

# How does generalization behave under suitable model capacities in modern machine learning

- A new  $\varphi$ -curve under norm-based capacity
- 

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at Department of Mathematics, The University of Hong Kong



The  
Alan Turing  
Institute

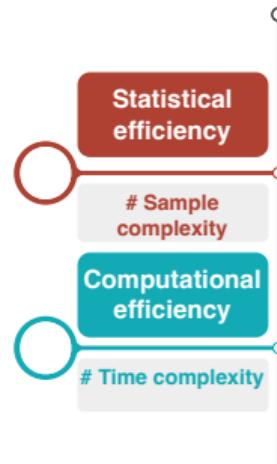
THE  
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# My research

## ❑ Research interests

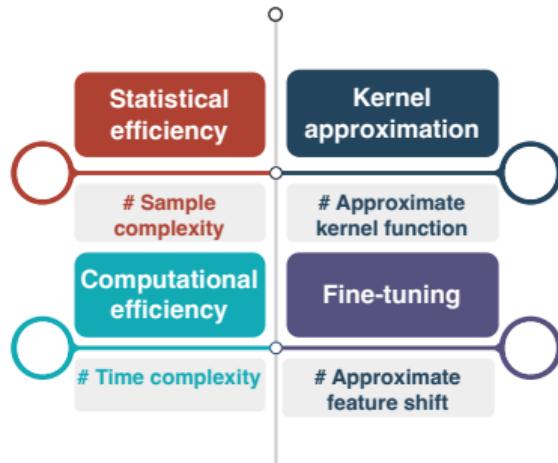
- Foundations of machine learning (ML)
- Theory-grounded efficient algorithm design
- Trustworthy ML



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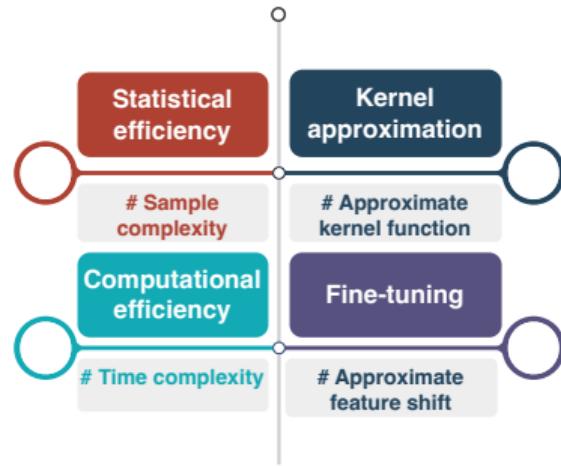
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## ❑ Research goal

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



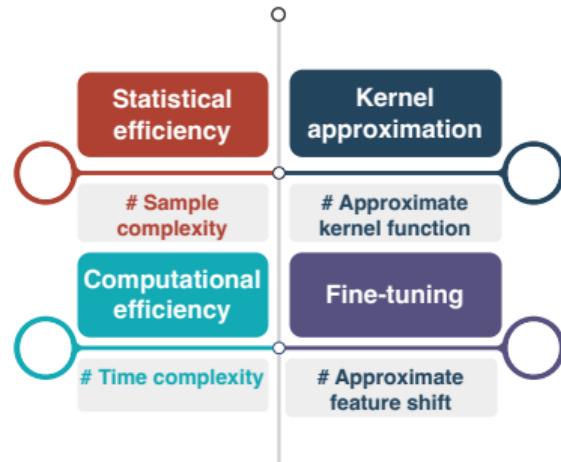
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## Learning efficiency (Curse of Dimensionality, CoD)

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

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

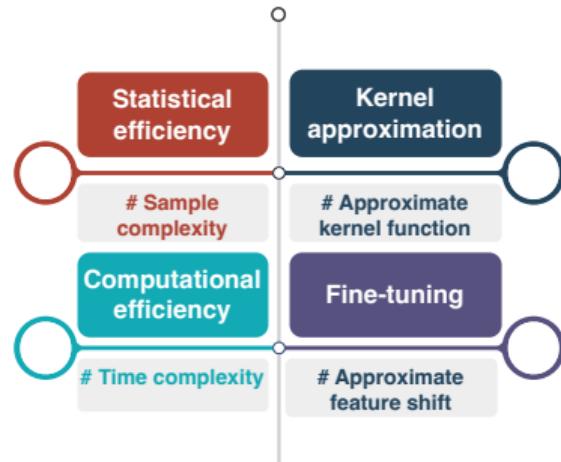
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Data



Model



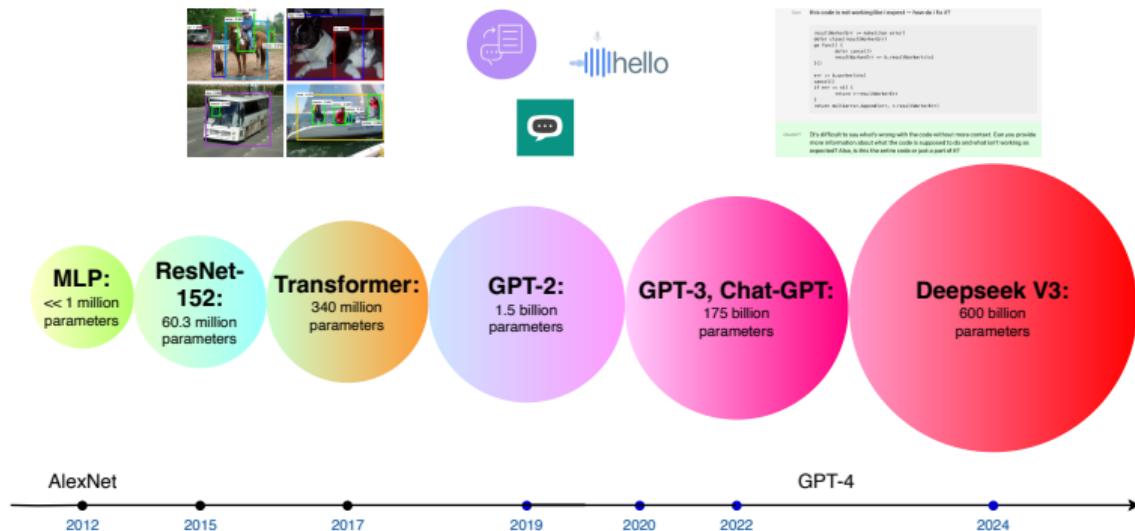
Algorithm



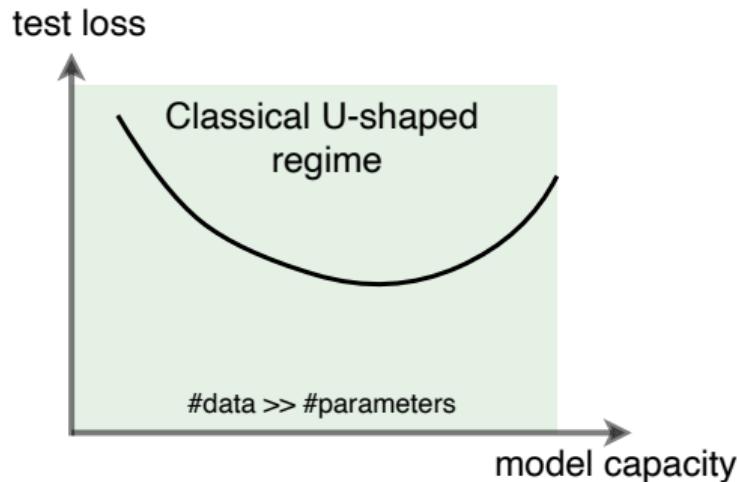
Compute

# In the era of machine learning

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

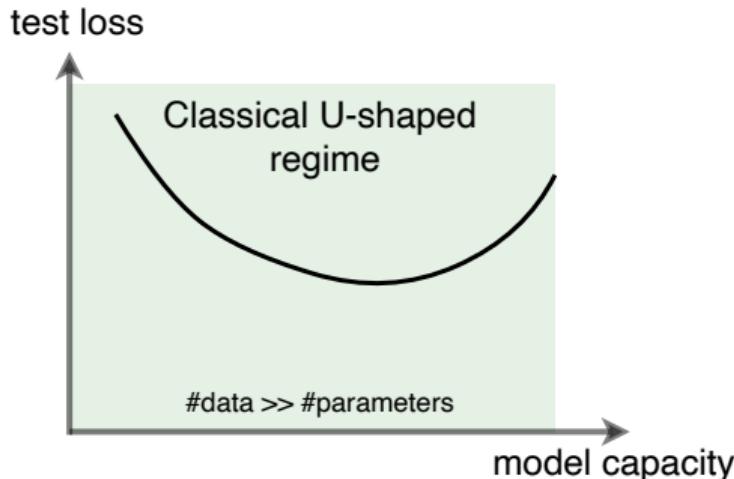


ML textbooks: Larger models tend to overfit!

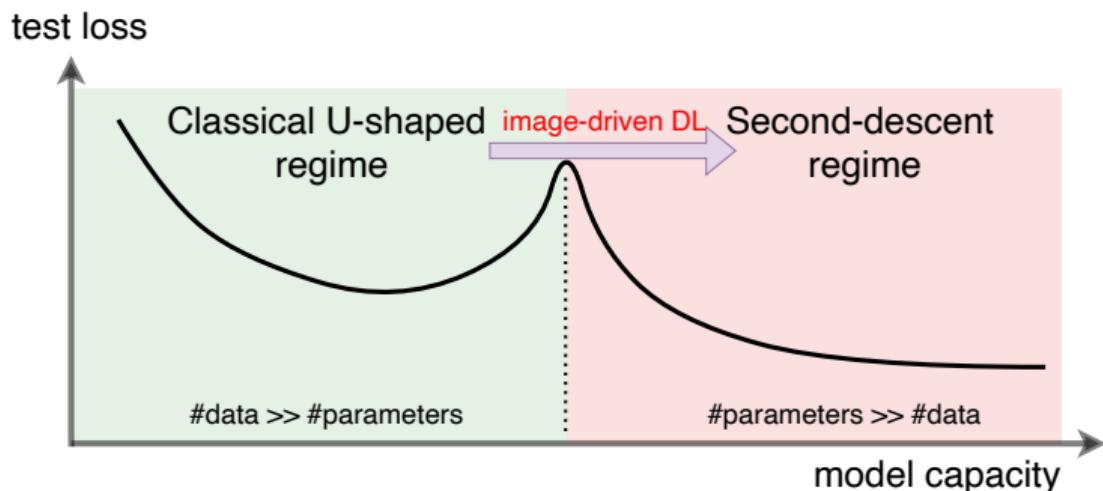


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Practice of deep learning: bigger models perform better!

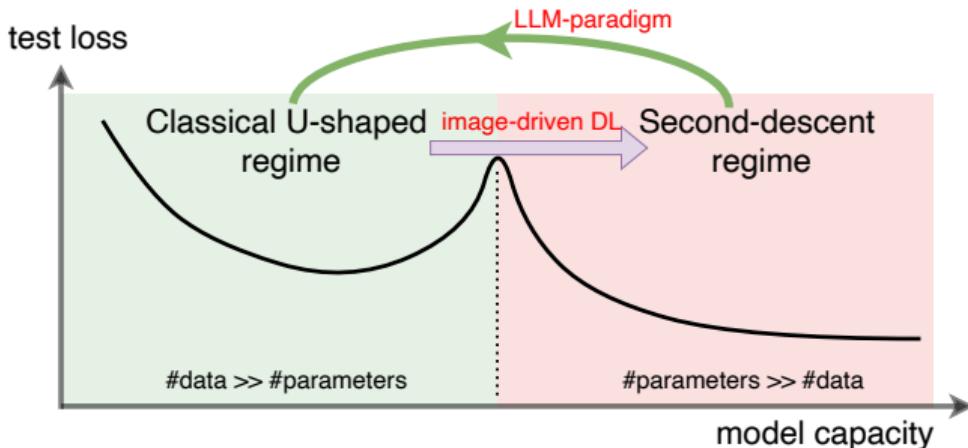


Practice of deep learning: bigger models perform better!



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

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

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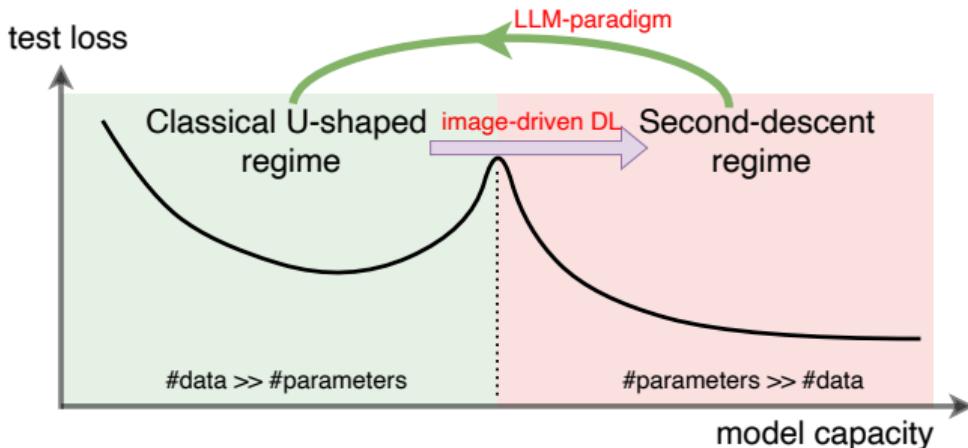


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# A fundamental concept in machine learning: model capacity

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](#))

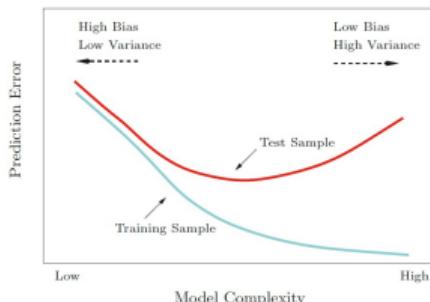
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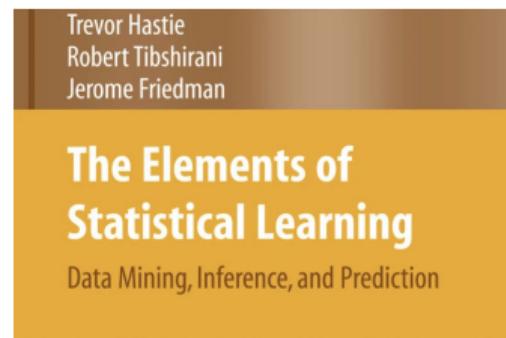
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## Bias-variance decomposition

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



([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.

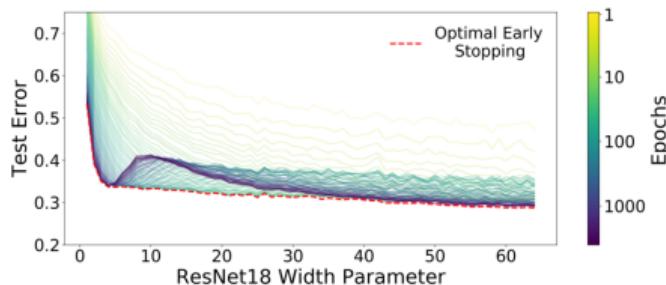
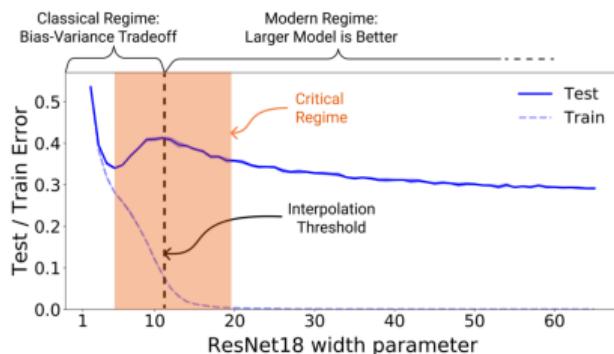
— Ben Recht, 2025

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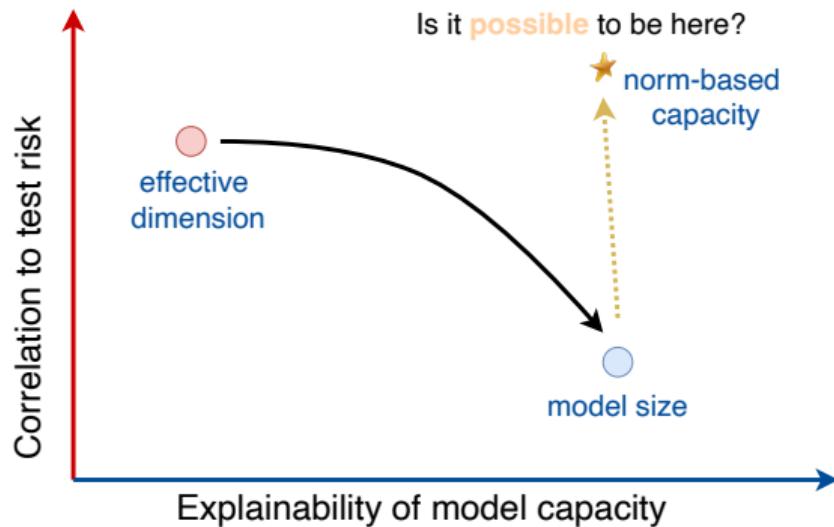
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Double descent can disappear for the same architecture!



(a) Results on ResNet18 (Nakkiran et al., 2019) (b) Optimal early stopping (Nakkiran et al., 2019).

# Today's talk: Norm-based capacity via deterministic equivalence



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(Bartlett, 1998)

"The size of the weights is more important than the size of the network!"

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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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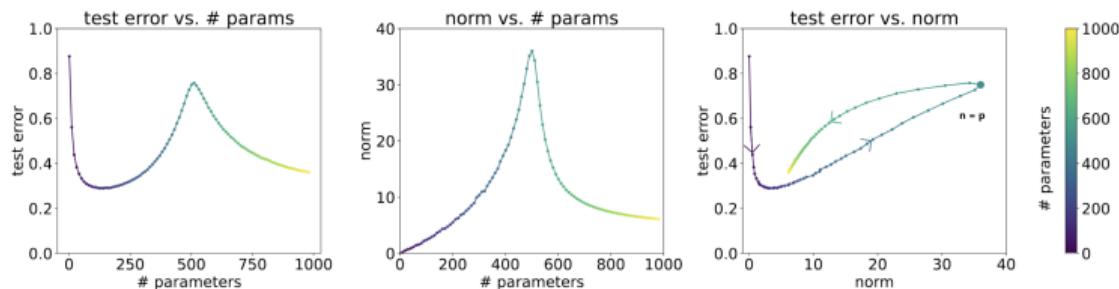


Figure 3: Stanford CS229 lecture notes (Ng and Ma, 2023, Figure 8.12).

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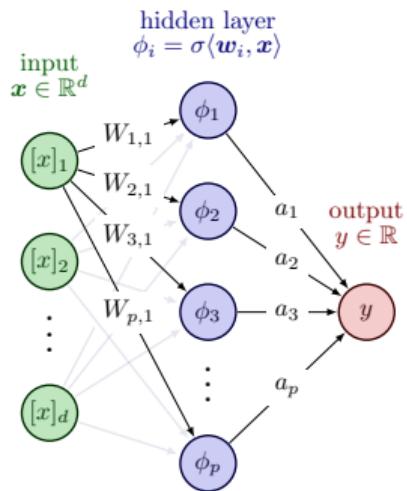
- How to precisely characterize the relationship under norm-based model capacity?
  - Reshape bias-variance trade-offs, double descent, scaling law under  $\ell_2$  norm-based capacity!
  - Yichen Wang, Yudong Chen, Lorenzo Rosasco, Fanghui Liu. *The shape of generalization through the lens of norm-based capacity control.* 2025. [arXiv](#)

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



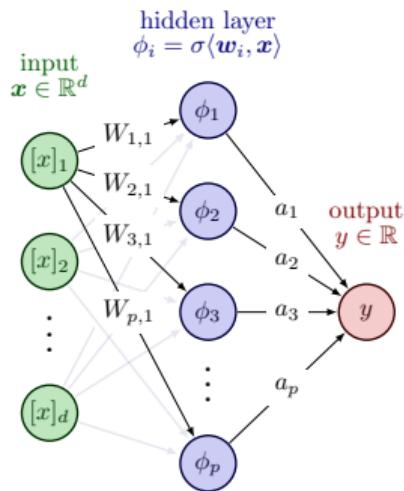
$$f_p(\mathbf{x}; \boldsymbol{\theta}) = \sum_{i=1}^p a_i \phi(\mathbf{x}, \mathbf{w}_i), \quad \boldsymbol{\theta} := \{(a_i, \mathbf{w}_i)\}_{i=1}^p$$

- $\phi : \mathcal{X} \times \mathcal{W} \rightarrow \mathbb{R}$ , e.g., ReLU:  
$$\phi(\mathbf{x}, \mathbf{w}) = \max(\langle \mathbf{x}, \mathbf{w} \rangle, 0)$$
- Random features models (RFMs) (Rahimi and Recht, 2007; Liu et al., 2021):
  - $\{\mathbf{w}_i\}_{i=1}^p \stackrel{iid}{\sim} \mu$  for a given  $\mu \in \mathcal{P}(\mathcal{W})$
  - only train the second layer

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

- $\mathbf{Z} \in \mathbb{R}^{n \times p}$  with  $[\mathbf{Z}]_{ij} = \frac{1}{\sqrt{m}} \phi(\mathbf{x}_i, \mathbf{w}_j)$ .
- Norm over the first-layer (untrained)  $\|\mathbf{W}\|_{\text{F}}$
- Norm over the second-layer  $\|\hat{\mathbf{a}}\|_2^2$

# Background: Random features ridge regression



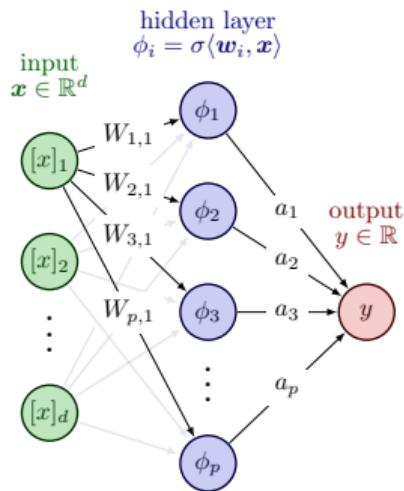
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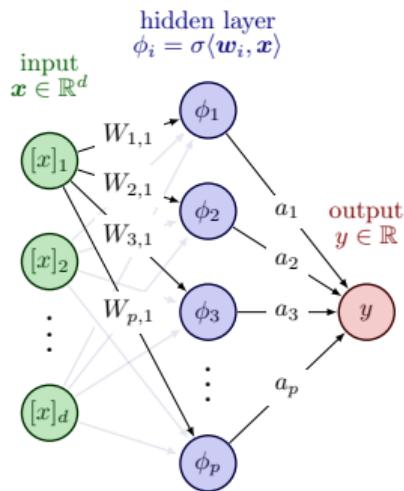
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## Background: Test risk of random features model

- A **compact** integral operator  $\mathbb{T} : L^2(\rho_X) \rightarrow L^2(\mu_W)$  for any  $f \in L_2(\rho_X)$  (Defilippis et al., 2024)

$$(\mathbb{T}f)(\mathbf{w}) := \int_{\mathbb{R}^d} \phi(\mathbf{x}, \mathbf{w}) f(\mathbf{x}) d\rho(\mathbf{x}), \quad \mathbb{T} = \sum_{k=1}^{\infty} \xi_k \psi_k \varphi_k^*.$$

- Covariate feature matrix  $\mathbf{G} := [\mathbf{g}_1, \dots, \mathbf{g}_n]^\top \in \mathbb{R}^{n \times \infty}$  with  $\mathbf{g}_i := (\psi_k(\mathbf{x}_i))_{k \geq 1}$
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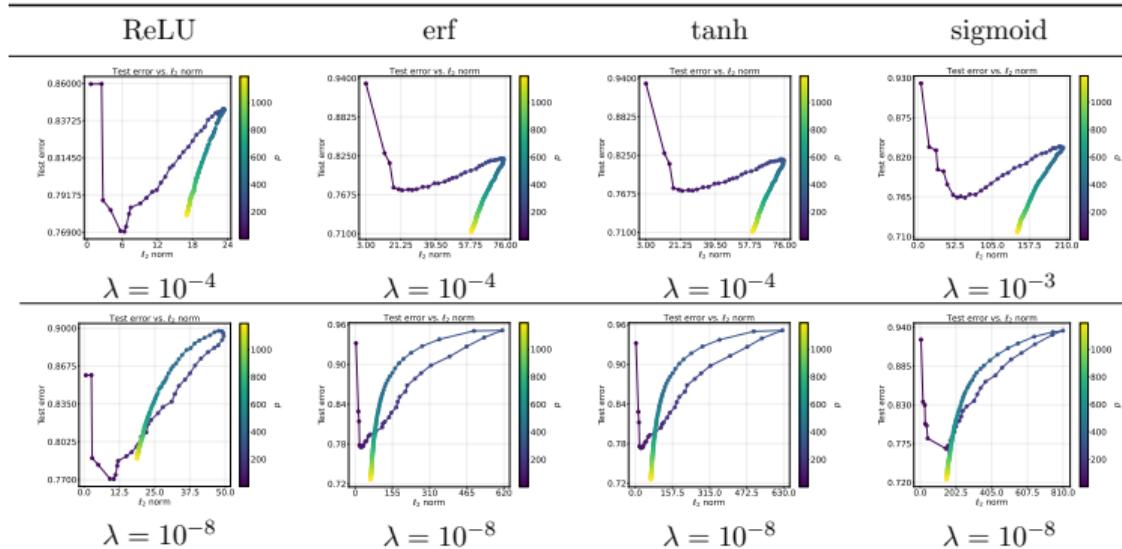
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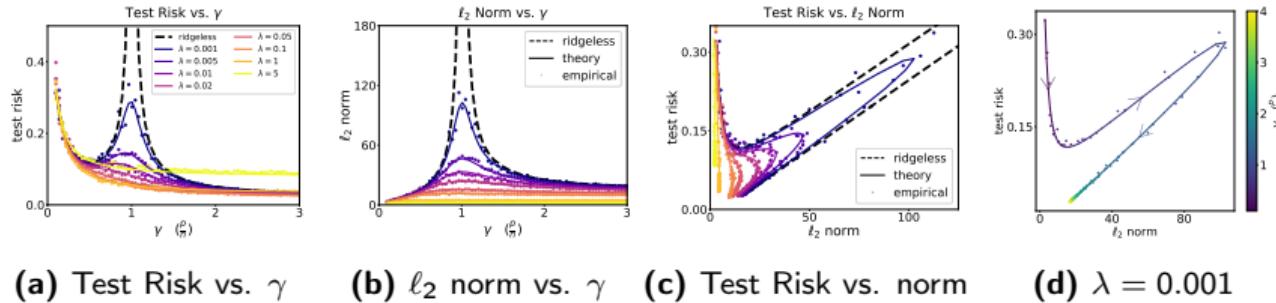
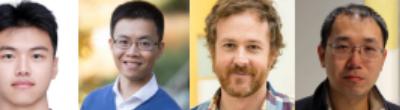
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# Empirical observation under real-world dataset



**Figure 3:** Results for RFMs under FasionMNIST.

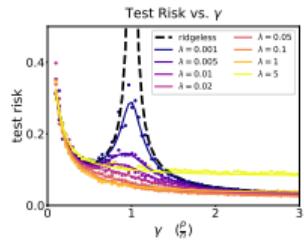
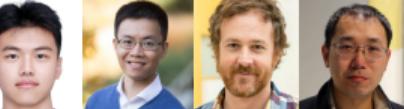
# Our results under well-behaved data



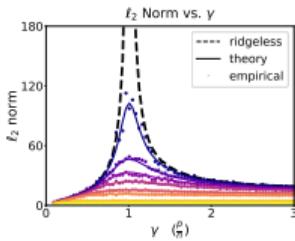
**(a)** Test Risk vs.  $\gamma$     **(b)**  $\ell_2$  norm vs.  $\gamma$     **(c)** Test Risk vs. norm    **(d)**  $\lambda = 0.001$

- $\gamma := p/n$ ,  $p$  : model size (width),  $n$  : data size

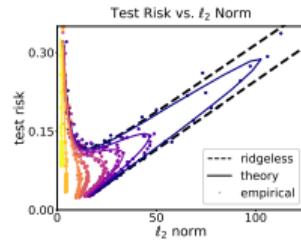
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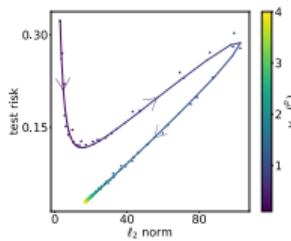
(a) Test Risk vs.  $\gamma$



(b)  $\ell_2$  norm vs.  $\gamma$



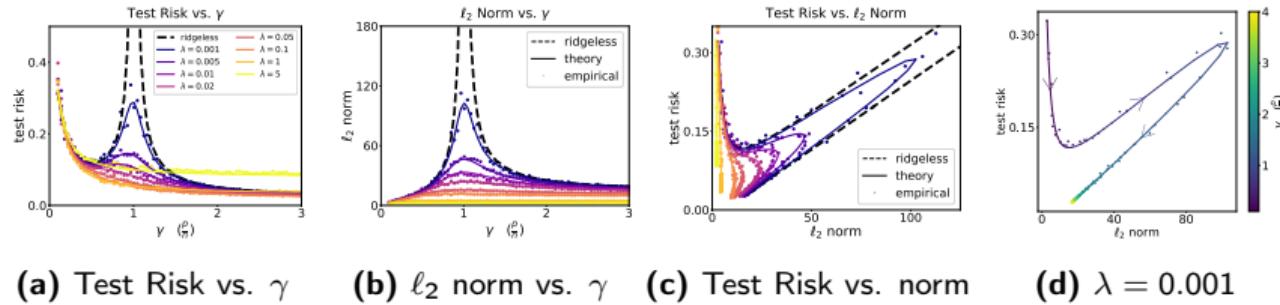
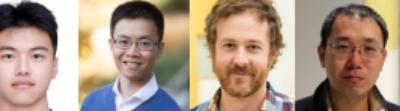
(c) Test Risk vs. norm



(d)  $\lambda = 0.001$

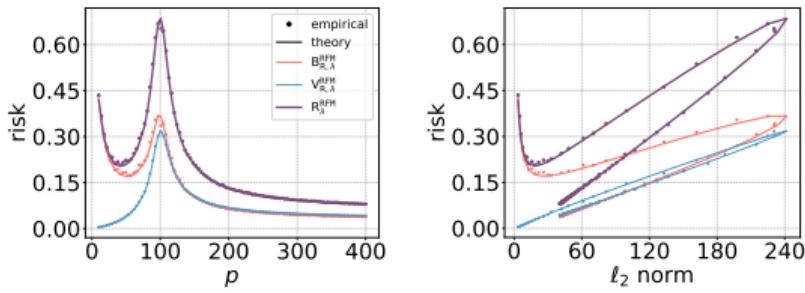
- $\gamma := p/n$ ,  $p$ : model size (width),  $n$ : data size
- Phase transition exists but double descent does not exist
- More close to **U-shaped** instead of double descent: **A  $\varphi$  paradigm**
- Over-parameterization is still **better than** under-parameterization

# Our results under well-behaved data

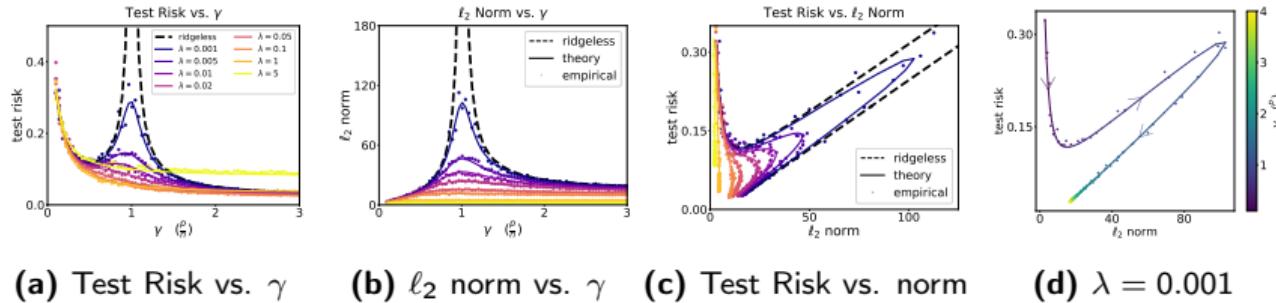
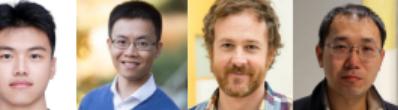


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$$\text{Test error} = \text{Bias}^2 + \text{Variance}$$

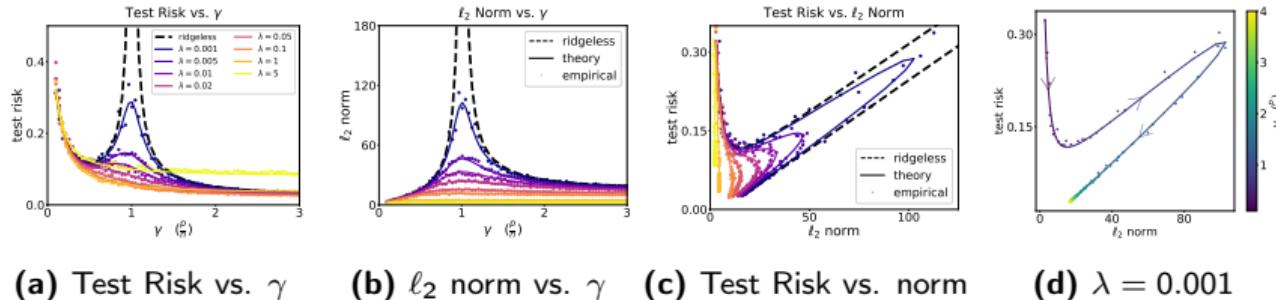
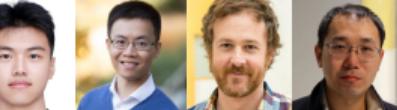


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- $\gamma := p/n$ ,  $p$ : model size (width),  $n$ : data size
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 with  $a > 0$  and  $b \in \mathbb{R}$

## Control norm by tuning $\lambda$ : L-curve (Hansen, 1992)

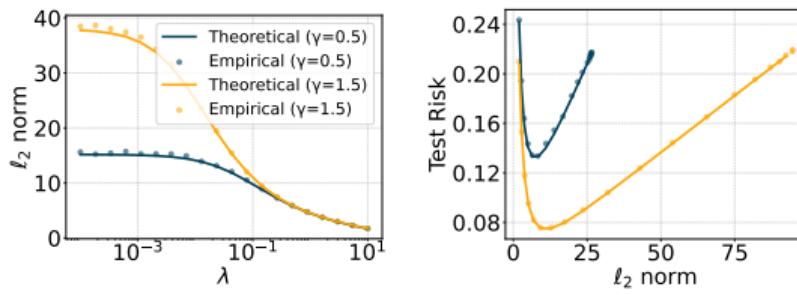
### Explicit (model size) vs. Implicit (norm)

One-to-one mapping between norm and  $\lambda$

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**(a)** Norm vs.  $\lambda$  (varying  $\lambda$ )

**(b)** Risk vs. Norm (varying  $\lambda$ )

## An example of linear regression: Textbook level and beyond

- $n$  i.i.d. samples  $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$  with  $\mathbf{x}_i \in \mathbb{R}^d$ ,  $y_i \in \mathbb{R}$
- $y = \langle \boldsymbol{\beta}_*, \mathbf{x} \rangle + \varepsilon$ ,  $\mathbb{E}(\varepsilon) = 0$  and  $\mathbb{V}(\varepsilon) = \sigma^2$ , covariance matrix  $\Sigma = \mathbb{E}[\mathbf{x}\mathbf{x}^\top]$
- ridge regression:  $\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$

Target: precise analysis

The expected test risk  $\mathbb{E}_\varepsilon \|\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_*\|_\Sigma^2$  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](#); [Bach, 2024](#))

The empirical spectral measure converges to a deterministic limit.

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$$\text{Tr}(\mathbf{X}^\top \mathbf{X} (\mathbf{X}^\top \mathbf{X} + \lambda)^{-1}) \sim \text{Tr}(\Sigma(\Sigma + \lambda_*)^{-1}), \text{w.h.p.}$$

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

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- Deterministic equivalence (Cheng and Montanari, 2024; Misiakiewicz and Saeed, 2024; Bach, 2024)
- Bias-variance decomposition on the test risk

- $\mathcal{B}_{\mathcal{R}, \lambda}^{\text{LS}} = \lambda^2 \langle \boldsymbol{\beta}_*, (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \Sigma (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \boldsymbol{\beta}_* \rangle$
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# Our results

## Theorem (asymptotic/non-asymptotic results)

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 and  $\Sigma$ , we have  $\mathcal{B}_{\mathcal{N},\lambda} \sim B_{\mathcal{N},\lambda}$  and  $\mathcal{V}_{\mathcal{N},\lambda} \sim V_{\mathcal{N},\lambda}$ , w.h.p.

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- Test risk  $R_\lambda$  and norm  $N_\lambda$  formulates a cubic curve (complex but precise).

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

$$R_0 = \begin{cases} N_0 - \|\beta_*\|_2^2; & \text{in under-parameterized regimes} \\ \sqrt{[N_0 - (\|\beta_*\|_2^2 - \sigma^2)]^2 + 4\|\beta_*\|_2^2\sigma^2} - \sigma^2. \end{cases}$$

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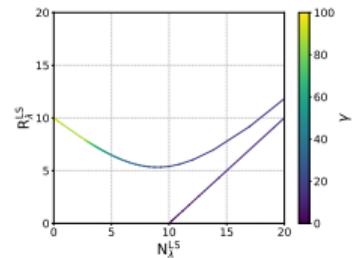
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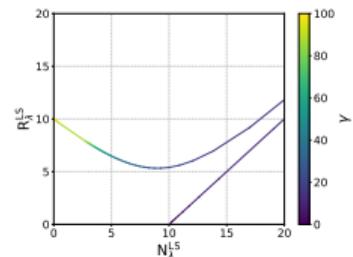
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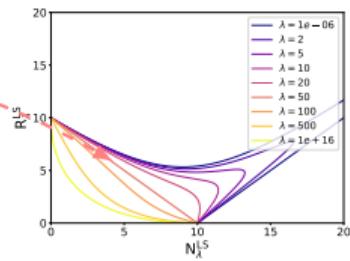
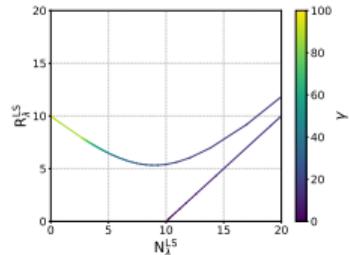
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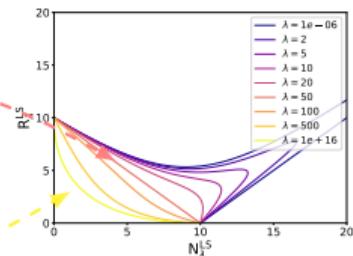
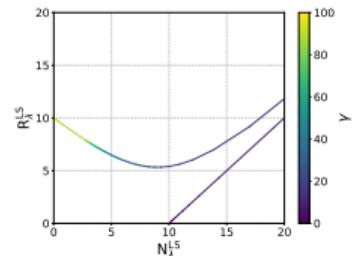
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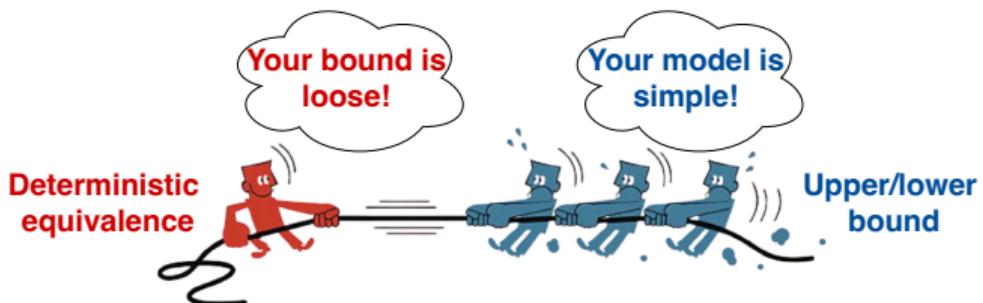


## Precise analysis via deterministic equivalence

- Precisely describe the learning curve.
  - phase transitions, (non-)monotonicity, etc.
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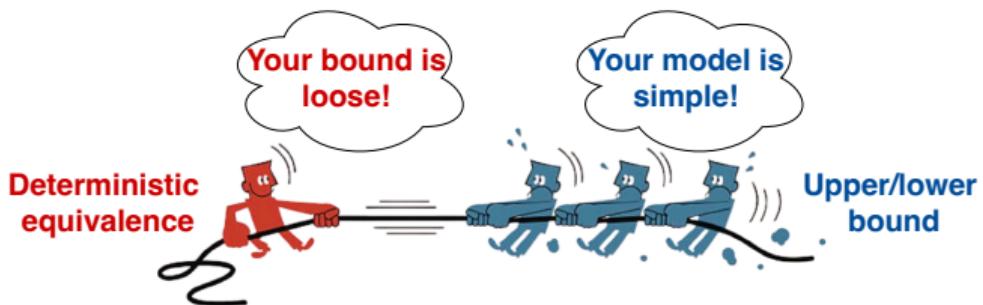
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Is  $\ell_2$  norm-based capacity **best** for characterizing generalization?

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

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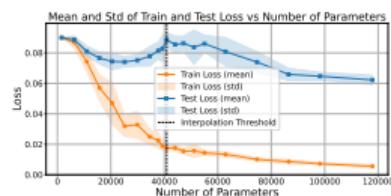
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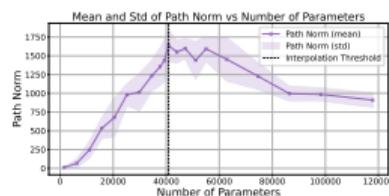
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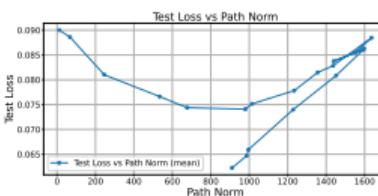
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(a) Test (training) Loss vs.  $p$



(b) Path-norm vs.  $p$



(c) Test Loss vs. Path-norm

**Figure 6:** Experiments on two-layer neural networks.

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**Table 2:** Complexity measures compared in the empirical study (Jiang et al., 2020), and their correlation with generalization.

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Spectral complexity	$\prod_{i=1}^L \ W_i\  \left( \sum_{i=1}^L \frac{\ W_i\ _{2,1}^{3/2}}{\ W_i\ ^{3/2}} \right)^{2/3}$	-0.537
Fisher-Rao	$\frac{(L+1)^2}{n} \sum_{i=1}^n \langle W, \nabla_W \ell(h_W(x_i), y_i) \rangle$	0.078
Path-norm	$\sum_{(i_0, \dots, i_L)} \prod_{j=1}^L (W_{i_j, i_{j-1}})^2$	0.373

# Which model capacity is suitable (for neural networks)?

**Table 2:** Complexity measures compared in the empirical study (Jiang et al., 2020), and their correlation with generalization.

name	definition	rank correlation
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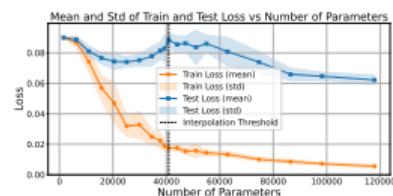
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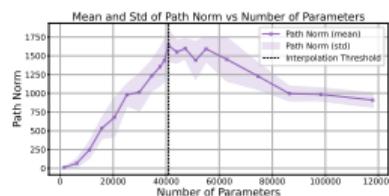
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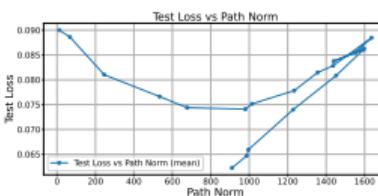
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(a) Test (training) Loss vs.  $p$



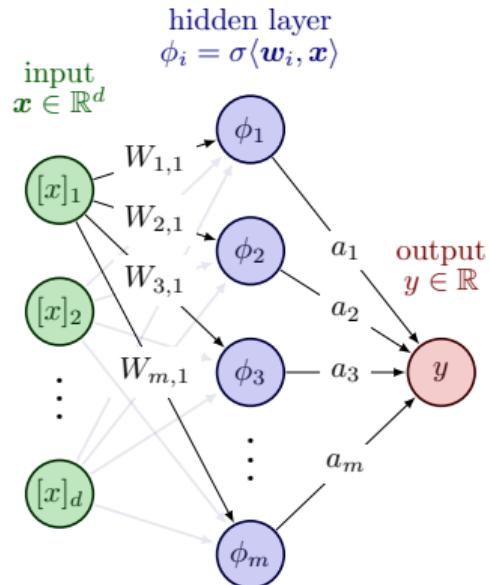
(b) Path-norm vs.  $p$



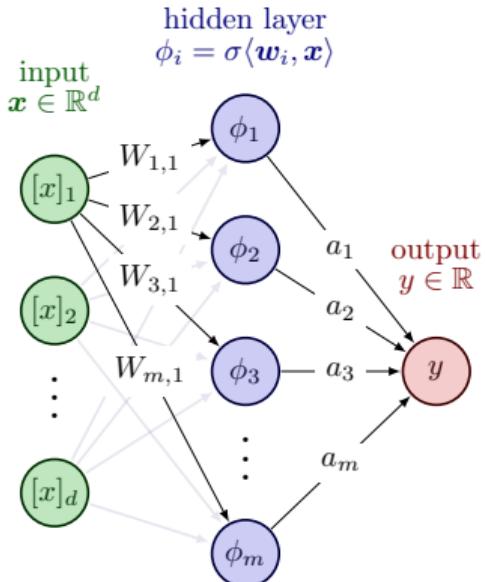
(c) Test Loss vs. Path-norm

**Figure 7:** Experiments on two-layer neural networks.

## Two-layer neural networks, path norm



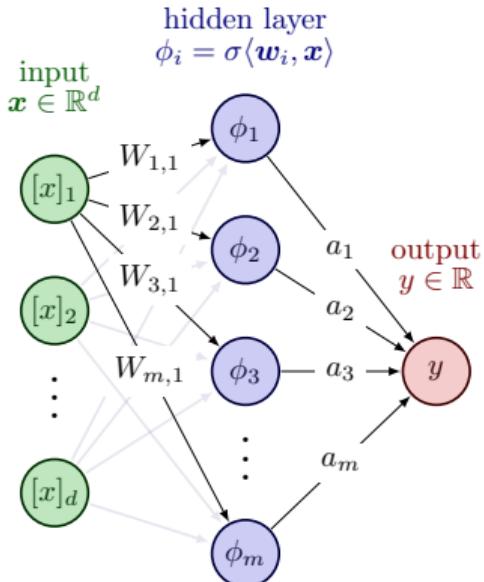
## Two-layer neural networks, path norm



$\ell_1$ -path norm (Neyshabur et al., 2015)

$$\|\boldsymbol{\theta}\|_{\mathcal{P}} := \frac{1}{m} \sum_{k=1}^m |a_k| \|\mathbf{w}_k\|_1$$

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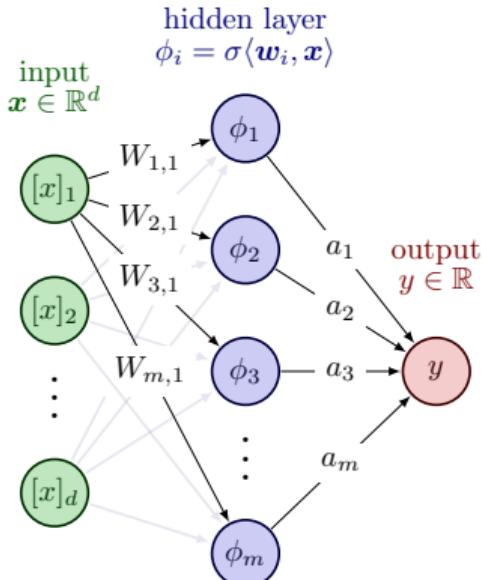
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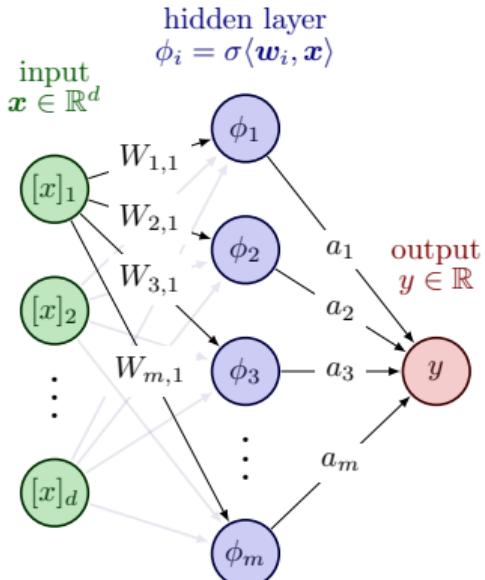
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- Variation in only a few directions  
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Can neural networks identify this structure?



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

To achieve  $\epsilon$ -excess risk,

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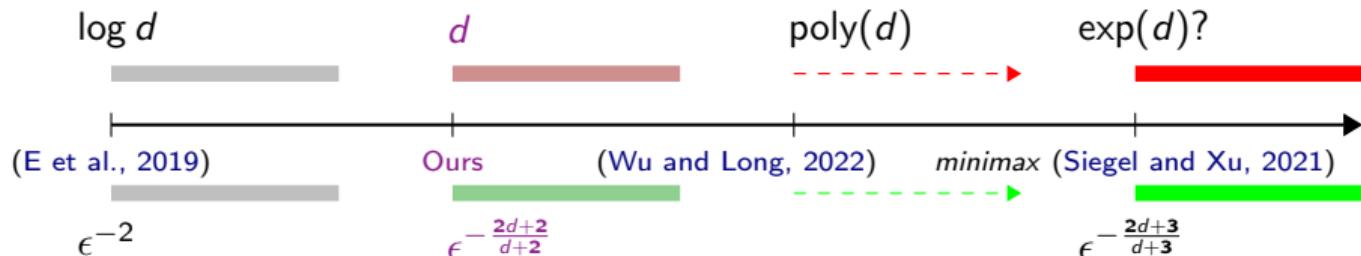
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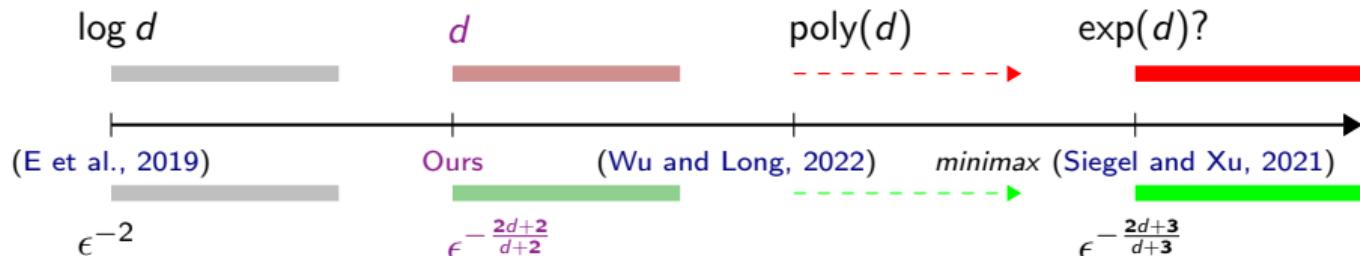
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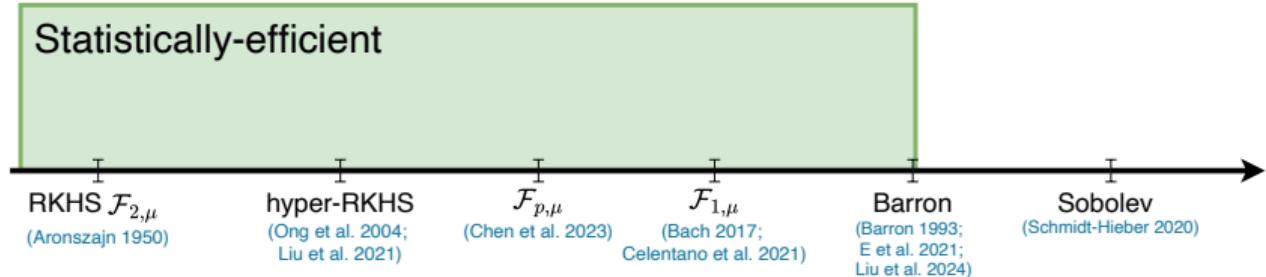
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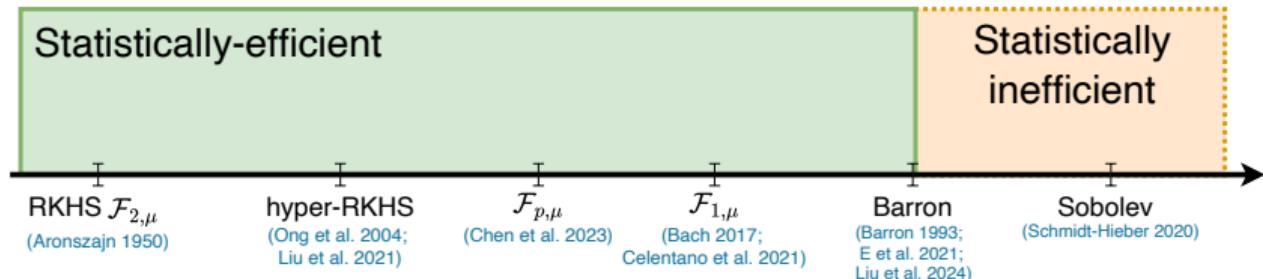


The “best” trade-off between  $\epsilon$  and  $d$ .

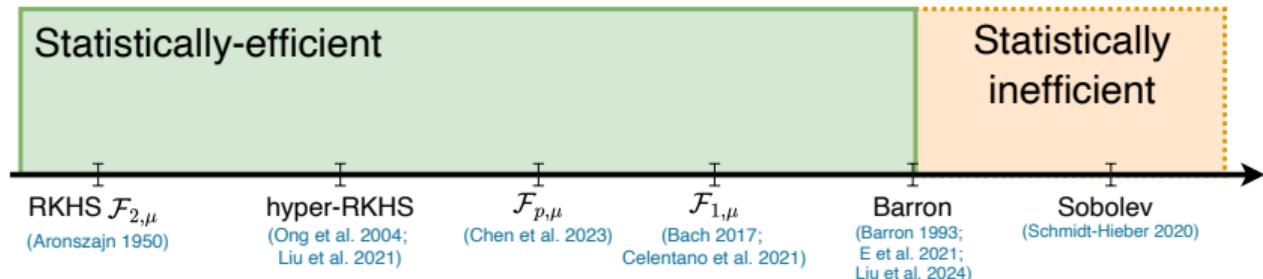
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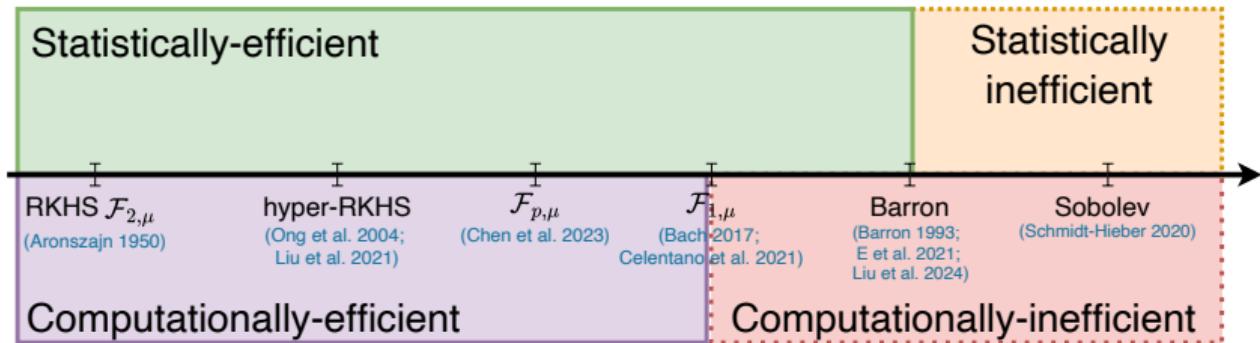


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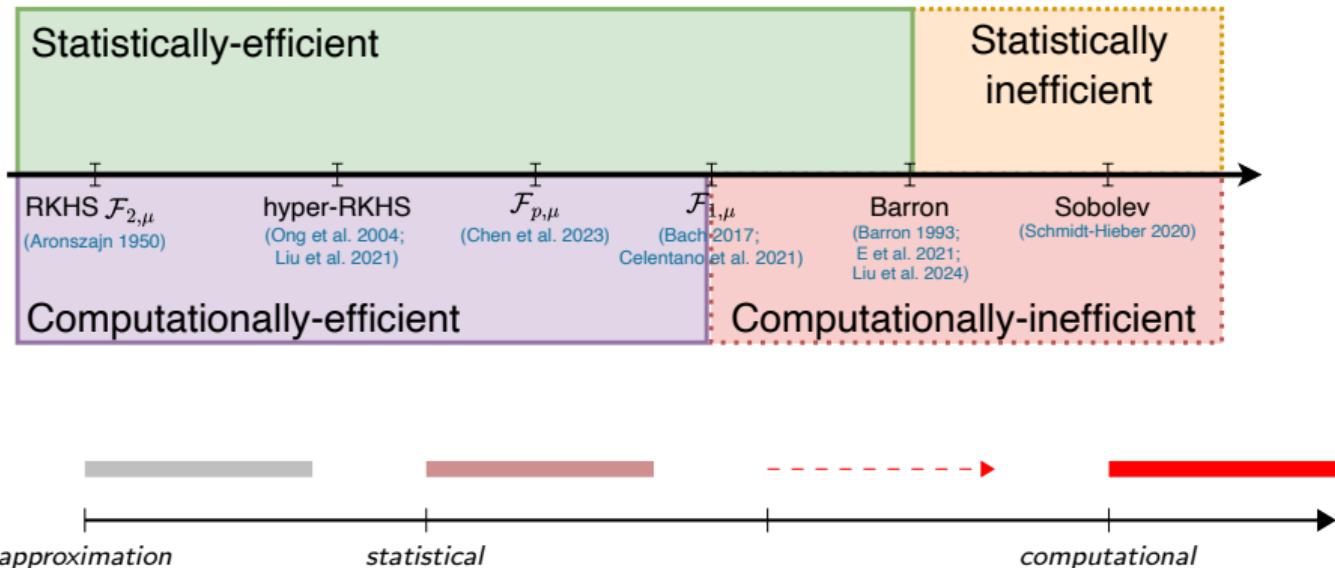


Optimization in Barron spaces is NP hard: curse of dimensionality!  
(Bach, 2017)

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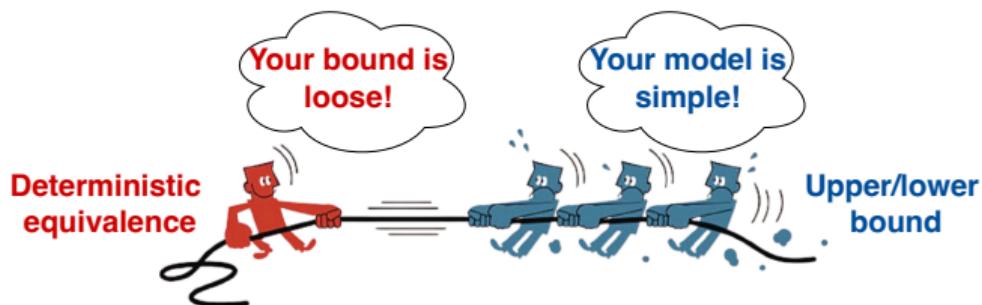


- ReLU neurons (Chen and Narayanan, 2023)
- Low-dimensional polynomials (Arous et al., 2021; Lee et al., 2024)

## **Deep learning phenomena $\Rightarrow$ interesting mathematical problems**

### Be aware of model capacity! A new paradigm of $\varphi$ curve!

- Reshape bias-variance trade-offs, double descent, scaling law under proper  $\ell_2$  norm-based capacity via **deterministic equivalence**.

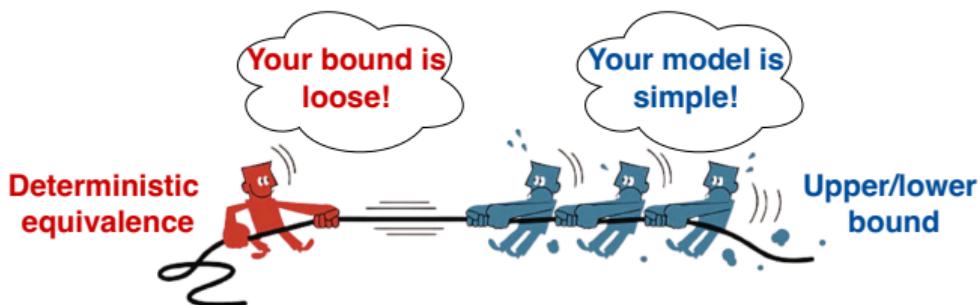


# Takeaway messages

## Deep learning phenomena $\Rightarrow$ interesting mathematical problems

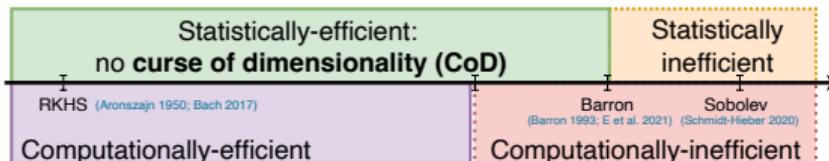
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### Which function class can be **efficiently** learned by neural networks?

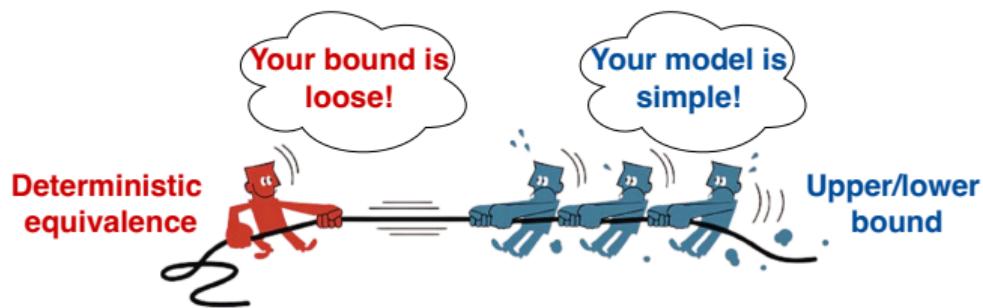
- Neural networks can adapt to low-dimensional structure and avoid CoD!



## Takeaway messages

### Deep learning phenomena $\Rightarrow$ interesting mathematical problems

- Be aware of model capacity! A new paradigm of  $\varphi$  curve!
  - Reshape bias-variance trade-offs, double descent, scaling law under proper  $\ell_2$  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 theory contribute to practical fine-tuning problems?
  - One-step full gradient can be sufficient! [ICML'25 oral]

## References

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- Gerard Ben Arous, Reza Gheissari, and Aukosh Jagannath. Online stochastic gradient descent on non-convex losses from high-dimensional inference. *Journal of Machine Learning Research*, 22(106):1–51, 2021.
- Francis Bach. Breaking the curse of dimensionality with convex neural networks. *Journal of Machine Learning Research*, 18(1):629–681, 2017.
- Francis Bach. High-dimensional analysis of double descent for linear regression with random projections. *SIAM Journal on Mathematics of Data Science*, 6(1):26–50, 2024.

- Andrew R Barron. Universal approximation bounds for superpositions of a sigmoidal function. *IEEE Transactions on Information theory*, 39(3):930–945, 1993.
- Peter Bartlett. The sample complexity of pattern classification with neural networks: the size of the weights is more important than the size of the network. *IEEE Transactions on Information Theory*, 44(2):525–536, 1998.
- Mikhail Belkin, Daniel Hsu, Siyuan Ma, and Soumik Mandal. Reconciling modern machine-learning practice and the classical bias–variance trade-off. *the National Academy of Sciences*, 116(32):15849–15854, 2019.
- Hongrui Chen, Jihao Long, and Lei Wu. A duality framework for generalization analysis of random feature models and two-layer neural networks. *arXiv preprint arXiv:2305.05642*, 2023.

- Sitan Chen and Shyam Narayanan. A faster and simpler algorithm for learning shallow networks. *arXiv preprint arXiv:2307.12496*, 2023.
- Chen Cheng and Andrea Montanari. Dimension free ridge regression. *The Annals of Statistics*, 52(6):2879–2912, 2024.
- Leonardo Defilippis, Bruno Loureiro, and Theodor Misiakiewicz. Dimension-free deterministic equivalents for random feature regression. In *Advances in Neural Information Processing Systems*, 2024.
- Weinan E, Chao Ma, and Lei Wu. A priori estimates of the population risk for two-layer neural networks. *Communications in Mathematical Sciences*, 17(5):1407–1425, 2019.
- Weinan E, Chao Ma, and Lei Wu. The barron space and the flow-induced function spaces for neural network models. *Constructive Approximation*, pages 1–38, 2021.

- Jonathan Frankle and Michael Carbin. The lottery ticket hypothesis: Finding sparse, trainable neural networks. In *International Conference on Learning Representations*, 2019.
- Stuart Geman, Elie Bienenstock, and René Doursat. Neural networks and the bias/variance dilemma. *Neural computation*, 4(1):1–58, 1992.
- Per Christian Hansen. Analysis of discrete ill-posed problems by means of the l-curve. *SIAM Review*, 34(4):561–580, 1992.
- Trevor Hastie, Robert Tibshirani, Jerome H Friedman, and Jerome H Friedman. *The elements of statistical learning: data mining, inference, and prediction*, volume 2. Springer, 2009.
- Trevor Hastie, Andrea Montanari, Saharon Rosset, and Ryan J Tibshirani. Surprises in high-dimensional ridgeless least squares interpolation. *Annals of Statistics*, 50(2):949–986, 2022.

- Yiding Jiang, Behnam Neyshabur, Hossein Mobahi, Dilip Krishnan, and Samy Bengio. Fantastic generalization measures and where to find them. In *International Conference on Learning Representations*, 2020.
- Jared Kaplan, Sam McCandlish, Tom Henighan, Tom B Brown, Benjamin Chess, Rewon Child, Scott Gray, Alec Radford, Jeffrey Wu, and Dario Amodei. Scaling laws for neural language models. *arXiv preprint arXiv:2001.08361*, 2020.
- Jason D Lee, Kazusato Oko, Taiji Suzuki, and Denny Wu. Neural network learns low-dimensional polynomials with sgd near the information-theoretic limit. *arXiv preprint arXiv:2406.01581*, 2024.
- Tengyuan Liang, Alexander Rakhlin, and Xiyu Zhai. On the multiple descent of minimum-norm interpolants and restricted lower isometry of kernels. In *Conference on Learning Theory*, pages 2683–2711, 2020.

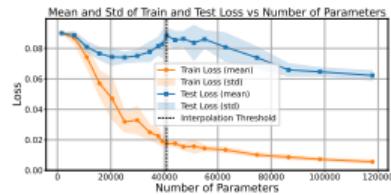
- Fanghui Liu, Xiaolin Huang, Yudong Chen, and Johan AK Suykens. Random features for kernel approximation: A survey on algorithms, theory, and beyond. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 44(10):7128–7148, 2021.
- Theodor Misiakiewicz and Basil Saeed. A non-asymptotic theory of kernel ridge regression: deterministic equivalents, test error, and gcv estimator. *arXiv preprint arXiv:2403.08938*, 2024.
- Pavlo Molchanov, Stephen Tyree, Tero Karras, Timo Aila, and Jan Kautz. Pruning convolutional neural networks for resource efficient inference. In *International Conference on Learning Representations*, 2017.
- Preetum Nakkiran, Gal Kaplun, Yamini Bansal, Tristan Yang, Boaz Barak, and Ilya Sutskever. Deep double descent: Where bigger models and more data hurt. In *International Conference on Learning Representations*, 2019.

- Brady Neal. On the bias-variance tradeoff: Textbooks need an update. *arXiv preprint arXiv:1912.08286*, 2019.
- Behnam Neyshabur, Ryota Tomioka, and Nathan Srebro. Norm-based capacity control in neural networks. In *Conference on Learning Theory*, pages 1376–1401. PMLR, 2015.
- Andrew Ng and Tengyu Ma. CS229 lecture notes. 2023. URL [https://cs229.stanford.edu/main\\_notes.pdf](https://cs229.stanford.edu/main_notes.pdf).
- Elliot Paquette, Courtney Paquette, Lechao Xiao, and Jeffrey Pennington. 4+3 phases of compute-optimal neural scaling laws. *arXiv preprint arXiv:2405.15074*, 2024.
- Rahul Parhi and Robert D Nowak. Near-minimax optimal estimation with shallow ReLU neural networks. *IEEE Transactions on Information Theory*, 2022.

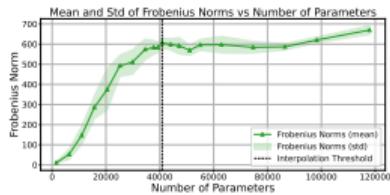
- Ali Rahimi and Benjamin Recht. Random features for large-scale kernel machines. In *Advances in Neural Information Processing Systems*, pages 1177–1184, 2007.
- Pedro Savarese, Itay Evron, Daniel Soudry, and Nathan Srebro. How do infinite width bounded norm networks look in function space? In *Conference on Learning Theory*, pages 2667–2690. PMLR, 2019.
- Jonathan W Siegel and Jinchao Xu. Sharp bounds on the approximation rates, metric entropy, and  $n$ -widths of shallow neural networks. *arXiv preprint arXiv:2101.12365*, 2021.
- Aad W Van Der Vaart, Adrianus Willem van der Vaart, Aad van der Vaart, and Jon Wellner. *Weak convergence and empirical processes: with applications to statistics*. Springer Science & Business Media, 1996.

- Vladimir N. Vapnik. *The Nature of Statistical Learning Theory*. Springer, 1995.
- Andrew Gordon Wilson. Deep learning is not so mysterious or different. *arXiv preprint arXiv:2503.02113*, 2025.
- Denny Wu and Ji Xu. On the optimal weighted  $\ell_2$  regularization in overparameterized linear regression. In *Advances in Neural Information Processing Systems*, pages 10112–10123, 2020.
- Lei Wu and Jihao Long. A spectral-based analysis of the separation between two-layer neural networks and linear methods. *Journal of Machine Learning Research*, 119:1–34, 2022.

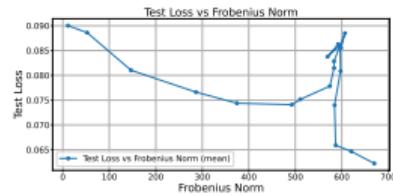
# Experimental results



(a) Test (training) Loss vs.  $p$



(b) Fro-norm vs.  $p$



(c) Test Loss vs. Fro-norm

**Figure 8:** 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

- $\{(\mathbf{x}_i, y_i)\}_{i=1}^n \stackrel{i.i.d.}{\sim} \mu, \mathbf{x}_i \in \mathbb{R}^d, y_i \in \mathbb{R}$ , covariance matrix  $\Sigma = \mathbb{E}[\mathbf{x}\mathbf{x}^\top]$
- $y = \langle \boldsymbol{\beta}_*, \mathbf{x} \rangle + \varepsilon$  with  $\mathbb{E}(\varepsilon) = 0$  and  $\mathbb{V}(\varepsilon) = \sigma^2$
- ridge regression:  $\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$
- min- $\ell_2$ -norm interpolation:  $\hat{\boldsymbol{\beta}}_{\min} = \operatorname{argmin}_{\boldsymbol{\beta}} \|\boldsymbol{\beta}\|_2$ , s.t.  $\mathbf{X}\boldsymbol{\beta} = \mathbf{y}$
- expected test risk: bias-variance decomposition

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

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- \*Intuitive fact: for i.i.d. sub-Gaussian data  $\mathbf{X}$ , we have

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- $y = \langle \boldsymbol{\beta}_*, \mathbf{x} \rangle + \varepsilon$  with  $\mathbb{E}(\varepsilon) = 0$  and  $\mathbb{V}(\varepsilon) = \sigma^2$
- ridge regression:  $\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$
- min- $\ell_2$ -norm interpolation:  $\hat{\boldsymbol{\beta}}_{\min} = \operatorname{argmin}_{\boldsymbol{\beta}} \|\boldsymbol{\beta}\|_2$ , s.t.  $\mathbf{X}\boldsymbol{\beta} = \mathbf{y}$
- expected test risk: bias-variance decomposition

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

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

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

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

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

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

**Theorem (Deterministic equivalence (Cheng and Montanari, 2024))**

For sub-Gaussian data, assume  $\Sigma$  is well-behaved, w.h.p.

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

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

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

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

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

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

- 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

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

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# Proof sketch: convex hull technique and its constant!

- Consider the following function space

$$\mathcal{F} = \{\sigma(\langle \tilde{\mathbf{w}}, \cdot \rangle) : \tilde{\mathbf{w}} \in \mathcal{W}\} \cup \{0\} \cup \{-\sigma(\langle \tilde{\mathbf{w}}, \cdot \rangle) : \tilde{\mathbf{w}} \in \mathbb{S}_1^{d-1} \text{ with the } \ell_1 \text{ ball}\}$$

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

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

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

$$\log \mathcal{N}_2(\mathcal{G}_1, \epsilon) \leq \log \mathcal{N}_2(\bar{\mathcal{F}}, \epsilon, \mu) \leq \textcolor{red}{C} \left( \frac{1}{\epsilon} \right)^{\frac{2d}{d+2}}.$$

- control the constant  $\textcolor{red}{C}$

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

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