Learning structured data with random features and kernel methods

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ML lunch

Joint work with Behrooz Ghorbani (Google Research), Song Mei (UC Berkeley) and Andrea Montanari (Stanford)

- 'Mysteries' of Deep Learning:
  - **Optimization:** training is a *highly non-convex* problem, but we are still able to find near global optimizers.
  - **Generalization:** *overparametrized* models. The solution often interpolates the training data while generalizing well on test data.
- In this talk, I will focus on the connection between neural networks (NNs) and kernel machines.

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- In this talk, I will focus on the connection between neural networks (NNs) and kernel machines.

Neural Tangent (NT) model

- Neural network: $\mathrm{NN}_p(\boldsymbol{x}; \boldsymbol{\theta})$, $\boldsymbol{x} \in \mathbb{R}^d$, $\boldsymbol{\theta} \in \mathbb{R}^p$.
  e.g., fully-connected neural network:

$$\mathrm{NN}_p(\boldsymbol{x}; \boldsymbol{\theta}) = \langle \boldsymbol{a}, \sigma(\dots \boldsymbol{W}_2 \sigma(\boldsymbol{W}_1 \boldsymbol{x})) \rangle.$$

- Linearization around random initialization $\boldsymbol{\theta}_0$:

$$\mathrm{NN}_p(x; \theta) = \mathrm{NN}_p(x; \theta_0) + \underline{\langle \theta - \theta_0, \nabla_\theta \mathrm{NN}_p(x; \theta_0) \rangle} + o(\|\theta - \theta_0\|_2).$$

- Neural Tangent (NT) model: [Chizat et al.,'18], [Du et al.,'18]

$$\mathrm{NT}_p(x; \beta, \theta_0) = \langle \beta, \nabla_\theta \mathrm{NN}_p(x; \theta_0) \rangle.$$

- Finite-width approximation of limiting kernel ($p \to \infty$ + iid initialization):

$$K_{\mathrm{NT}}(x, y) = \mathbb{E}_{\theta_0}[\langle \nabla_\theta \mathrm{NN}_p(x; \theta_0), \nabla_\theta \mathrm{NN}_p(y; \theta_0) \rangle].$$

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GD trained NNs $\approx$ NT model in some regime

Coupled gradient descent on empirical squared loss:

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\theta}^t = -\nabla_{\boldsymbol{\theta}}\hat{\mathbb{E}}[(y - \mathrm{NN}_p(\boldsymbol{x};\boldsymbol{\theta}^t))^2], \qquad \boldsymbol{\theta}^0 = \boldsymbol{\theta}_0,$$
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Theorem (informal)

For any $\varepsilon > 0$, for large enough NNs and proper random initialization θ_0 (Xavier initialization), we have with high probability

$$\sup_{t\geq 0}\sup_{\|x\|_2=1} |\mathrm{NN}_p(x;\theta^t) - \mathrm{NT}_p(x;\beta^t,\theta_0)| \leq \varepsilon.$$

$\Longrightarrow$ Intuition: *weights do not change much* and $\|\theta^t - \theta_0\|_2$ remains small.

[Jacot, Gabriel, Hongler,'18] , [Du, Zhai, Poczos, Singh,'18], [Du, Lee, Li, Wang, Zhai,'18], [Allen-Zhu, Li, Song,'18] , [Zou, Cao, Zhou, Gu,'18], [Oymak, Soltanolkotabi,'18], [Chizat, Oyallon, Bach,'19], ...

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The 'Kernel Regime'

- Optimization success:

With sufficient over-parametrization and proper initialization, gradient descent on training loss of NN converges linearly to global minimum.

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  - **Lazy Training:** weights hardly change, there is 'no feature learning'. [Chizat et al.,'18]
  - Empirically, NNs perform often better than their linearized counterparts.

However, offer theoretical insights [Bartlett, Montanari, Rakhlin,'21]:

- Tractability via overparametrization.
- Explain some of the trade-off between overparametrization and generalization (benign overfitting, double descent).

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New approach for kernel engineering

- Progress on CIFAR-10:

Paper	Method	Accuracy
[Coates, Lee, Ng,'11]	feature learning + linear regression	77%
[Arora et al.,'19]	CNTK (data independent)	77%
[Li et al.,'19]	CRFK + data dependent preprocessing	89%
[Shankar et al.,'20]	CRFK (data independent)	90%
-	CNN	$> 99\%$

- NTK achieves near state-of-the-art results on UCI dataset [Arora et al.,'19].

Observations:

- NNs often outperform kernel methods.
- Kernel methods sometimes achieve comparable accuracy to NNs.
- Kernels induced by NNs perform much better than previous handcrafted kernels.

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Outline of the talk

Questions

- Why are kernel methods not as good as NNs in general?
- When can we expect kernel methods to perform well, comparable to NNs?
- Can we quantify the benefits of using convolutional kernels against inner-product kernels (e.g., Gaussian kernel)?

Three 'stylized' scenarios:

A. **Isotropic covariates model:**
   - large gap between NN and kernel methods.

B. **Spiked covariates model:**
   - smaller gap between NN and kernel methods.

C. **Invariant function estimation:**
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A. Isotropic covariates model

Setting

- Given n iid samples $\{(y_i, \boldsymbol{x}_i)\}_{i\in[n]}$:

$$y_i = f_\star(\boldsymbol{x}_i) + \varepsilon_i, \qquad \boldsymbol{x}_i \sim_{iid} \mathrm{Unif}(\mathbb{S}^{d-1}(\sqrt{d})), \qquad \varepsilon_i \sim_{iid} N(0, \tau^2).$$

- Two-layers neural networks: $\mathrm{NN}_N(\boldsymbol{x}; \theta) = \sum_{i=1}^N a_i \sigma(\langle \boldsymbol{w}_i, \boldsymbol{x}\rangle)$.

- Random Features model [Rahimi, Recht,'08]:

$$\mathrm{RF}_N(\boldsymbol{x}; \boldsymbol{a}, \boldsymbol{W}) = \sum_{i=1}^N a_i \sigma(\langle \boldsymbol{w}_i, \boldsymbol{x}\rangle) = \langle \boldsymbol{a}, \nabla_{\boldsymbol{a}} \mathrm{NN}_p(\boldsymbol{x}; \theta_0)\rangle.$$

- Ridge regression with RF model (with fixed $\boldsymbol{W} = (\boldsymbol{w}_i)_{i\in[N]} \sim_{iid} \mathrm{Unif}(\mathbb{S}^{d-1})$)

$$\hat{\boldsymbol{a}}(\lambda) = \arg\min_{\boldsymbol{a}} \left\{ \frac{1}{n} \sum_{i=1}^n \left(y_i - \sum_{j=1}^N a_j \sigma(\langle \boldsymbol{w}_j, \boldsymbol{x}_i\rangle) \right)^2 + \lambda \|\boldsymbol{a}\|_2^2 \right\}.$$

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Test error of RF model

Theorem (Mei, Misiakiewicz, Montanari, 2021)

Assume $d^{\ell+\delta} \le \min(n, N) \le d^{\ell+1-\delta}$ and $|\log(n/N)| \ge \delta \log d$, σ satisfies some generic conditions and λ is small enough. Then,

$$\|f_\star - \widehat{\mathrm{RF}}_{n,N,\lambda}\|_{L^2}^2 = \|\mathrm{P}_{>\ell} f_\star\|_{L^2}^2 + o_{d,\mathbb{P}}(\cdot).$$

$\mathrm{P}_{>\ell}$: projection orthogonal to the space of degree-ℓ polynomials.

- For d^ℓ parameters and samples, RF fits the best degree-ℓ polynomial approximation.
- n and N play a symmetric role:

$$\text{Test error}(n, N) = \max\Big\{\text{approx. error } (n = \infty, N), \text{statistical error } (n, N = \infty)\Big\}.$$

- Statistical error $(n, N = \infty)$: kernel method with an inner-product kernel $K(x_1, x_2) = h(\langle x_1, x_2\rangle/d)$ (e.g., NTK of fully-connected NNs of any depth).

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The truncated staircase decay

$$f = \mathsf{P}_0 f + \mathsf{P}_1 f + \mathsf{P}_2 f + \mathsf{P}_3 f + \mathsf{P}_4 f.$$

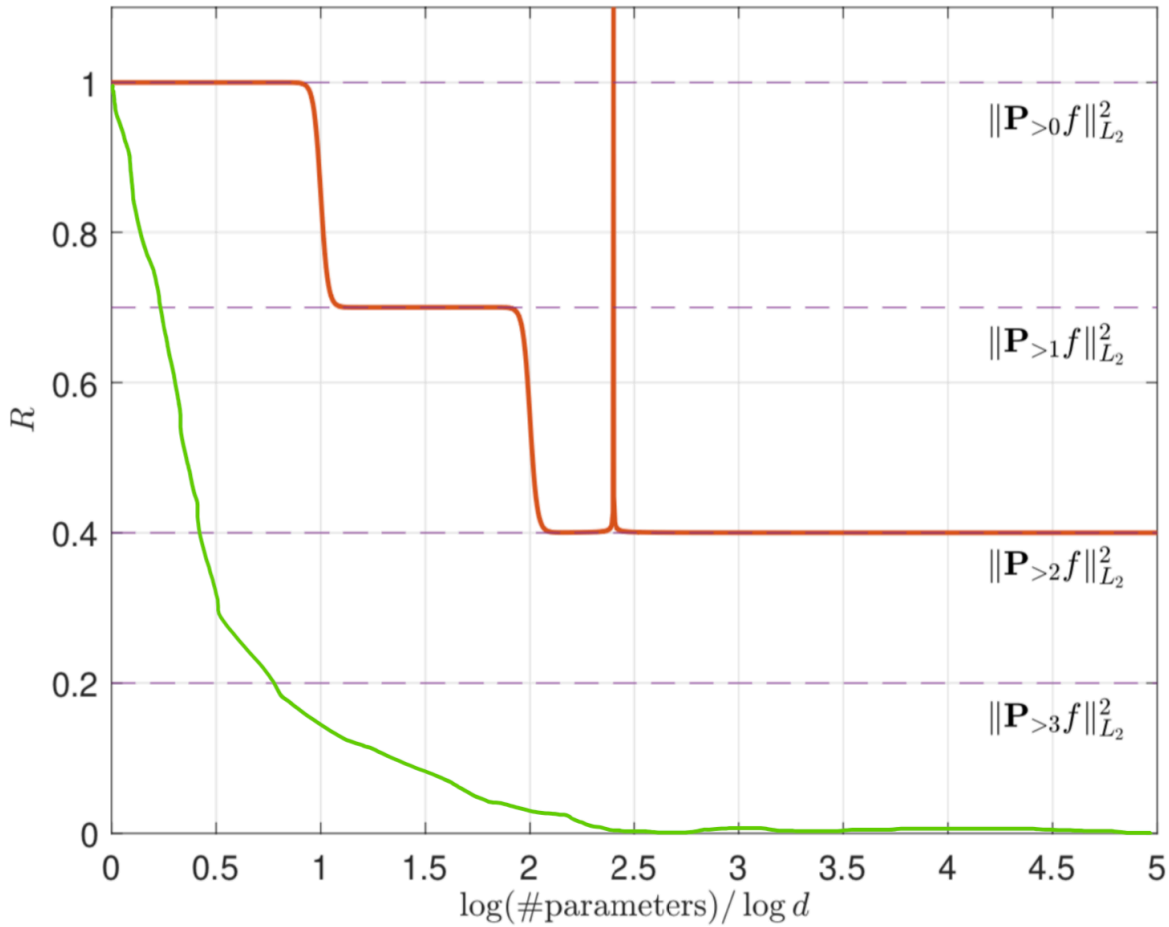

Figure: Test error (in red) v.s. $\log(N)/\log(d)$ for $n = d^{2.4}$ and $\lambda = 0^+$. Train error in green.

Performance gap between NN and kernel methods

- We expect NNs to perform way better on 'low complexity' functions

  E.g., $f_\star(\boldsymbol{x}) = \sigma(\langle \boldsymbol{w}_\star, \boldsymbol{x}\rangle)$: if $N \propto 1$ and $n \propto d$, then GD solution:

$$\|f_\star - \widehat{\mathrm{NN}}_{N,n}\|_{L^2}^2 = o_{d,\mathbb{P}}(\cdot) \qquad \text{[Bai et al.,'16]}$$

  while for KRR:

$$\|f_\star - \widehat{\mathrm{KR}}_{N,n}\|_{L^2}^2 = \|\mathrm{P}_{>1} f_\star\|_{L^2}^2 + o_{d,\mathbb{P}}(\cdot).$$

- More generally we expect NNs to vastly outperform kernel methods for target functions that only depend on a low dimensional subspace of the data [Bach,'17].

Intuition: fit $\varphi(x_1)$ using features $\sigma(\langle \boldsymbol{w}_i, \boldsymbol{x}\rangle)$

- For RF, $\boldsymbol{w}_i$'s are random, $\mathrm{corr}(x_1 \boldsymbol{e}_1, \langle \boldsymbol{w}_i, \boldsymbol{x}\rangle)^2 = \langle \boldsymbol{w}_i, \boldsymbol{e}_1\rangle^2 / \|\boldsymbol{w}_i\|_2^2$ is small in HD.
- For NN, $\boldsymbol{w}_i$'s can be chosen to have a large correlation with $\boldsymbol{e}_1$.

NN can 'adaptively learn' $\boldsymbol{w}_i$'s while RF cannot.

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NN can 'adaptively learn' $\boldsymbol{w}_i$'s while RF cannot.

Performance gap between NN and kernel methods

- We expect NNs to perform way better on 'low complexity' functions

  E.g., $f_\star(\boldsymbol{x}) = \sigma(\langle \boldsymbol{w}_\star, \boldsymbol{x}\rangle)$: if $N \propto 1$ and $n \propto d$, then GD solution:

$$\|f_\star - \widehat{\mathrm{NN}}_{N,n}\|_{L^2}^2 = o_{d,\mathbb{P}}(\cdot) \qquad \text{[Bai et al.,'16]}$$

  while for KRR:

$$\|f_\star - \widehat{\mathrm{KR}}_{N,n}\|_{L^2}^2 = \|\mathrm{P}_{>1} f_\star\|_{L^2}^2 + o_{d,\mathbb{P}}(\cdot).$$

- More generally we expect NNs to vastly outperform kernel methods for target functions that only depend on a low dimensional subspace of the data [Bach,'17].

Intuition: fit $\varphi(x_1)$ using features $\sigma(\langle \boldsymbol{w}_i, \boldsymbol{x}\rangle)$

- For RF, $\boldsymbol{w}_i$'s are random, $\mathrm{corr}(x_1 \boldsymbol{e}_1, \langle \boldsymbol{w}_i, \boldsymbol{x}\rangle)^2 = \langle \boldsymbol{w}_i, \boldsymbol{e}_1\rangle^2 / \|\boldsymbol{w}_i\|_2^2$ is small in HD.
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In the isotropic covariates model:

- Kernel methods suffer from the **curse of dimensionality**.

- For target functions that depend on a **low dimensional projection** of the data, NNs can **adaptively learn a good representation** of the data and vastly outperform kernel methods.

B. Spiked covariates model

Spiked covariates model

Covariate vector: orthogonal matrix $[\boldsymbol{U}, \boldsymbol{U}^\perp]$

$$\boldsymbol{x} = \boldsymbol{U}\boldsymbol{z}_1 + \boldsymbol{U}^\perp \boldsymbol{z}_2, \qquad \boldsymbol{z}_1 \in \mathbb{R}^{d_s}, \boldsymbol{z}_2 \in \mathbb{R}^{d-d_s}.$$

Signal part: $\boldsymbol{z}_1 \sim \text{Unif}\left(\mathbb{S}^{d_s-1}\left(\sqrt{\text{snr}_c \cdot d_s}\right)\right)$.

Noise part: $\boldsymbol{z}_2 \sim \text{Unif}\left(\mathbb{S}^{d-d_s-1}\left(\sqrt{d-d_s}\right)\right)$

d_s = signal dimension.

snr_c = covariate SNR.

Target function: $f_\star(\boldsymbol{x}) = \varphi(\boldsymbol{z}_1)$.

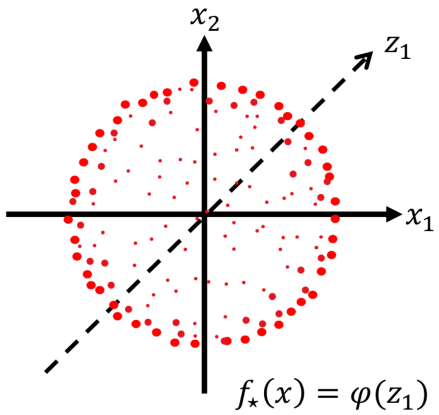

Figure: Isotropic covariates: $\text{snr}_c = 1$.

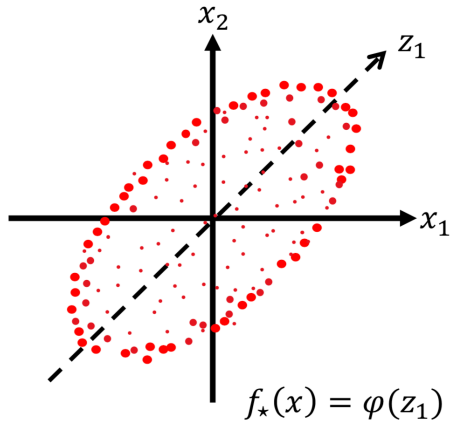

Figure: Anisotropic covariates: $\text{snr}_c > 1$.

Test error of KRR in the spiked covariates model

- Given iid samples $(\{\boldsymbol{x}_i, y_i\})_{i\in[n]}$ from the spiked covariates model.
- Effective dimension: $d_{\text{eff}} = d_s \vee (d/\text{snr}_c)$.

Theorem (Ghorbani, Mei, Misiakiewicz, Montanari, 2020)

Assume ${d_{\text{eff}}}^{\ell+\delta} \le \min(n, N) \le {d_{\text{eff}}}^{\ell+1-\delta}$ and $|\log(n/N)| \ge \delta \log d_{\text{eff}}$, σ satisfies some generic conditions and λ is small enough. Then,

$$\|f_\star - \widehat{\text{RF}}_{n,N,\lambda}\|_{L^2}^2 = \|\text{P}_{>\ell} f_\star\|_{L^2}^2 + o_{d,\mathbb{P}}(\cdot).$$

- d_{eff} capture the 'effective low-dimensionality' of the data.
- d_{eff} decreases with snr_c (data more anisotropic) and kernel methods will perform better.
- On the contrary, we expect NNs to learn features $\boldsymbol{w}_i$ aligned with $\boldsymbol{z}_1$ and to depend mildly on snr_c.

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NNs vs kernel methods in the spiked covariates model

Effective dimension: $d_{\text{eff}} = d_s \vee (d/\text{snr}_c)$.

In the spiked covariates model, we expect the generalization error of:

- Kernel methods to depend on d_{eff};
- NNs to depend on d_s.

- $d_s \le d_{\text{eff}} \le d$:

  Test error: NN $\le$ Kernel methods

- d_{eff} decreases with snr_c:
  - Isotropic features: $d_{\text{eff}} = d$ (low covariate SNR)

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Intuition for the gap: anisotropic case

Goal: fitting $\varphi(x_1)$ using features $\sigma(\langle \boldsymbol{w}_i, \boldsymbol{x} \rangle)$.

Consider $\mathbb{E}[\boldsymbol{x}\boldsymbol{x}^\mathsf{T}] = \mathrm{diag}(\mathsf{snr}_c, \mathrm{Id}_{d-1})$.

- To fit $\varphi(x_1)$, we need to use features $\sigma(\langle \boldsymbol{w}_i, \boldsymbol{x} \rangle)$ that are correlated to x_1, i.e.,

$$\mathrm{corr}(x_1 \boldsymbol{e}_1, \langle \boldsymbol{w}_i, \boldsymbol{x} \rangle) = \mathsf{snr}_c \cdot \frac{\langle \boldsymbol{w}_i, \boldsymbol{e}_1 \rangle^2}{\|\Sigma^{1/2} \boldsymbol{w}_i\|_2^2} = \mathsf{snr}_c \cdot O_{d,\mathbb{P}}(d^{-1}) = O_{d,\mathbb{P}}(d_{\mathsf{eff}}{}^{-1}).$$

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Insight

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Lower covariate SNR (data more isotropic) should lead to larger generalization gap between NNs and kernel methods.

How to test this insight?

In *image classification*, we expect

- Images to have most of their spectrum concentrated on low-frequencies (z_1 part);
- The labels to depend predominantly on the low-frequencies ($y = f_\star(x) = \varphi(z_1)$).

Experiment: add noise to the high frequency components (z_2 part) of the images (i.e., decreasing the snr_c).

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Numerical simulations

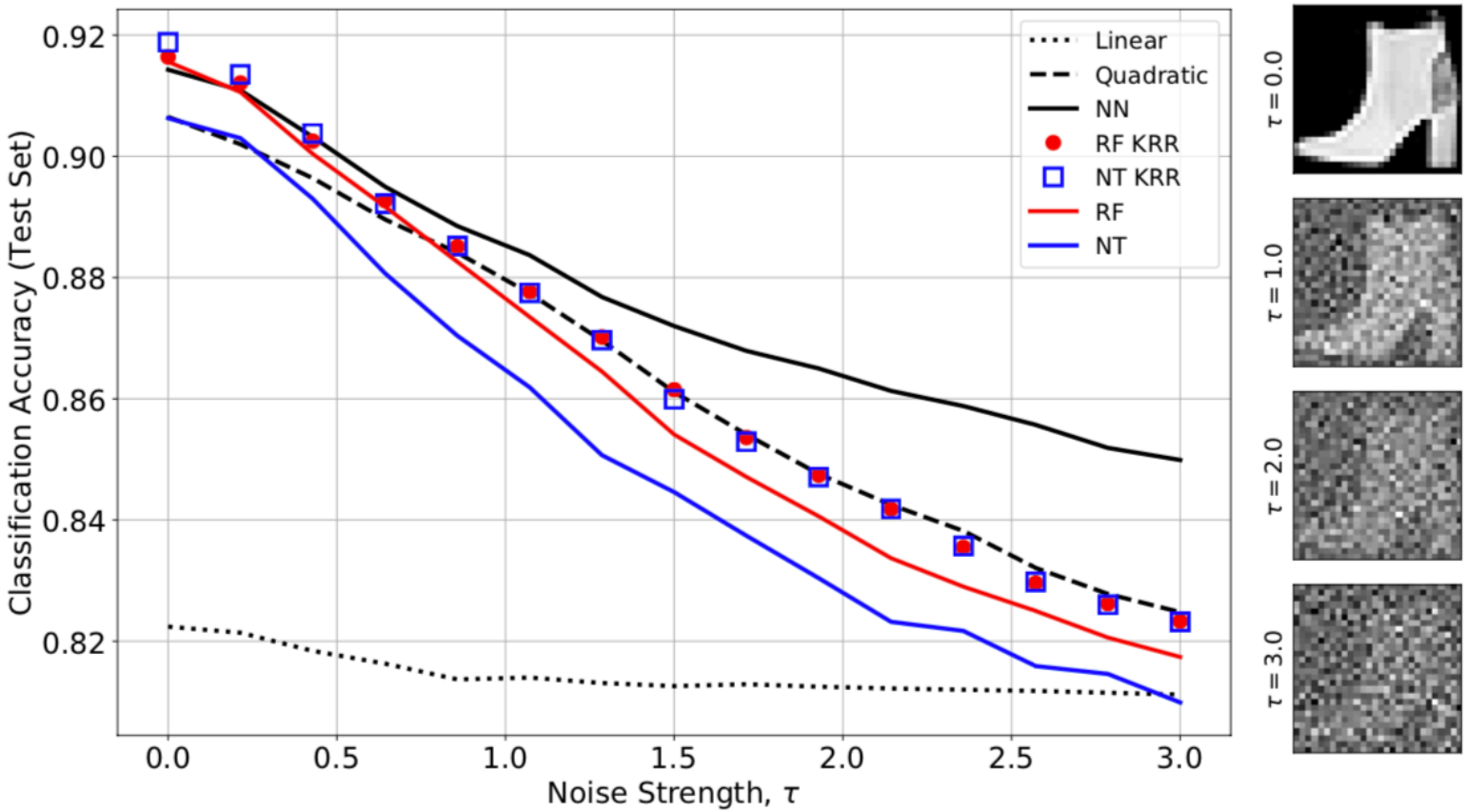

Figure: Test accuracy on FMNIST: adding noise to the high frequency components.

Spiked covariates model:
A controlling parameter of the performance gap between NN and kernel methods is

$$\mathrm{snr}_c = \text{Covariate SNR} = \frac{\text{Signal covariates variance}}{\text{Noise covariates variance}}.$$

- Small snr_c: large separation.
- Large snr_c: kernel methods perform closer to NN.

Intuition:

- When snr_c is small, RF fail to find the signal covariates.
- When snr_c is big, RF automatically find the signal covariates.
- NNs always look for the signal covariates.

C. Invariant function estimation on the sphere

Symmetries in the data

- In many learning tasks, the target function present some **natural symmetries**.

  E.g., image classification: labels **invariant under translation** of the images.

- Effectiveness of NNs architectures is often loosely attributed to their ability to encode various symmetries present in the data.

  E.g., **CNNs with translation invariance.**

- CNNs perform better than fully-connected networks.

  Convolutional kernels perform better than inner-product kernels.

- **Can we quantify this gain?**

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Cyclic function estimation on the sphere

- Data $\boldsymbol{x} \sim \text{Unif}(\mathbb{S}^{d-1}(\sqrt{d}))$.
- Consider $\mathcal{G}_d = \{g_0, g_1, \ldots, g_{d-1}\}$ the cyclic group:

$$g_i \cdot \boldsymbol{x} = (x_{d-i+1}, x_{d-i+2}, \ldots, x_d, x_1, x_2, \ldots, x_{d-i}).$$

- **Goal:** learn a cyclic invaeriant function $f_\star$:

$$\text{i.e., } f_\star(g \cdot \boldsymbol{x}) = f_\star(\boldsymbol{x}) \text{ for all } g \in \mathcal{G}_d.$$

E.g., $f(\boldsymbol{x}) = \sum_{i=1}^{d} x_i x_{i+1}$.

Stylized model for an image label $y = f_\star(\boldsymbol{x})$ invariant by translation of image $\boldsymbol{x}$.

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Invariant random features and kernels

- Invariant RF model:

$$\mathrm{RF}_N^{\mathrm{inv}}(x; a, W) = \sum_{i=1}^{N} a_i \int_{g \in \mathcal{G}_d} \sigma(\langle w_i, g \cdot x \rangle) \pi(\mathrm{d}g) = \frac{1}{d} \sum_{i=1}^{N} a_i \sum_{k=1}^{d} \sigma(\langle w_i, g_k \cdot x \rangle).$$

Neural tangent model of a CNN with N filters $w_i \in \mathbb{R}^d$.
Associated invariant kernel:

$$K_{\mathrm{inv}}(x, y) = \int_{g \in \mathcal{G}_d} h(\langle g \cdot x, y \rangle / d) \pi(\mathrm{d}g).$$

- Compared to standard RF model:

$$\mathrm{RF}_N(x; a, W) = \sum_{i=1}^{N} a_i \sigma(\langle x, w_i \rangle),$$

and associated 'standard' (inner-product) kernel:

$$K(x, y) = h(\langle x, y \rangle / d).$$

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$$K_{\mathrm{inv}}(\boldsymbol{x}, \boldsymbol{y}) = \int_{g \in \mathcal{G}_d} h(\langle g \cdot \boldsymbol{x}, \boldsymbol{y} \rangle / d) \pi(\mathrm{d}g).$$

- Compared to standard RF model:

$$\mathrm{RF}_N(\boldsymbol{x}; \boldsymbol{a}, \boldsymbol{W}) = \sum_{i=1}^{N} a_i \sigma(\langle \boldsymbol{x}, \boldsymbol{w}_i \rangle),$$

  and associated 'standard' (inner-product) kernel:

$$K(\boldsymbol{x}, \boldsymbol{y}) = h(\langle \boldsymbol{x}, \boldsymbol{y} \rangle / d).$$

Test error of KRR with invariant kernel

- Cyclic invariant $f_\star$: given iid samples $\{(y_i, \boldsymbol{x}_i)\}_{i\in[n]}$,

$$y_i = f_\star(\boldsymbol{x}_i) + \varepsilon_i, \qquad \boldsymbol{x}_i \sim_{iid} \mathrm{Unif}(\mathbb{S}^{d-1}(\sqrt{d})), \quad \varepsilon_i \sim_{iid} N(0, \tau^2).$$

Theorem (Mei, Misiakiewicz, Montanari, 2021)

Assume $d^{\ell-1+\delta} \le \min(n, N) \le d^{\ell-\delta}$ and $|\log(n/N)| \ge \delta \log d$, σ satisfies some generic conditions and λ is small enough. Then,

$$\|f_\star - \widehat{\mathrm{RF}}^{\mathrm{inv}}_{n,N,\lambda}\|_{L^2}^2 = \|\mathrm{P}_{>\ell} f_\star\|_{L^2}^2 + o_{d,\mathbb{P}}(\cdot).$$

- Standard RF model:

$$\text{For } d^{\ell+\delta} \le \min(n, N) \le d^{\ell+1-\delta}, \qquad \|f_\star - \widehat{\mathrm{RF}}_{n,N,\lambda}\|_{L^2}^2 = \|\mathrm{P}_{>\ell} f_\star\|_{L^2}^2 + o_d(\cdot).$$

  Gain a factor d in features and sample complexity by using invariant RF.

- More generally, for $\mathcal{G}_d$ with 'degeneracy α', we gain a factor d^α.

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Numerical simulations

$$f_{\text{lin}} = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} x_i, \qquad f_{\text{quad}} = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} x_i x_{i+1}, \qquad f_{\text{cube}} = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} x_i x_{i+1} x_{i+2}.$$

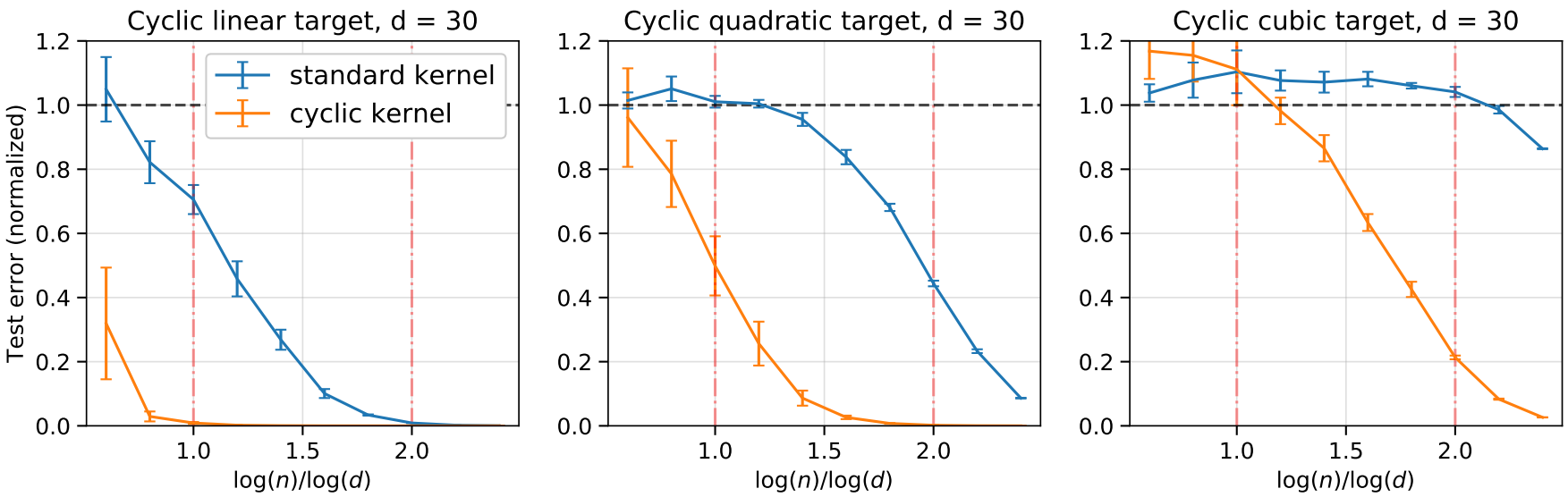
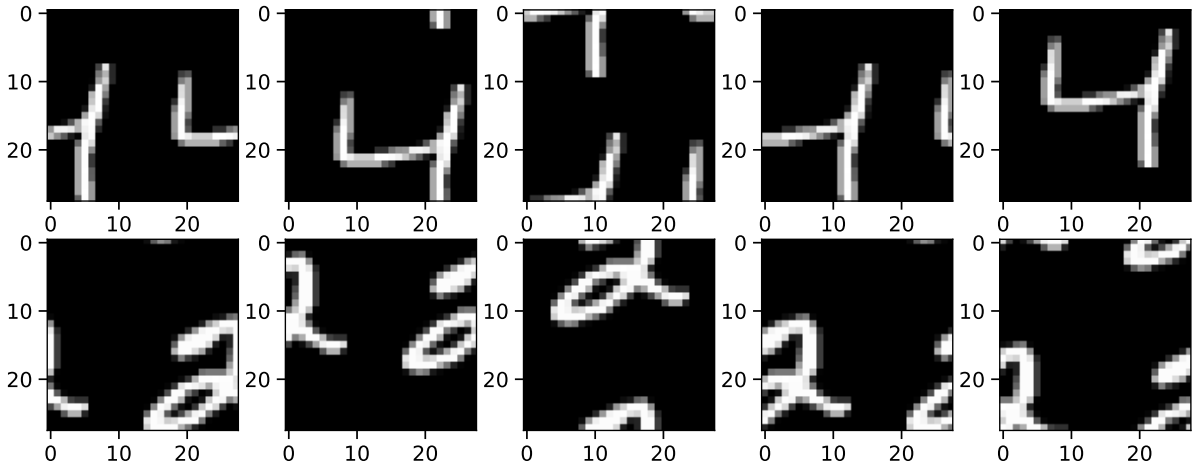


Figure: Test error of KRR with invariant kernel and inner-product kernel.

Cyclic invariant MNIST



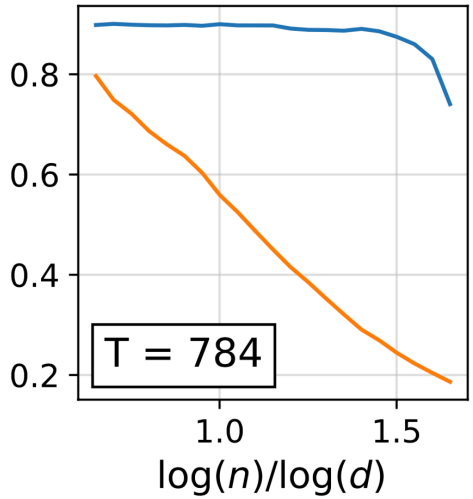


Figure: Test accuracy against number of samples (orange: cyclic kernel, blue: standard kernel).

Summary

What I illustrated in this talk:

- **Isotropic covariates model:**
  Kernel methods suffer from the *curse of dimensionality* and perform inferior to NNs due to **lack of feature learning.**

- **Spiked covariates model:**
  For large covariate SNR, **feature learning is unecessary** and kernel methods can also perform well.

- **Invariant function estimation:**
  Invariant kernels outperform standard kernels and we quantify the gain in statistical efficiency.

All the results in this talk can be derived from a general framework for getting high-dimensional asymptotics of test error of random features and kernel methods.

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Open problems

- Show that NNs trained by gradient descent overcome the curse of dimensionality in the spiked covariates model (using mean-field dynamics, see [Chizat, Bach, '20]).
- What are other latent low-dimensional structure that we can study? (other than the spiked covariates model)
- Using our general framework to study more complicated kernels.
- Data dependent kernel methods?
- Practical advantages of using kernel methods vs NNs? Transfer learning, robustness...
- ...

Thank you!