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.

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Neural Tangent (NT) model

- Neural network: $\mathrm{NN}_p(x; \ ), \ x \ 2 \ \mathrm{R}^d, \quad 2 \ \mathrm{R}^p$.
  e.g., fully-connected neural network:

$$\mathrm{NN}_p(x; \ ) = ha; \ (:::W_2 \ (W_1 x))i:$$

- Linearization around random initialization $_0$:

$$\mathrm{NN}_p(x; \ ) = \mathrm{NN}_p(x; \ _0) + h \quad _0; r \ \mathrm{NN}_p(x; \ _0)i + o(k \quad _0k_2):$$

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

$$\mathrm{NT}_p(x; \ ; \ _0) = h \ ; r \ \mathrm{NN}_p(x; \ _0)i:$$

- Finite-width approximation of limiting kernel ($p \ ! \ 1$ + iid initialization):

$$K_{\mathrm{NT}}(x; y) = \mathrm{E}_{\ _0}[h r \ \mathrm{NN}_p(x; \ _0); r \ \mathrm{NN}_p(y; \ _0)i]:$$

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Coupled gradient descent on empirical squared loss:

$$\frac{\mathrm{d}}{\mathrm{d}t}\ ^{t} = \quad r\ \hat{E}[(y \quad \mathrm{NN}_p(x;\ ^{t}))^2]; \qquad ^{0} = \ _{0};$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\ ^{t} = \quad r\ \hat{E}[(y \quad \mathrm{NT}_p(x;\ ^{t};\ _{0}))^2]; \qquad ^{0} = 0:$$

Theorem (informal)

For any $" > 0$, for large enough NNs and proper random initialization $_0$ (Xavier initialization), we have with high probability

$$\sup_{t} \sup_{0\ kxk_2=1} j\mathrm{NN}_p(x;\ ^{t}) \quad \mathrm{NT}_p(x;\ ^{t};\ _{0})j \quad ":$$

$=)$ Intuition: *weights do not change much* and $k\ ^{t} \quad _0k_2$ remains small.

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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.

- $\therefore$ but:
  - 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-o 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%
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- 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.
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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 $f(y_i; x_i)g_{i\,2[n]}$:

$$y_i = f_\star(x_i) + "_i; \qquad x_i \quad _{iid} \text{Unif}(S^{d\ \ 1}(^{p}\overline{d})); \qquad "_i \quad _{iid} N(0; \ \ ^2):$$

- Two-layers neural networks: $\text{NN}_N(x; \ \ ) = \sum_{i=1}^{N} a_i \ \ (hw_i; x\,i)$.

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

$$\text{RF}_N(x; a; W) = \sum_{i=1}^{N} a_i \ \ (hw_i; x\,i) = ha; \ r_{\ a}\text{NN}_p(x; \ \ _0)i:$$

- Ridge regression with RF model (with fixed $W = (w_i)_{i\,2[N]} \quad _{iid} \text{Unif}(S^{d\ \ 1})$)

$$\hat{a}(\ \ ) = \arg\min_a \left\{ \frac{1}{n}\sum_{i=1}^{n}\left(y_i \quad \sum_{j=1}^{N} a_j \ \ (hw_j; x_i\,i)\right)^2 + \ \ kak_2^2 \right\}:$$

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Test error of RF model

Theorem (Mei, Misiakiewicz, Montanari, 2021)

Assume $d^{\ell+\delta}$ $\min(n; N)$ $d^{\ell+1}$ $^{\delta}$ and $j \log(n/N)j$ $\log d$, satisfies some generic conditions and is small enough. Then,

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

$\mathrm{P}_{>\ell}$: 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:

$$\text{Test error}(n; N) = \max\left\{\text{approx. error } (n = 1; N); \text{statistical error } (n; N = 1)\right\}.$$

- Statistical error $(n; N = 1)$: 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

$$f = P_0 f + P_1 f + P_2 f + P_3 f + P_4 f :$$

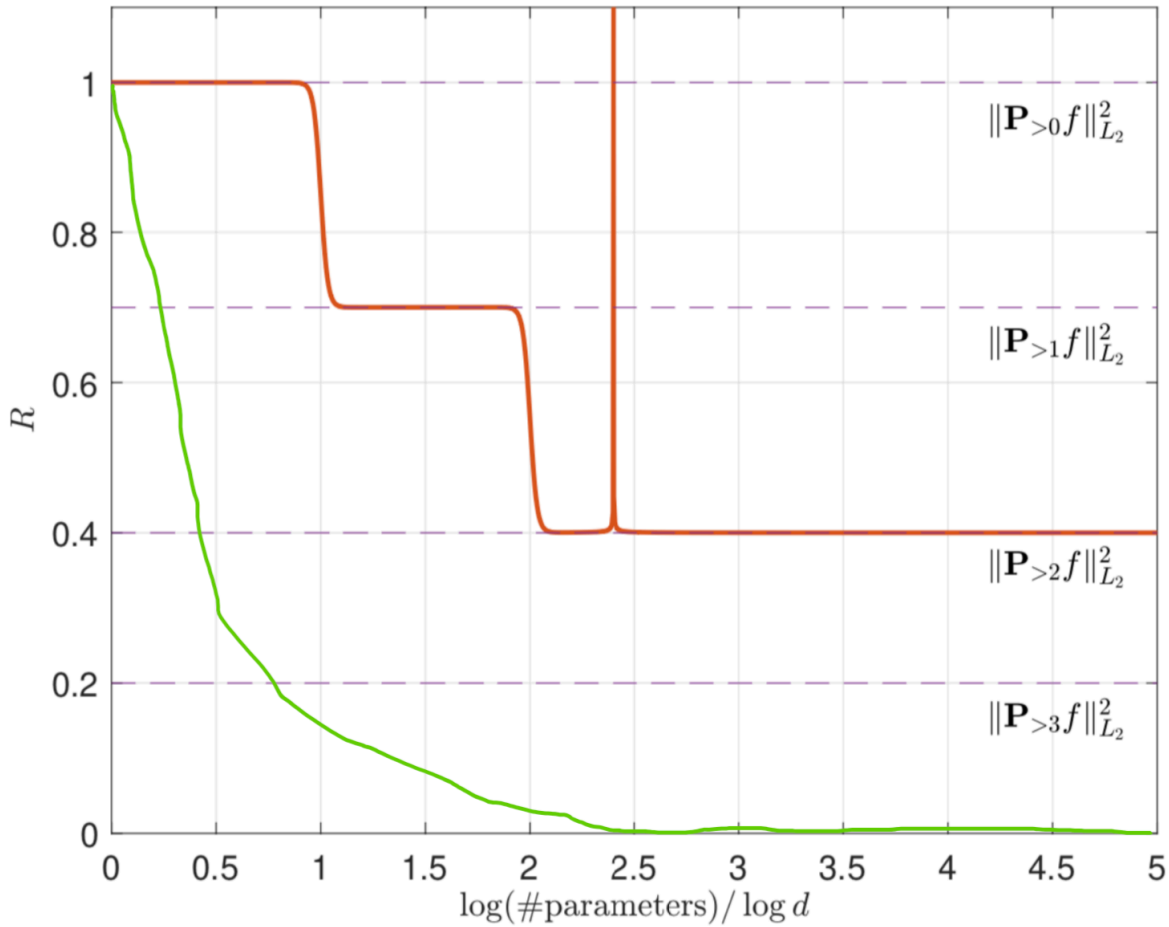

Figure: Test error (in red) v.s. $\log(N)/\log(d)$ for $n = d^{2.4}$ and $\quad = 0^+$. Train error in green.

Performance gap between NN and kernel methods

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

  E.g., $f_\star(x) = \quad (\langle w_\star, x\rangle)$: if $N \;/\; 1$ and $n \;/\; d$, then GD solution:

$$\|f_\star - \widehat{\mathrm{NN}}_{N,n}\|_{L^2}^2 = o_{d,\mathrm{P}}(1) \qquad \text{[Bai et al.,'16]}$$

  while for KRR:

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

- 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 $\sigma'(x_1)$ using features $\sigma(\langle w_i, x\rangle)$

- For RF, w_i's are random, $\mathrm{corr}(x_1 e_1, \langle w_i, x\rangle)^2 = \langle w_i, e_1\rangle^2 / \|w_i\|_2^2$ is small in HD.
- For NN, w_i's can be chosen to have a large correlation with e_1.

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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 $[U; U^?]$

$$x = Uz_1 + U^? z_2; \qquad z_1 \; 2 \; \mathrm{R}^{d_s}; z_2 \; 2 \; \mathrm{R}^{d \;\; d_s}:$$

Signal part: $z_1 \quad \mathrm{Unif}\left(\mathrm{S}^{d_s \;\; 1}\left(\sqrt{\mathrm{snr}_c \;\; d_s}\right)\right)$.

Noise part: $z_2 \quad \mathrm{Unif}\left(\mathrm{S}^{d \;\; d_s \;\; 1}\left(\sqrt{d \;\;\; d_s}\right)\right)$

d_s = signal dimension.

snr_c = covariate SNR.

Target function: $f_\star(x) = \;'(z_1)$.

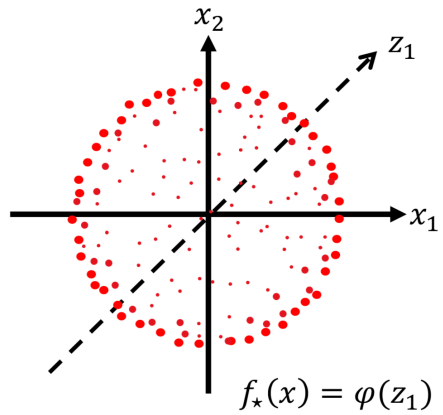

Figure: Isotropic covariates: $\mathrm{snr}_c = 1$.

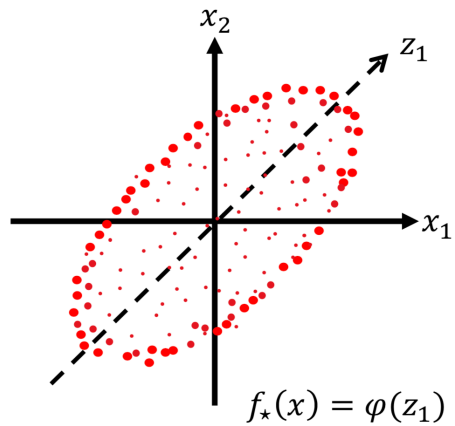

Figure: Anisotropic covariates: $\mathrm{snr}_c > 1$.

Test error of KRR in the spiked covariates model

- Given iid samples $(f x_i ; y_i g)_{i 2 [n]}$ from the spiked covariates model.
- Effective dimension: $d_{\text{eff}} = d_s \_ (d = \text{snr}_c)$.

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

Assume $d_{\text{eff}}{}^{\ell+\delta}$ $\min(n; N)$ $d_{\text{eff}}{}^{\ell+1}{}^{\ \delta}$ and $j \log(n=N) j$ $\log d_{\text{eff}}$, satisfies some generic conditions and is small enough. Then,

$$k f_\star \quad \widehat{\text{RF}}_{n,N,\lambda} k_{L^2}^2 = k \text{P}_{>\ell} f_\star k_{L^2}^2 + o_{d,\text{P}}(\ ):$$

- d_{eff} capture the 'effective low-dimensionality' of the data.
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- On the contrary, we expect NNs to learn features w_i aligned with z_1 and to depend mildly on snr_c.

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NNs vs kernel methods in the spiked covariates model

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

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 d_{eff} d:

  Test error: NN Kernel methods

- d_{eff} decreases with snr_c:
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Intuition for the gap: anisotropic case

Goal: fitting $'(x_1)$ using features $(hw_i; x\,i)$.

Consider $\mathsf{E}[xx^{\mathsf{T}}] = \mathrm{diag}(\mathrm{snr}_c; \mathrm{Id}_{d\ \ 1})$.

- To fit $'(x_1)$, we need to use features $(hw_i; x\,i)$ that are correlated to x_1, i.e.,

$$\mathrm{corr}(x_1 e_1; hw_i; x\,i) = \mathrm{snr}_c \ \frac{hw_i; e_1 i^2}{k^{\ 1/2} w_i k_2^2} = \mathrm{snr}_c \ \ O_{d,\mathsf{P}}(d^{\ 1}) = O_{d,\mathsf{P}}(d_{\mathrm{eff}}^{\ 1}):$$

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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 ($y = f_\star(x) = \ '(z_1)$).

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

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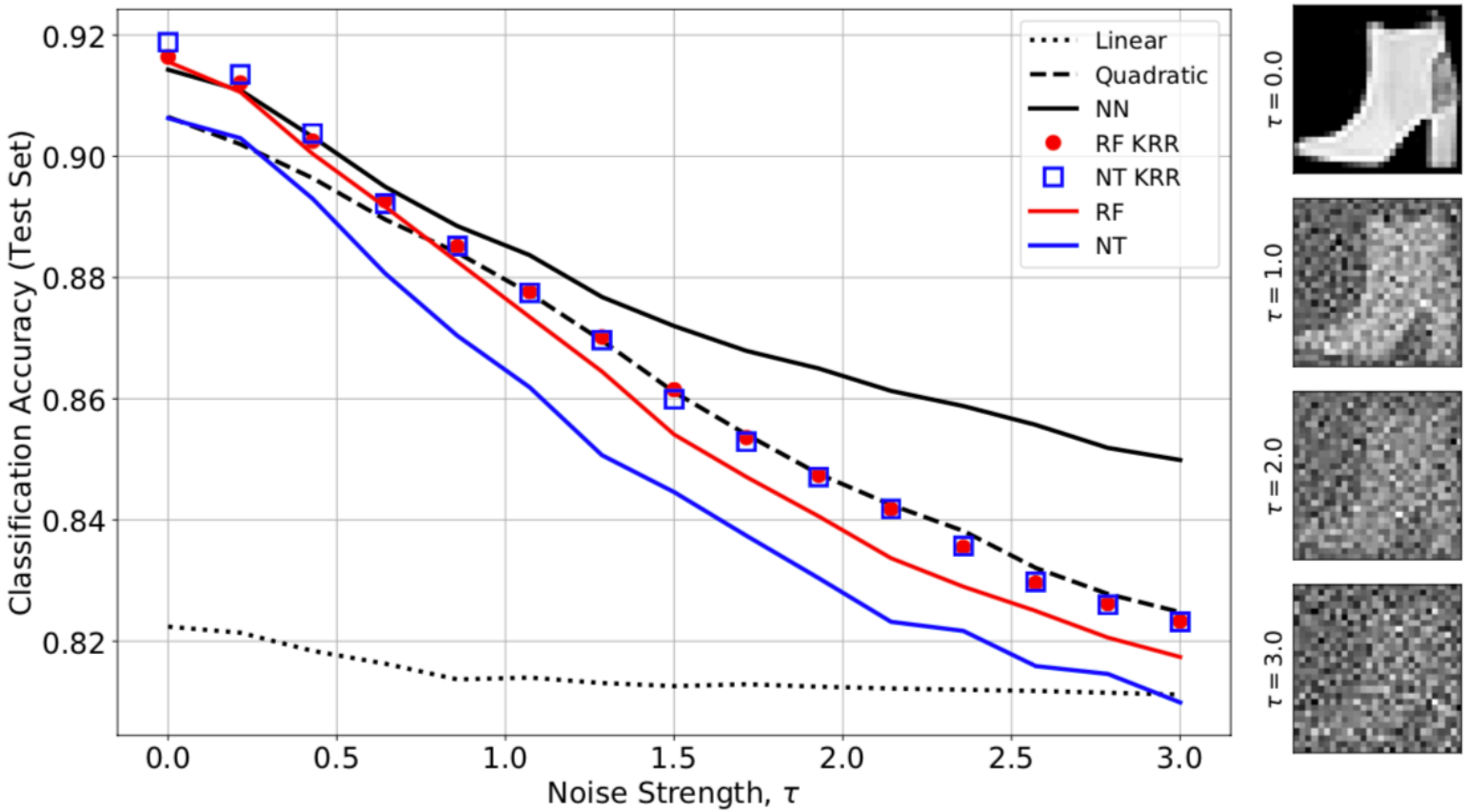

Figure: Test accuracy on FMNIST: adding noise to the high frequency components.

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.

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Cyclic function estimation on the sphere

- Data x Unif($S^{d\ 1}(\sqrt{p}\overline{d})$).
- Consider $G_d = fg_0; g_1; : : : ; g_{d\ 1}g$ the cyclic group:

$$g_i\ x = (x_{d\ i+1}; x_{d\ i+2}; : : : ; x_d; x_1; x_2; : : : ; x_{d\ i}):$$

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

$$\text{i.e., } f_\star(g\ x) = f_\star(x) \text{ for all } g\ 2\ G_d.$$

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

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

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Invariant random features and kernels

- Invariant RF model:

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

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

$$K_{\mathrm{inv}}(x;y) = \int_{g \in G_d} h(\langle g \cdot x; y \rangle / d)\ (\mathrm{d}g).$$

- Compared to standard RF model:

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

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Test error of KRR with invariant kernel

- Cyclic invariant $f_\star$: given iid samples $f(y_i; x_i)g_{i\,2[n]}$,

$$y_i = f_\star(x_i) + "_i; \qquad x_i \quad _{iid} \text{Unif}(S^{d\ 1}(^{p}\overline{d})); \quad "_i \quad _{iid} N(0; \ ^2):$$

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

- More generally, for G_d with 'degeneracy ', we gain a factor d^α.

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Numerical simulations

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

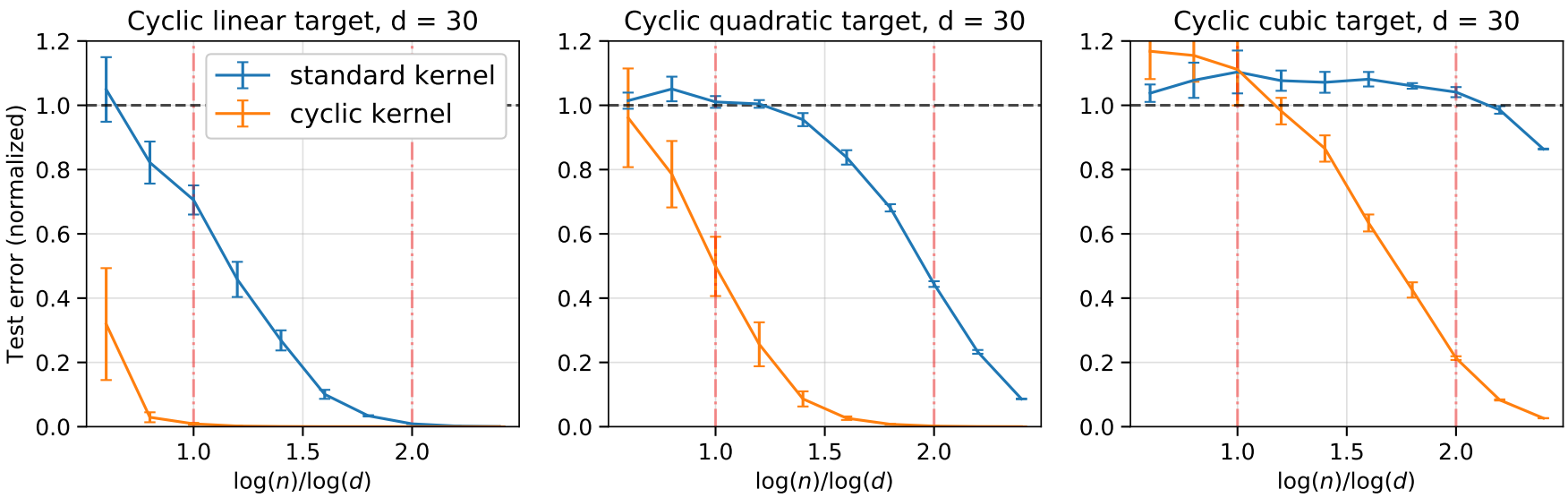
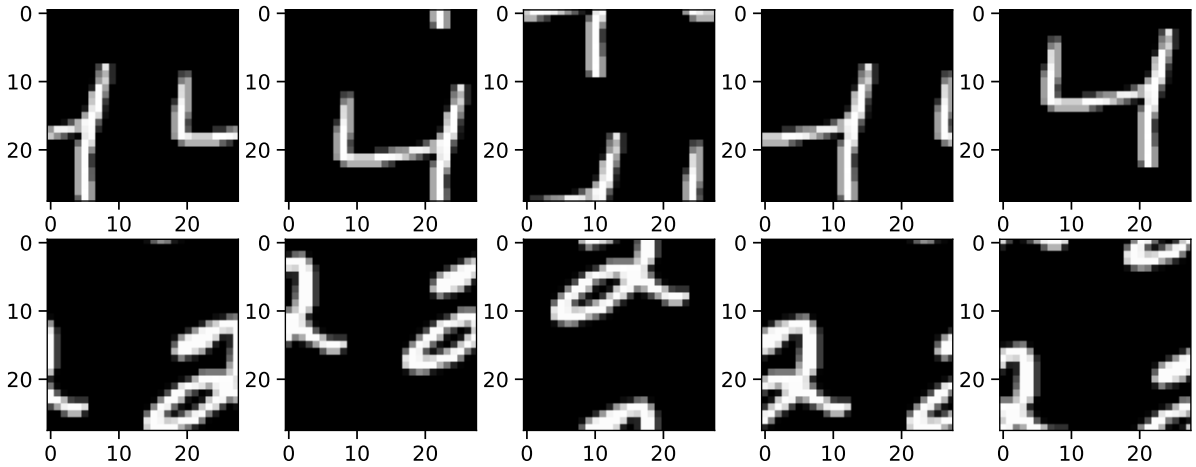


Figure: Test error of KRR with invariant kernel and inner-product kernel.

Cyclic invariant MNIST



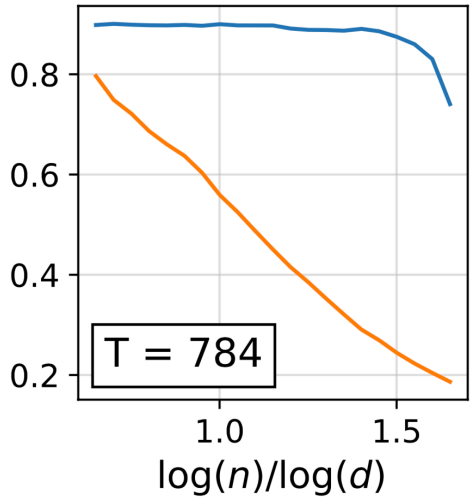


Figure: Test accuracy against number of samples (orange: cyclic kernel, blue: standard kernel).

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!