



A random matrix analysis of random fourier features

beyond the Gaussian kernel, a precise phase transition, and the corresponding double descent

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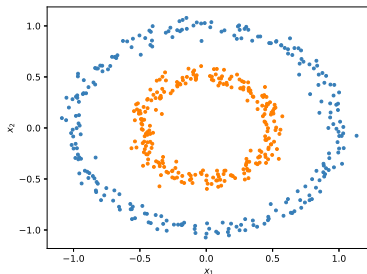
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Linear Classification with Non-linear Input

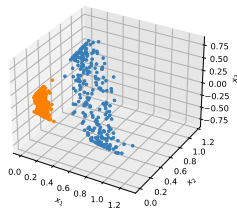
Consider a binary classification problem with non-linear (e.g. polynomial) samples. This is not separable with linear function.

$$\text{(e.g. } \mathbf{X} = \begin{bmatrix} x_{1,1} & x_{1,2} \\ x_{2,1} & x_{2,2} \\ \vdots & \vdots \\ x_{N,1} & x_{N,2} \end{bmatrix} \in \mathbb{R}^{N \times 2}.)$$



Lifting

One idea is to **LIFT** the samples into a higher dimensional space in which the samples are linearly separable.



The Lifting function in this case is $\phi(\mathbf{X}) = \begin{bmatrix} x_{1,1}^2 & x_{1,2}^2 & \sqrt{2}x_{1,1}x_{1,2} \\ x_{2,1}^2 & x_{2,2}^2 & \sqrt{2}x_{2,1}x_{2,2} \\ \vdots & \vdots & \vdots \\ x_{N,1}^2 & x_{N,2}^2 & \sqrt{2}x_{N,1}x_{N,2} \end{bmatrix}$.

Curse of Dimensionality

Consider solving the above problem with *support vector machine* (SVM).

$$\mathcal{L}(\mathbf{w}, \alpha) = \sum_{n=1}^N \alpha_n - \frac{1}{2} \sum_n^N \sum_m^N \alpha_n \alpha_m y_n y_m (\mathbf{x}_n^T \mathbf{x}_m).$$

The \mathbf{w} is the linear decision boundary and α is a vector of Lagrange multipliers.



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We need to use lifting function $\phi(X)$ to make the samples linearly separable. Specifically, we replace $(\mathbf{x}_n^\top \mathbf{x}_m)$ with $(\phi(\mathbf{x}_n)^\top \phi(\mathbf{x}_m))$.

$$\begin{aligned} \phi(\mathbf{x}_n)^\top \phi(\mathbf{x}_m) &= \begin{bmatrix} x_{n,1}^2 & x_{n,2}^2 & \sqrt{2}x_{n,1}x_{n,2} \end{bmatrix} \begin{bmatrix} x_{m,1}^2 & x_{m,2}^2 & \sqrt{2}x_{m,1}x_{m,2} \end{bmatrix}^\top \\ &= x_{n,1}^2 x_{m,1}^2 + x_{n,2}^2 x_{m,2}^2 + 2x_{n,1}x_{n,2}x_{m,1}x_{m,2} \end{aligned}$$



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Calculate the inner product in the \mathbb{R}^3 across all N pairs of samples is acceptable. However, the lifting function $\phi(X)$ is usually very high dimensional.

Kernel Trick

Consider the following derivation,

$$\begin{aligned}(\mathbf{x}_n^\top \mathbf{x}_m)^2 &= ([x_{n,1} \ x_{n,2}][x_{m,1} \ x_{m,2}]^\top)^2 \\&= (x_{n,1}x_{m,1} + x_{n,2}x_{m,2})^2 \\&= x_{n,1}^2x_{m,1}^2 + x_{n,2}^2x_{m,2}^2 + 2x_{n,1}x_{n,2}x_{m,1}x_{m,2} \\&= \phi(\mathbf{x}_n)^\top \phi(\mathbf{x}_m)\end{aligned}$$



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Instead of computing inner product in the high dimensional space, we compute the inner product in the original space.

The function

$$K(\mathbf{x}_n, \mathbf{x}_m) = (\mathbf{x}_n^\top \mathbf{x}_m)^2 = \phi(\mathbf{x}_n)^\top \phi(\mathbf{x}_m)$$

is called a **kernel function**.

There must be disadvantages...

Given training data $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_N, y_N) \in \mathcal{X} \times \mathcal{Y}$, where $\mathcal{X} \subseteq \mathbb{R}^d$ and $\mathcal{Y} \subseteq \mathbb{R}$. Consider *Kernel Ridge Regression* (KRR), with $\phi(\mathcal{X}) \subseteq \mathbb{R}^k$, where $k \rightarrow \infty$

$$\mathcal{L}(\mathbf{w}, \lambda) = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_n^N (y_n - \mathbf{w}^\top \phi(\mathbf{x}_n))^2 + \lambda \mathbf{w}^\top \mathbf{w}.$$

Solving it with Lagrange multipliers α , which is the solution of

$$(\mathbf{K} + \lambda \mathbf{I}_k) \alpha = \mathbf{y},$$

requires $\Theta(k^3)$ time and $\Theta(k^2)$ memory. Here $\mathbf{K} \in \mathbb{R}^{k \times k}$ is the kernel matrix or Gram matrix defined by $\mathbf{K}_{nm} \equiv K(\mathbf{x}_n, \mathbf{x}_m)$.

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Intuition: Can we find a kernel function which lifts \mathcal{X} to \mathbb{R}^s , where $d < s \ll k$, while not sacrifices model performance?

Some Prerequisites

Shift Invariant Kernel (Radial Basis Function (RBF))

A kernel function $K(\mathbf{x}_n, \mathbf{x}_m)$ is called **shift invariant** if it can be written as $K(\mathbf{x}_n, \mathbf{x}_m) = g(\mathbf{x}_n - \mathbf{x}_m)$ for some function $g(\cdot)$ (e.g. $K_{Gaussian}(\mathbf{x}_n, \mathbf{x}_m) = \exp(-\gamma \|\mathbf{x}_n - \mathbf{x}_m\|_2^2)$).

Mercer's Theorem

A continuous function $K(\mathbf{x}_n, \mathbf{x}_m)$ is a valid kernel function if and only if the kernel matrix \mathbf{K} is **positive semi-definite**.

Bochner's Theorem

A continuous function $g(\cdot)$ is **positive semi-definite** if and only if it is the Fourier transform of a non-negative measure.



Random Fourier Features

Conclusion

A continuous **shift invariant** kernel $K(\mathbf{x}_n, \mathbf{x}_m)$, which is **positive semi-definite** (Mercer's Theorem), is the Fourier transform of a non-negative measure $p(\cdot)$.

$$\phi(\mathbf{x}_n)^\top \phi(\mathbf{x}_m) = K(\mathbf{x}_n, \mathbf{x}_m) = K(\mathbf{x}_n - \mathbf{x}_m) \quad (1)$$

$$= \int_{\mathbb{R}^d} p(\omega) \exp(i\omega^\top (\mathbf{x}_n - \mathbf{x}_m)) d\omega \quad (2)$$

$$= \mathbb{E}_\omega [\xi_\omega(\mathbf{x}_n)^* \xi_\omega(\mathbf{x}_m)] \quad (3)$$

Here $\xi_\omega(\mathbf{x}) = \exp(i\omega^\top \mathbf{x}) = \begin{bmatrix} \cos(\omega^\top \mathbf{x}) \\ \sin(\omega^\top \mathbf{x}) \end{bmatrix}$ and hence $\xi_\omega(\mathbf{x}_n)^* \xi_\omega(\mathbf{x}_m)$ is an unbiased estimator of $K(\mathbf{x}_n, \mathbf{x}_m)$ when ω is drawn from $p(\cdot)$.



Random Fourier Features

Since both the $p(\cdot)$ and $K(\Delta)$ are real-valued, we can replace $\xi_\omega(\mathbf{x})$ with $z_\omega(\mathbf{x}) = [\sqrt{2} \cos(\omega^\top \mathbf{x} + b)]$ where ω is drawn from $p(\omega)$ and b is uniformly drawn from $[0, 2\pi]$. Then eq. (3) becomes $\mathbb{E}_\omega [z_\omega(\mathbf{x}_n)^\top z_\omega(\mathbf{x}_m)]$



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Note: $z_\omega(\mathbf{x}_n)^\top z_\omega(\mathbf{x}_m)$ is an unbiased estimator of $\phi(\mathbf{x}_n)^\top \phi(\mathbf{x}_m)$.
The $z_\omega(\mathbf{x})$ is not a lifting function.



Random Fourier Features

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Note: $z_\omega(\mathbf{x}_n)^\top z_\omega(\mathbf{x}_m)$ is an unbiased estimator of $\phi(\mathbf{x}_n)^\top \phi(\mathbf{x}_m)$. The $z_\omega(\mathbf{x})$ is not a lifting function.

Note: To further reduce the variance of the estimator, we can randomly draw s samples of ω and normalize each corresponding $z_\omega(\mathbf{x})$ by \sqrt{s} . Then the inner product $z(\mathbf{x}_n)^\top z(\mathbf{x}_m) = \frac{1}{s} \sum_{j=1}^s z_{\omega_j}(\mathbf{x}_n)^\top z_{\omega_j}(\mathbf{x}_m)$

Algorithm

Algorithm 1 Random Fourier Features

Require: A shift invariant kernel $K(\mathbf{x}_n, \mathbf{x}_m) = K(\mathbf{x}_n - \mathbf{x}_m)$.

Ensure: A randomized feature map $z(\mathbf{x}) : \mathbb{R}^d \rightarrow \mathbb{R}^s$ so that

$$z(\mathbf{x}_n)^\top z(\mathbf{x}_m) \approx K(\mathbf{x}_n, \mathbf{x}_m).$$

Compute the Fourier transform $p(\cdot)$ of the kernel $K : p(\omega) = \frac{1}{2\pi} \int \exp(-i\omega^\top \Delta) K(\Delta) d\Delta$

Draw s i.i.d. samples $\omega_1, \omega_2, \dots, \omega_s \in \mathbb{R}^d$ from $p(\cdot)$ and s i.i.d. samples $b_1, b_2, \dots, b_s \in [0, 2\pi]$.

$$\text{Let } z(\mathbf{x}) \equiv \sqrt{\frac{2}{s}} [\cos(\omega_1^\top \mathbf{x} + b_1) \quad \cos(\omega_2^\top \mathbf{x} + b_2) \quad \dots \quad \cos(\omega_s^\top \mathbf{x} + b_s)]^\top$$

Convergence

Bound for a *fixed* pair of samples \mathbf{x}_n and \mathbf{x}_m

Given z_ω is bounded random variable between $[-\sqrt{2}, \sqrt{2}]$, with Hoeffding's Inequality, we have

$$\mathbb{P}(|z(\mathbf{x}_n)^\top z(\mathbf{x}_m) - K(\mathbf{x}_n, \mathbf{x}_m)| \geq \epsilon) \leq 2 \exp\left(-\frac{s\epsilon^2}{4}\right).$$

Convergence



Bound for *all* pair of samples \mathbf{x}_n and \mathbf{x}_m

Let \mathcal{M} be a compact subset of \mathbb{R}^d with diameter $\text{diam}(\mathcal{M})$. Then, for the mapping z defined in Algorithm 1, we have

$$\begin{aligned} & \mathbb{P}\left(\sup_{x,y \in \mathcal{M}} |z(\mathbf{x}_n)^\top z(\mathbf{x}_m) - K(\mathbf{x}_n, \mathbf{x}_m)| \geq \epsilon\right) \\ & \leq 2^8 \left(\frac{\sigma_{p(\cdot)} \text{diam}(\mathcal{M})}{\epsilon}\right)^2 \exp\left(-\frac{s\epsilon^2}{4(d+2)}\right). \end{aligned}$$



Common RFF

Kernel	$K(\Delta)$	$p(\omega)$
Gaussian	$\exp(-\gamma \ \Delta\ _2^2)$	$(2\pi)^{-\frac{s}{2}} \exp(-\gamma \ \omega\ _2^2)$
Laplacian	$\exp(-\ \Delta\ _1)$	$\prod_d (\pi(1 + \omega_d^2))^{-1}$
Cauchy	$\prod_d 2(1 + \Delta_d^2)^{-1}$	$\exp(-\ \Delta\ _1)(?)$



The challenge that RFF faces in the learning regime

Consider a machine learning system with d parameters, trained on a dataset of size N , asymptotic analysis has

Classical regime: either focuses on the (statistical) population $N \rightarrow \infty$ limit, for d fixed, or the over-parameterized $d \rightarrow \infty$ limit, for a given N .

Modern regime: modern learning system (e.g. Neural Network) usually has model complexity and data size increase together. A double asymptotic regime where $N, d \rightarrow \infty, d/N \rightarrow c$ is established.

RFF has been shown that entry-wise the Gram matrix $\xi(\mathbf{x})$ converges to the Gaussian kernel matrix as $s \rightarrow \infty$ and this property remains in modern regime.

However, the convergence $\|\Xi^T \Xi / s - \mathbf{K}\| \rightarrow 0$ no longer holds in spectral norm (blow-up). Here Ξ is the matrix formed by stacking $\xi(\mathbf{x})$ for all samples.

Setup

$$0 < \liminf_N \min\left\{\frac{s}{N}, \frac{d}{N}\right\} \leq \limsup_N \max\left\{\frac{s}{N}, \frac{d}{N}\right\} < \infty.$$

$$\limsup_N \|\mathbf{X}\|_2 < \infty \quad \limsup_N \|\mathbf{y}\|_\infty < \infty$$

In classical regime $\|\mathbf{\Xi}^\top \mathbf{\Xi} / s\| \equiv \mathbf{K} \equiv \mathbf{K}_{\cos} + \mathbf{K}_{\sin}$

Training MSE: $\mathcal{L}_{train} = \frac{1}{N} \|\mathbf{y} - \mathbf{\Xi}^\top \mathbf{w}\|_2^2 = \frac{\lambda^2}{N} \|\mathbf{Q}(\lambda) \mathbf{y}\|_2^2$ where

$$\mathbf{Q}(\lambda) \equiv \left(\frac{1}{N} \mathbf{\Xi}^\top \mathbf{\Xi} + \lambda \mathbf{I}_N \right)^{-1}$$

We want to assess the asymptotic \mathcal{L}_{train} by expectation which is equivalent to assess the asymptotic $\mathbb{E}_\Omega \{\mathbf{Q}(\lambda)\}$ where Ω is the matrix form of ω , which is numerically hard.

Object: Find an asymptotic “alternative” for $\mathbb{E}_\Omega \{\mathbf{Q}(\lambda)\}$ when $d, s, N \rightarrow \infty$.



Some Vague Idea from me...

We want to show that with consideration of d, s, N

$$\begin{aligned}\|\mathbb{E}_{\Omega}\{\mathbf{Q}(\lambda)\} - \hat{\mathbf{Q}}(\lambda)\|_2 &\rightarrow 0 \\ \hat{\mathbf{Q}}(\lambda) &\equiv \left(\frac{s}{N} \left(\frac{\mathbf{K}_{\cos}}{1 + \delta_{\cos}} + \frac{\mathbf{K}_{\sin}}{1 + \delta_{\sin}} \right) + \lambda \mathbf{I}_N \right)^{-1} \\ \delta_{\cos} &= \frac{1}{N} \text{tr}(\mathbf{K}_{\cos} \hat{\mathbf{Q}}) \quad \delta_{\sin} = \frac{1}{N} \text{tr}(\mathbf{K}_{\sin} \hat{\mathbf{Q}})\end{aligned}$$

When $\frac{s}{N} \rightarrow \infty$, $\delta_{\cos}, \delta_{\sin} \rightarrow 0$ and thus $\hat{\mathbf{Q}} \simeq (\frac{s}{N} \mathbf{K})^{-1}$