RANDOM FOURIER FEATURES
FOR KERNEL RIDGE REGRESSION:
APPROXIMATION BOUNDS AND STATISTICAL GUARANTEES

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ICML 2017.
Our Contributions:

- Analyze the random Fourier features method (Rahimi Recht '07) for kernel approximation using leverage score-based techniques.
- Concrete: Introduce new sampling distribution that gives statistical guarantees for kernel ridge regression when used to approximate the Gaussian kernel.
- High Level: Hope that Fourier leverage scores will have further applications in kernel approximation, function approximation, and sparse Fourier transform methods.
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Kernel approximation

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- Other operations require even more. A single iteration of a linear system solver takes $\Omega(n^2)$ time.
- For $n = 100,000$, $K$ has 10 billion entries. Takes 80 GB of storage if each is a double.
Employ classic solution: low-rank approximation

\[ K \rightarrow Z \rightarrow Z^T \]

- Storing \( Z \) uses \( O(n_s) \) space and computing \( ZZ^T \) takes \( O(n_s) \) time.
- Orthogonalization, eigendecomposition, and pseudo-inversion of \( ZZ^T \) all take just \( O(n_s^2) \) time.
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- Storing $Z$ uses $O(ns)$ space and computing $ZZ^T x$ takes $O(ns)$ time. Orthogonalization, eigendecomposition, and pseudo-inverse of $ZZ^T$ all take just $O(ns^2)$ time.
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- Many faster methods have been studied: incomplete Cholesky factorization (Fine & Scheinberg ‘02, Bach & Jordan ‘02), entrywise sampling (Achlioptas, McSherry, & Schölkopf ‘01), Nyström approximation (Williams & Seeger ‘01), random Fourier features (Rahimi & Recht ‘07)
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Rahimi & Recht NIPS ‘07:

• For any shift-invariant \( k(x_i, x_j) = k(x_i - x_j) \) let \( p(\cdot) \) be the Fourier transform of \( k(\cdot) \). By Bochner’s theorem, \( p(\eta) \geq 0 \) for all \( \eta \).

• Sample \( \eta_1, \ldots, \eta_s \in \mathbb{R}^d \) with probabilities proportional to \( p(\eta) \).

• Set \( z_i = \frac{1}{\sqrt{s}} [e^{-2\pi i \eta_1^T x_i}, \ldots, e^{-2\pi i \eta_s^T x_i}] \).
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- Sample $\eta_1, ..., \eta_s \in \mathbb{R}^d$ with probabilities proportional to $p(\eta)$.

\[
k(x_i - x_j) = e^{-\|x_i - x_j\|^2/\sigma} \quad \text{and} \quad p(\eta) \propto e^{-\|\eta\|^2 \sigma/4}
\]
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- $\int_{\eta \in \mathbb{R}^d} \Phi_i(\eta) p(\eta) \Phi_j(\eta)^* d\eta = \int_{\eta \in \mathbb{R}^d} e^{-2\pi i \eta^T (x_i - x_j)} p(\eta) d\eta = k(x_i - x_j) = K_{i,j}$.

- Set $\bar{\Phi} = \Phi P^{1/2}$. So $K = \bar{\Phi} \bar{\Phi}^T$.
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**Diagram:**

- $K = \Phi \Phi^T$
- $\Phi_i(\eta) = e^{-2\pi i \eta^T x_i}$
- $x_1, x_2, ..., x_n$
- $\eta \in \mathbb{R}^d$
- Kernel Fourier transform
- Fourier matrix
- $\bar{\Phi} = \Phi P^{1/2}$
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- Set $\Phi = \Phi P^{1/2}$. So $K = \Phi \Phi^T$. 

VIEW AS MATRIX SAMPLING METHOD
• $Z(j) = \frac{1}{\sqrt{\text{sp}(\eta)}} \bar{\Phi}(\eta)$ with probability $p(\eta)$. So $E[ZZ^T] = K$.

$z_i = \frac{1}{\sqrt{s}} [e^{-2\pi i \eta^T x_1}, \ldots, e^{-2\pi i \eta^T x_s}]$ for $\eta_1, \ldots, \eta_s$ sampled according to $p(\eta)$. 
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\[
\mathbf{K} = \mathbf{\Phi} \mathbf{\Phi}^T = \mathbf{\Phi}_\mathbf{P} \mathbf{P}^{-1} / 2
\]

- \(\mathbf{Z}\) is a sample of \(\mathbf{\Phi} = \mathbf{P} \mathbf{\Phi}_1\), columns are sampled with probability \(\propto p(\eta)\), i.e., their squared column norms.

- It is well known from work on randomized methods in linear algebra that there are better sampling probabilities (in both theory and practice): the column leverage scores.

- Also noted by Bach '17, implicit in Rudi et al. '16.
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Column Norm Sampling: \( s = \tilde{O}(d/\epsilon^2) \) samples ensure that 
\[ (ZZ^T)_{i,j} = K_{i,j} \pm \epsilon \] for all \( i,j \) with high probability [RR07].
**Column Norm Sampling:** \( s = \tilde{O}(d/\epsilon^2) \) samples ensure that \((ZZ^T)_{i,j} = K_{i,j} \pm \epsilon\) for all \(i,j\) with high probability [RR07].

**Ridge Leverage Score Sampling:** \( s = \tilde{O}(s_\lambda/\epsilon^2) \) samples gives spectral approximation:

\[
(1 - \epsilon)(ZZ^T + \lambda I) \preceq K + \lambda I \preceq (1 + \epsilon)(ZZ^T + \lambda I).
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where \( s_\lambda = tr(K(K + \lambda I)^{-1}) \) is the statistical dimension.
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- Spectral approximation gives statistical guarantees for kernel ridge regression (this work), and approximation bounds for kernel PCA and k-means clustering (Cohen, Musco, Musco ‘16,‘17)
The ridge leverage score for frequency \( \eta \) is given by:

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\tau_\lambda(\eta) = \Phi(\eta)^T (K + \lambda I)^{-1} \Phi(\eta).
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$$

- Expensive to invert $K + \lambda I$. But even if you could do that efficiently, it is not at all clear you could efficiently sample from the leverage score distribution.
**Main goal:** Get a handle on the Fourier ridge leverage scores for common kernels by upper bounding them with simple distributions.
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1. Improve random Fourier features.
2. Bound statistical dimension by the sum of leverage scores.
3. Connections with sparse Fourier transforms, Fourier interpolation, and other problems.
Ridge leverage score $\tau_\lambda(\eta) = \Phi(\eta)^T (K + \lambda I)^{-1} \Phi(\eta)$ also equals:

$$\tau_\lambda(\eta) = \min_y \lambda^{-1} \| \Phi y - \Phi(\eta) \|_2^2 + \| y \|_2^2.$$
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**Intuition:** \( \tau_\lambda(\eta) \) is small iff there exists a function \( y : \mathbb{R}^d \to \mathbb{C} \) with low energy (\( \|y\|_2^2 \) small) whose (\( \sqrt{p(\eta)} \) weighted) Fourier transform is close to the frequency \( e^{-2\pi i x_j^T \eta} \) at each data point.
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**Intuition:** $\tau_\lambda(\eta)$ is small iff there exists a function $y : \mathbb{R}^d \to \mathbb{C}$ with low energy ($\| y \|^2_2$ small) whose ($\sqrt{p(\eta)}$ weighted) Fourier transform is close to the frequency $e^{-2\pi i x_j^T \eta}$ at each data point.

- $y$ reconstructs frequency $\eta$ from other frequencies. The easier it is to reconstruct, the less important it is to sample.
Assume data points are 1-dimensional and bounded: $x_1, \ldots, x_n \in [-\delta, \delta]$. One possibility is to choose $y$ with $(\sqrt{p(\eta)}$ weighted) Fourier transform equal to $e^{-2\pi i x \eta}$ for all $x \in [-\delta, \delta]$. 

Achieved by the shifted sinc function weighted by $\frac{1}{\sqrt{p(\eta)}}$.
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FREQUENCY RECONSTRUCTION FOR BOUNDED DATA
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- Achieved by the shifted sinc function weighted by $1/\sqrt{p(\eta)}$. 

![Diagram showing $e^{-2\pi ix\eta}$ and sinc function](image.png)
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- **Solution:** Dampen the sinc by multiplying with a Gaussian, keeping Fourier transform nearly identical.
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- **Solution**: Dampen the sinc by multiplying with a Gaussian, keeping Fourier transform nearly identical.
**Upshot:** easy to sample from approximate leverage distribution for the Gaussian kernel with $x_1, ..., x_n \in [-\delta, \delta]^d$:

\[
\bar{\tau}_\lambda(\eta) = \begin{cases} 
\tilde{O}(\delta^d) & \text{when } \|\eta\|_\infty \leq \sqrt{\log n/\lambda} \\
p(\eta) = e^{-\|\eta\|_2^2/2} & \text{otherwise.}
\end{cases}
\]
Example of approximating a synthetic ‘wiggly function’:

CRF = classic random Fourier features ‘column norm’ sampling,  
MRF = our modified sampling distribution.
Questions?