z_{+N_{-1}^T} \circ z_{+N_{-1}^T} \right] \in \mathbb{R}^{J_+ \times N^2} \). Notice,

\[
\frac{1}{N^2} \|Z_+ Z_+^T - Z(w) Z(w)^T\|_F^2 = (1 - w)^T \frac{R^* R^T}{N} (1 - w).
\]

We approximate Eq. (28) with \( (1 - w)^T \frac{R^*}{\sqrt{S}} \frac{R^T}{\sqrt{S}} (1 - w) \) and bound the error. Suppose

\[
D^* := \max_{i,j \in [J_+]} \left| \left( \frac{R^*}{\sqrt{S}} \frac{R^T}{\sqrt{S}} \right)_{ij} - \left( \frac{R}{\sqrt{S}} \frac{R^T}{\sqrt{S}} \right)_{ij} \right| \leq \epsilon / 2.
\]

Then,

\[
(1 - w)^T \frac{R^*}{N} \frac{R^T}{N} (1 - w) - (1 - w)^T \frac{R}{\sqrt{S}} \frac{R^T}{\sqrt{S}} (1 - w) \leq \sum_{i,j \in [J_+]} |w_i - 1||w_j - 1|D^* \leq \|w - 1\|^2 \frac{\epsilon}{2}.
\]

Notice,

\[
\mathbb{E}_{i,S, js} \left[ \left( \frac{R}{\sqrt{S}} \frac{R^T}{\sqrt{S}} \right)_{ij} \right] = \mathbb{E}_{i,S, js} \left[ \frac{1}{S} \sum_{s=1}^{S} c_{is} c_{js} \right] = \mathbb{E}_{i,S, js} \left[ c_{is} c_{js} \right] = \mathbb{E}_{i,S, js} \left[ c_{is} c_{js} \right] = \left( \frac{R^*}{N} \frac{R^T}{N} \right)_{ij}.
\]
Hence, the i.i.d. collection of random variables \( \{c_isc_j\}_{s=1}^S \) yields an unbiased estimate of \( \left( \frac{R^*}{N} \frac{\mu^T}{N} \right)_{ij} \). Each \( c_isc_j \) is bounded by \( \frac{1}{J^*} \). Therefore, by Hoeffding’s inequality and a simple union bound,

\[
P (D^* \geq \frac{\epsilon}{2}) \leq 2 J_+^2 \exp \left( -2 S J_+^4 \epsilon^2 \right).
\]  

(31)

Setting the right-hand side to \( \frac{\epsilon}{2} \) and solving for \( \frac{\epsilon}{2} \) implies with probability at least \( 1 - \frac{\epsilon^*}{2} \),

\[
\frac{\epsilon}{2} \leq \frac{1}{\sqrt{S J_+^2}} \log \left[ \frac{4 J_+^2}{\delta^*} \right]^{\frac{1}{2}}.
\]  

(32)

Hence, with probability at least \( 1 - \frac{\epsilon^*}{2} \),

\[
\frac{1}{N^2} \| Z_+ Z_+^T - Z(w) Z(w)^T \|^2_f \leq (1 - w)^T \frac{R}{\sqrt{S}} \frac{R^T}{\sqrt{S}} (1 - w) + \| 1 - w \|^2_1 \frac{1}{\sqrt{S J_+^2}} \log \left[ \frac{4 J_+^2}{\delta^*} \right]^{\frac{1}{2}}
\]

\[
= \frac{1}{S} \| r - r(w) \|^2_2 + \| 1 - w \|^2_1 \frac{1}{\sqrt{S J_+^2}} \log \left[ \frac{4 J_+^2}{\delta^*} \right]^{\frac{1}{2}}.
\]

Lemma A.1 implies that there exists a \( 0 \leq \nu < 1 \) such that \( \frac{1}{S} \| r - r(w) \|^2_2 \leq \nu^{2J - 2} \). Since \( \nu \) depends on the pairs \( i_1, j_1 \) picked, we can take \( \nu^a \) to be the largest \( \nu \) possible. Since the set of all possible \( S \) pairs is finite, that implies \( 0 \leq \nu^a < 1 \). Hence, setting \( J = \frac{1}{2} \log_{\frac{1}{0.1}} \frac{2.4 J}{\delta^*} + 2 \) guarantees that \( \frac{1}{S} \| r - r(w) \|^2_2 \leq \frac{\epsilon}{2} \) for any collection of drawn \( i_1, j_1 \), \( 1 \leq l \leq S \). Assume for any \( a \in (0, 1] \) and \( \delta > 0 \), we can find an \( M \) such that

\[
P (\max_j \sigma_j^2 (J_i^2, \sigma_i^2) > M) < a \delta.
\]  

(33)

If Eq. (33) holds, we may assume \( \max_j \sigma_j^2 (J_i^2, \sigma_i^2) < M \) by setting \( M \) large enough since we just need a \( 1 - \delta \) probabilistic guarantee. By the polytope constraint in Eq. (34), \( w_i^* \leq \frac{\epsilon}{\delta^*} \) for all \( i \in [J_+] \). Without loss of generality, assume the first \( J \) components of \( w^* \) can be the only non-zero values since \( w^* \) is at least \( J \) sparse. For \( S \geq 8 \frac{M^2}{\sigma^2} \log \left( \frac{2 J_+ \delta^*}{\delta^2} \right) \), Lemma B.1 implies with probability at least \( 1 - \frac{\epsilon^*}{2} \),

\[
\| 1 - w^* \|^2_1 \leq \left( \frac{\delta^*}{\delta^i} J + (J_+ - J) \right)^2
\]

\[
\leq (J M J_+ + J_+)^2
\]

\[
\leq (2 J M \sqrt{S} J_+)^2
\]

\[
\leq 10 J_+^2 M^2 J^2
\]

\[
\leq 10 J_+^2 M^2 (\log \frac{\nu}{\delta})^2 (\log \nu)^2
\]

Therefore, with probability at least \( 1 - \frac{\epsilon^*}{2} \),

\[
\frac{1}{N^2} \| Z_+ Z_+^T - Z(w) Z(w)^T \|^2_f \leq \frac{\epsilon}{2} + \frac{10 M^2 (\log \frac{\nu}{\delta})^2}{\sqrt{\log \nu}^2} \log \left[ \frac{4 J_+^2}{\delta^*} \right]^{\frac{1}{2}}.
\]  

(35)

Finally, setting \( S \geq \max \left( \frac{100}{\epsilon} \left( J M \log \frac{\nu}{\delta} \right)^4 \log \left[ \frac{4 J_+^2}{\delta^*} \right], 8 \frac{M^4}{\sigma^2} \left( \frac{2 J_+ \delta^*}{\delta^2} \right) \right) \) implies \( \frac{1}{N^2} \| Z_+ Z_+^T - Z(w) Z(w)^T \|^2_f \leq \epsilon \) with probability at least \( 1 - \frac{\epsilon^*}{2} \) which matches the rate provided in Theorem 3.2.

It remains to show Eq. (33). Notice that

\[
\frac{\sigma}{J_+ \sigma_j} = \frac{1}{J_+} + \frac{1}{J_+} \sum_{i \neq j} \sigma_{ij},
\]  

(36)
where \( \sigma_{ij} := \frac{\sigma_i}{\sigma_j} \). Notice that each \( \sigma_{ij} \) are i.i.d. for \( i \neq j \). Let the \( \mu_j = \mathbb{E}\sigma_{ij} \) and \( s_j \) be the standard deviation of \( \sigma_{ij} \). Since each \( \sigma_i \) is i.i.d. that implies \( \mu_j \) and \( s_j \) are both constant across \( j \) so we drop the subscript. By a union bound, it suffices to show for any \( \tau > 0 \) we can find an \( M \) such that

\[
\mathbb{P} \left( \max_{1 \leq j \leq J_+} \frac{1}{J_+} \sum_{i \neq j} \sigma_{ij} > M \right) < \tau. \tag{37}
\]

By Chebyshev’s inequality,

\[
\mathbb{P} \left( \frac{1}{J_+} \sum_{i \neq j} \sigma_{ij} - \mu > \frac{cs}{J_+} \right) \leq \frac{1}{e^c}. \tag{38}
\]

Take \( c = J_+ \tau \). Then,

\[
\mathbb{P} \left( \frac{1}{J_+} \sum_{i \neq j} \sigma_{ij} - \mu > \frac{cs}{J_+} \right) \leq \frac{1}{J_+^2 \tau} < \tau. \tag{39}
\]

By a union bound, Eq. (38) implies

\[
\mathbb{P} \left( \max_{1 \leq j \leq J_+} \frac{1}{J_+} \sum_{i \neq j} \sigma_{ij} > M \right) < \frac{1}{\tau J_+} < \tau
\]

for \( M = \mu + s\tau \) as desired.

The proof of

\[
0 < \limsup_{J_+ \to \infty} \nu_{J_+} < 1
\]

is the same as the proof Theorem 3.4

\[ \square \]

C Runtime analysis of methods

The ridge regression and PCA runtimes depend on the number of features used, as specified in Table 1 and therefore follow from the first column of the table.

First, we show that RFM with \( J_+ = O \left( \frac{1}{\epsilon^2} \log \frac{1}{\epsilon^2} \right) \) number of random features ensures that \( \frac{1}{n} \| K - \hat{K} \|^2_F = O(\epsilon) \) with high probability. Notice that \( \mathbb{P} \left( \frac{1}{n} \| K - \hat{K} \|^2_F \leq \epsilon \right) \geq \mathbb{P} \left( \max_{i,j \in [n]} | K_{ij} - \hat{K}_{ij} | \leq \sqrt{\epsilon} \right) \). Now, Claim 1 of [33] implies that

\[
\mathbb{P} \left( \max_{i,j \in [n]} | K_{ij} - \hat{K}_{ij} | \geq \sqrt{\epsilon} \right) = O \left( \frac{1}{\epsilon} e^{-J_+ \epsilon} \right), \tag{40}
\]

Setting the right-hand side above to some fixed probability threshold \( \delta^* \) implies \( J_+ = O \left( \frac{1}{\epsilon^2} \log \left( \left( \frac{1}{\epsilon^2} \right) \right) \right) = O \left( \frac{1}{\epsilon^2} \log \frac{1}{\epsilon^2} \right) \) suffices. We use \( J_+ = O \left( \frac{1}{\epsilon} \log \frac{1}{\epsilon} \right) \) as the up-projection dimension for both RFM-FW and RFM-JL.

To prove the bounds for RFM-FW, take \( S = O \left( J_+^2 \log J_+ \right)^2 \). It is straightforward to check that this choice of \( S \) satisfies the requirements of Theorem 3.2. Since \( J_+ \geq O \left( \frac{1}{\epsilon} \right) \), we may apply Theorem 3.2 with \( J = O \left( \log J_+ \right) \) iterations. Since the output number of random features of RFM-FW has to be less than \( J \), we have shown the first column of RFM-FW in Table 2. Algorithm I takes \( O \left( J_+ \log J_+ \text{RFM} \right) \) to construct the random features and weights. Finally, it takes \( O \left( N \log J_+ \text{RFM} \right) \) to apply these \( O \left( \log J_+ \text{RFM} \right) \) weighted random features to the \( N \) datapoints.

Denote \( \tilde{x}_i \in \mathbb{R}^{J_+} \) as the mapped datapoints from RFM and \( A \in \mathbb{R}^{k \times J_+}, k \leq J_+ \) a matrix filled with i.i.d. \( N(0, \frac{1}{\epsilon}) \) random variables for the JL compression step. Let \( f(x) := Ax \). It suffices to pick a \( k \) such that

\[
\mathbb{P} \left( \max_{1 \leq j \leq n} | \tilde{x}_i^T \tilde{x}_j - f(\tilde{x}_i)^T f(\tilde{x}_j) | \geq \sqrt{\epsilon} \right) \leq \delta^* \tag{41}
\]

for RFM-JL. We use the following corollary from [24 Corollary 2.1] to bound the above probability.
Lemma C.1. Let \( u, v \in \mathbb{R}^d \) and such that \( \|u\| \leq 1 \) and \( \|v\| \leq 1 \). Let \( f(x) = Ax \), where \( A \) is a \( k \times d, k \leq d \) matrix of i.i.d. \( N(0, \frac{1}{k}) \) random variables. Then,

\[
P\left( |u^T v - f(u)^T f(v)| \right) \leq 4e^{-\frac{1}{2}(\epsilon^2 - \epsilon^3)}k.
\] (42)

Notice that \( \|\tilde{x}_i\| = 1 \) since \( \tilde{x}_i = \frac{1}{\sqrt{J_+}}(\cos(\omega^T_i x + b), \cdots, \cos(\omega^T_{J_+} x + b)) \). By a union bound and an application of Lemma C.1 Eq. (41) is bounded by \( O\left( N^2 e^{-\kappa \epsilon k} \right) \). Setting \( N^2 e^{-\kappa \epsilon k} \) equal to \( \delta^* \) and solving for \( k \) implies that \( k \geq O\left( \frac{J_+}{\epsilon^2 \log \frac{N^2}{\delta^*}} \right) = O\left( \frac{J_+}{\epsilon^2 \log N} \right) \). Now, \( O\left( \frac{1}{\epsilon} \right) = O\left( \frac{J_+}{\log \frac{N}{\epsilon}} \right) \) which implies \( k = O\left( \frac{J_+ \log N}{\log \frac{1}{\epsilon}} \right) \). Since \( N > J_+ > O\left( \frac{1}{\epsilon} \right) \), \( k \) can therefore only be set to \( O\left( J_+ \right) \) which shows the first column of Table 2 for RFM-JL. While the JL algorithm typically takes \( O\left( NJ_+ k \right) \) time to map a \( N \times J_+ \) matrix to a \( N \times k \) matrix, the techniques in [18 Section 3.5] show that only \( O\left( NJ_+ \log k \right) \) time is needed for RFM-JL.

D Impact of kernel approximation

Here we provide the precise error bound and runtimes for kernel ridge regression, kernel SVM, and kernel PCA when using a low-rank factorization \( ZZ^T \) of \( K \). We denote \( X \subset \mathbb{R}^p \) as the input space and define \( c > 0 \) such that \( K(x, x) \leq c \) and \( \tilde{K}(x, x) \leq c \) for all \( x \in X \). This condition is verified with \( c = 1 \) for Gaussian kernels for example. All the bounds provided follow from [11, 46], where we simply replace the spectral norm with the Frobenius norm since the Frobenius norm upper bounds the spectral norm.

D.1 Kernel ridge regression

Exact kernel ridge regression takes \( O(N^3) \) since \( K \) must be inverted. Suppose \( K \approx ZZ^T := \tilde{K} \), where \( Z \) could be found using RFM for example. Running ridge regression with the feature matrix \( Z \) just requires computing and inverting the covariance matrix \( Z^T Z \in \mathbb{R}^{J \times J} \) which takes \( \Theta(\max(J^3, NJ^2)) \) time. Proposition D.1 quantifies the error between the regressor obtained from \( K \) and the one from \( \tilde{K} \).

Proposition D.1. (Proposition 1 of [17]) Let \( \hat{f} \) denote the regression function returned by kernel ridge regression when using the approximate kernel matrix \( \tilde{K} \in \mathbb{R}^{N \times M} \), and \( f^* \) the function returned when using the exact kernel matrix \( K \). Assume that every response \( y \) is bounded in absolute value by \( M \) for some \( 0 < M < \infty \). Let \( \lambda := n\lambda_0 > 0 \) be the ridge parameter. Then, the following inequality holds for all \( x \in X \):

\[
|\hat{f}(x) - f^*(x)| \leq \frac{cM}{\lambda_0^2 N} \|\tilde{K} - K\|_2
\]

\[
\leq \frac{cM}{\lambda_0 N} \|\tilde{K} - K\|_F
\]

\[
= O\left( \frac{1}{N} \|\tilde{K} - K\|_F \right)
\]

D.2 Kernel SVM

Kernel SVM regression takes \( O(N^3) \) using \( K \) since \( K \) must be inverted. Again suppose \( K \approx ZZ^T := \tilde{K} \). Then, training a linear SVM via dual-coordinate decent on \( Z \) has time complexity \( O(NJ \log \rho) \), where \( \rho \) is the optimization tolerance [21].

Proposition D.2. (Proposition 2 of [17]) Let \( \hat{f} \) denote the hypothesis returned by SVM when using the approximate kernel matrix \( \tilde{K} \), \( f^* \) the hypothesis returned when using the exact kernel matrix \( K \),
We follow [46] to understand the effect matrix approximation has on kernel PCA. For a more in-depth analysis, see pg. 92-98 of [46]. Without loss of generality, we assume the data are mean zero.

Let $\Phi(\cdot)$ be the unique feature map such that $k(x, y) = \langle \Phi(x), \Phi(y) \rangle$. Let the feature covariance matrix $\Sigma_\Phi = \Phi(X_N)\Phi(X_N)^T$, where $\Phi(X_N) := [\Phi(x_1) \cdots \Phi(x_n)]$. Since the rank of $\Sigma_\Phi$ is at most $N$, let $v_i$ $1 \leq i \leq N$ be the $N$ singular vectors of $\Sigma_\Phi$. For certain kernels, e.g. the Gaussian kernel, the $v_i$ are infinite dimensional. However, the projection of $\Phi(x), x \in X$, onto $v_i$ is tractable to compute:

$$
\Phi(x)^T v_i = \Phi(x)^T \Phi(X_N) u_i = \frac{k_x u_i}{\sqrt{\sigma_i}},
$$

where $k_x := (K(x_1, x), \cdots, K(x_n, x))$ and $u_i$ is the $i$th singular vector of $K$ with associated eigenvalue $\sigma_i$. Often, the goal is to project $\Phi(x)$ onto the first $l$ eigenvectors of $\Sigma_\Phi$ for dimensionality reduction. To analyze the error of the projection, let $P_{V_l}$ be defined as the subspace $V_l$ spanned by the top $l$ eigenvectors of $\Sigma_\Phi$. Then, the average empirical residual $R_l(K)$ of a kernel matrix $K$ is defined as,

$$
R_l(K) := \frac{1}{N} \sum_{n=1}^{N} \|\Phi(x_i)\|^2 - \frac{1}{N} \sum_{n=1}^{N} \|P_{V_l} (\Phi(x_i))\|^2
$$

$$
= \sum_{i>l} \sigma_i
$$

(44)

$R_l(K)$ is simply the spectral error of a low-rank decomposition of $\Sigma_\Phi$ using the SVD. If we instead use $\hat{K}$ for the eigendecomposition, the following proposition bounds the difference between $R_l(K)$ and $R_l(\hat{K})$.

**Proposition D.3.** (Proposition 5.4 of [46]) For $R_l(K)$ and $R_l(\hat{K})$ defined as above,

$$
|R_l(K) - R_l(\hat{K})| \leq \left(1 - \frac{l}{N}\right) \|K - \hat{K}\|_2
$$

$$
\leq \left(1 - \frac{l}{N}\right) \|K - \hat{K}\|_F.
$$

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