Be aware of model capacity when talking about generalization in modern machine learning

Fanghui Liu

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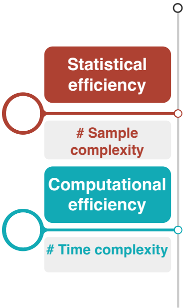
Centre for Discrete Mathematics and its Applications (DIMAP), Warwick

My research

❐ Research interests

- Foundations of machine learning (ML)
- Theory-grounded efficient algorithm design
- Trustworthy ML



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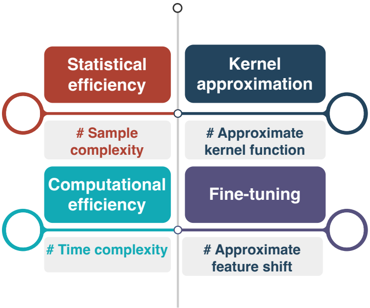

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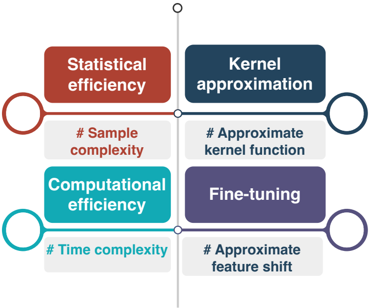
- characterize **learning efficiency** in theory
- contribute to practice



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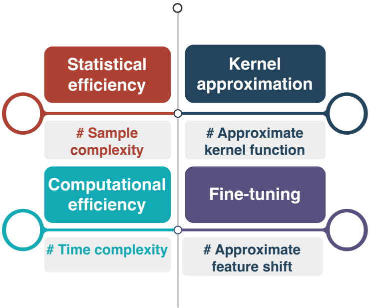

Learning efficiency (Curse of Dimensionality, CoD)

Machine learning works in **high dimensions** that can be a **curse**!

— David Donoho, 2000. (Richard E. Bellman, 1957)

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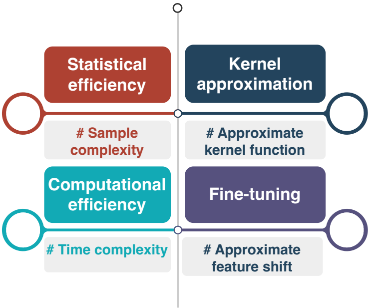

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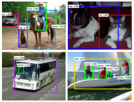
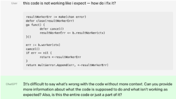
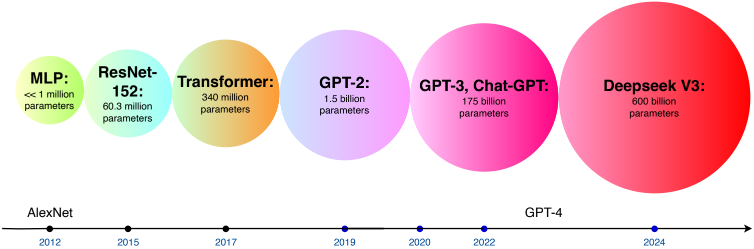
In the era of machine learning

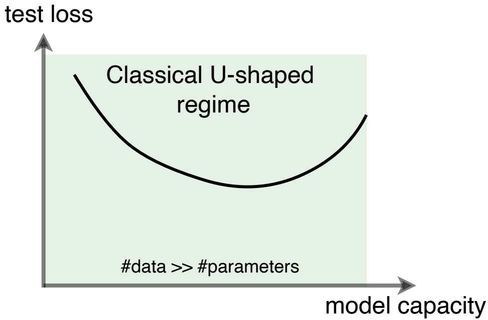
Prefer more data and larger model to obtain better performance...







ML textbooks: Larger models tend to overfit!



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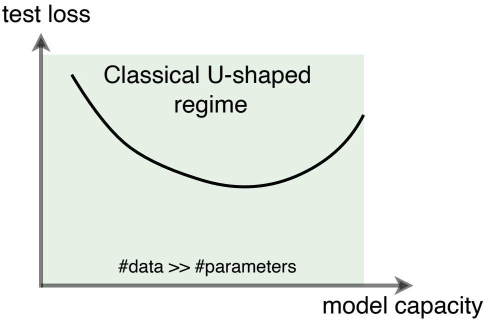
Practice of deep learning: bigger models perform better!



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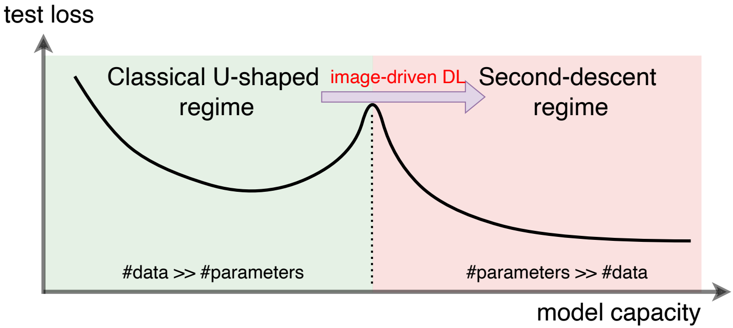


Proposed explanation: double descent (Belkin et al., 2019)

Learning paradigm in the past twenty years

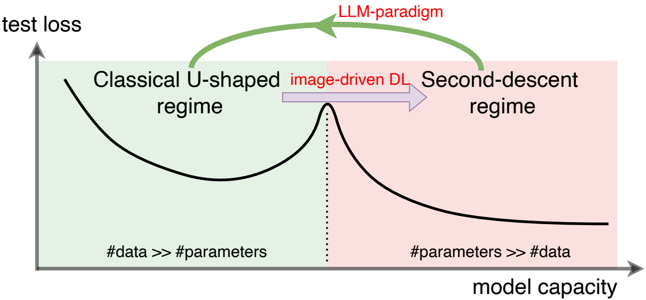
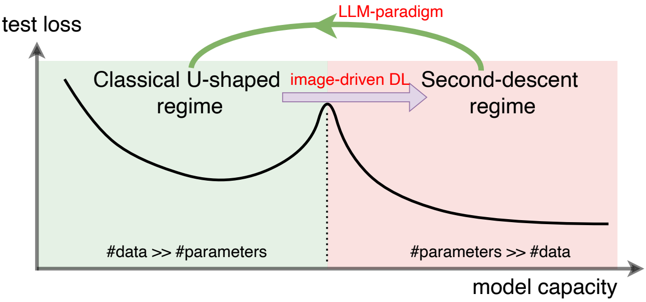


Figure 1: Paradigm among test loss, data, and model capacity.

Scaling law (Kaplan et al., 2020) in the era of LLMs

test loss $= A \times \text{Model Size}^{-a} + B \times \text{Data Size}^{-b} + C$



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A fundamental concept in machine learning: model capacity

Too many learning curves...

- U-shaped curve (bias-variance trade-offs) (Vapnik, 1995; Hastie et al., 2009)
- double (multiple) descent (Belkin et al., 2019; Liang et al., 2020)
- scaling law (Kaplan et al., 2020; Paquette et al., 2024)

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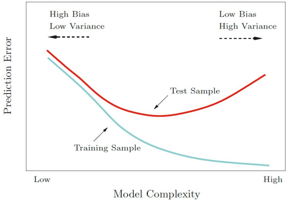
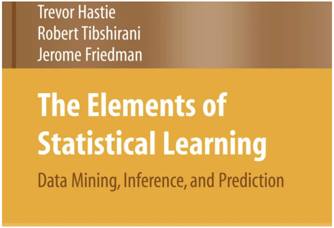
Bias-variance decomposition

$$\text{Test error} = \text{Bias}^2 + \text{Variance}$$



(Hastie et al., 2009, Figure 2.11)



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“Remove bias-variance trade-offs from ML textbooks"

Trade-off is a **misnomer**, by Geman et al. (1992); Neal (2019); Wilson (2025).

I can define **model capacity** at random and see whatever curve I want to see.

— Ben Recht, 2025

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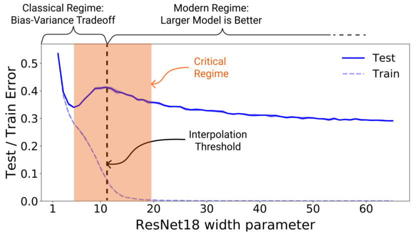
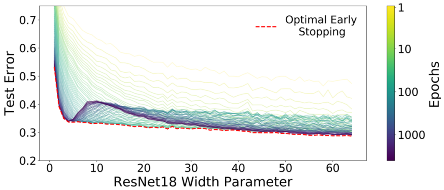
Double descent can disappear for the same architecture!



(a) Results on ResNet18 (Nakkiran et al., 2019)



(b) Optimal early stopping (Nakkiran et al., 2019).

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- Theoretical studies (Neyshabur et al., 2015; Savarese et al., 2019)
- Min-norm solution (Hastie et al., 2022)
- Applications: neural networks pruning (Molchanov et al., 2017), lottery ticket hypothesis (Frankle and Carbin, 2019)

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How these learning curves behave under a more suitable model capacity?

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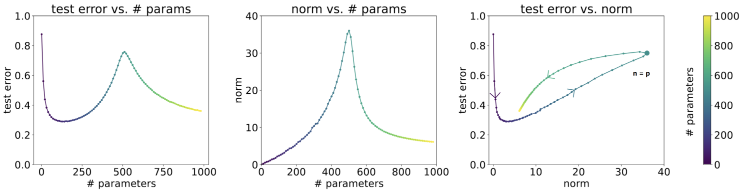

Figure 3: Stanford CS229 lecture notes (Ng and Ma, 2023, Figure 8.12).

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❒ How to **precisely** characterize the relationship under norm-based model capacity?

- Reshape bias-variance trade-offs, double descent, scaling law under ℓ_2 norm-based capacity!
- Yichen Wang, Yudong Chen, Lorenzo Rosasco, **Fanghui Liu**. *The shape of generalization through the lens of norm-based capacity control.* 2025. arXiv

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- What is the induced function space and statistical/computational efficiency under norm-based capacity?

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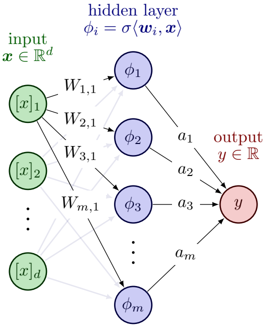
❒ What is the induced function space and statistical/computational efficiency under norm-based capacity?

- Which function class can be **efficiently** learned by neural networks?
- **Fanghui Liu**, Leello Dadi, and Volkan Cevher. *Learning with norm constrained, over-parameterised, two-layer neural networks.* JMLR 2024.

Background: Random features ridge regression



$$f_m(\boldsymbol{x};\boldsymbol{\theta}) = \sum_{i=1}^{m} a_i \phi(\boldsymbol{x}, \boldsymbol{w}_i), \quad \boldsymbol{\theta} := \{(a_i, \boldsymbol{w}_i)\}_{i=1}^m$$

- $\phi : \mathcal{X} \times \mathcal{W} \to \mathbb{R}$, e.g., ReLU: $\phi(\boldsymbol{x}, \boldsymbol{w}) = \max(\langle \boldsymbol{x}, \boldsymbol{w} \rangle, 0)$
- Random features models (RFMs) Rahimi and Recht (2007):
  - $\{\boldsymbol{w}_i\}_{i=1}^m \overset{iid}{\sim} \mu$ for a given $\mu \in \mathcal{P}(\mathcal{W})$
  - only train the second layer

$$\hat{\boldsymbol{a}} := \operatorname*{argmin}_{\boldsymbol{a} \in \mathbb{R}^p} \left\{ \sum_{i=1}^{n} (y_i - f(\boldsymbol{x}_i; \boldsymbol{a}))^2 + \lambda \|\boldsymbol{a}\|_2^2 \right\} = \left(\boldsymbol{Z}^\top \boldsymbol{Z} + \lambda \boldsymbol{I}_p \right)^{-1} \boldsymbol{Z}^\top \boldsymbol{y} \,.$$

- $\boldsymbol{Z} \in \mathbb{R}^{n \times p}$ with $[\boldsymbol{Z}]_{ij} = \frac{1}{\sqrt{p}} \phi(\boldsymbol{x}_i, \boldsymbol{w}_j)$.

- Norm over the first-layer (untrained) $\|\boldsymbol{W}\|_{\mathrm{F}}$
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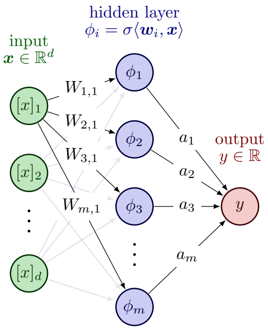

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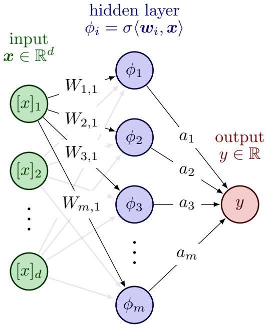

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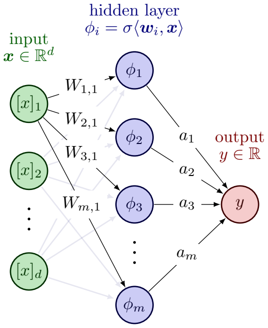

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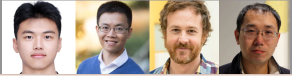

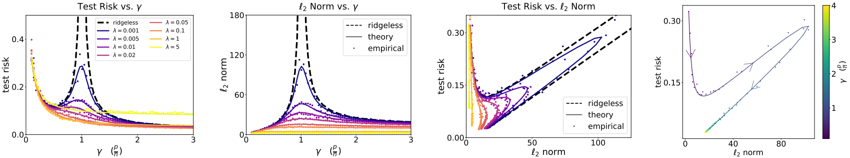

(a) Test Risk vs. γ **(b)** ℓ_2 norm vs. γ **(c)** Test Risk vs. norm **(d)** $\lambda = 0.001$

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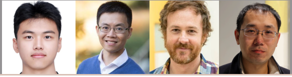

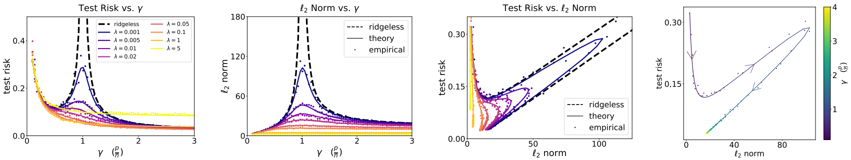

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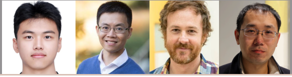
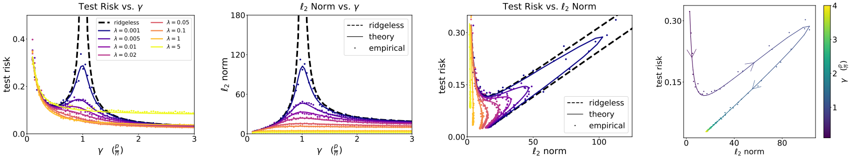
- Phase transition exists but double descent does not exist
- More close to **U-shaped** instead of double descent
- Over-parameterization is still **better than** under-parameterization

(Wang, Chen, Rosasco, Liu, 2025)





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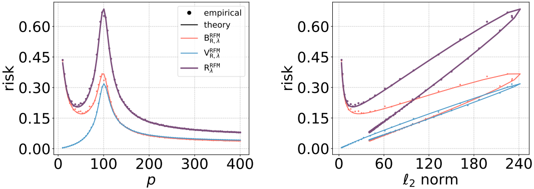
Test error = Bias^2 + Variance



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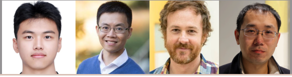

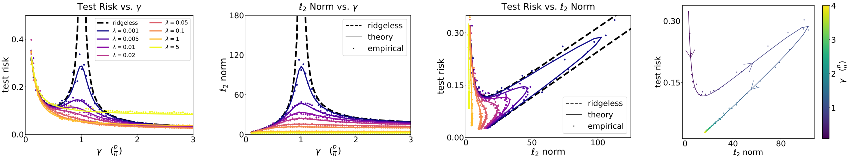

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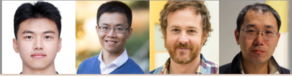

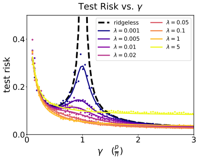

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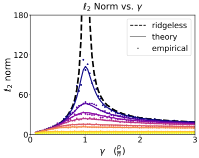

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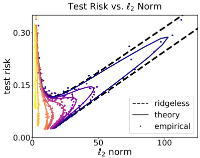

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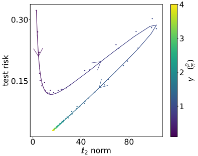

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  test loss $=$ A $\times$ Data Size^{-a} $\times$ **Norm Capacity**$^{-b}$ with $a > 0$ and $b \in \mathbb{R}$

Control norm by tuning λ: L-curve (Hansen, 1992)

Explicit (model size) *vs.* Implicit (norm)

One-to-one mapping between norm and λ

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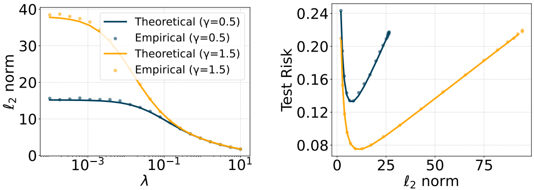

(a) Norm vs. λ (varying λ) **(b)** Risk vs. Norm (varying λ)

An example of linear regression: Textbook level and beyond

- n i.i.d. samples $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ with $\boldsymbol{x}_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$
- $y = \langle \boldsymbol{\beta}_*, \boldsymbol{x} \rangle + \varepsilon$, $\mathbb{E}(\varepsilon) = 0$ and $\mathbb{V}(\varepsilon) = \sigma^2$, covariance matrix $\boldsymbol{\Sigma} = \mathbb{E}[\boldsymbol{x}\boldsymbol{x}^\top]$
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The expected test risk $\mathbb{E}_\varepsilon \|\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_*\|_{\boldsymbol{\Sigma}}^2$ vs. the norm $\mathbb{E}_\varepsilon \|\hat{\boldsymbol{\beta}}\|_2^2$

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❒ Deterministic equivalence (Cheng and Montanari, 2024; Misiakiewicz and Saeed, 2024): law of large samples/dimensions in random matrix theory

The empirical spectral measure converges to a deterministic limit.

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$$\mathrm{Tr}\left(\boldsymbol{X}^\top \boldsymbol{X} (\boldsymbol{X}^\top \boldsymbol{X} + \lambda)^{-1}\right) \sim \mathrm{Tr}\left(\boldsymbol{\Sigma}(\boldsymbol{\Sigma} + \lambda_*)^{-1}\right), w.h.p.$$

- $\sim$ can be **asymptotic** or **non-asymptotic** at the rate of $\mathcal{O}(1/\sqrt{n})$.
- λ_* is the non-negative solution to the self-consistent equation $n - \frac{\lambda}{\lambda_*} = \mathrm{Tr}(\boldsymbol{\Sigma}(\boldsymbol{\Sigma} + \lambda_*)^{-1})$.

Theorem (Deterministic equivalence of estimator's norm)

We have a bias-variance decomposition $\mathbb{E}_\varepsilon \|\hat{\beta}\|_2^2 = \mathcal{B}_{\mathcal{N},\lambda} + \mathcal{V}_{\mathcal{N},\lambda}$.

For well-behaved data, we have

$$\mathsf{B}_{\mathsf{N},\lambda} := \langle \beta_*, \Sigma^2(\Sigma+\lambda_*)^{-2}\beta_* \rangle + \frac{\operatorname{Tr}(\Sigma(\Sigma+\lambda_*)^{-2})}{n} \frac{\lambda_*^2 \langle \beta_*, \Sigma(\Sigma+\lambda_*)^{-2}\beta_* \rangle}{1 - \frac{1}{n}\operatorname{Tr}(\Sigma^2(\Sigma+\lambda_*)^{-2})},$$

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Remark: Which model capacity suffices to characterize the test risk?

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Example: Relationship under isotropic features ($\Sigma = I_d$)

❐ Test risk R_λ and norm N_λ formulates a cubic curve (complex but precise).

- min-norm interpolator ($\lambda = 0$):

$$\mathsf{R}_0 = \begin{cases} \mathsf{N}_0 - \|\beta_*\|_2^2; \text{ in under-parameterized regimes} \\ \sqrt{\left[\mathsf{N}_0 - (\|\beta_*\|_2^2 - \sigma^2)\right]^2 + 4\|\beta_*\|_2^2\sigma^2} - \sigma^2 . \end{cases}$$

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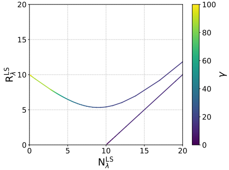

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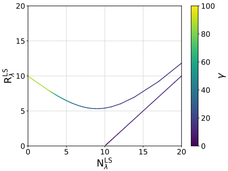

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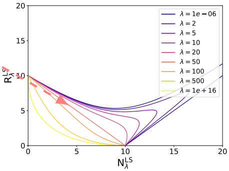

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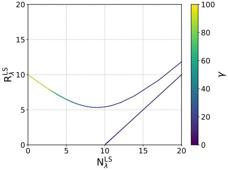

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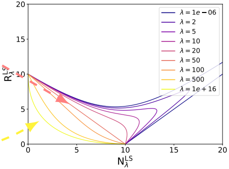

Precise analysis via deterministic equivalence

- Precisely describe the learning curve.
  - phase transitions, (non-)monotonicity, etc.
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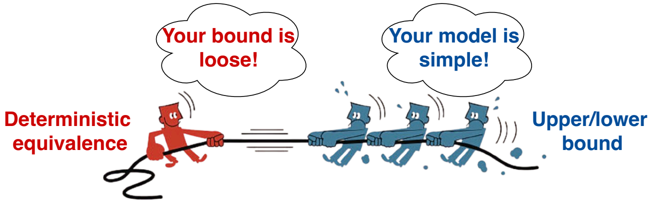

Which model capacity is suitable (for neural networks)?

Table 1: Complexity measures compared in the empirical study (Jiang et al., 2020), and their correlation with generalization.

name	definition	rank correlation
Parameter Frobenius norm	$\sum_{i=1}^{L} \|\boldsymbol{W}_i\|_F^2$	0.073
Frobenius distance to initialization	$\sum_{i=1}^{L} \|\boldsymbol{W}_i - \boldsymbol{W}_i^0\|_{\mathrm{F}}^2$	-0.263
Spectral complexity	$\prod_{i=1}^{L} \|\boldsymbol{W}_i\| \left(\sum_{i=1}^{L} \frac{\|\boldsymbol{W}_i\|_{2,1}^{3/2}}{\|\boldsymbol{W}_i\|^{3/2}} \right)^{2/3}$	-0.537
Fisher-Rao	$\frac{(L+1)^2}{n} \sum_{i=1}^{n} \langle \boldsymbol{W}, \nabla_{\boldsymbol{W}} \ell(h_{\boldsymbol{W}}(\boldsymbol{x}_i), y_i) \rangle$	0.078
Path-norm	$\sum_{(i_0,\dots,i_L)} \prod_{j=1}^{L} \left(\boldsymbol{W}_{i_j, i_{j-1}} \right)^2$	0.373

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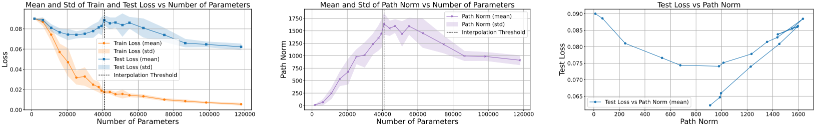
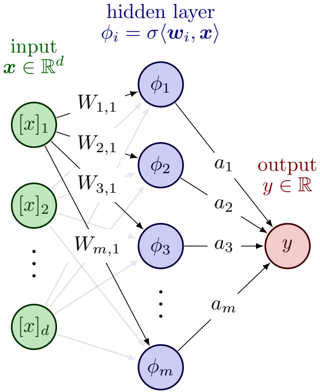
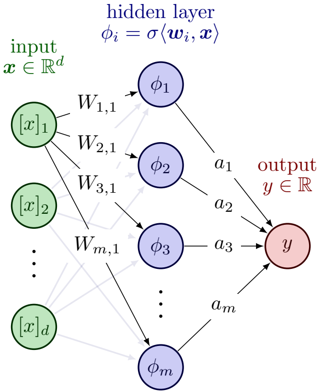


(a) Test (training) Loss vs. p **(b)** Path-norm vs. p **(c)** Test Loss vs. Path-norm

Figure 5: Experiments on two-layer neural networks.

Two-layer neural networks, path norm





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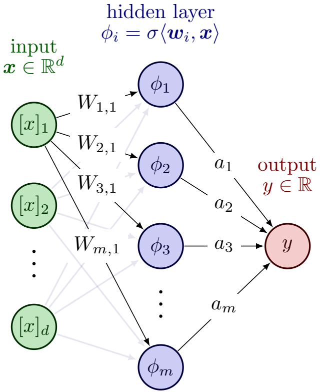

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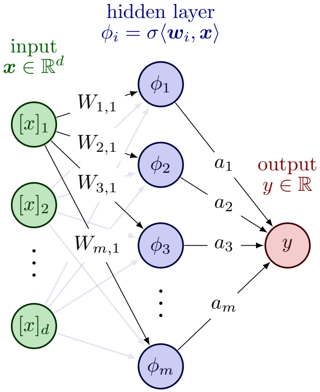

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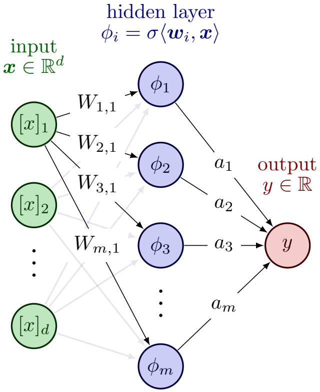

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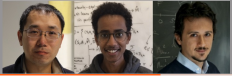
Can neural networks identify this structure?

(Liu, Dadi, Cevher, JMLR'24)



Theorem (Informal, sample complexity of learning $f^\star \in \mathcal{B}$)

To achieve ϵ-excess risk,

- *Kernel methods require $\Omega(\epsilon^{-d})$ samples.*
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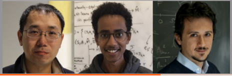

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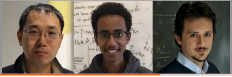

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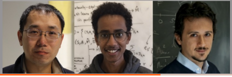

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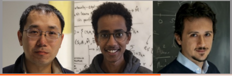

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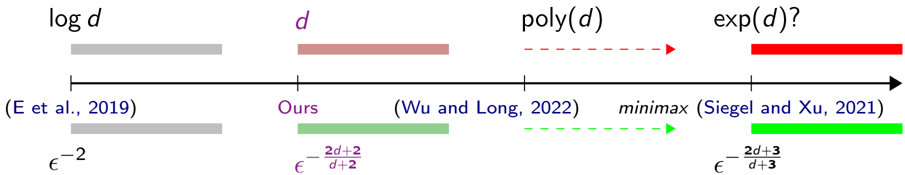
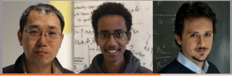


(Liu, Dadi, Cevher, JMLR'24)



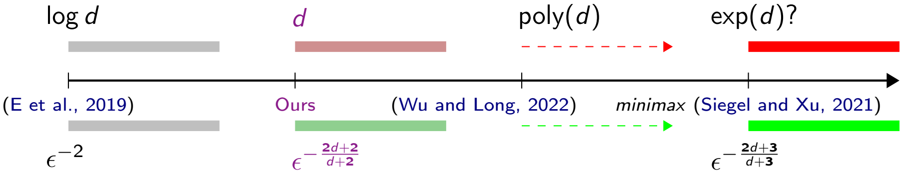
Theorem (Informal, sample complexity of learning $f^\star \in \mathcal{B}$)

To achieve ϵ-excess risk,

- *Kernel methods require $\Omega(\epsilon^{-d})$ samples.*
- *Two-layer neural networks require $\Omega(\epsilon^{-\frac{2d+2}{d+2}})$ samples. smaller than ϵ^{-2}*

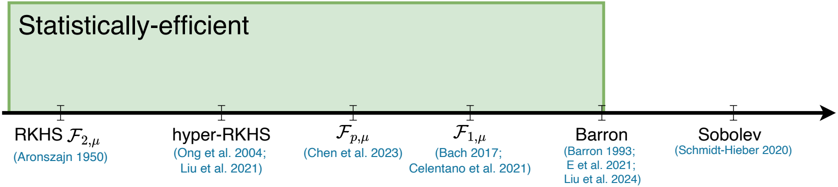
No **Curse of Dimensionality**: NNs adapt to directional smoothness.

❒ Track sample complexity (via metric entropy) and dimension dependence



The "best" trade-off between ϵ and d.

Which function class can be efficiently learned by neural networks



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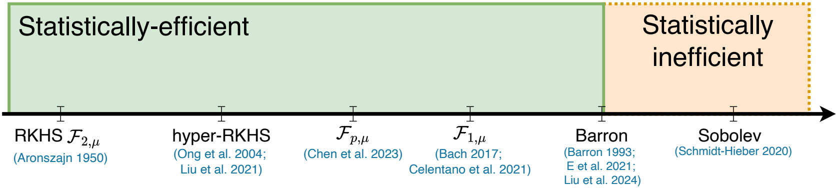

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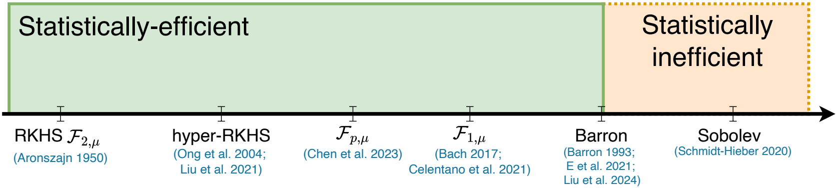
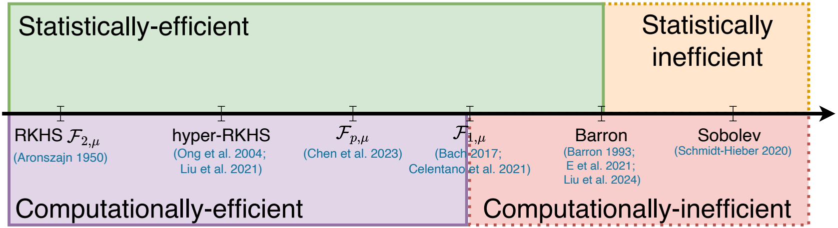


Optimization in Barron spaces is NP hard: curse of dimensionality!
(Bach, 2017)

Which function class can be efficiently learned by neural networks



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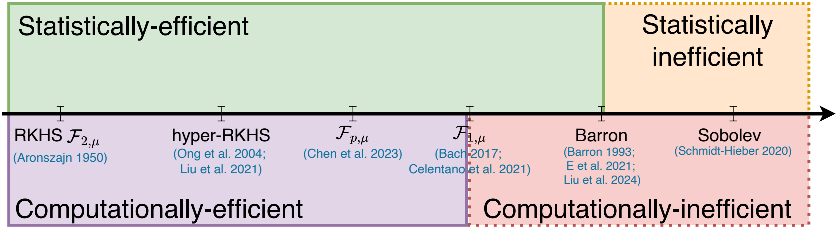
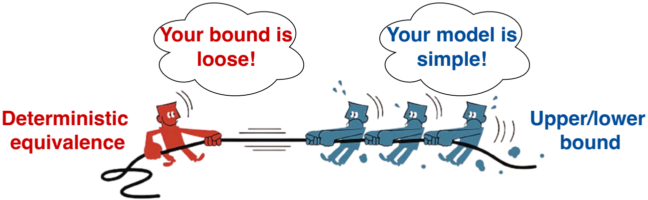


- ReLU neurons (Chen and Narayanan, 2023)
- Low-dimensional polynomials (Arous et al., 2021; Lee et al., 2024)

Deep learning phenomena $\Rightarrow$ interesting mathematical problems

- Be aware of model capacity!
  - Reshape bias-variance trade-offs, double descent, scaling law under proper ℓ_2 norm-based capacity via deterministic equivalence.



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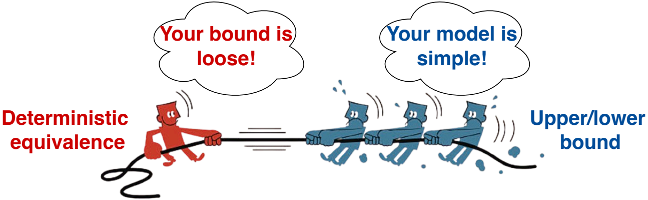
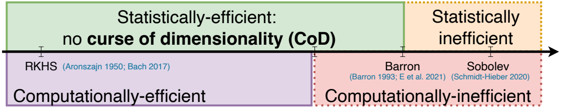


❒ Which function class can be **efficiently** learned by neural networks?

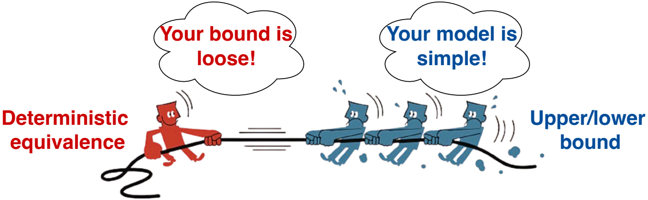
- Neural networks can adapt to low-dimensional structure and avoid CoD!



Takeaway messages

Deep learning phenomena $\Rightarrow$ interesting mathematical problems

- ❒ Be aware of model capacity!
  - Reshape bias-variance trade-offs, double descent, scaling law under proper ℓ_2 norm-based capacity via deterministic equivalence.



- ❒ Which function class can be **efficiently** learned by neural networks?
  - Neural networks can adapt to low-dimensional structure and avoid CoD!

Theoretical advances $\Rightarrow$ principled guidance in practical problems

- ❒ How does our theory contribute to practical fine-tuning problems?
  - One-step full gradient can be sufficient! [GitHub]

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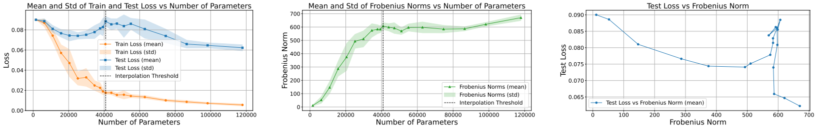

(a) Test (training) Loss vs. p **(b)** Fro-norm vs. p **(c)** Test Loss vs. Fro-norm

Figure 6: Experiments on two-layer fully connected neural networks with noise level $\eta = 0.2$. The **left** figure shows the relationship between test (training) loss and the number of the parameters p. The **middle** figure shows the relationship between the Frobenius norm and p. The **right** figure shows the relationship between the test loss and Fro-norm.

An example of linear model: a textbook level

- $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n \overset{i.i.d.}{\sim} \mu$, $\boldsymbol{x}_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$, covariance matrix $\boldsymbol{\Sigma} = \mathbb{E}[\boldsymbol{x}\boldsymbol{x}^\top]$
- $y = \langle \boldsymbol{\beta}_*, \boldsymbol{x} \rangle + \varepsilon$ with $\mathbb{E}(\varepsilon) = 0$ and $\mathbb{V}(\varepsilon) = \sigma^2$
- ridge regression: $\hat{\boldsymbol{\beta}} = (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I})^{-1} \boldsymbol{X}^\top \boldsymbol{y}$
- min-ℓ_2-norm interpolation: $\hat{\boldsymbol{\beta}}_{\text{min}} = \operatorname{argmin}_{\boldsymbol{\beta}} \|\boldsymbol{\beta}\|_2, \text{s.t. } \boldsymbol{X}\boldsymbol{\beta} = \boldsymbol{y}$
- expected test risk: bias-variance decomposition

$$\mathcal{R}^{\mathrm{LS}} := \mathbb{E}_\varepsilon \|\beta_* - \hat{\beta}\|_{\Sigma}^2 = \underbrace{\|\beta_* - \mathbb{E}_\varepsilon[\hat{\beta}]\|_{\Sigma}^2}_{:=\mathcal{B}^{\mathrm{LS}}_{\mathcal{R},\lambda}} + \underbrace{\mathrm{tr}(\boldsymbol{\Sigma}\mathrm{Cov}_\varepsilon(\hat{\beta}))}_{:=\mathcal{V}^{\mathrm{LS}}_{\mathcal{R},\lambda}} .$$

- $\mathcal{B}^{\mathrm{LS}}_{\mathcal{R},\lambda} = \lambda^2 \langle \beta_*, (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I})^{-1} \Sigma (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I})^{-1} \beta_* \rangle$
- $\mathcal{V}^{\mathrm{LS}}_{\mathcal{R},\lambda} = \sigma^2 \mathrm{Tr}(\Sigma \boldsymbol{X}^\top \boldsymbol{X} (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I})^{-2})$
- *Intuitive fact: for i.i.d. sub-Gaussian data $\boldsymbol{X}$, we have

$$\|\frac{1}{n}\boldsymbol{X}^\top \boldsymbol{X} - \Sigma\|_{op} = \Theta(\sqrt{d/n}) \, , w.h.p \, .$$

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Beyond textbook level: deterministic equivalence (Cheng and Montanari, 2024)

$$\mathrm{Tr}\left(\boldsymbol{X}^\top \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X} + \lambda)^{-1}\right) \sim \mathrm{Tr}\left(\boldsymbol{\Sigma}(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I})^{-1}\right).$$

- $\sim$ can be **asymptotic** or **non-asymptotic** at the rate of $\mathcal{O}(1/\sqrt{n})$.
- λ_* is the non-negative solution to the self-consistent equation $n - \frac{\lambda}{\lambda_*} = \mathrm{Tr}(\boldsymbol{\Sigma}(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I}_d)^{-1})$.

Theorem (Deterministic equivalence (Misiakiewicz and Saeed, 2024))

For sub-Gaussian data, assume Σ is **well-behaved**, *w.h.p.*

$$\underbrace{\|\boldsymbol{\beta}_* - \mathbb{E}_\varepsilon[\hat{\boldsymbol{\beta}}]\|_{\boldsymbol{\Sigma}}^2}_{:=\mathcal{B}^{\mathrm{LS}}_{\mathcal{R},\lambda}} \sim \mathrm{B}^{\mathrm{LS}}_{\mathrm{R},\lambda} := \frac{\lambda_*^2 \langle \boldsymbol{\beta}_*, \boldsymbol{\Sigma}(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I}_d)^{-2} \boldsymbol{\beta}_* \rangle}{1 - n^{-1}\mathrm{tr}(\boldsymbol{\Sigma}^2(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I}_d)^{-2})}$$

$$\underbrace{\mathrm{tr}(\boldsymbol{\Sigma}\mathrm{Cov}_\varepsilon(\hat{\boldsymbol{\beta}}))}_{:=\mathcal{V}^{\mathrm{LS}}_{\mathcal{R},\lambda}} \sim \mathrm{V}^{\mathrm{LS}}_{\mathrm{R},\lambda} := \frac{\sigma^2 \mathrm{tr}(\boldsymbol{\Sigma}^2(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I}_d)^{-2})}{n - \mathrm{tr}(\boldsymbol{\Sigma}^2(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I}_d)^{-2})}.$$

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Proof of sketch on bias

$$\mathcal{B}^{\mathtt{LS}}_{\mathcal{N},\lambda} = \mathtt{Tr}\left(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{X}^\top \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X} + \lambda)^{-1}\right) - \lambda \mathtt{Tr}\left(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{X}^\top \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X} + \lambda)^{-2}\right)$$

- first term

$$\mathtt{Tr}\left(\boldsymbol{A}\boldsymbol{X}^\top \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X} + \lambda)^{-1}\right) \sim \mathtt{Tr}\left(\boldsymbol{A}\boldsymbol{\Sigma}(\boldsymbol{\Sigma} + \lambda_*)^{-1}\right), \forall \boldsymbol{A}$$

- second term

$$\lambda \mathtt{tr}\left(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{X}^\top \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X} + \lambda)^{-2}\right) \sim \lambda \cdot \frac{\mathtt{Tr}\left(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{\Sigma}^2(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I})^{-2}\right)}{n - \mathtt{Tr}(\boldsymbol{\Sigma}^2(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I})^{-2})}$$

$$\leq \mathtt{Tr}(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{\Sigma}(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I})^{-1}) - \mathtt{Tr}(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{\Sigma}^2(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I})^{-2})$$

$$\leq \left(1 - \frac{1}{C}\right)\mathtt{Tr}(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{\Sigma}(\boldsymbol{\Sigma} + \lambda_*)^{-1})$$

Proof of sketch on bias

$$\mathcal{B}^{\mathtt{LS}}_{\mathcal{N},\lambda} = \mathtt{Tr}\left(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{X}^\top\boldsymbol{X}(\boldsymbol{X}^\top\boldsymbol{X}+\lambda)^{-1}\right) - \lambda\mathtt{Tr}\left(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{X}^\top\boldsymbol{X}(\boldsymbol{X}^\top\boldsymbol{X}+\lambda)^{-2}\right)$$

- first term

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$$\begin{aligned}
&\lambda\mathtt{tr}\left(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{X}^\top\boldsymbol{X}(\boldsymbol{X}^\top\boldsymbol{X}+\lambda)^{-2}\right) \sim \lambda \cdot \frac{\mathtt{Tr}\left(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{\Sigma}^2(\boldsymbol{\Sigma}+\lambda_*\boldsymbol{I})^{-2}\right)}{n - \mathtt{Tr}\left(\boldsymbol{\Sigma}^2(\boldsymbol{\Sigma}+\lambda_*\boldsymbol{I})^{-2}\right)} \\
&\leq \mathtt{Tr}(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{\Sigma}(\boldsymbol{\Sigma}+\lambda_*\boldsymbol{I})^{-1}) - \mathtt{Tr}(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{\Sigma}^2(\boldsymbol{\Sigma}+\lambda_*\boldsymbol{I})^{-2}) \\
&\leq \left(1 - \frac{1}{C}\right)\mathtt{Tr}(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{\Sigma}(\boldsymbol{\Sigma}+\lambda_*)^{-1})
\end{aligned}$$

Proof of sketch on bias

$$\mathcal{B}^{\mathrm{LS}}_{\mathcal{N},\lambda} = \mathtt{Tr}\left(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{X}^\top \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X} + \lambda)^{-1}\right) - \lambda \mathtt{Tr}\left(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{X}^\top \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X} + \lambda)^{-2}\right)$$

- first term

$$\mathtt{Tr}\left(\boldsymbol{A}\boldsymbol{X}^\top \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X} + \lambda)^{-1}\right) \sim \mathtt{Tr}\left(\boldsymbol{A}\boldsymbol{\Sigma}(\boldsymbol{\Sigma} + \lambda_*)^{-1}\right), \forall \boldsymbol{A}$$

- second term

$$\begin{aligned}
\lambda \mathtt{tr}\left(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{X}^\top \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X} + \lambda)^{-2}\right) &\sim \lambda \cdot \frac{\mathtt{Tr}\left(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{\Sigma}^2(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I})^{-2}\right)}{n - \mathtt{Tr}(\boldsymbol{\Sigma}^2(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I})^{-2})} \\
&\leq \mathtt{Tr}(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{\Sigma}(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I})^{-1}) - \mathtt{Tr}(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{\Sigma}^2(\boldsymbol{\Sigma} + \lambda_* \boldsymbol{I})^{-2}) \\
&\leq \left(1 - \frac{1}{C}\right)\mathtt{Tr}(\boldsymbol{\beta}_*\boldsymbol{\beta}_*^\top \boldsymbol{\Sigma}(\boldsymbol{\Sigma} + \lambda_*)^{-1})
\end{aligned}$$

*Path norm, Barron spaces, RKHS (Chen et al., 2023)

Consider a random features model (RFM) (Rahimi and Recht, 2007)

- first layer: $\boldsymbol{w} \overset{iid}{\sim} \mu \in \mathcal{P}(\mathcal{W})$; only train the second layer

infinite many features $f_a(\boldsymbol{x}) = \int_{\mathcal{W}} a(\boldsymbol{w})\phi(\boldsymbol{x}, \boldsymbol{w})\mathrm{d}\mu(\boldsymbol{w})$

$$\mathcal{F}_{p,\mu} := \{f_a : \|\boldsymbol{a}\|_{L^p(\mu)} < \infty\}, \quad \|f\|_{\mathcal{F}_{p,\mu}} := \inf_{f=f_a} \|\boldsymbol{a}\|_{L^p(\mu)}$$

- RFMs $\equiv$ kernel methods by taking $p = 2$ using Representer theorem
- RFMs $\not\equiv$ kernel methods if $p < 2$
- function space: $\mathcal{F}_{\infty,\mu} \subseteq \mathcal{F}_{p,\mu} \subseteq \mathcal{F}_{q,\mu} \subseteq \mathcal{F}_{1,\mu}$ if $p \geq q$

For any $1 \leq p \leq \infty$, define

$$\mathcal{B} = \cup_{\mu \in \mathcal{P}(\mathcal{W})} \mathcal{F}_{p,\mu}\,, \quad \|f\|_{\mathcal{B}} = \inf_{\mu \in \mathcal{P}(\mathcal{W})} \|f\|_{\mathcal{F}_{p,\mu}}$$

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Proof sketch: convex hull technique and its constant!

- Consider the following function space

  $\mathcal{F} = \{\sigma(\langle \widetilde{\boldsymbol{w}}, \cdot \rangle) : \widetilde{\boldsymbol{w}} \in \mathcal{W}\} \cup \{0\} \cup \{-\sigma(\langle \widetilde{\boldsymbol{w}}, \cdot \rangle) : \widetilde{\boldsymbol{w}} \in \mathbb{S}_1^{d-1}$ with the ℓ_1 ball$\}$

- the convex hull of $\mathcal{F}$ is

$$\overline{\mathrm{conv}}\mathcal{F} = \left\{ \sum_{i=1}^{m} \alpha_i f_i \middle| f_i \in \mathcal{F}, \sum_{i=1}^{m} \alpha_i = 1, \alpha_i \geqslant 0, m \in \mathbb{N} \right\}.$$

- convex hull technique (Van Der Vaart et al., 1996, Theorem 2.6.9)

$$\log \mathcal{N}_2(\mathcal{G}_1, \epsilon) \leqslant \log \mathcal{N}_2(\overline{\backslash}\mathcal{F}, \epsilon, \mu) \leqslant C \left(\frac{1}{\epsilon}\right)^{\frac{2d}{d+2}}.$$

- control the constant C

$$C := \underbrace{D_k}_{=\Theta(d)} [\underbrace{C_k}_{=\Theta(1)} (2^{d+1} + 1)^{\frac{1}{d}}]^{\frac{2d}{d+2}} \leq 10^7 d \quad \text{if } d > 5$$

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