Nonlinear Dimensionality Reduction for Faster Kernel Methods in Machine Learning

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“Random Fourier Features for Kernel Ridge Regression: Approximation Bounds and Statistical Guarantees”

Joint work with:

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- Michael Kapralov (EPFL)
- Cameron Musco (MIT)
- Ameya Velingker (EPFL)
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Main idea:

Study **Fourier kernel approximation methods** from a **matrix sampling point of view**.
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Specifics:

- Analyze *Random Fourier Features method* (Rahimi, Recht NIPS ’07) using techniques based on *leverage scores*.
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- Analyze **Random Fourier Features method** (Rahimi, Recht NIPS ’07) using techniques based on **leverage scores**.
- Develop an **improved Random Fourier Features method** based on this analysis (better in theory and experiments).
Main idea:
Study Fourier kernel approximation methods from a matrix sampling point of view.

Specifics:
- Analyze Random Fourier Features method (Rahimi, Recht NIPS ’07) using techniques based on leverage scores.
- Develop an improved Random Fourier Features method based on this analysis (better in theory and experiments).

Lots of open questions and directions for future work.
Opportunities to combine techniques from randomized linear algebra and Fourier methods.
QUICK REFRESHER ON KERNEL METHODS
Adapt standard linear learning methods (least squares regression, support vector machines, PCA, k-means clustering) to learn nonlinear relationships.
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(therefore well-understood, multipurpose, widely used)
“Lift” data points to a higher dimensional feature space. E.g.

\[ x = \begin{bmatrix}
  x_1 \\
  x_2 \\
  \vdots \\
  x_d
\end{bmatrix} \]
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\[
\begin{bmatrix}
    x_1 \\
    x_2 \\
    \vdots \\
    x_d
\end{bmatrix}
\implies
\phi(x) =
\begin{bmatrix}
    x_1 \\
    \vdots \\
    x_d \\
    x_1x_1 \\
    x_1x_2 \\
    \vdots \\
    x_dx_d
\end{bmatrix}
\]
Kernel Methods in Machine Learning

Linear Classifier

\[ x_1 + 2x_2 \geq 6 \]

Kernel Classifier

\[ x_1^2 + x_2^2 \geq 10 \]
Kernel methods in machine learning

Linear Classifier

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Kernel Classifier

\[ x_1^2 + x_2^2 \geq 10 \]
\[ \phi(x)_3 + \phi(x)_4 \geq 10 \]
Main computational issue: Forming $\phi(x)$ is intractable even for moderately complex kernels.

E.g. degree $q$ polynomials $\implies O(d^q)$ dimensional vectors.
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Fix: For common linear learning methods, we only need the kernel dot product for each pair of data points $x, y$:

$$k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle.$$
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Fix: For common linear learning methods, we only need the kernel dot product for each pair of data points $x, y$:

$$k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle.$$ 

Can often be computed much more quickly than $\phi(x_i), \phi(x_j)$. 
Input: Data $X = [x_1, \ldots, x_n]^T$, responses $b = [b_1, \ldots, b_n]^T$. 
### Example: Least Squares Regression

**Input:** Data $X = [x_1, \ldots, x_n]^T$, responses $b = [b_1, \ldots, b_n]^T$.

**Solve:**

$$w^* = \arg \min_w \|Xw - b\|_2^2 + \lambda \|w\|_2^2$$

**Predict:**

$$b_{new} = w^*^T x_{new}$$
**Input:** Data $X = [x_1, \ldots, x_n]^T$, responses $b = [b_1, \ldots, b_n]^T$.

**Solve:**

$$w^* = \arg \min_w \|Xw - b\|_2^2 + \lambda \|w\|_2^2$$

$$y^* = \arg \min_y \|XX^Ty - b\|_2^2 + \lambda \|X^Ty\|_2^2$$

**Predict:**

$$b_{new} = w^{*T}x_{new}$$

$$b_{new} = y^{*T}Xx_{new}$$
For training, we compute \((K + \lambda I)^{-1}\) for the kernel matrix \(K\):

\[
\begin{pmatrix}
X
\end{pmatrix} = \begin{pmatrix}
X^T
\end{pmatrix} = K
\]
For training, we compute $(K + \lambda I)^{-1}$ for the kernel matrix $K$:

If we replace each $x_i$ with $\phi(x_i)$ for nonlinear learning, we just need to alternatively compute:

$$K_{i,j} = \langle \phi(x_i), \phi(x_j) \rangle = k(x_i, x_j).$$
Kernel dot product can often be computed implicitly without forming $\phi(x)$ and $\phi(y)$. For example:

\[
(1 + \langle x, y \rangle)^2 = (1 + x_1 y_1 + \ldots + x_d y_d)^2 \\
= (1 + x_1 y_1 + x_1^2 y_1^2 + 2x_1 y_1 x_2 y_2 + \ldots) \\
= \langle [1, x_1, x_1^2, \sqrt{2}x_1 x_2, \ldots], [1, y_1, y_1^2, \sqrt{2}y_1 y_2, \ldots] \rangle \\
= \langle \phi(x), \phi(y) \rangle
\]
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$$= (1 + x_1y_1 + x_1^2y_1^2 + 2x_1y_1x_2y_2 + \ldots)$$

$$= \left\langle [1, x_1, x_1^2, \sqrt{2}x_1x_2, \ldots], [1, y_1, y_1^2, \sqrt{2}y_1y_2, \ldots] \right\rangle$$

$$= \langle \phi(x), \phi(y) \rangle$$

The kernel function $k(x, y) = (1 + x^Ty)^2$ provides an alternative similarity metric to the standard dot product.
Kernel learning pipeline for data points $x_1, \ldots, x_n$:

1. Choose kernel function $k(x_i, x_j)$:
   
   $$(1 + x_i^T x_j)^q, \ e^{-\|x_i - x_j\|^2}, \ e^{-\|x_i - x_j\|_1}, \ \text{etc.}$$

2. Form $n \times n$ kernel matrix $K$ with:

   $$K_{i,j} = k(x_i, x_j)$$

3. Compute model using $K$: compute $(K + \lambda I)^{-1} b$ for kernel regression, eigendecomposition of $K$ for kernel PCA, etc.
ALGORITHMIC CHALLENGE

Even if we avoid explicit feature expansion, kernel methods are slow. Quadratic dependence on the number of data points.
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- \( n = 100,000 \) \( \Rightarrow \) 10 billion entries \( \Rightarrow \) 80 GB to store \( \mathbf{K} \).
- Just writing down \( \mathbf{K} \) requires \( \Omega(n^2) \) time.
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- \( n = 100,000 \Rightarrow 10 \text{ billion entries} \Rightarrow 80 \text{ GB to store } K. \\
- \text{Just writing down } K \text{ requires } \Omega(n^2) \text{ time.} \\
- \text{Other operations require even more. A single iteration for a linear system solver takes } \Omega(n^2) \text{ time.}
New algorithmic ideas are needed to scale kernel methods. Even for moderately large datasets.
Find approximation $\tilde{K} = ZZ^T$ for $K$ (which is symmetric and positive semidefinite):
STANDARD APPROACH: LOW-RANK APPROXIMATION

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$$K \xrightarrow{\text{low-rank approximation}} \begin{bmatrix} n \times n & \text{Z} \\ \text{Z}^T & n \times s \end{bmatrix}$$

We can typically set $s \ll n$.

- $Z$ takes $O(ns)$ space to store.
- Orthogonalization, eigendecomposition, and inversion of $ZZ^T$ all take just $O(ns^2)$ time.
- $ZZ^Tx$ can be computed in $O(ns)$ time.
All standard low-rank approximation algorithms take $\Omega(n^2)$ time for kernel matrices: we at least need to compute $K$.

**Goal**: Find methods that avoid explicit access to the $K$. 
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Example: Nyström approximation.

Construct $\tilde{K}$ from subsample of $K$'s columns and rows.
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Can match optimal $k$-rank approximation to $(1 + \epsilon)$ factor with $O(nk/\epsilon)$ total samples [Musco, Musco, NIPS 2017].
Suppose $k(x, y)$ is shift invariant.
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- Laplace kernel: $k(x, y) = e^{-\|x-y\|_1}$
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- Laplace kernel: $k(x, y) = e^{-\|x-y\|_1}$
- Matern kernel, Cauchy kernel, rational quadratic, etc.
Write $k(\Delta)$ using its inverse Fourier transform,

$$p(\eta) = \mathcal{F}^{-1}k(\Delta) \quad k(\Delta) = \int_{\eta \in \mathbb{R}^d} p(\eta) e^{-i \pi \eta^T \Delta} d\eta$$
Write \( k(\Delta) \) using its inverse Fourier transform,

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\]

Approximate with finite sum for any \( \Delta \):

\[
k(\Delta) \approx \frac{1}{s} \sum_{j=1}^{s} c_j e^{-i\pi \eta_j^T \Delta}
\]
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Approximate with finite sum for any $\Delta$:

$$k(\Delta) \approx \frac{1}{s} \sum_{j=1}^{s} c_j e^{-i\pi \eta_j^T \Delta}$$

Immediately gives low-rank approximation:

$$Z(x)Z(y)^* = \sum_j \frac{c_j}{s} e^{-i\pi \eta_j^T (x-y)} \approx k(x - y)$$
How do we choose the frequencies in the finite sum?

\[
\int_{\eta \in \mathbb{R}^d} p(\eta) e^{-i \pi \eta^T \Delta} d\eta \approx \frac{1}{s} \sum_{j=1}^{s} c_j e^{-i \pi \eta_j^T \Delta}
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How do we choose the frequencies in the finite sum?

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**Bochner’s Theorem:** For shift-invariant, positive semidefinite kernel functions, \( p(\eta) \geq 0 \) for all \( \eta \).
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Example (Gaussian kernel):

\[
k(x - y) = e^{-\|x-y\|^2} \quad \text{and} \quad p(\eta) \propto e^{-\|\eta\|^2/4}
\]
Sample frequencies from distribution $p(\eta)$. 
Random Fourier Features (RFF) Algorithm

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$$\mathbb{E} \left[ \frac{1}{s} \sum_{j=1}^{s} e^{-i\pi \eta_j^T \Delta} \right] = \mathbb{E} \left[ e^{-i\pi \eta^T \Delta} \right]$$
Sample frequencies from distribution $p(\eta)$.

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• Random Fourier Features (RFF) Algorithm

$$k(x - y) = e^{-\|x - y\|^2}$$

$$p(\eta) \propto e^{-\|\eta\|^2/4}$$

• Sampling frequencies by $$p(\eta)$$ is correct in expectation.
RANDOM FOURIER FEATURES (RFF) ALGORITHM

\[ k(x - y) = e^{-\|x-y\|^2} \]

\[ p(\eta) \propto e^{-\|\eta\|^2/4} \]

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- Final sum \( \frac{1}{s} \sum_{j=1}^{s} e^{-i\pi \eta_j^T \Delta} \approx k(\Delta) \) only has terms with magnitude \( |e^{-i\pi \eta_j^T \Delta}| = 1 \). Real part \( \leq 1 \). Imaginary part \( \leq 1 \).
Random Fourier Features (RFF) Algorithm

- Sampling frequencies by $p(\eta)$ is correct in expectation.
- Final sum $\frac{1}{s} \sum_{j=1}^{s} e^{-i\pi \eta_j^T \Delta} \approx k(\Delta)$ only has terms with magnitude $|e^{-i\pi \eta_j^T \Delta}| = 1$. Real part $\leq 1$. Imaginary part $\leq 1$.
- By Chernoff bound, if we take $O\left(\frac{\log n}{\epsilon^2}\right)$ samples, we approximate every entry in $K$ to error $\pm \epsilon$ w.h.p.
Super simple algorithm. For Gaussian kernel $k(x, y) = e^{-\|x-y\|^2_2}$:

$$ Z = \exp(-i\pi X) \text{ for } \eta_1 \ldots \eta_s $$

$$ Z_{x,j} = e^{-i\pi x^T \eta_j} \text{ for } \eta_j \sim \mathcal{N}$$
Super simple algorithm. For Gaussian kernel \( k(x, y) = e^{-\|x-y\|^2} \):

\[
Z = \exp\left(-i\pi X \right) \begin{pmatrix} \eta_1 & \ldots & \eta_s \end{pmatrix}
\]

random gaussians

\[
Z_{x,j} = e^{-i\pi x^T \eta_j} \quad \text{for} \quad \eta_j \sim \mathcal{N}
\]

\[
G = \text{randn}(d, s);
\]

\[
Z = \exp(-\sqrt{-1} \pi X G)/\sqrt{s};
\]
Super simple algorithm. For Gaussian kernel $k(x, y) = e^{-\|x - y\|^2}$:

$$Z = \exp\left( -i\pi x \right) \eta_1 \ldots \eta_s$$

This is a so-called oblivious sketch.
Want to improve the approximation guarantee:

\[ Z \approx Z^* = K + E \]

- Does not give bounds on \( \|Z\| \) unless we take \( \Omega(n^2) \) samples.
- No clear implications for downstream learning tasks. E.g., does \( (Z^* + I) \) approximate \( (K + I) \)?
- Faster but less accurate than a Nyström approximation with the same number of samples in practice.
Want to improve the approximation guarantee:

- Does not give bounds on $\|ZZ^* - K\|$ unless we take $\Omega(n^2)$ samples.

$Z \cdot Z^* = K + E$

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Want to improve the approximation guarantee:

- Does not give bounds on $\|ZZ^* - K\|$ unless we take $\Omega(n^2)$ samples.
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- No clear implications for downstream learning tasks. E.g., does $(ZZ^* + \lambda I)^{-1}$ approximate $(K + \lambda I)^{-1}$?
- Faster but less accurate than a Nyström approximation with the same number of samples in practice.
We want matrix-like error bounds, not entrywise bounds.
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**Key Idea:** Analyze the random Fourier features algorithm as a matrix sampling process.
$k(x_u - x_v) = \int_{\eta \in \mathbb{R}^d} p(\eta) e^{-i\pi \eta^T(x_u - x_v)} d\eta$
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Kernel Fourier Transform
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Kernel Fourier Transform

\[ \Phi_u(\eta) = \sqrt{p(\eta)} e^{-i\pi \eta^T x_u} \]

K = \Phi

weighted Fourier matrix

\[ \Phi^* \]
Standard RFF selects column with probability \( \frac{1}{p^2} \).

Simple matrix Chernoff already gives better bounds:

\[ \|KZZ\|_2 \leq \epsilon \text{ with } \sim O\left(\frac{n}{\epsilon^2}\right) \text{ samples.} \]
Standard RFF selects column $\Phi(\eta)$ with probability $\propto p(\eta)$. 

\[ \Phi_u(\eta) = \sqrt{p(\eta)} e^{-\pi \eta^T x_u} \]

\[ K = \begin{pmatrix} \eta_1 & \eta_2 & \eta_s \end{pmatrix} \begin{pmatrix} \Phi & \Phi^* \end{pmatrix} \]

Simplified matrix Chernoff already gives better bounds: $\|KZZ\|_2 \leq \epsilon$ with $\tilde{O}(n \epsilon^{-2})$ samples.
Standard RFF selects column $\Phi(\eta)$ with probability $\propto p(\eta)$. (with probability proportional to the column’s squared norm).
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(with probability proportional to the column’s squared norm).

Simple matrix Chernoff already gives better bounds:
$\|K - ZZ^*\|_2 \leq \epsilon$ with $\tilde{O}(n/\epsilon^2)$ samples.
LEVERAGE SCORE SAMPLING

For matrix approximation, norm based sampling probabilities are known to be suboptimal!
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We can obtain better theoretical bounds and empirical performance if we sample by column leverage scores.
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We can obtain better theoretical bounds and empirical performance if we sample by column leverage scores.

[See work on effective resistances for spectral graph sparsification, randomized linear algebra, etc.]
λ-Ridge Leverage Score Sampling:

\[(1 - \epsilon)(ZZ^* + \lambda I) \preceq K + \lambda I \preceq (1 + \epsilon)(ZZ^* + \lambda I).\]
\( \lambda \)-Ridge Leverage Score Sampling:

\[(1 - \epsilon)(ZZ^* + \lambda I) \preceq K + \lambda I \preceq (1 + \epsilon)(ZZ^* + \lambda I).\]

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- Spectral approximation also gives bounds for kernel PCA, k-means, CCA, etc. (Cohen, Musco, Musco ‘16,’17)
\(\lambda\)-Ridge Leverage Score Sampling:

\[ (1 - \epsilon)(\mathbf{ZZ}^* + \lambda \mathbf{I}) \preceq \mathbf{K} + \lambda \mathbf{I} \preceq (1 + \epsilon)(\mathbf{ZZ}^* + \lambda \mathbf{I}). \]

- Since \( \mathbf{A} \preceq \mathbf{B} \Rightarrow \mathbf{B}^{-1} \preceq \mathbf{A}^{-1} \), \( (\mathbf{Z} \mathbf{Z}^* + \lambda \mathbf{I})^{-1} \approx (\mathbf{K} + \lambda \mathbf{I})^{-1} \)
- Spectral approximation also gives bounds for kernel PCA, k-means, CCA, etc. (Cohen, Musco, Musco ‘16,’17)

Need \( \tilde{O}(s_\lambda/\epsilon^2) \) samples where \( s_\lambda \) is the statistical dimension:

\[ s_\lambda = \text{tr}(\mathbf{K}(\mathbf{K} + \lambda \mathbf{I})^{-1}) \]
λ-Ridge Leverage Score Sampling:

\[(1 - \epsilon)(\mathbf{ZZ}^* + \lambda \mathbf{I}) \preceq \mathbf{K} + \lambda \mathbf{I} \preceq (1 + \epsilon)(\mathbf{ZZ}^* + \lambda \mathbf{I}).\]

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Need \(\tilde{O}(s_\lambda/\epsilon^2)\) samples where \(s_\lambda\) is the statistical dimension:

\[s_\lambda = \text{tr}(\mathbf{K}(\mathbf{K} + \lambda \mathbf{I})^{-1}) = \sum_{i=1}^{n} \frac{\sigma_i(\mathbf{K})}{\sigma_i(\mathbf{K}) + \lambda}\]
λ-Ridge Leverage Score Sampling:

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- Since \(A \preceq B \Rightarrow B^{-1} \preceq A^{-1}\), \((ZZ^* + \lambda I)^{-1} \approx (K + \lambda I)^{-1}\)
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\[
s_\lambda = \text{tr}(K(K + \lambda I)^{-1}) = \sum_{i=1}^{n} \frac{\sigma_i(K)}{\sigma_i(K) + \lambda}
\]

Roughly the number of singular values \(\geq \lambda\) plus a term depending on the tail singular values.
What are the ridge leverage scores?

\[ \tau_\lambda(\eta) = \Phi(\eta)^* (K + \lambda I)^{-1} \Phi(\eta). \]
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\[ \tau_{\lambda}(\eta) = \Phi(\eta)^* (K + \lambda I)^{-1} \Phi(\eta). \]

Expensive to invert \( K + \lambda I \). Even if you could, not at all clear how to efficiently sample from the leverage score distribution.
Goal: Upper bound Fourier ridge leverage scores for common kernels with simple distributions.
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More closely match leverage score sampling to improve random Fourier features.
**First observation:** Scaled by $\frac{n}{\lambda}$, the standard Rahimi Recht distribution upper bounds the $\lambda$-ridge leverage scores.
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Basic Result: Sampling $O\left(\frac{n}{\lambda} \cdot \frac{1}{\epsilon^2}\right)$ frequencies with RFF gives spectral guarantees.
Ridge leverage score $\tilde{\Phi}(\eta)^*(K + \lambda I)^{-1}\tilde{\Phi}(\eta)$ solves:

$$\tau_\lambda(\eta) = \min_y \left[ \frac{1}{\lambda} \|\tilde{\Phi}y - \tilde{\Phi}(\eta)\|_2^2 + \|y\|_2^2 \right].$$

Intuition: $y$ reconstructs frequency from other frequencies. If $\eta$ is "easy" to reconstruct, it is less important to sample.
Ridge leverage score $\Phi(\eta)^* (K + \lambda I)^{-1} \Phi(\eta)$ solves:

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**Intuition:** $y$ reconstructs frequency $\eta$ from other frequencies. If $\eta$ is “easy” to reconstruct, it is less important to sample.
Approach: Obtain closed form upper bound on leverage scores by exhibiting simple candidate vector $\tilde{y}$ and noting that:

$$\tau_\lambda(\eta) \leq \frac{1}{\lambda} \| \Phi \tilde{y} - \Phi(\eta) \|_2^2 + \|\tilde{y}\|_2^2.$$
$\Phi y$ is just the Fourier transform of $\sqrt{P} y$ evaluated at $x_1, \ldots, x_n$!
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We want a function whose Fourier transform matches frequency \( \eta \) on these data points.
Need to bound: \( \frac{1}{\lambda} \| \tilde{\Phi} \tilde{y} - \tilde{\Phi}(\eta) \|_2^2 + \| \tilde{y} \|_2^2 \).
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Set \( \sqrt{P\tilde{y}} \) to be a **shifted sinc function**.
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\[ \frac{1}{\lambda} \| \Phi\tilde{y} - \Phi(\eta) \|_2^2 = 0! \]
First Attempt

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\| \sqrt{P\tilde{y}} \|_2^2 = O(\delta).
\]

$\| \tilde{y} \|_2^2$ is much larger!
\[ \tilde{y} = P^{-1/2} P^{1/2} y = P^{-1/2} \cdot \text{sinc function} \]

Sinc falls off as \( O(1/f) \), but \( \frac{1}{\sqrt{p(f)}} \) grows as \( e^{O(f^2)} \), so \( \|y\|_2^2 \) explodes.
Solution: Dampen sinc with a narrow Gaussian.
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(as long as \( \eta \) is not too large)
Easy to sample from approximate leverage distribution for the Gaussian kernel with $x_1, ..., x_n \in [-\delta, \delta]^d$:

$$
\tilde{\tau}_\lambda(\eta) = \begin{cases} 
\tilde{O}(\delta) & \text{when } \eta \leq \sqrt{\log n / \lambda} \\
\rho(\eta) = e^{-\|n\|_2^2 / 2} & \text{otherwise.}
\end{cases}
$$
Easy to sample from approximate leverage distribution for the Gaussian kernel with $x_1, \ldots, x_n \in [-\delta, \delta]^d$:

$$\bar{\tau}_\lambda(\eta) = \begin{cases} \tilde{O}(\delta) \text{ when } \eta \leq \sqrt{\log n / \lambda} \\ p(\eta) = e^{-\|n\|_2^2/2} \text{ otherwise.} \end{cases}$$
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Requires $O(\delta \sqrt{\log(n/\lambda)}) \cdot \frac{1}{\epsilon^2}$ samples for spectral guarantee. 

(vs. $O(n/\lambda) \cdot \frac{1}{\epsilon^2}$ for standard random Fourier features.)
Gaussian kernel for two clusters:
Gaussian kernel for two clusters:

Standard RFF element error.  Modified RFF element error.
Gaussian kernel for two clusters:

$$\frac{1}{\sqrt{2\pi \sigma^2}} e^{-\frac{x^2}{2\sigma^2}}$$

Standard RFF element error.  Modified RFF element error.

$$\left(1 - \epsilon\right)(ZZ^* + \lambda I) \preceq K + \lambda I \preceq \left(1 + \epsilon\right)(ZZ^* + \lambda I).$$

Sampling low frequencies relatively less biases error to align with large eigenvectors.
Example of approximate kernel ridge regression to interpolate a synthetic function:

CRF = classic random Fourier features ‘column norm’ sampling,
MRF = our modified sampling distribution.
In higher dimensions:

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MRF = our modified sampling distribution.
1. Viewed random Fourier features methods as a matrix sampling problem.
2. Used optimization perspective on leverage scores to certify upper bounds on these scores. Reduced score computation to Fourier approximation problem.
3. New sampling distribution under-samples lower frequencies to obtain better kernel approximations.
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**Major open question:** Can we achieve our spectral guarantee with $O(s^\lambda)$ samples in high dimensions for any data set.
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**Conjecture:** Yes, although maybe with polynomial loss (i.e. $\text{poly}(s_\lambda)$ samples).
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I.e. can we match data-adaptive methods like Nyström obliviously?
Duel view of leverage scores:

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Immediately get leverage score bounds from bounds on smoothness of sparse Fourier functions, e.g. [Chen, Kane, Price, Song FOCS 2016].
Vague open question: Why does this all actually matter for function fitting?
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We were surprised to beat random Fourier features on a kernel regression task.
THANK YOU!