Fast Sketching of Polynomial Kernels of Polynomial Degree

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Abstract

Kernel methods are fundamental in machine learning, and faster algorithms for kernel approximation provide direct speedups for many core tasks in machine learning. The polynomial kernel is especially important as other kernels can often be approximated by the polynomial kernel via a Taylor series expansion. Recent techniques in oblivious sketching reduce the dependence in the running time on the degree $q$ of the polynomial kernel from exponential to polynomial, which is useful for the Gaussian kernel, for which $q$ can be chosen to be polylogarithmic. However, for more slowly growing kernels, such as the neural tangent and arc-cosine kernels, $q$ needs to be polynomial, and previous work incurs a polynomial factor slowdown in the running time. We give a new oblivious sketch which greatly improves upon this running time, by removing the dependence on $q$ in the leading order term. Combined with a novel sampling scheme, we give the fastest algorithms for approximating a large family of slow-growing kernels.

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1 Introduction

Kernel methods are a powerful tool for solving non-parametric learning problems, such as kernel regression, support vector machines (SVM), principal component analysis (PCA), and many others. A typical burden for kernel methods is that they suffer from scalability, since computing a kernel matrix requires computing a quadratic (in the number of input points) number of entries in the matrix. A direction that has received less attention but still of particular interest is the regime where the dimension $d$ of the data points is large. Typically, applying the kernel function to each pair of data points takes $O(d)$ time. This is especially undesirable in applications for natural language processing [DL20] and computational biology [TPK02], where $d$ can be as large as $\text{poly}(n)$, with $n$ being the number of data points. To compute the kernel matrix, the algorithm does have to read the $d \times n$ input matrix. Therefore, algorithms that have a nearly linear dependence on $nd$ are of particular interest.

To accelerate the computation of kernel matrices from the naive $O(n^2d)$ time algorithm, a lot of work has focused on finding a good approximation to a kernel matrix efficiently [RR07, AM15, MM17, AKK+20, WZ20]. All of these methods make use of randomized algorithmic primitives such as sampling or sketching. Roughly speaking, the idea is to randomly generate a “sketching matrix" with a small number of rows, multiply the sketching matrix with the input matrix, and show that the resulting matrix approximately preserves the length of vectors in the row or column space of the original matrix.

The polynomial kernel is of interest, since any kernel can be written as a sum of polynomial kernels through a Taylor expansion. If we can efficiently approximate the polynomial kernel, then we will be able to efficiently approximate many types of kernels. In [ANW14], Avron, Nguyen and Woodruff approximate the polynomial kernel with a sketching matrix in time that depends exponentially on the degree $p$ of the polynomial kernel. Recent works of [AKK+20, WZ20] have improved the dependence on $p$ to polynomial. However, their algorithms mainly focus on optimizing the dependence on $n$ and reducing the exponential dependence on $p$ to polynomial. If $X \in \mathbb{R}^{d \times n}$ is the input matrix and is dense, then these algorithms have runtime $\tilde{O}(pnd + \epsilon^{-2}n^3p^2)$.

Thus, a natural question to ask is:

Does there exist a sketch for polynomial kernels of degree $p$, such that the runtime is nearly linear in $nd$, and with an improved dependence on $p$? Notice this is especially desirable for kernels such as the neural tangent kernel (NTK) [JGH18] and the arc-cosine kernel [CS09], whose Taylor series have a much slower decay rate ($1/n^c$ for some $c$) compared to the Gaussian kernel (which is $1/n!$).

We list our contributions as follows:

- We develop an efficient algorithm that computes a sketch of the polynomial kernel of degree $p$ in time linear in $p^2$ and nearly linear in $nd$.

- Our algorithm only uses two distinct sketches compared to the $O(p)$ independent sketches of [AKK+20]. This enables us to use repeated powering to compute our sketch very efficiently.

- We characterize kernel matrices by considering their Taylor series, and provide different algorithmic schemes to solve them. Our characterization includes a family of interesting and

\footnote{We use $\tilde{O}(\cdot), \tilde{\Omega}(\cdot), \tilde{\Theta}(\cdot)$ to suppress $\text{poly}(\log(nd/\epsilon \delta))$ factors.}
popular kernels. We also use this sketch as a preconditioner for solving linear systems involving a kernel matrix, and we extend our sketch to solve kernel ridge regression, by composing it with another sketch that depends on the statistical dimension.

1.1 Related Work

**Kernel regression**  Classical regression has the form \( \min_w \| Y - Xw \|_2^2 \), where \( X \) and \( Y \) are a given dataset and corresponding labels, respectively. Kernel regression \([\text{Bac}13, \text{ZDW}15, \text{AM}15, \text{ACW}17b, \text{AKM}+17, \text{ZNV}+20, \text{LSS}+20, \text{ACSS}20]\) allows for \( X \) to be a kernel matrix \( K \in \mathbb{R}^{n \times n} \), where each entry is the application of a kernel function to a pair of data points in \( X \). Kernel regression \( \min_w \| Y - Kw \|_2^2 \) enables fitting non-linear data into a hyperplane by transforming the data into a high-dimensional space.

**Sketching techniques for tensor-related problems** Sketching techniques have been used extensively in tensor-related problems, e.g., for linear-algebraic problems involving polynomial kernels \([\text{ANW}14, \text{AKK}+20, \text{WZ}20]\), for tensor low-rank approximation \([\text{SWZ}19]\), and for tensor regression \([\text{HLW}17, \text{DSSW}18, \text{DJS}+19]\).

**Subspace embeddings**  An (oblivious) subspace embedding is a useful concept in randomized numerical linear algebra introduced by Sárosi \([\text{Sar}06]\). Many applications rely on subspace embeddings or their variants, such as linear regression, low-rank approximation \([\text{CW}13, \text{NN}13, \text{MM}13, \text{BW}14, \text{BWZ}16, \text{SWZ}17, \text{ALS}+18]\), tensor decomposition \([\text{SWZ}19]\), cutting plane methods \([\text{JLSW}20]\), and linear programming \([\text{LSZ}19, \text{JSWZ}21, \text{SY}21]\).

**Roadmap** In Section 2, we introduce definitions, notations and some basic facts. In Section 3, we present a technical overview of our results. In Section 4, we propose an efficient algorithm to generate a sketch and apply it to a polynomial kernel of arbitrary positive integer degree \( p \). In Section 5, we analyze our algorithm with a specific sketching matrix. In Section 6, we present applications to the Gaussian kernel and a more general class of kernels, which can be characterized through the coefficients of their Taylor expansion. We also discuss how to use our sketch as a preconditioner for solving kernel linear systems, and solve sketched kernel ridge regression.

2 Preliminaries

For an integer \( n \), let \([n]\) denote the set \( \{1, 2, \cdots, n\} \). For two scalars \( a \) and \( b \), we say \( a \approx_\epsilon b \) if \((1 - \epsilon)b \leq a \leq (1 + \epsilon)b\). We say a square symmetric matrix \( A \) is positive semi-definite (PSD) if \( \forall x, x^\top Ax \geq 0 \). For two PSD matrices \( A \) and \( B \), we define \( A \approx_\epsilon B \) if \((1 - \epsilon)B \preceq A \preceq (1 + \epsilon)B\), where \( A \preceq B \) means \( B - A \) is PSD. For a matrix \( A \), we use \( \| A \|_F = (\sum_{i,j} A_{i,j}^2)^{1/2} \) to denote its Frobenius norm and use \( \| A \|_{\text{op}} \) to denote its operator (spectral) norm. For a square symmetric matrix \( A \), we use \( \text{tr}[A] \) to denote the trace of \( A \). For a square symmetric matrix \( A \), we use \( \lambda_{\text{min}}(A), \lambda_{\text{max}}(A) \) to denote its smallest and largest eigenvalues, respectively. For a rectangular matrix \( A \), we use \( \sigma_{\text{min}}(A), \sigma_{\text{max}}(A) \) to denote its smallest and largest singular values, respectively, and we use \( \kappa = \sigma_{\text{max}}(A) / \sigma_{\text{min}}(A) \) to denote its condition number.

2.1 Definitions

We define an oblivious subspace embedding (\([\text{Sar}06]\)) as follows:
Definition 2.1 (Oblivious Subspace Embedding (OSE)). Let $\epsilon, \delta \in (0, 1)$ and $d, n \geq 1$ be integers. An $(\epsilon, \delta, d, n)$-Oblivious Subspace Embedding (OSE) is a distribution over $m \times d$ matrices with the guarantee that for any fixed matrix $A \in \mathbb{R}^{d \times n}$, we have

$$\Pr_{\Pi \sim D}[((\Pi A)^\top \Pi A) \approx_\epsilon (A^\top A)] \geq 1 - \delta.$$  

We also introduce tensor products of vectors and Kronecker products of matrices.

Definition 2.2 (Vector tensor product). Given two vectors $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^m$, we define the tensor product between $x$ and $y$, denoted by $x \otimes y$, to be $\text{vec}(xy^\top)$. We will use $x^{\otimes p}$ to denote the self-tensoring of the vector $x$ a total of $p$ times.

The Kronecker product of matrices is a natural extension of the tensor product of vectors:

Definition 2.3. Given $A_1 \in \mathbb{R}^{m_1 \times n_1}, A_2 \in \mathbb{R}^{m_2 \times n_2}, \ldots, A_k \in \mathbb{R}^{m_k \times n_k}$, we define $A_1 \times A_2 \times \cdots \times A_k$ to be the matrix in $\mathbb{R}^{m_1 m_2 \ldots m_k \times n_1 n_2 \ldots n_k}$ whose element at row $(i_1, \ldots, i_k)$ and column $(j_1, \ldots, j_k)$ is $A_1(i_1, j_1) \cdots A_k(i_k, j_k)$.

An important property of the Kronecker product is the so-called mixed product property:

Claim 2.4 (Mixed product). For matrices $A, B, C, D$ with appropriate sizes, the following holds:

$$(A \cdot B) \times (C \cdot D) = (A \times C) \cdot (B \times D).$$

One consequence is the following claim:

Claim 2.5. Let $A_1 \in \mathbb{R}^{m_1 \times n_1}, A_2 \in \mathbb{R}^{m_2 \times n_2}, \ldots, A_k \in \mathbb{R}^{m_k \times n_k}$ and $v_1 \in \mathbb{R}^{n_1}, v_2 \in \mathbb{R}^{n_2}, \ldots, v_k \in \mathbb{R}^{n_k}$. Then,

$$(A_1 \times A_2 \times \cdots \times A_k)(v_1 \times v_2 \times \cdots \times v_k) = (A_1 v_1) \times (A_2 v_2) \times \cdots \times (A_k v_k).$$

We will extensively use the following notation:

Definition 2.6. Given $A_1 \in \mathbb{R}^{m_1 \times n_1}, A_2 \in \mathbb{R}^{m_2 \times n_2}, \ldots, A_k \in \mathbb{R}^{m_k \times n_k}$, we define $A_1 \otimes A_2 \otimes \cdots \otimes A_k$ to be the matrix in $\mathbb{R}^{m_1 m_2 \ldots m_k \times n_1 n_2 \ldots n_k}$ whose $j^{th}$ column is $A_1^j \times A_2^j \times \cdots \times A_k^j$ for every $j \in [n]$, where $A_l^{j}$ is the $j^{th}$ column of $A_l$ for every $l \in [k]$.

2.2 Sketching Matrices

We recall the Subsampled Randomized Hadamard Transform (SRHT), which is a Fast Johnson-Lindenstrauss transform [AC06].

Definition 2.7 (Subsampled Randomized Hadamard Transform (SRHT), see [LDFU13, Woo14]). The SRHT matrix $S \in \mathbb{R}^{m \times d}$ is defined as $S = \frac{1}{\sqrt{m}} \text{PHD}$, where each row of matrix $P \in \{0, 1\}^{m \times d}$ contains exactly one 1 at a random position, $H$ is the $d \times d$ Hadamard matrix, and $D$ is a $d \times d$ diagonal matrix with each diagonal entry being a value in $\{-1, +1\}$ with equal probability.

Remark 2.8. Using the Fast Fourier Transform (FFT) [CT65], $S$ can be applied to a vector in time $O(d \log d)$.

We also introduce a sketching matrix for degree-2 tensors, which is a generalization of the SRHT.
We define the TensorSRHT $S : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^m$ as $S = \sqrt{m}P \cdot (HD_1 \times HD_2)$, where each row of $P \in \{0,1\}^{m \times d}$ contains only one 1 at a random coordinate, one can view $P$ as a sampling matrix. $H$ is a $d \times d$ Hadamard matrix, and $D_1, D_2$ are two $d \times d$ independent diagonal matrices with diagonals that are each independently set to be a Rademacher random variable (uniform in $\{-1, 1\}$).

Remark 2.10. By leveraging the FFT algorithm in the sketch space, $S(x \otimes 2)$ can be computed in time $O(d \log d + m)$.

We will use the following properties of the SRHT and TensorSRHT.

Lemma 2.11 (Theorem 2.4 in [Woo14]). Let $T$ be an SRHT matrix defined in Definition 2.7. If $m = O(n \log(nd/\delta)\epsilon^{-2})$, then $T$ is an $(\epsilon, \delta, d, n)$-OSE.

Lemma 2.12 (Lemma 21 in [AKK+20]). Let $S$ be a TensorSRHT matrix defined in Definition 2.9. If $m = O(n \log^3(nd/\epsilon \delta)\epsilon^{-2})$, then $S$ is an $(\epsilon, \delta, d, n)$-OSE for degree-2 tensors.

2.3 Kernels

We introduce several kernels that are widely-used in practice, e.g., see [GE08, CHC+10] for the polynomial kernel, and see [NJW01] for the Gaussian kernel.

Definition 2.13 (Polynomial Kernel). Given two data points $x, y \in \mathbb{R}^d$, the degree-$p$ polynomial kernel, $P$, between $x$ and $y$ is defined as $P(x, y) = (x, y)^p$. Let $X \in \mathbb{R}^{d \times n}$. The degree-$p$ polynomial kernel $P$, defined on matrix $X$, is the matrix $P_{i,j} = \langle x_i, x_j \rangle^p$, where $x_i, x_j$ are the $i$th and $j$th column of $X$, respectively.

Definition 2.14 (Gaussian Kernel). Given two data points $x, y \in \mathbb{R}^d$, the Gaussian kernel, $G$, between $x$ and $y$ is defined as $G(x, y) = \exp(-\|x - y\|_2^2/2)$. Let $X \in \mathbb{R}^{d \times n}$. The Gaussian kernel $G$, defined on matrix $X$, is the matrix $G_{i,j} = \exp(-\|x_i - x_j\|_2^2/2)$, where $x_i, x_j$ are the $i$th and $j$th column of $X$, respectively.

3 Technical Overview

We first consider one way to compute the polynomial kernel $P$ via the identity $P = (X \otimes p)^\top X \otimes p$. Our algorithm will try to compute $X \otimes p$ quickly.

Suppose we want to compute the $p$-fold tensoring of a vector $x$, and assume for simplicity that $p$ is a power of 2. Our algorithm is inspired by that of [AKK+20], which generates a complete binary tree with $2p - 1$ nodes, and thus leaves. For the $i$-th leaf node, it picks a sketch $T^i$ and applies it to $x$, obtaining $T^i x$. Each internal node $j$ then does the following: it picks a sketch $S^j$, and applies $S^j$ to the tensor product of its two children. $S^j$ is picked as a map from $\mathbb{R}^{m^2} \rightarrow \mathbb{R}^m$ for each $j$, so at each level of the binary tree, we reduce the number of vectors by half, while remaining in the low-dimensional space $\mathbb{R}^m$. One drawback of this algorithm is the usage of an independent sketch for each node of the tree, thus incurring a linear dependence on $p$ in the runtime.

Our algorithm instead uses a much smaller amount of randomness. We pick only a single $T$ and a single $S$, i.e., $T^1 = T^2 = \cdots = T^p$ for all leaf nodes, and we have $S^j = S$ for all internal nodes $j$. The challenge with this approach is of course that we have much less independence in our analysis, and consequently do not obtain the same guarantees for preserving the length of the tensor.

\footnote{A more standard definition is $P(x, y) = (x, y)^p + c$; we can simulate this by creating an extra dimension on all data points.}
product of an arbitrary set of vectors as in previous work. We stress that we compute a sketch that preserves the column span of $X^\otimes p$, and this is weaker than the guarantee we would get had we used full independence, which gives a sketch that is an oblivious subspace embedding, meaning that it can preserve the column span of any matrix in $\mathbb{R}^{dp \times n}$. However, the key point is that we can preserve the tensor product of a vector with itself $p$ times, and this will suffice for our applications.

This allows for a much faster way to compute $x^\otimes p$: “square” a vector by computing the tensor product with itself, then apply a sketch, and repeat this process. By doing so, we reduce the dependence on $p$ in the first level of the tree from linear to logarithmic. However, this will incur a $p^2$ factor in the dimension of the sketch, and so we will pay more for $p$ in levels other than the first level. Fortunately, levels other than the first level apply sketches to lower dimensional vectors. By carefully balancing the complexity of applying $T$ and $S$, we achieve an improved running time, which is useful when the degree $p$ is large.

4 Fast Sketching Algorithm for the Polynomial Kernel

We introduce our algorithm that sketches a single vector $x^\otimes p$ and extend it to each column of a matrix. In Section 4.1 we give some definitions. In Section 4.2 we prove several technical tools related to tensors. In Section 4.3 we show our sketch preserves the column space of the polynomial kernel. In Section 4.4 we prove our main result for this section.

4.1 Definitions

We define the sketching matrix formed by Algorithm 1 as follows:

**Definition 4.1.** Let $q$ be a power of 2 and $\Pi^q : \mathbb{R}^{d^q} \to \mathbb{R}^m$ be defined as the following matrix:

$$\Pi^q = Q^q \cdot T^q,$$

where $T^q = T \times T \times \ldots \times T$ and $Q^q = S^1 \cdot S^2 \cdot S^4 \cdot \ldots \cdot S^{q/2}$, and $S^l = S \times S \times \ldots \times S$.

We will design an algorithm that achieves the following goal:

**Case 1** If $p$ is a power of 2, then it computes $\Pi^p X^\otimes p$ efficiently.

**Case 2** If $p$ is not a power of 2, then let $b$ be its binary representation and let

$$E = \{i : b_i = 1, i \in \{0, \ldots, \log_2 p\}\}.$$ 

We will iterate through all indices in $E$ and continue tensoring two vectors where $b_i = 1$, and apply $S$ to them.

**Definition 4.2.** Let $S \in \mathbb{R}^{m^2} \to \mathbb{R}^m$ and $T : \mathbb{R}^d \to \mathbb{R}^m$ be base sketches. Let $X \in \mathbb{R}^{d \times n}$ be an input matrix. We define $Z(S, T, X)$ to be the matrix for which we apply Algorithm 1 on each column of $X$, with base sketches $S$ and $T$.

4.2 Equivalence Results for Tensors

We provide two technical tools for handling tensors.

**Lemma 4.3 (The output guarantee of Algorithm 1).** Let $p$ be a power of 2 and $\Pi^p$ be defined as in Definition 4.1. Let $x \in \mathbb{R}^d$. Then the output vector $z$ generated by Algorithm 1 satisfies $z = \Pi^p (x^\otimes p)$. 

5
Algorithm 1 Our algorithm for sketching the vector $x \otimes p$ with limited randomness.

1: procedure TensorSketchViaLimRand $(x \in \mathbb{R}^d, p \in (1, \infty), S \in \mathbb{R}^{m \times m^2}, T \in \mathbb{R}^{m \times d})$ \triangleright Theorem 4.8 and 5.1
2: Let $q = 2^{\log_2 p}$
3: Let $w_0 = Tx$ \triangleright $T$ can be SRHT (Definition 2.7)
4: for $l = 1$ to $\log_2 q$ do
5: Compute $w_l = S(w_{l-1} \otimes 2^l)$ \triangleright $S$ can be TensorSRHT (Definition 2.9)
6: end for
7: Let $b$ be the binary representation of $p$, and let $E = \{ i : b_i = 1, i \in \{0, \ldots, \log_2 p\} \}$
8: Let $z = w_j$, where $j$ is the lowest bit of $b$ where $b_j = 1$
9: for $i$ in $E \setminus \{j\}$ do
10: $z = S(z \times w_i)$
11: end for
12: return $z$ \triangleright $z \in \mathbb{R}^m$
13: end procedure

Proof. If $p$ is a power of 2, then Algorithm 1 will output $z$ on line 8. We will exploit the fact that although Algorithm 1 only computes one vector at a time, we can view it as computing $p/2^i$ identical vectors in the $i^{th}$ iteration. On line 3, we can treat it as computing $p$ copies of $w_0$, and therefore, by Claim 2.5, we have

$$w_0 \otimes p = (Tx) \otimes p = (T \times T \times \ldots \times T)(x \times x \times \ldots \times x) = T^p x \otimes p.$$ 

We can apply the same line of reasoning to line 4 of the algorithm. In the $i^{th}$ iteration, we can treat it as

$$S(w_{i-1} \otimes 2^i) \times S(w_{i-1} \otimes 2^i) \times \ldots \times S(w_{i-1} \otimes 2^i)$$

a total of $p/2^i$ times. Again, using Claim 2.5, we have

$$w_i \otimes p/2^i = S(w_{i-1} \otimes 2^i) \otimes S(w_{i-1} \otimes 2^i) \otimes \ldots \otimes S(w_{i-1} \otimes 2^i)$$

$$= (S(w_{i-1} \otimes 2^i)) \otimes S(w_{i-1} \otimes 2^i) \otimes \ldots \otimes S(w_{i-1} \otimes 2^i)$$

$$= (S \times S \times \ldots \times S)(w_{i-1} \otimes 2^i) \otimes 2^i$$

$$= S(p/2^i \cdot w_{i-1} \otimes 2^i).$$

Recursively applying this identity, we will end up with

$$z = S^1 \cdot S^2 \cdot S^4 \cdot \ldots \cdot S^{p/2} \cdot T^p x \otimes p = \Pi^p (x \otimes p). \square$$

Next, we wish to show that if $p$ is a power of 2, then $\Pi^p$ preserves the subspace spanned by the columns of $X \otimes p$ within a factor of $1 \pm \varepsilon_{2^p}$. Notice this is weaker than $\Pi^p$ being an OSE, but sufficient for our application to polynomial kernels. We will show that

$$(\Pi^p X \otimes p)^\top \Pi^p X \otimes p \approx \varepsilon (X \otimes p)^\top X \otimes p.$$
The following lemma outlines the main technique in our proof of this property. It establishes a one-to-one mapping between a vector in the column span of $X^\otimes p$ and a matrix. We then use this equivalence to inductively prove that $\Pi^p$ preserves the target subspace.

**Lemma 4.4** (From Vector Tensor to Matrix Tensor). Let $X \in \mathbb{R}^{d \times n}$. Consider $u = X^\otimes p y$ for some $y \in \mathbb{R}^n$ and positive integer $p$. Then,

$$\|u\|_2 = \|X^{\otimes (p-1)} Y X^\top\|_F,$$

where $Y = \text{diag}(y) \in \mathbb{R}^{n \times n}$ is a diagonal matrix where the $i$-th entry on the diagonal is $y_i$, $\forall i \in [n]$.

**Proof.** We will use $X_{\ell,j}$ to denote the $i$-th row and $j$-th column of $X$. We observe that a fixed column $X_{s,j}^{\otimes p}$ is equivalent to taking the outer product $X_{s,j}^{\otimes p-1} X_{s,j}^\top$, then flattening the matrix into a long vector. If we use a double index to indicate an entry of $X_{s,j}^{\otimes p}(a,b)$, then we have $X_{s,j}^{\otimes p}(a,b) = X_{s,j}^{\otimes (p-1)}(a)X(b)$, where $a$ ranges from 1 to $d^{p-1}$ and $b$ ranges from 1 to $d$. Consider the $\ell_2$ norm $u$:

$$\|u\|_2^2 = \|X^{\otimes p} y\|_2^2 = \sum_{a=1}^{d^{p-1}} \sum_{b=1}^d \left( \sum_{i=1}^n y_i(X_{s,i}^{\otimes p})(a,b) \right)^2.$$

On the other hand, we can write $X^{\otimes (p-1)}$ in its column form:

$$
\begin{bmatrix}
X_{s,1}^{\otimes (p-1)} & X_{s,2}^{\otimes (p-1)} & \cdots & X_{s,n}^{\otimes (p-1)}
\end{bmatrix}.
$$

Recall that $Y$ is a diagonal matrix and therefore, the product $X^{\otimes (p-1)} Y$ can be expressed as

$$
\begin{bmatrix}
y_1 X_{s,1}^{\otimes (p-1)} & y_2 X_{s,2}^{\otimes (p-1)} & \cdots & y_n X_{s,n}^{\otimes (p-1)}
\end{bmatrix}.
$$

Using the outer product definition of matrix product, we have

$$X^{\otimes (p-1)} Y X^\top = \sum_{i=1}^n y_i X_{s,i}^{\otimes (p-1)} X_{s,i}^\top.$$

This is a matrix of size $d^{p-1} \times d$. Therefore, we can write its Frobenius norm as

$$\|X^{\otimes (p-1)} Y X^\top\|_F^2 = \|\sum_{i=1}^n y_i X_{s,i}^{\otimes (p-1)} X_{s,i}^\top\|_F^2 = \sum_{a=1}^{d^{p-1}} \sum_{b=1}^d \left( \sum_{i=1}^n y_i(X_{s,i}^{\otimes p})(a,b) \right)^2.$$

This completes the proof. \(\square\)
4.3 Preserving the Polynomial Kernel Subspace

We prove the sketch generated by Algorithm 1 preserves the column space of the polynomial kernel.

Lemma 4.5 (\(T^p\) Preserves Polynomial Kernel Subspace). Let \(X \in \mathbb{R}^{d \times n}\), \(y \in \mathbb{R}^n\) and \(u = X^\otimes p y\), where \(p\) is a positive integer. If \(T\) is an \((\epsilon, \delta, d, n)\) OSE, then with probability at least \(1 - \delta\),

\[
\| (TX)^\otimes p y \|^2_2 = (1 \pm \epsilon)^p \| X^\otimes p y \|^2_2
\]

Proof. We proceed by induction on \(p\). For \(p = 1\), by Definition 2.1, we have

\[
\| TXy \|^2_2 = (1 \pm \epsilon) \| Xy \|^2_2.
\]

For the inductive step, we will prove this for a general positive integer \(p > 1\). We break \(p\) into \(p - 1\) and 1. By Lemma 4.4, we have

\[
\| (TX)^\otimes (p-1) Y X^\top T^\top \|^2_F = (1 \pm \epsilon) \| (TX)^\otimes (p-1) Y X^\top \|^2_F.
\]

Recall that \(T\) is an \((\epsilon, \delta, d, n)\) OSE for \(X\). This means right multiplying by \(T^\top\) preserves the length of all columns of \((TX)^\otimes (p-1) Y X^\top\), and therefore we have

\[
\| (TX)^\otimes (p-1) Y X^\top \|^2_F = (1 \pm \epsilon)^{p-1} \| X^\otimes (p-1) Y X^\top \|^2_F.
\]

Using the inductive hypothesis, for any vector \(z \in \mathbb{R}^n\), we have

\[
\| (TX)^\otimes (p-1) z \|^2_2 = (1 \pm \epsilon')^{p-1} \| X^\otimes (p-1) z \|^2_2.
\]

Applying this to each column of \(Y X^\top\), we have

\[
\| (TX)^\otimes p Y X^\top \|^2_F = (1 \pm \epsilon)^p \| X^\otimes p Y X^\top \|^2_F
\]

\[
= (1 \pm \epsilon)^{p-1} \| X^\otimes p y \|^2_2.
\]

This enables us to conclude that

\[
\| (TX)^\otimes p y \|^2_2 = (1 \pm \epsilon)^p \| X^\otimes p y \|^2_2
\]

\(\square\)

Remark 4.6. As we motivated in Section 3, if we view Algorithm 1 as a binary tree, Lemma 4.5 effectively proves that the bottom layer of the tree preserves the column space of \(X^\otimes p\). We then pick \(S\) to be an OSE for degree-2 tensors, and inductively establish our embedding.

Lemma 4.7 (\(\Pi^p\) Preserves the Polynomial Kernel Subspace). Let \(S : \mathbb{R}^{m^2} \to \mathbb{R}^m\) be an \((\epsilon, \delta, d, n)\)-OSE for degree-2 tensors, and let \(T : \mathbb{R}^d \to \mathbb{R}^m\) be an \((\epsilon, \delta, d, n)\)-OSE (Definition 2.1). Let \(p\) be a power of 2. Let \(\Pi^p\) be the sketching matrix defined as in Definition 4.1. Then we have for any \(y \in \mathbb{R}^n\), with probability at least \(1 - \delta\),

\[
(1 - \epsilon)^{2p} \| X^\otimes p y \|^2_2 \leq \| \Pi^p X^\otimes p y \|^2_2 \leq (1 + \epsilon)^{2p} \| X^\otimes p y \|^2_2.
\]
Proof. We will prove this by induction on the number of iterations of Algorithm 1. Let $k = \log_2 p$; we will induct on the parameter $l$ from 1 to $k$. Let $\mathbf{Y}^{2l}$ denote the sketching matrix at level $l$: $\mathbf{Y}^{2l} = S^{p/2l} \cdot S^{p/2l-1} \cdot \ldots \cdot S^{p/2} \cdot T^p$, for all $l \in [k]$ and $\mathbf{Y}^0 = T^p$. We will prove the following statement: For the base case, note that Lemma 4.5 automatically gives our desired result. For the inductive step, we assume it holds for some $l - 1$, so

$$\|\mathbf{Y}^{2l-1} X^{\oplus p} y\|_2 \leq (1 + \epsilon)\sum_{i=0}^{p/2l} \|X^{\oplus p} y\|_2.$$

Note that when $l = k$, we have $\mathbf{Y}^{2k} = \Pi^p$, and therefore it gives us the desired result.

For the base case, note that Lemma 4.5 automatically gives our desired result. For the inductive step, we assume it holds for some $l - 1$, so

$$\|\mathbf{Y}^{2l-1} X^{\oplus p} y\|_2 \leq (1 + \epsilon)\sum_{i=0}^{p/2l} \|X^{\oplus p} y\|_2.$$

Notice that $\mathbf{Y}^{2l} = S^{p/2l} \cdot \mathbf{Y}^{2l-1}$. Let $Z$ be defined as the matrix

$$Z = \begin{bmatrix}
(x^1_1)^{\otimes 2} & (x^2_1)^{\otimes 2} & \ldots & (x^n_1)^{\otimes 2} \\
(x^1_{l-1})^{\otimes 2} & (x^2_{l-1})^{\otimes 2} & \ldots & (x^n_{l-1})^{\otimes 2} \\
\vdots & \vdots & \ddots & \vdots \\
(x^1_{l-1})^{\otimes 2} & (x^2_{l-1})^{\otimes 2} & \ldots & (x^n_{l-1})^{\otimes 2}
\end{bmatrix},$$

where we use $x^i_j$ to denote the $i$th column of $X$ after the $j$th iteration. From Algorithm 1, we have that $Z = \mathbf{Y}^{2l} X^{\oplus p}$, and so the product $S^{p/2l} \cdot \mathbf{Y}^{2l-1} X^{\oplus p}$ can be written as $(SZ)^{\oplus p/2l}$.

If $p/2l > 1$, then similar to Lemma 4.5,

$$\|(SZ)^{\oplus p/2l} y\|_2^2 = \|(SZ)^{\oplus (p/2l-1)} \cdot \mathbf{diag}(y)Z^T S^T \|_F^2 = (1 + \epsilon)\|(SZ)^{\oplus (p/2l-1)} \cdot \mathbf{diag}(y)Z^T \|_F^2 = (1 + \epsilon)\|Z^{\oplus p/2l} y\|_2^2 = (1 + \epsilon)\|Z^{\oplus p/2l} y\|_2^2 = (1 + \epsilon)\sum_{i=0}^{p/2l} \|X^{\oplus p} y\|_2^2.$$

The third step uses the same reasoning as Lemma 4.5, i.e., we can pull out $S$ by paying an extra $(1 + \epsilon)^{p/2l-1}$ factor. The last line uses the inductive hypothesis.

If $p/2l = 1$, then we will end up with $SZy$, and can simply use the fact that $S$ is an OSE to argue that $SZy$ preserves the length of $Zy$. We then use the inductive hypothesis on $Z$ to conclude the proof. 

Below, we state and prove a theorem that establishes the correctness of Algorithm 1 without instantiating the sketching matrix $T$ and $S$. This enables us to use different sketches with various trade-offs.

### 4.4 Main Result

We prove the main result of this section, which establishes the correctness of Algorithm 1.

**Theorem 4.8 (Main Result, Correctness Part).** Let $S : \mathbb{R}^{m^2} \rightarrow \mathbb{R}^m$ be an $(\epsilon, \delta, 0, d, n)$-OSE for degree-2 tensors and $T : \mathbb{R}^d \rightarrow \mathbb{R}^m$ be an $(\epsilon, \delta, d, n)$-OSE. Let $p$ be a positive integer. Let $Z = Z(S, T, X)$ be the matrix as defined in Def. 4.2. Then for any $y \in \mathbb{R}^n$, we have

$$(1 - \epsilon)^{3p} \|X^{\oplus p} y\|_2 \leq \|Zy\|_2 \leq (1 + \epsilon)^{3p} \|X^{\oplus p} y\|_2$$
Proof. Let \( b \) be the binary representation of \( p \), and let \( E = \{ i : b_i = 1, i \in \{ 0, 1, \ldots, \log_2 p \} \} \). If \( p \) is a power of 2, by Lemma 4.7, we are done. So suppose \( p \) is not a power of 2. Let \( q = 2^{\lceil \log_2 p \rceil} \). Algorithm 1 computes \( \Pi^q X \otimes q \) and combines intermediate results with indices in \( E \) to form the final result. We will again prove this by induction on the indices in \( E \), from smallest to largest. For the base case, let \( i_1 \) be an index in \( E \) and let \( q_1 = 2^{i_1} \). Since \( q_1 \) is a power of 2, Lemma 4.7 establishes this case.

For the inductive step, suppose this holds for \( i_1, i_2, \ldots, i_{j-1} \in E \), and let \( q_1 = 2^{i_1}, q_2 = 2^{i_2}, \ldots, q_{j-1} = 2^{i_{j-1}} \). We will prove this holds for \( q_j = 2^{i_j} \). Let \( Z \) denote the matrix after the \((j-1)\)th application of this recursive process. We will show that

\[
\| S \left( (\Pi^{q_j} X^{\otimes q_j}) \otimes Z \right) y \|_2^2 = (1 + \epsilon)^j \sum_{i=1}^{q_j} \| X^{\otimes (\sum_{i=1}^{q_j} q_i)} \|_F^2.
\]

(1)

We first use the fact \( S \) is an OSE to obtain

\[
\| S \left( (\Pi^{q_j} X^{\otimes q_j}) \otimes Z \right) y \|_2^2 = (1 + \epsilon) \| (\Pi^{q_j} X^{\otimes q_j}) \otimes Z \|_F^2.
\]

(2)

By Lemma 4.4, we have

\[
\| (\Pi^{q_j} X^{\otimes q_j}) \otimes Z \|_F^2 = \| \Pi^{q_j} X^{\otimes q_j} \|_F^2 \|	ext{diag}(y) Z^T \|_F^2.
\]

\[
= (1 + \epsilon)^{q_j + \sum_{i=1}^{q_j-1} 2q_i} \| X^{\otimes (\sum_{i=1}^{q_j-1} q_i)} \|_F^2 \|	ext{diag}(y) Z^T \|_F^2.
\]

\[
= (1 + \epsilon)^{q_j + \sum_{i=1}^{q_j-1} 2q_i} \| X^{\otimes (\sum_{i=1}^{q_j-1} q_i)} Y \|_2^2.
\]

(3)

Combining Eq. (2) and Eq. (3), we obtain Eq. (1), which is our desired result. \( \square \)

5 Analysis of Sketching Matrices: SRHT and TensorSRHT

In this section, we analyze the runtime of Algorithm 1 with \( T \) being an SRHT sketch (Definition 2.7) and \( S \) being a TensorSRHT sketch (Definition 2.9).

5.1 Main Result

The goal of this section is to give a runtime analysis of Algorithm 1 using SRHT as \( T \) and TensorSRHT as \( S \).

Theorem 5.1 (Main Result, Running Time). Let \( p \in \mathbb{N}_+ \) and \( \epsilon, \delta \in (0,1) \). Then for every \( X \in \mathbb{R}^{d \times n} \), there exists a distribution over oblivious linear sketches \( \Pi : \mathbb{R}^{dp} \to \mathbb{R}^m \) such that if \( m = \tilde{O}(\epsilon^{-2}np^2) \), we have

\[
(\Pi X^{\otimes p})^\top \Pi X^{\otimes p} \approx \epsilon \left( X^{\otimes p} \right)^\top X^{\otimes p}.
\]

Moreover, using Algorithm 1, \( \Pi X^{\otimes p} = Z(S, T, X) \) can be computed in time \( \tilde{O}(nd + \epsilon^{-2}n^2p^2) \).

Proof. We will use an SRHT for \( T \) and a TensorSRHT for \( S \). We pick both of these sketches to be \((\hat{\epsilon}, \delta, d, n)\)-OSEs where \( \hat{\epsilon} = \frac{\epsilon}{3p} \). Let \( Z = Z(S, T, X) \) be the matrix generated by Algorithm 1 with these parameters. By Theorem 4.8, we have

\[
(1 - \hat{\epsilon})^{3p} (X^{\otimes p})^\top X^{\otimes p} \leq Z^\top Z \leq (1 + \hat{\epsilon})^{3p} (X^{\otimes p})^\top X^{\otimes p}.
\]
By Taylor expanding $(1 + x/n)^n$ around $x = 0$, we have

$$(1 + \frac{\epsilon}{3p})^{3p} = 1 + \epsilon + O(\epsilon^2).$$

Thus, by picking $\tilde{\epsilon} = \frac{\epsilon}{3p}$, we have

$$Z^\top Z \approx \epsilon (X\otimes p)^\top X\otimes p.$$ 

For both SRHT and TensorSRHT to be $(\epsilon/3p, \delta, d, d, n)$ OSEs, we need $m = \tilde{\Theta}(n/(\epsilon/3p)^2) = \tilde{\Theta}(p^2n/\epsilon^2)$.

We now analyze the runtime of Algorithm 1 under SRHT and TensorSRHT. On line 2, we compute $TX$ in time $\tilde{O}(nd)$ since $T$ is an SRHT. We then enter a loop with $O(\log p)$ iterations, where in each iteration we apply $S$ to the tensor product of a column with itself resulting from the previous iteration. Since $S$ is a TensorSRHT, this takes $O(m) = \tilde{O}(p^2n/\epsilon^2)$ time per column, and there are $n$ columns, so $\tilde{O}(p^2n^2/\epsilon^2)$ time in total for this step. We also compute each bit in the binary representation, which incurs an $O(\log p)$ factor in the final runtime. So it takes Algorithm 1 $\tilde{O}(nd + p^2n^2/\epsilon^2)$ time to compute $Z(S, T, X)$. This completes the proof. □

5.2 Discussion

We compare our result with the results obtained in [AKK+20, WZ20]. The setting we are considering is 1) matrix $X$ is dense, i.e., $\text{nnz}(X) \approx nd$, and 2) $d \gg n$. In such a scenario, [AKK+20] obtains a sketching dimension $m = \Omega(\epsilon^{-2}n^{-2}p)$ and the runtime of applying the sketch to $X$ is $O(pmd + \epsilon^{-2}n^3p^2)$, so our result improves the dependence on the $nd$ term and pays only $n^2$ instead of $n^3$ on the second term. Another result from [WZ20] has $m = \Theta(\epsilon^{-2}n)$ but the time to apply sketching is $\tilde{O}(p^2 n^2d + \text{poly}(\epsilon^{-1}, p)n^3)$, which is much worse in the leading $nd$ term, compared to our result. However, we also point out the results obtained in these two works are more general than ours in the sense that their sketches have the OSE property, while our sketch only preserves the column space of $X\otimes p$. Nevertheless, the latter suffices for our applications. We use Table 1 to summarize and compare the different results.

| Reference   | Sketch Dimension | Running Time              |
|-------------|------------------|----------------------------|
| [AKK+20]    | $\Theta(\epsilon^{-2}n^{-2}p)$ | $O(pmd + \epsilon^{-2}n^3p^2)$ |
| [WZ20]      | $\Theta(\epsilon^{-2}n)$       | $O(p^2 n^2d + \text{poly}(\epsilon^{-1}, p)n^3)$ |
| Theorem 5.1 | $\Theta(\epsilon^{-2}np^2)$    | $O(nd + \epsilon^{-2}n^2p^2)$ |

Table 1: Comparison of different algorithms. We assume $\text{nnz}(X) \approx nd$ and $d \gg n$. We also assume there is no regularization, i.e., $\lambda = 0$.

Also, the prior results mentioned are stated in terms of the statistical dimension, while we do not directly obtain bounds in terms of the statistical dimension, though our sketches can be composed with sketches that do. Therefore, we consider the case when there is no regularization ($\lambda = 0$) and $X\otimes p$ is of full rank. In this case, the statistical dimension reduces to $n$.

6 Applications

In this section, we introduce various applications using our sketch. In Section 6.1, we study approximating the Gaussian kernel using our algorithm. In Section 6.2 we extend the analysis to a class
of slow-decaying kernels. In Section 6.3 we illustrate an efficient algorithm to solve kernel linear systems. In Section 6.4 we show how to solve kernel ridge regression using our sketch.

6.1 Gaussian Kernels

We provide the fastest algorithm to preserve the column space of a Gaussian kernel when \( d \) is large.

**Theorem 6.1** (Gaussian Kernel, informal version of Theorem A.1). Let \( X \in \mathbb{R}^{d \times n} \) be the data matrix and \( r \in \mathbb{R}_+ \) be the radius of \( X \), i.e., \( \| x_i \|_2 \leq r \) for all \( i \in [n] \), where \( x_i \) is the \( i \)-th column of \( X \). Suppose \( G \in \mathbb{R}^{n \times n} \) is the Gaussian kernel matrix given in Definition 2.14. There exists an algorithm that computes a matrix \( W_g(X) \in \mathbb{R}^{m \times n} \) in time \( \tilde{O}(\epsilon^{-2} n^2 q^3 + nd) \), such that for every \( \epsilon > 0 \),

\[
\Pr[|W_g(X)^\top W_g(X) - G| \geq 1 - 1/\operatorname{poly}(n)],
\]

where \( m = \Theta(q^3 n / \epsilon^2) \) and \( q = \Theta(r^2 + \log(n/\epsilon)) \).

We provide a sketch of the proof here, and further details can be found in the appendix. The Taylor expansion of the Gaussian kernel can be written as

\[
G = \sum_{l=0}^{\infty} \frac{(X^{\otimes l}D)^\top X^{\otimes l}D}{l!}
\]

where \( D \) is a diagonal matrix with \( D_{i,i} = \exp(-\|x_i\|_2^2/2) \). Let

\[
K = \sum_{l=0}^{\infty} \frac{(X^{\otimes l})^\top X^{\otimes l}}{l!}.
\]

If we set \( q = \Omega(r^2 + \log(n/\epsilon)) \) and just use the first \( q \) terms of \( K \):

\[
Q = \sum_{l=0}^{q} \frac{(X^{\otimes l})^\top X^{\otimes l}}{l!},
\]

then we have that \( \|K - Q\|_{\infty} \leq \frac{\epsilon}{2} \). Our algorithm applies Algorithm 1 on each term of \( Q \). This gives us the desired runtime and dimension. The complete proof is in Appendix A.

6.2 General \( p \)-convergent Kernels

A key advantage of Algorithm 1 is its moderate dependence on the degree \( p \), which gives it more leverage when \( p \) is large. We introduce a characterization of kernels, based on the series of the coefficients in the Taylor expansion of the kernel. As we will later see in the proof of Theorem B.2, the decay rate of coefficients has a direct relation with the degree \( p \) we need for approximating a kernel.

**Definition 6.2** (\( p \)-convergent kernel, informal version of Definition B.1). We say the kernel matrix \( K \) for data matrix \( X \) is \( p \)-convergent if its corresponding Taylor expansion series can be written as follows:

\[
K = \sum_{l=0}^{\infty} C_l \cdot (X^{\otimes l})^\top X^{\otimes l},
\]

where the coefficients \( C_l = (l + 1)^{-\Theta(p)} \).

**Theorem 6.3** (Sketch \( p \)-convergent Kernels, informal version of Theorem B.2). Let \( X \in \mathbb{R}^{d \times n} \) be the data matrix with radius \( r \) for some \( r \in \mathbb{R}_+ \). Let \( p > 1 \) be an integer, suppose \( K \) is a \( p \)-convergent matrix. Let \( m = \Theta(\epsilon^{-2} n^q q^3) \) and \( q = \Theta(r^2 + (n/\epsilon)^{1/p}) \). There exists an algorithm that computes a matrix \( W_k(X) \in \mathbb{R}^{m \times n} \) in time \( \tilde{O}(\epsilon^{-2} n^2 q^3 + nd) \) such that

\[
\Pr[|W_k(X)^\top W_k(X) - K| \geq 1 - 1/\operatorname{poly}(n)].
\]
For the sake of illustration, suppose \( r = 1 \). Then the first term in the running time becomes \( e^{-2} n^{2 + \frac{2}{3}} \). When \( p \) is large, Theorem 6.3 gives a fast algorithm for approximating the kernel, but the runtime becomes much slower when \( p \in (1, 3) \). Therefore, we propose a novel sampling scheme to deal with small values of \( p \). Roughly speaking, we exactly compute the first \( s \) terms in the Taylor expansion, while for the remaining \( q - s \) terms we sample only \( s \) of them proportional to their coefficient. Using a matrix Bernstein bound (Theorem B.4), we obtain an even faster algorithm.

We apply our result to the neural tangent kernel (NTK), which is a 1.5-convergent kernel.

Corollary 6.4 (Approximate NTK, informal version of Corollary C.3). Let \( X \in \mathbb{R}^{d \times n} \) be a data matrix with unit radius. Suppose \( K \in \mathbb{R}^{n \times n} \) is the NTK matrix. There exists an algorithm that computes a matrix \( W_k(X) \) in time

\[
\tilde{O}(\epsilon^{-3} n^{11/3} + nd)
\]

such that

\[
\Pr \left[ W_k(X)^\top W_k(X) \approx \epsilon K \right] \geq 1 - 1/\text{poly}(n).
\]

Remark 6.5. We remark that our definition of \( p \)-convergent kernels captures a wide range of kernels that have slow decay rate in their coefficients in their Taylor expansion, such as NTK and arc-cosine kernels. Typically, the coefficients are of the form \( 1/n^c \) for some \( c > 1 \). In contrast, Gaussian kernels enjoy a much faster decay rate, and therefore, designing algorithm for the Gaussian kernel is considerably simpler, since the number of terms we need to approximate it with in its Taylor expansion is small, and no sampling is necessary.

6.3 Kernel Linear Systems

Another interesting application of our sketching scheme is to constructing a preconditioner for solving PSD systems involving a kernel matrix [COCF16]. In order to apply algorithms such as Conjugate Gradient [She94], one has to obtain a good preconditioner for a potentially ill-conditioned kernel system.

Theorem 6.6 (Sketching as a Preconditioner, informal version of Theorem D.1). Let \( G \in \mathbb{R}^{n \times n} \) be the Gaussian kernel matrix for \( X \in \mathbb{R}^{d \times n} \) and suppose \( \|x_i\|_2 \leq 1, \forall i \in [n] \), where \( x_i \) is the \( i \)th column of \( X \). Let \( G = Z^\top Z \) and \( \kappa \) denote the condition number of \( Z \). There exists an algorithm that, with probability at least \( 1 - \delta \), computes an \( \epsilon \)-approximate solution \( \hat{x} \) satisfying

\[
\|G\hat{x} - y\|_2 \leq \epsilon \|y\|_2
\]

in \( \tilde{O}(\epsilon^{-3} n^{2} \log(\kappa/\epsilon) + n^\omega + nd) \) time, where \( \omega \) is the exponent of matrix multiplication (currently \( \omega \approx 2.373 \) [Wil12, LG14]).

Remark 6.7. In certain NLP [DL20] and biological tasks [TPK02] where \( d = n^c \) for a positive integer \( c \), Theorem 6.6 provides a fast algorithm for which the running time depends nearly linearly on \( nd \). We also remark that the algorithm we use for Theorem 6.6 is inspired by the idea of [BPSW21] (their situation involves \( c = 4 \)). It is also interesting that in their applications, regularization is not needed since solving a kernel system is equivalent to training an over-parametrized ReLU network without regularization.
6.4 Kernel Ridge Regression

Kernel ridge regression (KRR) is a popular method to model the relationship between data points and labels. Let $K = A^\top A$ denote the kernel matrix. Instead of solving the ordinary regression
\[
\min_{x \in \mathbb{R}^n} \| Kx - y \|_2^2,
\]
which is equivalent to solving a linear system, we focus on solving the following ridge regression problem:
\[
\min_{x \in \mathbb{R}^n} \| Kx - y \|_2^2 + \lambda \| Ax \|_2^2,
\]
for $\lambda > 0$. A relevant notion is the statistical dimension:

**Definition 6.8 (Statistical Dimension).** Let $\lambda > 0$, and $K \in \mathbb{R}^{n \times n}$ be a positive semi-definite matrix. We define the $\lambda$-statistical dimension of $K$ to be
\[
s_\lambda(K) := \text{tr}[K(K + \lambda I_n)^{-1}].
\]

One drawback of our sketch is that we cannot obtain a dimension depending on $s_\lambda(K)$ instead of $n$, since it does not have the approximate matrix product property. To mitigate this effect, we propose the following composition of sketches.

**Theorem 6.9 (Kernel Ridge Regression, informal version of Theorem E.2).** Let $\epsilon \in (0, 1)$, $p > 1$ be an integer and $X \in \mathbb{R}^{d \times n}$. If $K$ is its degree-$p$ polynomial kernel with statistical dimension $s_\lambda(K)$, where $\lambda \leq \epsilon^{-2} \lambda_{\text{max}}(K)$, then we can compute $Z$ such that $Z^\top Z$ is a $(1 \pm \epsilon)$-spectral approximation to $K$, in $\tilde{O}(\epsilon^{-2} p^2 n^2 + nd)$ time. Moreover, there exists a matrix $S$ with $m = \tilde{O}(\epsilon^{-1} s_\lambda(K))$ rows such that the optimal solution $x^*$ to
\[
\| S(Z^\top Zx - y) \|_2^2 + \lambda \| Zx \|_2^2
\]
satisfies
\[
\| Kx^* - y \|_2^2 + \lambda \| X^\otimes p x^* \|_2^2 \leq (1 + \epsilon) \cdot \text{OPT},
\]
where $\text{OPT}$ is $\min_{x \in \mathbb{R}^n} \| Kx - y \|_2^2 + \lambda \| X^\otimes p x \|_2^2$. The time to solve the above KRR is
\[
\tilde{O}(\epsilon^{-2} p^2 n (n + m^2) + n^\omega).
\]

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References

[AC06] Nir Ailon and Bernard Chazelle. Approximate nearest neighbors and the fast johnson-lindenstrauss transform. In STOC, pages 557—563, 2006.

[ACSS20] Josh Alman, Timothy Chu, Aaron Schild, and Zhao Song. Algorithms and hardness for linear algebra on geometric graphs. In FOCS, 2020.

[ACW17a] H. Avron, K. Clarkson, and D. Woodruff. Sharper bounds for regularized data fitting. In APPROX-RANDOM, 2017.

[ACW17b] Haim Avron, Kenneth L Clarkson, and David P Woodruff. Faster kernel ridge regression using sketching and preconditioning. SIAM Journal on Matrix Analysis and Applications, 38(4):1116–1138, 2017.

[AKK+20] Thomas D Ahle, Michael Kapralov, Jakob BT Knudsen, Rasmus Pagh, Ameya Velingker, David P Woodruff, and Amir Zandieh. Oblivious sketching of high-degree polynomial kernels. In Proceedings of the Fourteenth Annual ACM-SIAM Symposium on Discrete Algorithms (SODA), pages 141–160. SIAM, 2020.

[AKM+17] Haim Avron, Michael Kapralov, Cameron Musco, Christopher Musco, Ameya Velingker, and Amir Zandieh. Random fourier features for kernel ridge regression: Approximation bounds and statistical guarantees. In ICML, 2017.

[ALS+18] Alexandr Andoni, Chengyu Lin, Ying Sheng, Peilin Zhong, and Ruiqi Zhong. Subspace embedding and linear regression with orlicz norm. In International Conference on Machine Learning (ICML), pages 224–233. PMLR, 2018.

[AM15] Ahmed Alaoui and Michael W Mahoney. Fast randomized kernel ridge regression with statistical guarantees. In Advances in Neural Information Processing Systems (NeurIPS), pages 775–783, 2015.

[ANW14] Haim Avron, Huy Nguyen, and David Woodruff. Subspace embeddings for the polynomial kernel. In Z. Ghahramani, M. Welling, C. Cortes, N. D. Lawrence, and K. Q. Weinberger, editors, Advances in Neural Information Processing Systems 27, pages 2258–2266. 2014.

[AZLS19a] Zeyuan Allen-Zhu, Yuanzhi Li, and Zhao Song. A convergence theory for deep learning via over-parameterization. In ICML, 2019.

[AZLS19b] Zeyuan Allen-Zhu, Yuanzhi Li, and Zhao Song. On the convergence rate of training recurrent neural networks. In NeurIPS, 2019.

[Bac13] Francis Bach. Sharp analysis of low-rank kernel matrix approximations. In Conference on Learning Theory (COLT), pages 185–209, 2013.

[BPSW21] Jan van den Brand, Bingshu Peng, Zhao Song, and Omri Weinstein. Training (over-parametrized) neural networks in near-linear time. In ITCS, 2021.

[BW14] Christos Boutsidis and David P Woodruff. Optimal cur matrix decompositions. In Proceedings of the 46th Annual ACM Symposium on Theory of Computing (STOC), pages 353–362. ACM, 2014.
[BWZ16] Christos Boutsidis, David P Woodruff, and Peilin Zhong. Optimal principal component analysis in distributed and streaming models. In Proceedings of the forty-eighth annual ACM symposium on Theory of Computing (STOC), pages 236–249, 2016.

[CHC+10] Yin-Wen Chang, Cho-Jui Hsieh, Kai-Wei Chang, Michael Ringgaard, and Chih-Jen Lin. Training and testing low-degree polynomial data mappings via linear svm. Journal of Machine Learning Research, pages 1471–1490, 2010.

[COCF16] Kurt Cutajar, Michael A. Osborne, John P. Cunningham, and Maurizio Filippone. Preconditioning kernel matrices, 2016.

[CS09] Youngmin Cho and Lawrence K Saul. Kernel methods for deep learning. In Advances in neural information processing systems (NIPS), pages 342–350, 2009.

[CT65] James W Cooley and John W Tukey. An algorithm for the machine calculation of complex fourier series. Mathematics of computation, 19(90):297–301, 1965.

[CW13] Kenneth L. Clarkson and David P. Woodruff. Low rank approximation and regression in input sparsity time. In Symposium on Theory of Computing Conference (STOCâ), pages 81–90, 2013.

[DDH07] James Demmel, Ioana Dumitriu, and Olga Holtz. Fast linear algebra is stable. Numerische Mathematik, 108(1):59–91, Oct 2007.

[DJS+19] Huaian Diao, Rajesh Jayaram, Zhao Song, Wen Sun, and David P Woodruff. Optimal sketching for kronecker product regression and low rank approximation. In NeurIPS, 2019.

[DL20] Reza Drikvandi and Olamide Lawal. Sparse principal component analysis for natural language processing. Annals of data science., 2020.

[DSSW18] Huaian Diao, Zhao Song, Wen Sun, and David Woodruff. Sketching for kronecker product regression and p-splines. In International Conference on Artificial Intelligence and Statistics, pages 1299–1308. PMLR, 2018.

[DZPS19] Simon S Du, Xiyu Zhai, Barnabas Poczos, and Aarti Singh. Gradient descent provably optimizes over-parameterized neural networks. In ICLR. arXiv preprint arXiv:1810.02054, 2019.

[GE08] Yoav Goldberg and Michael Elhadad. splitSVM: Fast, space-efficient, non-heuristic, polynomial kernel computation for NLP applications. In Proceedings of ACL-08: HLT, Short Papers, pages 237–240, Columbus, Ohio, June 2008. Association for Computational Linguistics.

[HLSY21] Baihe Huang, Xiaoxiao Li, Zhao Song, and Xin Yang. Fl-ntk: A neural tangent kernel-based framework for federated learning convergence analysis. In ICML, 2021.

[HLW17] Jarvis Haupt, Xingguo Li, and David P Woodruff. Near optimal sketching of low-rank tensor regression. In NeurIPS, 2017.

[JGH18] Arthur Jacot, Franck Gabriel, and Clément Hongler. Neural tangent kernel: Convergence and generalization in neural networks. In Advances in neural information processing systems (NeurIPS), pages 8571–8580, 2018.
[JLSW20] Haotian Jiang, Yin Tat Lee, Zhao Song, and Sam Chiu-wai Wong. An improved cutting plane method for convex optimization, convex-concave games and its applications. In *STOC*, 2020.

[JSWZ21] Shunhua Jiang, Zhao Song, Omri Weinstein, and Hengjie Zhang. Faster dynamic matrix inverse for faster lps. In *STOC*, 2021.

[LDFU13] Yichao Lu, Paramveer Dhillon, Dean P Foster, and Lyle Ungar. Faster ridge regression via the subsampled randomized hadamard transform. In *Advances in neural information processing systems*, pages 369–377, 2013.

[LG14] François Le Gall. Powers of tensors and fast matrix multiplication. In *Proceedings of the 39th international symposium on symbolic and algebraic computation (ISSAC)*, pages 296–303. ACM, 2014.

[LL18] Yuanzhi Li and Yingyu Liang. Learning overparameterized neural networks via stochastic gradient descent on structured data. In *NeurIPS*, 2018.

[LSS+20] Jason D Lee, Ruoqi Shen, Zhao Song, Mengdi Wang, and Zheng Yu. Generalized leverage score sampling for neural networks. In *NeurIPS*, 2020.

[LSZ19] Yin Tat Lee, Zhao Song, and Qiuyi Zhang. Solving empirical risk minimization in the current matrix multiplication time. In *COLT*, 2019.

[MM13] Xiangrui Meng and Michael W Mahoney. Low-distortion subspace embeddings in input-sparsity time and applications to robust linear regression. In *Proceedings of the forty-fifth annual ACM symposium on Theory of computing (STOC)*, pages 91–100, 2013.

[MM17] Cameron Musco and Christopher Musco. Recursive sampling for the nyström method. In *Advances in Neural Information Processing Systems (NeurIPS)*, pages 3833–3845, 2017.

[MOSW21] Alexander Munteanu, Simon Omlor, Zhao Song, and David P. Woodruff. A new initialization technique for reducing the width of neural networks. *manuscript*, 2021.

[NJW01] Andrew Ng, Michael Jordan, and Yair Weiss. On spectral clustering: Analysis and an algorithm. *Advances in neural information processing systems*, 14:849–856, 2001.

[NN13] Jelani Nelson and Huy L Nguyén. Osnap: Faster numerical linear algebra algorithms via sparser subspace embeddings. In *2013 IEEE 54th Annual Symposium on Foundations of Computer Science (FOCS)*, pages 117–126. IEEE, 2013.

[RR07] Ali Rahimi and Benjamin Recht. Random features for large-scale kernel machines. In *NIPS*, volume 3, page 5. Citeseer, 2007.

[Sar06] Tamas Sarlos. Improved approximation algorithms for large matrices via random projections. In *2006 47th Annual IEEE Symposium on Foundations of Computer Science (FOCS)*, pages 143–152. IEEE, 2006.

[SGV98] Craig Saunders, Alexander Gammerman, and Volodya Vovk. Ridge regression learning algorithm in dual variables. In *Proceedings of the Fifteenth International Conference on Machine Learning*, ICML ’98, page 515–521, San Francisco, CA, USA, 1998. Morgan Kaufmann Publishers Inc.
[She94] Jonathan Richard Shewchuk. An introduction to the conjugate gradient method without the agonizing pain. Technical report, Carnegie Mellon University, 1994.

[SWZ17] Zhao Song, David P Woodruff, and Peilin Zhong. Low rank approximation with entrywise $\ell_1$-norm error. In Proceedings of the 49th Annual Symposium on the Theory of Computing (STOC), 2017.

[SWZ19] Zhao Song, David P Woodruff, and Peilin Zhong. Relative error tensor low rank approximation. In SODA. arXiv preprint arXiv:1704.08246, 2019.

[SY19] Zhao Song and Xin Yang. Quadratic suffices for over-parametrization via matrix chernoff bound. arXiv preprint arXiv:1906.03593, 2019.

[SY21] Zhao Song and Zheng Yu. Oblivious sketching-based central path method for solving linear programming problems. In 38th International Conference on Machine Learning (ICML), 2021.

[TPK02] Miguel L. Teodoro, G. Phillips, and L. Kavraki. A dimensionality reduction approach to modeling protein flexibility. In RECOMB ’02, 2002.

[Tro15] Joel A Tropp. An introduction to matrix concentration inequalities. Foundations and Trends® in Machine Learning, 8(1-2):1–230, 2015.

[Wil12] Virginia Vassilevska Williams. Multiplying matrices faster than coppersmith-winograd. In Proceedings of the forty-fourth annual ACM symposium on Theory of computing (STOC), pages 887–898. ACM, 2012.

[Woo14] David P. Woodruff. Sketching as a tool for numerical linear algebra. Foundations and Trends in Theoretical Computer Science, 10(1–2):1–157, 2014.

[WZ20] David P Woodruff and Amir Zandieh. Near input sparsity time kernel embeddings via adaptive sampling. In ICML. arXiv preprint arXiv:2007.03927, 2020.

[XLS17] Bo Xie, Yingyu Liang, and Le Song. Diverse neural network learns true target functions. In Artificial Intelligence and Statistics (AISTATS), pages 1216–1224, 2017.

[ZDW15] Yuchen Zhang, John Duchi, and Martin Wainwright. Divide and conquer kernel ridge regression: A distributed algorithm with minimax optimal rates. The Journal of Machine Learning Research, 16(1):3299–3340, 2015.

[ZNV+20] Amir Zandieh, Navid Nouri, Ameya Velingker, Michael Kapralov, and Ilya Razenshteyn. Scaling up kernel ridge regression via locality sensitive hashing. In AISTATS, 2020.
Appendix

Roadmap In Section A, we give an algorithm to compute a subspace embedding for the Gaussian kernel using Theorem 4.8. In Section B, we characterize a large class of kernels based on the coefficients in their Taylor expansion, and develop fast algorithms for different scenarios. In Section C, we apply our results in Section B to the Neural Tangent kernel. In Section D, we use our sketch in conjunction with another sketch to compute a good preconditioner for the Gaussian kernel. In Section E, we compose our sketch with our sketching matrices to solve Kernel Ridge Regression.

Notation We use $\widetilde{O}(f)$ to denote $f \cdot \text{poly}(\log f)$ and use $\widetilde{\Omega}(f)$ to denote $f / \text{poly}(\log f)$.

For an integer $n$, let $[n]$ denote the set $\{1, 2, \cdots, n\}$. For two scalars $a$ and $b$, we say $a \approx b$ if $(1 - \epsilon)b \leq a \leq (1 + \epsilon)b$. We say a square symmetric matrix $A$ is positive semidefinite (PSD) if $\forall x, x^\top A x \geq 0$. For two PSD matrices $A$ and $B$, we define $A \approx B$ if $(1 - \epsilon)B \preceq A \preceq (1 + \epsilon)B$. For a matrix $A$, we use $\|A\|_F = (\sum_{i,j} A_{i,j}^2)^{1/2}$ to denote its Frobenius norm and use $\|A\|_{\text{op}}$ to denote its operator (spectral) norm. For a square matrix $A$, we use $\text{tr}[A]$ to denote the trace of $A$. For a square symmetric matrix $A$, we use $\lambda_{\min}(A), \lambda_{\max}(A)$ to denote its smallest and largest eigenvalues, respectively. For a rectangular matrix $A$, we use $\sigma_{\min}(A), \sigma_{\max}(A)$ to denote its smallest and largest singular values.

A Gaussian Kernel

We apply Algorithm 1 to compute a subspace embedding to the Gaussian kernel matrix $G \in \mathbb{R}^{n \times n}$ defined over $n$ data points of dimension $d$, denoted by $X \in \mathbb{R}^{d \times n}$. Our method has the advantage that when $d$ is large and the matrix $X$ is dense, its leading factor depends nearly linearly on $nd$, which makes it useful for certain biological and NLP tasks.

We remark that our construction of a sketch for the Gaussian kernel and its corresponding analysis is inspired by [AKK+20], and is thus similar to the proof of Theorem 5 in their paper. For completeness, we include a proof here.

Theorem A.1 (Gaussian Kernel, formal version of Theorem 6.1). Let $X \in \mathbb{R}^{d \times n}$ and $r \in \mathbb{R}_+$ be the radius of $X$. Suppose $G \in \mathbb{R}^{n \times n}$ is the Gaussian kernel matrix given in Definition 2.14. For any accuracy parameter $\epsilon \in (0, 1)$ and for any failure probability $\delta \in (0, 1)$, there exists an algorithm running in time:

$$O(\epsilon^{-2}n^2q^3 \cdot \log^3(nd/\epsilon\delta) + nd \log(nd/\epsilon\delta))$$

and outputting a matrix $W_g(X) \in \mathbb{R}^{m \times n}$ such that

$$\Pr [W_g(X)^\top W_g(X) \approx G] \geq 1 - \delta$$

where $m = \Omega(\epsilon^{-2}nq^3 \log^3(nd/\epsilon\delta))$ and $q = \Theta(r^2 + \log(n/\epsilon))$.

Proof. By definition of the Gaussian kernel matrix $G_{i,j} = \exp(-\|x_i - x_j\|^2/2)$, we can rewrite it as $G = DKD$, where $D$ is an $n \times n$ diagonal matrix with $i$th diagonal entry equal to $\exp(-\|x_i\|^2/2)$ and $K \in \mathbb{R}^{n \times n}$ is a positive definite kernel matrix defined as $K_{i,j} = \exp(x_i^\top x_j)$. Note the Taylor series expansion for kernel $K$ gives

$$K = \sum_{l=0}^\infty \frac{(X^\otimes l)^\top X^\otimes l}{l!}.$$
Let $q = C \cdot (r^2 + \log(n/\epsilon))$ for a sufficiently large constant $C$, and let $Q = \sum_{l=0}^{q} \frac{(X^{\otimes l})^T X^{\otimes l}}{l!}$ be the first $q$ terms of $K$. By the triangle inequality we have:

$$\|K - Q\|_{op} \leq \sum_{l>q} \left\| \frac{(X^{\otimes l})^T X^{\otimes l}}{l!} \right\|_{F} \leq \sum_{l>q} \frac{n \cdot r^2 l!}{l!} \leq \frac{\epsilon}{2}.$$ 

Then $Q$ is a positive definite kernel matrix and $\|D\|_{op} \leq 1$. Therefore, in order to preserve the subspace of $G$ it suffices to show the following with probability $1 - \delta$:

$$(1 - \epsilon/2) \cdot DQD \preceq W_g(X)^T W_g(X) \preceq (1 + \epsilon/2) \cdot DQD. \tag{4}$$

For each term $(X^{\otimes l})^T X^{\otimes l}$ in $Q$, we run Algorithm 1 to approximate $X^{\otimes l}$. Let $Z_l \in \mathbb{R}^{m_l \times n}$ be the resulting matrix $Z(S, T, X)$, where

$$m_l = \Omega(\epsilon^{-2} n l^2 \cdot \log^2(n d/\epsilon \delta) \cdot \log(n/\delta)).$$

Then by Theorem 5.1, we get

$$(1 - \epsilon/2)(X^{\otimes l} D)^T X^{\otimes l} D \preceq (\Pi^l X^{\otimes l} D)^T \Pi^l X^{\otimes l} D \preceq (1 + \epsilon/2)(X^{\otimes l} D)^T X^{\otimes l} D$$

with probability at least $1 - \frac{\delta}{q+1}$. Moreover, $Z_l$ can be computed in time

$$O(\epsilon^{-2} n^2 l^2 \cdot \log^2(n d/\epsilon \delta) \cdot \log(n/\delta)).$$

Our algorithm will simply compute $Z_l$ from $l = 0$ to $q$, normalize each $Z_l$ by $\frac{1}{\sqrt{l!}}$, and then multiply by $D$. More precisely, the approximation $W_g(X)$ will be

$$W_g(X) = \left( \bigoplus_{l=0}^{q} \frac{Z_l}{\sqrt{l!}} \right) D$$

where we use $A \oplus B$ to denote the matrix $\begin{bmatrix} A \\ B \end{bmatrix}$ if $A$ and $B$ have the same number of columns. Notice $W_g(X) \in \mathbb{R}^{m \times n}$. The following holds for $W_g(X)^T W_g(X)$:

$$W_g(X)^T W_g(X) = D \left( \sum_{l=0}^{q} \frac{Z_l^T Z_l}{l!} \right) D = \sum_{l=0}^{q} \frac{(Z_l D)^T Z_l D}{l!}.$$ 

By combining terms in (4) and using a union bound over all $0 \leq l \leq q$, we obtain that with probability at least $1 - \delta$, we have the following:

$$(1 - \epsilon/2) \cdot DQD \preceq W_g(X)^T W_g(X) \preceq (1 + \epsilon/2) \cdot DQD.$$
Thus, we conclude that
\[(1 - \epsilon) \cdot G \preceq W_g(X)^\top W_g(X) \preceq (1 + \epsilon) \cdot G.\]

Note the target dimension of \(W_g\) is
\[m = m_0 + m_1 + \cdots + m_q = \Omega(\epsilon^{-2} n q^3 \cdot \log^2(nd/\epsilon \delta) \cdot \log(n/\delta)).\]

Also, by Theorem 5.1, the time to compute \(W_g(X)\) is
\[t = t_0 + t_1 + \cdots + t_q = O(\epsilon^{-2} n^2 q^3 \cdot \log^2(nd/\epsilon \delta) \cdot \log(n/\delta)).\]

Notice we will have to pay an additive \(nd \log(nd/\epsilon \delta)\) due to line 2 of Algorithm 1, when applying the SRHT to \(X\). However, we only need to perform this operation once for the term with the highest degree, or the terms with lower degree that can be formed by combining nodes computed with the highest degree. Thus, the final runtime is
\[O(\epsilon^{-2} n^2 q^3 \cdot \log^2(nd/\epsilon \delta) \cdot \log(n/\delta) + nd \log(nd/\epsilon \delta)).\]

\begin{proof}
\end{proof}

\section*{B General \(p\)-Convergent Sequences}

We consider general \(p\)-convergent kernels defined below in Definition B.1. We apply our proposed Algorithm 1 to compute a subspace embedding with a fast running time.

\subsection*{B.1 General Theorem for \(p > 1\)}

In this section, we state a general theorem for \(p > 1\). The proof is similar to the proof for Theorem A.1. We start by restating the definition of a \(p\)-convergent kernel.

**Definition B.1** (\(p\)-convergent kernel matrix, formal version of Definition 6.2). Given an input matrix \(X \in \mathbb{R}^{d \times n}\), we say the kernel matrix \(K \in \mathbb{R}^{n \times n}\) is \(p\)-convergent if its corresponding Taylor expansion series can be written as follows:
\[K = \sum_{l=0}^{\infty} C_l \cdot (X^{\otimes l})^\top X^{\otimes l},\]
where the positive coefficients \(C_l > 0\) are a function of \(l\), and \(C_l\) satisfies
\[C_l = (l + 1)^{-\Theta(p)}.\]

**Theorem B.2** (Sketch for \(p\)-convergent Kernels, formal version of Theorem 6.3). Let \(X \in \mathbb{R}^{d \times n}\) with radius \(r\) for some \(r \in \mathbb{R}_+\). Suppose that \(K\) is a \(p\)-convergent kernel matrix where \(p > 1\) is an integer. Further, let choose \(m = \Omega(\epsilon^{-2} n q^3 \log^3(nd/\epsilon \delta))\) and \(q = \Theta(r^2 + (n/\epsilon)^{1/p})\). There exists an algorithm which computes a matrix \(W_g(X) \in \mathbb{R}^{m \times n}\) in time
\[O(\epsilon^{-2} n^2 q^3 \cdot \log^3(nd/\epsilon \delta) + nd \cdot \log(nd/\epsilon \delta))\]
such that
\[\Pr[W_g(X)^\top W_g(X) \approx_{\epsilon} G] \geq 1 - \delta.\]
Proof. Similar to the Gaussian kernel, here we use the first $q$ terms to approximate the kernel matrix $K$.

Let $q = C \cdot (r^2 + (n/\epsilon)^{1/p})$ for a sufficiently large constant $C$, and let $Q = \sum_{l=0}^{q} C_l (X^\otimes l)^\top X^\otimes l$ be the first $q$ terms of $K$. By the triangle inequality, we have

$$
\|K - Q\|_{op} \leq \sum_{l>q} C_l \left\| (X^\otimes l)^\top X^\otimes l \right\|_{op}
\leq \sum_{l>q} C_l \left\| (X^\otimes l)^\top X^\otimes l \right\|_F
\leq \sum_{l>q} C_l \cdot n \cdot r^{2l}
\leq \epsilon/2.
$$

The proof is identical to the proof of Theorem A.1, with the target dimension of $W_g$ being $m = m_0 + m_1 + \cdots + m_q = \Omega(\epsilon^{-2} n q^3 \log(n d/\epsilon \delta) \log(n/\delta))$.

Similar to Theorem A.1, we have to pay an extra $nd \log(n d/\epsilon \delta)$ term to apply the SRHT to $X$, so the final running time is

$$
t_0 + t_1 + \cdots + t_q + nd \log(n d/\epsilon \delta) = O(\epsilon^{-2} n^2 q^2 \log(n d/\epsilon \delta) \log(n/\delta) + nd \log(n d/\epsilon \delta)).
$$

\hfill \Box

Remark B.3. Recall our setting is when $d = \text{poly}(n)$, so if $p \geq 3$, Theorem B.2 gives a running time of $O(n^3/\epsilon^2 + nd)$, which is better than the classical result of $O(n^2 d)$ as long as $d > n/\epsilon^2$. However, if $p \in (1,3)$, Theorem B.2 gives a worse dependence on $n$, which can be further optimized.

### B.2 Sampling Scheme for $1 < p < 3$

We next describe a novel sampling scheme if $p \in (2,3)$, with a better dependence on $n$ compared to Theorem B.2. We first state some probability tools.

**Theorem B.4** (Matrix Bernstein Inequality[Tro15]). Let $S_1, \ldots, S_n$ be independent, zero-mean random matrices with common size $d_1 \times d_2$, and assume each one is uniformly bounded:

$$
\mathbb{E}[S_k] = 0, \|S_k\|_{op} \leq L, k \in [n]
$$

Let $Z = \sum_{k=1}^{n} S_k$, and let $\text{Var}[Z] = \max\{\|\mathbb{E}[Z^\top Z]\|_{op}, \|\mathbb{E}[ZZ^\top]\|_{op}\}$. Then for all $t > 0$,

$$
\text{Pr}[\|Z\|_{op} \geq t] \leq (d_1 + d_2) \cdot \exp \left( \frac{-t^2/2}{\text{Var}[Z] + Lt/3} \right).
$$

**Theorem B.5** (Sampling Scheme for $2 < p < 3$). Let $p > 1$ be an integer and $X \in \mathbb{R}^{d \times n}$ be a matrix with unit radius, suppose $K$ is a $p$-convergent kernel matrix. For any $p \in (2,3)$, there exists an algorithm which computes a matrix $W_g(X)$ with $n$ columns in expected running time

$$
O((n/\epsilon)^{2+6/(1+2p)} \cdot \text{poly}(\log(n d/\epsilon \delta)) + nd \log(n d/\epsilon \delta))
$$

such that

$$
\text{Pr}[W_g(X)^\top W_g(X) \approx \epsilon G] \geq 1 - \delta.
$$

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Proof. Let $q$ be the degree used in Theorem B.2 where $q = \Theta((n/\epsilon)^{1/p})$, and let $s$ be some positive integer smaller than $q$. We will consider the following scheme:

- For the first $s$ terms in the Taylor expansion, we approximate each term directly using Theorem B.2.
- For each of the next $q-s$ terms, we sample proportional to their coefficient $C_l$, taking only $s$ samples in total.

Correctness proof We will show that

\[ s = \Theta((n/\epsilon)^{2/(1+2p)} \cdot \text{poly}(\log(nd/\epsilon \delta))) \]

samples suffice. Let $P$ be the sum of the first $s$ terms in the Taylor expansion of $K$, and let $R$ be the remaining $q-s$ terms. Our goal is to have $\|R\|_\text{op} \leq \epsilon \|K\|_\text{op}$. We first calculate $\|R\|_\text{op}$:

\[
\|R\|_\text{op} \leq \sum_{l=s+1}^{q} C_l \cdot n = \sum_{l=s+1}^{q} \frac{1}{l^p} \cdot n \leq \frac{n}{s^p}.
\]

Notice that if $\|K\|_\text{op}$ is large, then it suffices to use the first $s$ terms. Specifically, if $\|K\|_\text{op} \geq \frac{n}{s^{2/p}}$, then we are done. Otherwise, suppose $\|K\|_\text{op} \leq \frac{n}{s^{2/p}}$. We will invoke Theorem B.4 to do the sampling. Let $T = \sum_{l=s+1}^{q} \frac{1}{l^p}$ and $p_i = \frac{C_l}{p_l}$. Define the random variable $S_i$ as follows: with probability $p_i$, we sample $R - \frac{C_l}{p_l} (X_{\otimes i})^\top X_{\otimes i}$ for $l = s+1, \ldots, q$. First notice that $S_i$ is unbiased:

\[
\mathbb{E}[S_i] = R - \sum_{i=s+1}^{q} p_i \frac{C_l}{p_l} (X_{\otimes i})^\top X_{\otimes i} = 0.
\]

Using the triangle inequality, we have

\[
\|S_i\|_\text{op} \leq T \cdot \|(X_{\otimes i})^\top X_{\otimes i}\|_\text{op} + \|R\|_\text{op} \\
\leq ns^{-p} + ns^{-p} \\
= 2ns^{-p}.
\]

We now consider the operator norm of the expectation of $S_i^\top S_i$:

\[
\|\mathbb{E}[S_i^\top S_i]\|_\text{op} = \left\| \frac{C_i^2}{p_i} (X_{\otimes i})^\top X_{\otimes i} (X_{\otimes i})^\top X_{\otimes i} + R^\top R - \frac{C_i}{p_i} (X_{\otimes i})^\top X_{\otimes i} R - \frac{C_i}{p_i} R (X_{\otimes i})^\top X_{\otimes i} \right\|_\text{op} \\
\leq \|C_i T (X_{\otimes i})^\top X_{\otimes i} (X_{\otimes i})^\top X_{\otimes i}\|_\text{op} + \|R^\top R\|_\text{op} + T \cdot (\|(X_{\otimes i})^\top X_{\otimes i} R\|_\text{op} + \|R (X_{\otimes i})^\top X_{\otimes i}\|_\text{op}) \\
\leq C_i T n^2 + (ns^{-p})^2 + 2T n \cdot ns^{-p} \\
= 4n^2 s^{-2p}.
\]
Let \( Z = \sum_{i=1}^{m} S_i \). Since each sample is sampled independently, we have

\[
\| \mathbb{E}[Z^\top Z] \|_{op} = \| \mathbb{E} \left[ \sum_{i=1}^{s} S_i^\top S_i \right] \|_{op} \\
\leq \sum_{i=1}^{s} \| \mathbb{E}[S_i^\top S_i] \|_{op} \\
\leq 4mn^2s^{-2p}.
\]

Let \( t = m\|K\|_{op} \). Applying Theorem B.4, we get that

\[
\Pr \left[ \|Z\|_{op} \geq m\|K\|_{op} \right] \leq 2n \cdot \exp \left( \frac{-m^2\epsilon^2\|K\|_{op}^2/2}{4mn^2s^{-2p} + 2m\epsilon\|K\|_{op}ns^{-p}/3} \right).
\]

Picking \( m = \Theta(\epsilon^{-2}n^2s^{-p} \log(n/\delta)) \), and then averaging over \( m \) samples, we get that

\[
\Pr \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} S_i \right\|_{op} \geq \epsilon \|K\|_{op} \right] \leq \delta, \tag{5}
\]

where we use the fact that the operator norm of \( K \) is at least 1, by our choice of \( s \). We now compute the expected running time of this algorithm.

**Runtime part 1: Computing the first \( s \) terms** For the first \( s \) terms, we can apply the same reasoning as in Theorem B.2 to get a running time of \( O(\epsilon^{-2}n^2s^3 \text{poly}(\log(nd/\epsilon\delta)) + nd\log(nd/\epsilon\delta)) \).

**Runtime part 2: Sampling the next \( s \) terms** For the sampling part, we consider the expected degree \( D \) of the sample we will be working with:

\[
D = \sum_{l=s+1}^{q} p_l \cdot l \\
= \sum_{l=s+1}^{q} l^{1-p} \\
\leq \frac{s^{1-p}}{s^{-p} - q^{-p}} \\
= s + \frac{s \cdot q^{-p}}{s^{-p} - q^{-p}} \\
= s + \frac{s}{q^p} - 1 \\
= \tilde{O}((n/\epsilon)^{2/(1+2p)})
\]

Now we are ready to compute the expected running time of the sampling phase:

\[
m \cdot D^2n^2/\epsilon^2 = (n/\epsilon)^{2+6/(1+2p)} \cdot \text{poly}(\log(nd/\epsilon\delta)).
\]

Additionally, we need to apply the SRHT to \( X \) at most twice, once for the initial phase, and once for the sampling phase, so the final running time is

\[
(n/\epsilon)^{2+6/(1+2p)} \cdot \text{poly}(\log(nd/\epsilon\delta)) + nd\log(nd/\epsilon\delta).
\]

\( \square \)
When \( p \in (1, 2] \), we use the largest degree \( q \) as an upper bound for analyzing our running time.

**Corollary B.6** (Sampling Scheme for \( 1 < p \leq 2 \)). Let \( p > 1 \) be an integer and \( X \in \mathbb{R}^{d \times n} \) with unit radius. Suppose \( K \) is a \( p \)-convergent kernel matrix. If \( p \in (1, 2] \), then there exists an algorithm which computes a matrix \( W_g(X) \) with \( n \) columns in time

\[
e^{-\left(2+6/(3+2p)\right)} n^{2+6(1+1/p)/(3+2p)} \cdot \text{poly}(\log(nd/\epsilon\delta)) + nd \log(nd/\epsilon\delta)
\]

such that

\[
\Pr [W_g(X)^\top W_g(X) \approx \epsilon G] \geq 1 - \delta.
\]

**Remark B.7.** In addition, using that \( p \in (1, 2] \), the first part of our running time can be upper bounded by

\[
e^{-3.2} n^{4.4} \cdot \text{poly}(\log(nd/\epsilon\delta)).
\]

**Proof.** The proof is almost identical to the proof of Theorem B.5. The only difference is when considering the expected degree \( D \), we use \( q \) as an upper bound. The number of terms \( s \) we approximate in the initial phase will be

\[
\tilde{\Theta}\left(\frac{n(2+2/p)/(3+2p)}{\epsilon^{2/(3+2p)}}\right).
\]

The final runtime will be

\[
\epsilon^{-2} n^2 \text{poly}(\log(nd/\epsilon\delta)) s^3 = (n^{2+3(2+2/p)/(3+2p)}/\epsilon^{2+6/(3+2p)}) \text{poly}(\log(nd/\epsilon\delta)) + nd \log(nd/\epsilon\delta).
\]

**Simplifying the Exponent** For the exponent of \( \epsilon \), we have

\[
(2 + 6/(3 + 2p)) = 4 - \frac{4p}{3 + 2p}.
\]

For any \( p \in (1, 2] \), we have

\[
4 - f_1(p) \in \left[2 + \frac{6}{7}, 3 + \frac{1}{5}\right).
\]

For the exponent on \( n \), we have

\[
2 + 6(1+1/p)/(3 + 2p) = 2 + \frac{6p + 6}{2p^2 + 3p}
\]

\[
= 5 - \frac{6p^2 + 3p - 6}{2p^2 + 3p}.
\]

For any \( p \in (1, 2] \), we have

\[
5 - f_2(p) \in \left[3 + \frac{2}{7}, 4 + \frac{2}{5}\right).
\]
C Properties of the Neural Tangent Kernel

We discuss an application of our sampling algorithm for \( p \in (1, 2] \) (Corollary B.6) to the Neural Tangent Kernel (NTK). We will first formally define the NTK, then consider its Taylor expansion, and then use a \( p \)-convergent kernel to bound it.

C.1 Taylor Expansion of NTK

In this section, we give the Taylor expansion of the NTK, by first examining its corresponding function in a single variable, and then extend it to the matrix case.

Consider a simple two-layer (an alternative name is one-hidden-layer) ReLU network with input layer initialized to standard Gaussians, activation function ReLU, and output layer initialized to uniform and independent Rademacher (\( \{-1, 1\} \)) random variables. Suppose we fix the output layer. Then the neural network can be characterized by a function

\[
f(W, x) = \frac{1}{\sqrt{m}} \sum_{r=1}^{m} a_r \sigma(w_r^\top x)
\]

where \( W \in \mathbb{R}^{d \times m} \), and \( w_r \in \mathbb{R}^d \) denotes the \( r \)-th column of \( W \), for each \( r \in [m] \).

The above formulation is standard for convergence analysis of neural networks [LL18, DZPS19, AZLS19b, AZLS19a, SY19, BPSW21, HLSY21, MOSW21].

The NTK ([JGH18]) is

\[
K(x, z) = \mathbb{E} \left[ \left( \frac{\partial f(W, x)}{\partial W}, \frac{\partial f(W, z)}{\partial W} \right) \right].
\]

For the sake of simplicity, assume all \( |a_r| = 1 \), \( \forall r \in [m] \), and consider an individual summand, which gives rise to

\[
K(x, z) = \int_{w \sim N(0, I)} \sigma'(w^\top x)\sigma'(w^\top z)x^\top z \, dw.
\]

If \( w \in \mathbb{R}^d \) is chosen uniformly on a sphere, then we will get the following closed-form for this kernel [CS09, XLS17]:

\[
K(x, z) = \left( \frac{1}{2} - \frac{\arccos x^\top z}{2\pi} \right) \cdot x^\top z.
\]

**Fact C.1.** Let function \( f : \mathbb{R} \to \mathbb{R} \) be defined as \( f(x) := (\frac{1}{2} - \frac{\arccos x}{2\pi}) \cdot x \). Then the Taylor expansion of \( f \) is

\[
f(x) = \frac{x}{4} + \sum_{n=0}^{\infty} \frac{(2n)!}{2^{2n}(n!)^2} \frac{x^{2n+2}}{(2n + 1)(2\pi)}
\]

\[
= \frac{x}{4} \left( \sum_{n=0}^{\infty} \frac{(2n)}{n} \frac{1}{2^{2n}} \frac{x^{2n+2}}{(2n + 1)(2\pi)} \right).
\]

**Fact C.2.** The Taylor expansion of the NTK is

\[
K = \frac{X^\top X}{4} \sum_{l=0}^{\infty} \binom{2l}{l} \frac{1}{2^{2l}} \frac{(X^{\otimes 2l+2})^\top X^{\otimes 2l+2}}{(2l + 1)2\pi}.
\]
C.2 Approximating the NTK

In this section, we will use a $p$-convergent kernel to bound the NTK, then apply Corollary B.6 to approximate it.

**Corollary C.3** (Fast Subspace Embedding for the NTK). Let $X \in \mathbb{R}^{d \times n}$ have unit radius Suppose $K \in \mathbb{R}^{n \times n}$ is the NTK matrix. Then there exists an algorithm which computes a matrix $W_g(X)$ in time

$$
\epsilon^{-3n^{11/3}} \cdot \text{poly}(\log(nd/\epsilon\delta)) + nd\log(nd/\epsilon\delta)
$$

such that

$$
\Pr\left[ W_g(X)\top W_g(X) \approx \epsilon K \right] \geq 1 - \delta.
$$

**Proof.** Let $C_l$ denote the coefficient of the $l^{th}$ term in the Taylor expansion of the NTK:

$$
C_l = \binom{2l}{l} \frac{1}{2^{2l}(2l+1)2\pi}.
$$

The term $\binom{2l}{l}$ is the central binomial coefficient. We will use the following bound on it:

$$
\frac{4^l}{\sqrt{4l}} \leq \binom{2l}{l} \leq \frac{4^l}{\sqrt{3l+1}}.
$$

This gives upper and lower bounds on $C_l$:

- Upper bound:

$$
C_l \leq \frac{4^l}{\sqrt{3l+1}} \cdot \frac{1}{2^{2l}(2l+1)2\pi}
$$

$$
= \frac{1}{\sqrt{3l+1}(2l+1)2\pi}.
$$

- Lower bound:

$$
C_l \geq \frac{1}{\sqrt{4l}(2l+1)2\pi}.
$$

Thus, $C_l = \Theta(\frac{1}{\sqrt{l}})$, and we can use a 1.5-convergent kernel for our approximation. Using Corollary B.6 with $p = 1.5$, we obtain an $\epsilon$-approximation in time

$$
\epsilon^{-3n^{11/3}} \cdot \text{poly}(\log(nd/\epsilon\delta)) + nd\log(nd/\epsilon\delta).
$$

D Preconditioning to Solve a Kernel Linear System

In this section, we illustrate how to construct a preconditioner for a kernel linear system. Specifically, we provide an algorithm to solve a Gaussian kernel linear system. Let $G = Z\top Z$ be the Gaussian kernel. By Theorem A.1, we can compute an approximation to $G$, denoted $W_g(X)\top W_g(X)$. In
In our result, we follow a similar approach as in [BPSW21] and the proof is similar to the proof of Lemma 4.2 in their paper. The main novelty of our framework is that we use a spectral approximation to the kernel matrix and analyze the error and runtime under our approximation. For completeness, we include a proof in this setting.

\textbf{Algorithm 2} Fast Regression for the Gaussian Kernel

\begin{algorithm}
\begin{algorithmic}[1]
\Procedure{PreconditionedGradientDescent}{$X, y$} \Comment{Theorem D.1}
\State $m \leftarrow O(n \log^2(nd/\epsilon \delta) \log(n/\delta)/\epsilon^2)$
\State $l \leftarrow \Omega(n \log(mn/\epsilon \delta) \log(n/\delta))$
\State Let $W_g(X) \in \mathbb{R}^{m \times n}$ be the approximate Gaussian kernel in Theorem A.1
\State Let $S \in \mathbb{R}^{1/\epsilon^2 \times m}$ be an SRHT matrix. Compute $SW_g(X)$
\State Compute $R$ such that $SW_g(X)R$ has orthonormal columns via a QR decomposition \Comment{$R \in \mathbb{R}^{n \times n}$}
\State $z_0 \leftarrow 0, n \in \mathbb{R}$
\While{$\|W_g(X)^\top W_g(X)Rz_t - y\|_2 \geq \epsilon$}
\State $z_{t+1} \leftarrow z_t - (R^\top W_g(X)^\top W_g(X)R)^\top (R^\top W_g(X)^\top W_g(X)Rz_t - R^\top y)$
\EndWhile
\State return $Rz_t$
\EndProcedure
\end{algorithmic}
\end{algorithm}

\textbf{Theorem D.1} (Sketching as a Preconditioner, formal version of Theorem 6.6). Let $G \in \mathbb{R}^{n \times n}$ be the Gaussian kernel matrix for $X \in \mathbb{R}^{d \times n}$. Write $G = Z^\top Z$, and let $\kappa$ denote the condition number of $Z$. If we assume for all $i \in [n]$ that $\|x_i\|_2 \leq 1$, then Algorithm 2, with probability at least $1 - \delta$, computes an $\hat{x}$ satisfying the following:

$$\|G \hat{x} - y\|_2 \leq \epsilon \|y\|_2.$$  

Moreover, $\hat{x}$ can be computed in time

$$\epsilon^{-2} n^2 \log(\kappa/\epsilon) \cdot \text{poly}(\log(nd/\epsilon \delta)) + n^\omega + nd \log(nd/\epsilon \delta),$$

where $\omega$ is the matrix multiplication exponent.

Before the proof, we define some notation and corresponding facts specifically about a PSD matrix.

\textbf{Fact D.2} (Inequality for condition numbers). Let $A, B$ be conforming square matrices. Then the following inequality holds:

$$\kappa(B) \leq \kappa(AB) \kappa(A),$$

where $\kappa(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}$ is the condition number of $A$.  

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We will make use of Lemma B.2 in [BPSW21].

**Lemma D.3** (Lemma B.2 in [BPSW21]). Consider the regression problem:
\[
\min_{x \in \mathbb{R}^n} \|Bx - y\|_2^2.
\]
Suppose \(B\) is a PSD matrix for which \(\frac{3}{4} \leq \|Bx\|_2 \leq \frac{5}{4}\) holds for all \(\|x\|_2 = 1\). Using gradient descent for \(t\) iterations, we obtain
\[
\|B(x_t - x^*)\|_2 \leq c\|B(x_0 - x^*)\|_2,
\]
where \(x_0\) is our initial guess, \(x^*\) is the optimal solution, and \(c \in (0, 0.9]\).

**Proof of Theorem D.1.** Throughout the proof, we will set \(\tilde{c} = \epsilon/4\). By Theorem A.1, we can compute an \(\epsilon\)-approximation to \(Z\) and \(W_g(X)\) in time
\[
O(\epsilon^{-2} n^2 \cdot \text{poly}(\log(nd/\epsilon\delta)) + nd \log(nd/\epsilon\delta)).
\]
If we solve the problem:
\[
\min_{x \in \mathbb{R}^n} \|W_g(X)^T W_g(X)x - y\|_2
\]
with solution \(\hat{x}\), then we have
\[
\|W_g(X)^T W_g(X)\hat{x} - y\|_2 \leq (1 + \tilde{c}) \min_{x \in \mathbb{R}^n} \|Z^T Zx - y\|_2.
\]
This means the optimal solution for the sketched problem gives an \(\tilde{c}\)-approximation to the optimal solution to the original problem. We will now show that Algorithm 2 computes the desired solution. By Theorem 2.11, with probability at least \(1 - \delta\), for any \(x \in \mathbb{R}^n\), we have
\[
\|SW_g(x)x\|_2 = (1 + \epsilon_0)\|W_g(x)x\|_2.
\]
Suppose \(R\) is the \(n \times n\) matrix computed via a QR decomposition, so that \(SW_g(X)R\) has orthonormal columns. Then for any \(\|x\|_2 = 1\), we have
\[
\|W_g(X)Rx\|_2 = (1 + \epsilon_0)\|SW_g(x)Rx\|_2 = 1 + \epsilon_0.
\]
Hence,
\[
\|R^T W_g(X)^T W_g(X)Rx\|_2 \leq (1 + \epsilon_0)^2.
\]
Now, pick \(\epsilon_0 = 0.1\) and solve the following regression problem:
\[
\min_{x \in \mathbb{R}^n} \|R^T W_g(X)^T W_g(X)Rz - R^Ty\|_2.
\]
Notice that Algorithm 2 implements gradient descent. Using Lemma D.3, after \(t = \log(1/\tilde{c})\) iterations, we have
\[
\|R^T W_g(X)^T W_g(X)R(z_t - z^*)\|_2 \leq \tilde{c}\|R^T W_g(X)^T W_g(X)R(z_0 - z^*)\|_2,
\]
where \(z^* = (R^T W_g(X)^T W_g(X)R)^{-1}R^Ty\) is the optimal solution to Equation (7). We will show the following for \(x_t = Rz_t\):
\[
\|W_g(X)^T W_g(X)x_t - y\|_2 \leq \kappa\tilde{c}\|y\|_2.
\]
Recalling that $z_0 = 0$, plugging into Eq. (8) we get
\[
\|R^T W_g(X) x_t - R^T y\|_2 \leq \tilde{c}\|R^T y\|_2 \leq \tilde{c} \cdot \sigma_{\text{max}}(R^T)\|y\|_2.
\]
On the other hand,
\[
\|R^T W_g(X)^T W_g(X) x_t - R^T y\|_2 = \|R^T (W_g(X)^T W_g(X) x_t - y)\|_2 \geq \sigma_{\text{min}}(R^T)\|W_g(X)^T W_g(X) x_t - y\|_2.
\]
Putting everything together, we get
\[
\|W_g^T W_g x_t - y\|_2 \leq \tilde{c}\kappa(R^T)\|y\|_2
\leq \tilde{c}\kappa(W_g(X)R)\|y\|_2
\leq 2\tilde{c}\kappa(W_g(X))\|y\|_2
\leq 2\tilde{c}\kappa \frac{1 + \tilde{c}}{1 - \tilde{c}} \|y\|_2
\leq 2\kappa\tilde{c} \|y\|_2.
\]
The second inequality uses that $R$ is a square matrix, the third inequality uses Fact D.2, and the second-to-last inequality uses that we have a $(1 \pm \tilde{c})$-subspace embedding. This means by setting the number of iterations to $t = \log(\kappa/\epsilon)$, we obtain
\[
\|W_g^T W_g x_t - y\|_2 \leq 2\tilde{c}\|y\|_2.
\]
Now, recall that for any $x, y \in \mathbb{R}^n$, we have
\[
\|W_g(X)^T W_g(X) x - y\|_2 \leq (1 + \tilde{c})\|Z^T Z x - y\|_2.
\]
As a consequence, we get
\[
\|Z^T Z x_t - y\|_2 \leq (1 + \tilde{c})\|W_g(X)^T W_g(X) x_t - y\|_2
\leq (1 + \tilde{c})2\tilde{c}\|y\|_2
\leq \epsilon \|y\|_2.
\]
Now we analyze the runtime.

- Computing $W_g(X)$, by Theorem A.1, takes time
\[
\epsilon^{-2}n^2 \cdot \text{poly}(\log(nd/\epsilon\delta)) + nd\log(nd/\epsilon\delta).
\]
- Applying $S$ to $W_g(X)$, using the FFT algorithm, takes time
\[
\epsilon^{-2}n^2 \cdot \text{poly}(\log(nd/\epsilon\delta)).
\]
- A QR decomposition algorithm, due to [DDH07], can be computed in time $n^{\omega}$.

The cost of each iteration is bounded by the cost of taking a matrix-vector product, which is at most $\tilde{O}(n^2/\epsilon^2)$, and there are $O(\log(\kappa/\epsilon))$ iterations in total. Thus, we obtain a final runtime of
\[
\epsilon^{-2}n^2 \cdot \text{poly}(\log(nd/\epsilon\delta)) \cdot \log(\kappa/\epsilon) + n^{\omega} + nd\log(nd/\epsilon\delta).
\]
\[\Box\]
E  Kernel Ridge Regression

In this section, we show how to compose our sketch with other sketches whose dimensions depend on the statistical dimension of $K$ instead of $n$. Before proceeding, we introduce the notion of the statistical dimension.

Definition E.1 (Statistical Dimension). Given $\lambda \geq 0$, for every positive semi-definite matrix $K \in \mathbb{R}^{n \times n}$, we define the $\lambda$-statistical dimension of $K$ to be

$$s_\lambda(K) := \text{tr}[K(K + \lambda I_n)^{-1}].$$

Solving ridge regression with runtime depending on the statistical dimension is done in a number of works, for example [RR07, AM15, AKM+17, ACW17a, MM17].

We state and prove our main result in this section below.

Theorem E.2 (Kernel Ridge Regression, formal version of Theorem 6.9). Let $\epsilon \in (0, 1)$, $p > 1$ be an integer, and $X \in \mathbb{R}^{d \times n}$. If $K$ is a degree-$p$ polynomial kernel with statistical dimension $s_\lambda(K)$ with $\lambda < \epsilon^{-2}\lambda_{\text{max}}(K)$, then we can compute $Z \in \mathbb{R}^{t \times n}$ such that $Z^\top Z$ is a $1 \pm \epsilon$ spectral approximation to $K$ in $\tilde{O}(\epsilon^{-2}p^2n^2 + nd)$ time and $t = \tilde{O}(\epsilon^{-2}p^2n)$.

Moreover, there exists a matrix $S$ with $m = \tilde{O}(\epsilon^{-1}s_\lambda(K))$ rows such that if $x^\ast$ is the optimal solution to $\|S(Z^\top z - y)\|_2^2 + \lambda\|z\|_2^2$, then

$$\|K x^\ast - y\|_2^2 + \lambda\|X^{\otimes p}x^\ast\|_2^2 \leq (1 + \epsilon) \min_{x \in \mathbb{R}^n} \|K x - y\|_2^2 + \lambda\|X^{\otimes p}x\|_2^2.$$

Finally, the time to solve above KRR is $\tilde{O}(\epsilon^{-2}p^2n(n + m^2) + n^2 \omega)$.

Before starting the proof, we introduce a key lemma regarding using the SRHT to approximate the solution of KRR.

Lemma E.3 (Corollary 15 of [ACW17a]). Let $A \in \mathbb{R}^{n \times t}$ and $\epsilon \in (0, 1)$. Suppose $\lambda < \epsilon^{-2}\sigma_{\text{max}}^2(A)$.

Suppose

$$m = \Omega(\epsilon^{-1}(s_\lambda(A) + \log(1/\epsilon)) \log(s_\lambda(A)/\epsilon))$$

and $S \in \mathbb{R}^{m \times n}$ is a SRHT matrix (Definition 2.7) and let $\hat{x} = \arg \min_{x \in \mathbb{R}^t} \|S(Ax - b)\|_2^2 + \lambda\|x\|_2^2$.

Then with probability at least 0.99, we have

$$\|A\hat{x} - b\|_2^2 + \lambda\|\hat{x}\|_2^2 \leq (1 + \epsilon) \min_{x \in \mathbb{R}^t} \|Ax - b\|_2^2 + \lambda\|x\|_2^2.$$

Proof of Theorem E.2. Throughout the proof, we assume $K$ has full rank and set $S$ to be a SRHT matrix with $m = \tilde{O}(\epsilon^{-1}s_\lambda(K))$ rows. We also use $A$ to denote $Z^\top Z$.

The proof consists of 3 parts:

- Part 1: Provide a construction of matrix $Z$;
- Part 2: Provide a sketching matrix $S$ with the solution guarantee;
- Part 3: Provide a runtime analysis for solving KRR.

Note that part 1 can be solved using Theorem 5.1. As a side note, since $Z^\top Z$ is a $1 \pm \epsilon$ approximation to $K$, with high probability it also has full rank. Consequently, $Z$ has full rank as well.

To show part 2, we will show the following:

- The optimal solution to $\|S(Z^\top z - y)\|_2^2 + \lambda\|z\|_2^2$ is a $(1 \pm \epsilon)$ approximation to the optimum of $\|Z^\top z - y\|_2^2 + \lambda\|z\|_2^2$;
- The optimum of $\|Z^\top z - b\|_2^2 + \lambda\|z\|_2^2$ is a $(1 \pm \epsilon)$ approximation to the optimum of $\|K z - y\|_2^2 + \lambda\|X^{\otimes p}z\|_2^2$. 

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From $\|S(Z^T x - y)\|_2^2 + \lambda \|Zx\|_2^2$ to $\|Z^T Zx - y\|_2^2 + \lambda \|Zx\|_2^2$ Recall that $Z$ has full rank. Therefore, we can set $z = Zx$ and the sketched problem becomes

$$\|S(Z^T z - y)\|_2^2 + \lambda \|z\|_2^2,$$

which can be solved using Lemma E.3. The only thing we need to justify is that the statistical dimension of $A$ gives a good approximation to the statistical dimension of $K$. Note that

$$s_\lambda(A) = \sum_{i=1}^n \frac{\lambda_i(A)}{\lambda_i(A) + \lambda} \leq \sum_{i=1}^n \frac{(1 + \epsilon)\lambda_i(K)}{(1 - \epsilon)\lambda_i(K) + \lambda} \leq \sum_{i=1}^n \frac{(1 + \epsilon)\lambda_i(K)}{1 - \epsilon(\lambda_i(K) + \lambda)} = \frac{1 + \epsilon}{1 - \epsilon} \cdot s_\lambda(K) \leq (1 + 3\epsilon) \cdot s_\lambda(K).$$

Thus, the dimension $O(\epsilon^{-1}s_\lambda(K)) = O(\epsilon^{-1}s_\lambda(A))$, which means we can invoke Lemma E.3.

From $\|Z^T Zx - y\|_2^2 + \lambda \|Zx\|_2^2$ to $\|Kx - y\|_2^2 + \lambda \|X^\otimes p x\|_2^2$ To prove this part, we define matrix $\hat{A}$ and $\hat{K}$:

$$\hat{A} := \left[ A \sqrt{\lambda Z} \right], \quad \hat{K} := \left[ K \sqrt{\lambda X^\otimes p} \right].$$

Similar to the first part, it suffices to show that for any $x \in \mathbb{R}^n$, we have

$$\|\hat{A}x\|_2 \leq (1 + \epsilon)\|\hat{K}x\|_2.$$

We start by computing the LHS:

$$\|\hat{A}x\|_2^2 = \|Ax\|_2^2 + \lambda x^T Z^T Zx \leq (1 + \epsilon)\|Kx\|_2^2 + (1 + \epsilon)\lambda\|X^\otimes p x\|_2^2.$$

This completes our proof for part 2.

For the final part, note that applying the sketch takes $\tilde{O}(\epsilon^2 p^2 n^2)$ time. To solve the regression problem, we instead solve:

$$\min_{z \in \mathbb{R}^t} \|SZ^T z - Sy\|_2^2 + \lambda \|z\|_2^2.$$

Since $Z$ has full rank, we know the argument $z$ realizing the minimum is the $x^*$ we are looking for. To output an $x$, we can simply solve the linear system $Zx = z$, which takes $\tilde{O}(nt + n^w)$ time. Finally, solving the above regression problem takes $\tilde{O}(m^2 t)$ time (see [SGV98]). This concludes our runtime analysis.\[\square\]