Lausanne Event on ML and NN Theory 2024

A Theory of Non-Linear Feature Learning with One Gradient Step in Two-Layer Neural Networks[1]

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May 31, 2024

[1] ICML 2024. Slide credit: Behrad Moniri

Collaborators

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Introduction

Deep Learning is *very* successful.

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- Why is it so successful? Despite fitting so many parameters and aiming to solve hugely non-convex problems?
- Vast range of theoretical explanations have been proposed... But still no definitive answer.

Some proposed explanations

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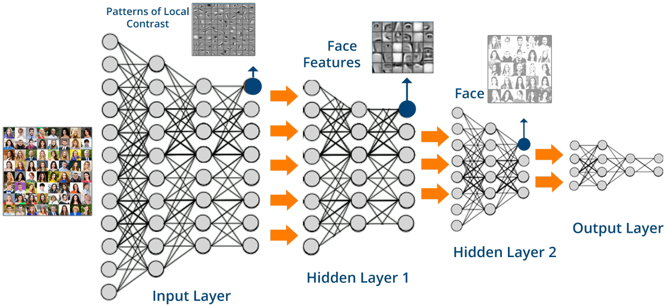
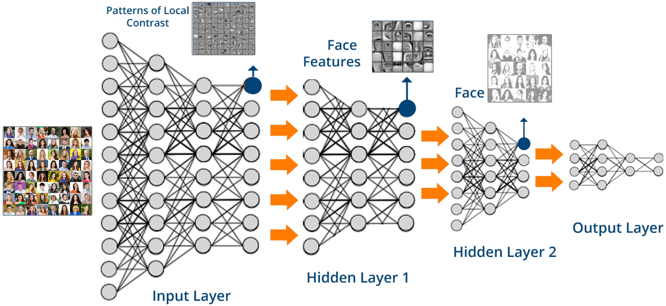
- Feature learning
- ...

Feature Learning



Feature Learning



People also ask

Why is deep learning more effective?

Unlike traditional machine learning techniques, deep learning algorithms can automatically extract intricate patterns and features from raw data, eliminating the need for manual feature engineering. This not only saves valuable time but also enhances the efficiency and accuracy of predictive models. Feb 29, 2024

Our work

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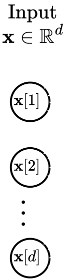
  1. Non-standard training, isotropic data

Two-Layer Neural Networks



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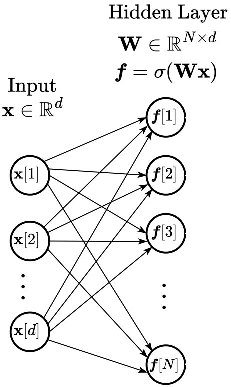

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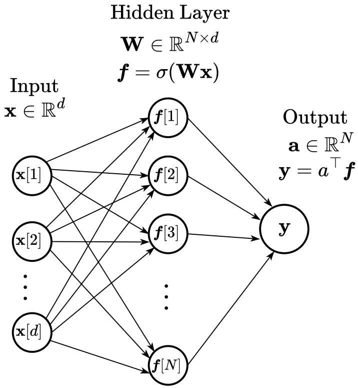

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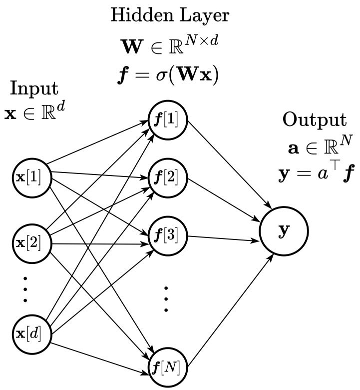
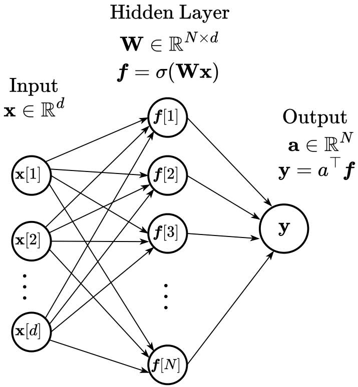


Proportional Asymptotic Regime: $n, d, N \to \infty$ with $d/n \to \phi$ and $d/N \to \psi$.

Training and Optimization



- **Simplest Version:**

  Random Feature Model.

  (Rahimi and Recht, 2007)

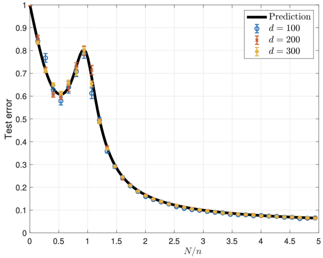
Random Feature Models

- Analysis of random feature models is popular:

Random Feature Models

- Analysis of random feature models is popular:
  - Used to study various aspects of deep learning such as double descent, robustness to adversarial attacks, privacy, fairness, OOD performance, calibration, etc.

See e.g., Mei and Montanari (2022); Gerace et al. (2020); Lin and Dobriban (2021); Lee et al. (2023); Hassani and Javanmard (2022); Bombari and Mondelli (2023); Bombari et al. (2023); Clarté et al. (2023), etc.



Double descent in random feature models (Mei and Montanari, 2022).

Random Feature Models

- Random feature models can only learn linear functions under proportional asymptotics.

  Ghorbani et al. (2021); Mei and Montanari (2022); Hu and Lu (2023),...

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$$\sigma(\mathbf{W}x) = c_1\mathbf{W}x + c_2 H_2(\mathbf{W}x) + \cdots$$

$$\approx c_1\mathbf{W}x + z$$

Random Feature Models

- Feature learning is absent in random feature models. How to go beyond random feature models?

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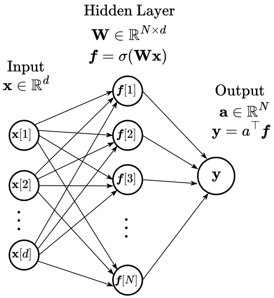
- Feature learning is absent in random feature models. How to go beyond random feature models?
- Realistic training is beyond reach (for now). Existing theoretical approaches:
  - Tensor programs. (Greg Yang et al., 2021+)
  - One step of gradient descent on first layer weights. Damian et al. (2022), Ba et al. (2022), Dandi et al. (2023), Cui et al. (2024), ...
  - ...

One Gradient Step

One Gradient Step Update

We train the network as follows:

Damian et al. (2022), Ba et al. (2022), Dandi et al. (2023), Cui et al. (2024), ...



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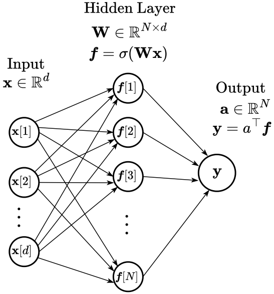
$$\boldsymbol{a} \sim \mathcal{N}\left(\mathbf{0}_N, \frac{1}{N}\mathbf{I}_N\right), \quad \text{and} \quad [\mathbf{W}_0]_{ij} \sim \mathcal{N}\left(0, \frac{1}{d}\right)$$



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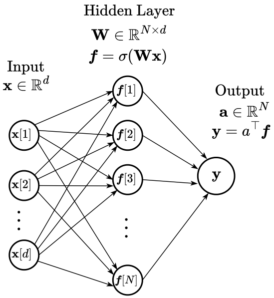
2. Take one gradient step on the empirical MSE loss $\mathcal{L}$:

$$\mathbf{W} = \mathbf{W}_0 - \eta \frac{\partial}{\partial \mathbf{W}} \left(\frac{1}{2n} \|\boldsymbol{y} - \sigma(\mathbf{X}\mathbf{W}^\top)\boldsymbol{a}\|_2^2 \right) \Big|_{\mathbf{W}_0, \boldsymbol{a}}$$



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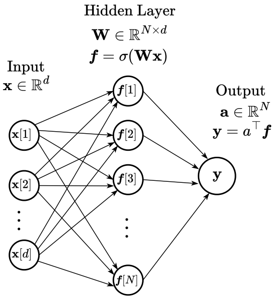
3. Fit $\boldsymbol{a}$ via ridge regression on independent dataset $\tilde{\mathbf{X}}, \tilde{\boldsymbol{y}}$ of same size:

$$\hat{\boldsymbol{a}} = \underset{\tilde{\boldsymbol{a}} \in \mathbb{R}^N}{\arg\min} \frac{1}{n}\|\tilde{\boldsymbol{y}} - \mathbf{F}\tilde{\boldsymbol{a}}\|_2^2 + \lambda\|\tilde{\boldsymbol{a}}\|_2^2, \quad \mathbf{F} = \sigma(\tilde{\mathbf{X}}\mathbf{W}^\top) \in \mathbb{R}^{n \times N}.$$



Data Generation

- **Data generation:**

$$x_i \overset{i.i.d.}{\sim} \mathsf{N}(0, \mathbf{I}_d), \quad y_i = f_\star(\boldsymbol{x}_i) + \varepsilon_i,$$

where $\varepsilon_i \overset{i.i.d.}{\sim} \mathsf{N}(0, \sigma_\varepsilon^2)$. Let $\mathbf{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n]^\top \in \mathbb{R}^{n \times d}$, $\boldsymbol{y} = (y_1, \ldots, y_n)^\top \in \mathbb{R}^n$ and $\tilde{\mathbf{X}} = [\boldsymbol{x}_{n+1}, \ldots, \boldsymbol{x}_{2n}]^\top \in \mathbb{R}^{n \times d}$, $\tilde{\boldsymbol{y}} = (y_{n+1}, \ldots, y_{2n})^\top \in \mathbb{R}^n$.

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- With one step, only a single-index approximation can be learned. (see e.g., Dandi et al. (2023), etc.) Thus, we let

$$f_\star(\boldsymbol{x}_i) = \sigma_\star(\boldsymbol{\beta}_\star^\top \boldsymbol{x}_i)$$

Prior Work

Partial understanding in prior work:

- Ba et al. (2022) show that if $\eta = O(1)$, still no nonlinear component of the teacher function can be learned. Performance is still worse than linear regression on full data.

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- Ba et al. (2022) show that if $\eta = O(1)$, still no nonlinear component of the teacher function can be learned. Performance is still worse than linear regression on full data.

- However, with $\eta = O(\sqrt{n})$ the one-step updated random features model can outperform linear and kernel predictors.

- How? What features are learned? By how much does performance improve?

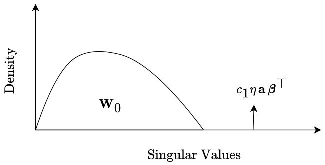
Spectral Analysis of the Feature Matrix

Spectrum of the Weights

$$\mathbf{W} = \mathbf{W}_0 - \eta \frac{\partial}{\partial \mathbf{W}} \left(\frac{1}{2n} \|\boldsymbol{y} - \sigma(\mathbf{X}\mathbf{W}^\top)\boldsymbol{a}\|_2^2 \right) \Big|_{\mathbf{W}_0, \boldsymbol{a}}$$

$$\approx \mathbf{W}_0 + \eta c_1 \boldsymbol{a} \left(\frac{\mathbf{X}^\top \boldsymbol{y}}{n} \right)^\top$$

Ba et al. (2022)

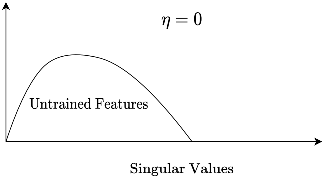


The vector $\boldsymbol{\beta} := \frac{\mathbf{X}^\top \boldsymbol{y}}{n}$ is aligned with $\boldsymbol{\beta}_\star$.

Spectrum of the Feature Matrix

Updated Weight Matrix: $\mathbf{W} \approx \mathbf{W}_0 + \eta c_1 \boldsymbol{a} \boldsymbol{\beta}^\top$

Feature Matrix: $\mathbf{F} = \sigma(\tilde{\mathbf{X}}\mathbf{W}^\top) \approx \sigma(\tilde{\mathbf{X}}\mathbf{W}_0^\top + c_1 \eta \tilde{\mathbf{X}} \boldsymbol{\beta} \boldsymbol{a}^\top) \in \mathbb{R}^{n \times N}$



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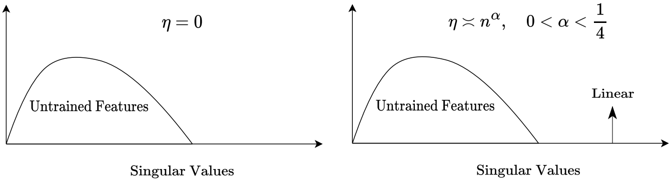

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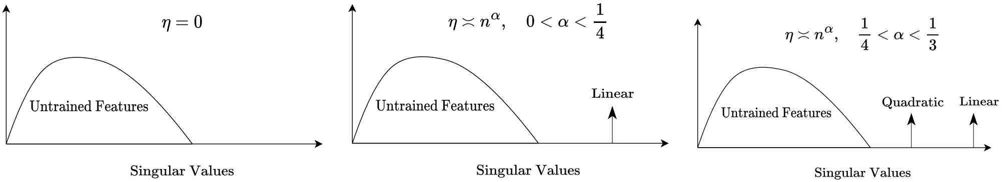

Non-linearity pushes spikes outside the spectrum of random features $\sigma(\tilde{\mathbf{X}}\mathbf{W}_0^\top)$, creating non-linear features.

Spectrum of Updated Feature Matrix

Recall $\mathbf{F}_0 = \sigma(\tilde{\mathbf{X}}\mathbf{W}_0^\top)$, $\mathbf{F} = \sigma(\tilde{\mathbf{X}}\mathbf{W}^\top) \approx \sigma(\tilde{\mathbf{X}}\mathbf{W}_0^\top + c_1\eta\tilde{\mathbf{X}}\boldsymbol{\beta}\boldsymbol{a}^\top)$. Hermite expansion in L^2 of activation function $\sigma : \mathbb{R} \to \mathbb{R}$, $c_1 \neq 0$:

$$\sigma(z) = \sum_{k=1}^{\infty} c_k H_k(z), \quad c_k = \frac{1}{k!}\mathbb{E}_{Z\sim\mathsf{N}(0,1)}[\sigma(Z)H_k(Z)].$$

Theorem

Let $\eta \asymp n^\alpha$ with $\frac{\ell-1}{2\ell} < \alpha < \frac{\ell}{2\ell+2}$ for some $\ell \in \mathbb{N}$. Under conditions,

$$\|\mathbf{F} - \mathbf{F}_\ell\|_{\mathrm{op}} = o_P(\sqrt{n}), \text{ with } \mathbf{F}_\ell := \mathbf{F}_0 + \sum_{k=1}^{\ell} c_1^k c_k \eta^k (\tilde{\mathbf{X}}\boldsymbol{\beta})^{\circ k}(\boldsymbol{a}^{\circ k})^\top.$$

Spectrum of Updated Feature Matrix

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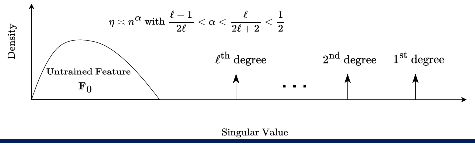

Some Intuition

- Recall

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- Consider $c_1^k c_k \eta^k (\tilde{\mathbf{X}}\boldsymbol{\beta})^{\circ k} (\boldsymbol{a}^{\circ k})^\top$. Its operator norm is of order

$$\eta^k \|(\tilde{\mathbf{X}}\boldsymbol{\beta})^{\circ k}\| \|\boldsymbol{a}^{\circ k}\| \approx n^{\alpha k} n^{1/2} n^{1/2-k/2} = n^{(\alpha-1/2)k+1}$$

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- We have $n^{(\alpha-1/2)k+1} \gg n^{1/2}$ iff $(1/2-\alpha)k < 1/2$ iff $\alpha > 1/2 - 1/(2k) = (k-1)/(2k)$

Training/Test Error

Universality

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    1. we replace $\mathbf{F} = \sigma(\tilde{\mathbf{X}}\mathbf{W}^\top)$ with

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  2. we replace $\mathbf{F}_0$ with $c_1 \tilde{\mathbf{X}}\mathbf{W}_0^\top + c_{>1}\mathbf{Z}$, $c_{>1} = (\sum_{k=2}^{\infty} k! c_k^2)^{1/2}$. (Gaussian equivalence; needs work here)

Training/Test Errors

Theorem

Let $\ell \in \mathbb{N}$ *and* $\eta \asymp n^{\alpha}$ *with* $\frac{\ell-1}{2\ell} < \alpha < \frac{\ell}{2\ell+2}$, *then under conditions, for the learned feature map* $\mathbf{F}$ *and the untrained feature map* $\mathbf{F}_0$, *we have*

$$\mathcal{L}_{\text{tr}}(\mathbf{F}_0) - \mathcal{L}_{\text{tr}}(\mathbf{F}) \to_P \Delta_{\text{tr}} \geq 0,$$

$$\mathcal{L}_{\text{te}}(\mathbf{F}_0) - \mathcal{L}_{\text{te}}(\mathbf{F}) \to_P \Delta_{\text{te}} \geq 0.$$

For test error, cover $\ell = 1, 2$.

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For test error, cover $\ell = 1, 2$.

Recent breakthrough: Test error for $\alpha = 1/$ via equivalent *spiked random features* model. Cui et al. (2024)

Details of Training/Test Error Analysis

Conditions:

1. We let $f_\star : \mathbb{R}^d \to \mathbb{R}$ be $f_\star(\boldsymbol{x}) = \sigma_\star(\boldsymbol{x}^\top \boldsymbol{\beta}_\star)$ for all $\boldsymbol{x}$, where $\boldsymbol{\beta}_\star \in \mathbb{R}^d$ is an unknown parameter with $\boldsymbol{\beta}_\star \sim \mathsf{N}(0, \frac{1}{d}\mathbf{I}_d)$ and $\sigma_\star : \mathbb{R} \to \mathbb{R}$ is a $\Theta(1)$-Lipschitz *teacher activation* function.
2. The teacher activation $\sigma_\star : \mathbb{R} \to \mathbb{R}$ has the following Hermite expansion in L^2:

$$\sigma_\star(z) = \sum_{k=1}^{\infty} c_{\star,k} H_k(z), \;\; c_{\star,k} = \frac{1}{k!} \mathbb{E}_{Z \sim \mathsf{N}(0,1)}[\sigma_\star(Z) H_k(Z)].$$

Also, we define $c_\star = (\sum_{k=1}^{\infty} k! c_{\star,k}^2)^{\frac{1}{2}}$.

Details of Training/Test Error Analysis

Conditions, ctd.:

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$$\sigma(z) = \sum_{k=1}^{\infty} c_k H_k(z), \quad c_k = \frac{1}{k!}\mathbb{E}_{Z\sim \mathsf{N}(0,1)}[\sigma(Z)H_k(Z)].$$

The coefficients satisfy $c_1 \neq 0$ and $c_k^2 k! \leq Ck^{-\frac{3}{2}-\omega}$ for some $C, \omega > 0$ and for all $k \geq 1$. Moreover, the first three derivatives of σ exist almost surely, and are bounded.

Special Case of Training Loss

Recall $n, d, N \to \infty$ with $d/n \to \phi$ and $d/N \to \psi$; c_i are Hermite coeffs of fitted RF nonlin. σ; $c_{\star,i}$ are Hermite coeffs of true nonlin. $\sigma_\star$

Proposition (Learning Linear & Quadratic Features)

If $c_1 \neq 0$ and $\eta \asymp n^\alpha$ with $0 < \alpha < \frac{1}{4}$, we have

$$\mathcal{L}_{\mathrm{tr}}(\mathbf{F}_0) - \mathcal{L}_{\mathrm{tr}}(\mathbf{F}) \to_P \Delta_1 := \frac{\psi \lambda c_{\star,1}^4 m_2}{\phi[c_{\star,1}^2 + \phi(c_\star^2 + \sigma_\varepsilon^2)]} \geq 0. \tag{1}$$

If also $c_2 \neq 0$ and $\eta \asymp n^\alpha$ with $\frac{1}{4} < \alpha < \frac{1}{3}$, we have

$$\mathcal{L}_{\mathrm{tr}}(\mathbf{F}_0) - \mathcal{L}_{\mathrm{tr}}(\mathbf{F}) \to_P \Delta_2 := \Delta_1 + \frac{4\psi \lambda c_{\star,1}^4 c_{\star,2}^2 m_1}{3\phi[\phi(c_\star^2 + \sigma_\varepsilon^2) + c_{\star,1}^2]^2} \geq 0. \tag{2}$$

Analysis of Training/Test Error

- **Limiting traces:** For $\mathbf{F}_0 = \sigma(\tilde{\mathbf{X}}_0 \mathbf{W}^\top)$, (Pennington and Worah, 2017; Adlam and Pennington, 2020)

$$m_1 := \frac{\phi}{\psi} \lim_{d,n,N\to\infty} \operatorname{tr}((\mathbf{F}_0\mathbf{F}_0^\top + \lambda n \mathbf{I}_n)^{-1}) > 0$$
$$m_2 := \frac{\phi}{\psi} \lim_{d,n,N\to\infty} \frac{1}{d} \operatorname{tr}(\tilde{\mathbf{X}}^\top (\mathbf{F}_0\mathbf{F}_0^\top + \lambda n \mathbf{I}_n)^{-1} \tilde{\mathbf{X}}) > 0.$$

- Unique solutions of the system of equations:

$$\phi\,(m_1 - m_2)\left(c_{>1}^2 m_1 + c_1^2 m_2\right) + \Psi(m_1, m_2) = 0,$$
$$\frac{\phi}{\psi}\left(c_1^2 m_1 m_2 + \phi\,(m_2 - m_1)\right) + \Psi(m_1, m_2) = 0,$$

where $\Psi(m_1, m_2) = c_1^2 m_1 m_2\,(\lambda \psi m_1/\phi - 1)$ and $c_{>1} = (\sum_{k=2}^{\infty} k! c_k^2)^{1/2}$.

Special Cases of Test Error

Proposition (Learning Linear & Quadratic Features)

If $c_1 \neq 0$ and $\eta \asymp n^\alpha$ with $0 < \alpha < \frac{1}{4}$, we have

$$\mathcal{L}_{\mathrm{te}}(\mathbf{F}_0) - \mathcal{L}_{\mathrm{te}}(\mathbf{F}) \to_P \Lambda_1 := \frac{c_{\star,1}^4}{[c_{\star,1}^2 + \phi(c_\star^2 + \sigma_\varepsilon^2)]} \left(-\frac{\partial m_2}{\partial \lambda}\right) \geq 0. \tag{3}$$

If also $c_2 \neq 0$ and $\eta \asymp n^\alpha$ with $\frac{1}{4} < \alpha < \frac{1}{3}$, we have

$$\mathcal{L}_{\mathrm{te}}(\mathbf{F}_0) - \mathcal{L}_{\mathrm{te}}(\mathbf{F}) \to_P \Lambda_1 + \frac{4c_{\star,1}^4 c_{\star,2}^2}{3[c_{\star,1}^2 + \phi(c_\star^2 + \sigma_\varepsilon^2)]^2 m_1^2} \left(-\frac{\partial m_1}{\partial \lambda}\right) \geq 0. \tag{4}$$

Training Error: General Case

Let $\xi_{i,j}$, $i,j \in \{0,1,\ldots\}$ s.t. for any $p \in \mathbb{N}$ and $x \in \mathbb{R}$, $x^p = \sum_{i=0}^{p} \xi_{p,i} H_i(x)$.

Theorem

Let $\ell \in \mathbb{N}$. If $c_1, \cdots, c_\ell \neq 0$, and $\eta \asymp n^\alpha$ with $\frac{\ell-1}{2\ell} < \alpha < \frac{\ell}{2\ell+2}$, then for the learned feature map $\mathbf{F}$ and the untrained feature map $\mathbf{F}_0$, we have $\mathcal{L}_{\mathrm{tr}}(\mathbf{F}_0) - \mathcal{L}_{\mathrm{tr}}(\mathbf{F}) \to_P \Delta_\ell \geq 0$, where

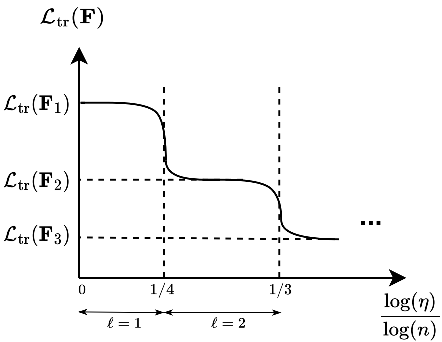
$$\Delta_\ell = \lambda \sum_{p=1}^{\ell} \sum_{q=1}^{\ell} c_{\star,p} c_{\star,q} r_p r_q \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \Omega_{i,j} \left(\phi(c_\star^2 + \sigma_\varepsilon^2) + c_{\star,1}^2 \right)^{(i+j)/2} \xi_{i,p} \xi_{j,q},$$

in which Ω is an invertible matrix with, $\forall i,j \in [\ell]$,

$$[\Omega^{-1}]_{i,j} = \left(c_{\star,1}^2 + \phi(c_\star^2 + \sigma_\varepsilon^2) \right)^{(i+j)/2} \frac{\psi}{\phi} \left[m_2 \xi_{i,1} \xi_{j,1} + m_1 \sum_{k=0,\ k\neq 1}^{\min(i,j)} k!\, \xi_{i,k} \xi_{j,k} \right],$$

and $r_p = \frac{p!\psi m_1}{\phi} \left(\frac{c_{\star,1}}{\sqrt{\phi(c_\star^2+\sigma_\varepsilon^2)+c_{\star,1}^2}} \right)^p, p \neq 1;\ r_p = \frac{\psi m_2}{\phi} \frac{c_{\star,1}}{\sqrt{\phi(c_\star^2+\sigma_\varepsilon^2)+c_{\star,1}^2}}, p = 1.$

Training Errors: “Staircase property"



Fit increasingly larger set of polynomial features. Consistent with *staircase property*. (Abbe et al., 2021, 2022; Berthier et al., 2023), . . .

Elements of the Proofs

- Training loss: $\mathcal{L}_{\rm tr}(\mathbf{F}) = \lambda \tilde{\boldsymbol{y}}^\top (\mathbf{F}\mathbf{F}^\top + \lambda n \mathbf{I}_n)^{-1} \tilde{\boldsymbol{y}}$.
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$$\mathbf{F}_0 = \sigma(\tilde{\mathbf{X}}\mathbf{W}_0^\top) \leftarrow c_1 \tilde{\mathbf{X}}\mathbf{W}_0^\top + c_{>1}\mathbf{Z}, \quad Z_{ij} \overset{i.i.d.}{\sim} \mathsf{N}(0,1).$$

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  The interaction between the first ℓ Hermite components of $\tilde{\boldsymbol{y}}$ and the spike terms is non-vanishing.
- Concentration + Adlam and Pennington (2020): find limits in terms of m_1, m_2.

Elements of the Proofs

- **Gaussian Equivalence:** Need to show that can replace

$$\mathbf{F}_0 = \sigma(\tilde{\mathbf{X}}\mathbf{W}_0^\top) \leftarrow c_1\tilde{\mathbf{X}}\mathbf{W}_0^\top + c_{>1}\mathbf{Z}, \quad Z_{ij} \overset{i.i.d.}{\sim} \mathsf{N}(0,1)$$

  w/o changing the limit of the nonlinear terms.
- We could not deduce this from existing results
- Adopt Lindeberg exchange method + concentration of QF + spectrum of kernel random matrices (El Karoui, 2010)

Simulations

Simulation Results

We consider

$$\textbf{Setting 1}: y = H_1(\boldsymbol{\beta}_\star^\top \boldsymbol{x}) + \varepsilon, \quad \varepsilon \sim \mathsf{N}(0,1),$$
$$\textbf{Setting 2}: y = H_1(\boldsymbol{\beta}_\star^\top \boldsymbol{x}) + \frac{1}{\sqrt{2}} H_2(\boldsymbol{\beta}_\star^\top \boldsymbol{x}).$$

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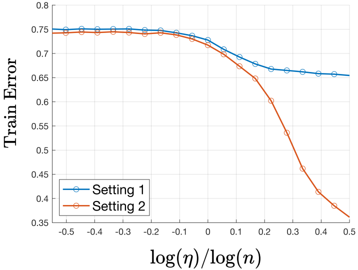

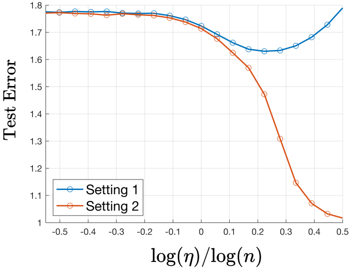

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- Thanks! Questions?

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