

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

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Fanghui Liu

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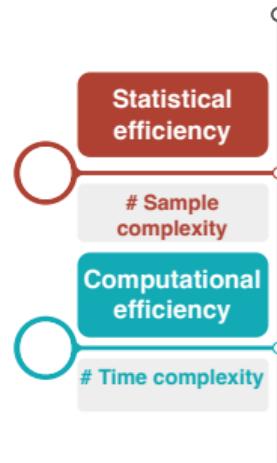
*Centre for Discrete Mathematics and its Applications (DIMAP), Warwick*



# My research

## ❑ Research interests

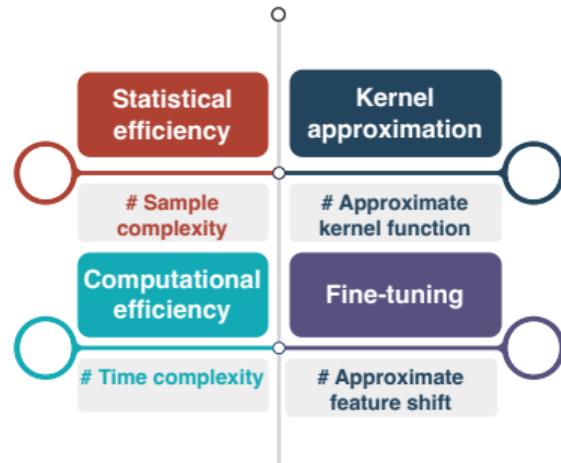
- Foundations of machine learning (ML)
- Theory-grounded efficient algorithm design
- Trustworthy ML



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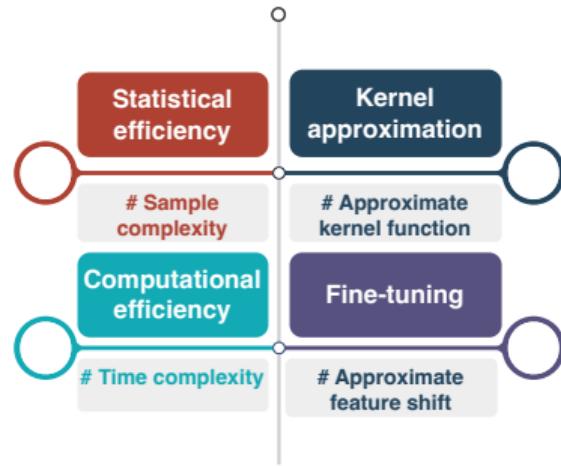
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- characterize **learning efficiency** in theory
- contribute to practice



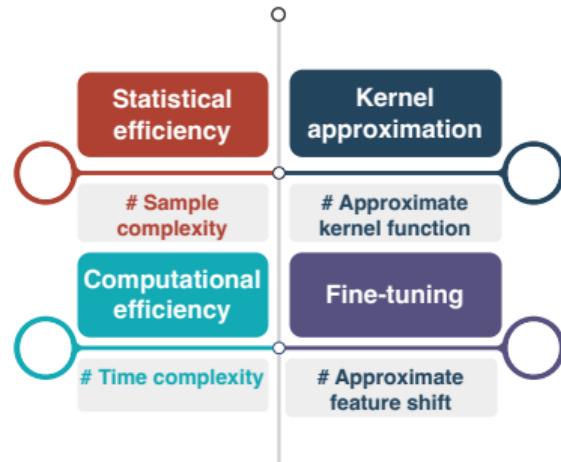
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## Learning efficiency (Curse of Dimensionality, CoD)

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

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

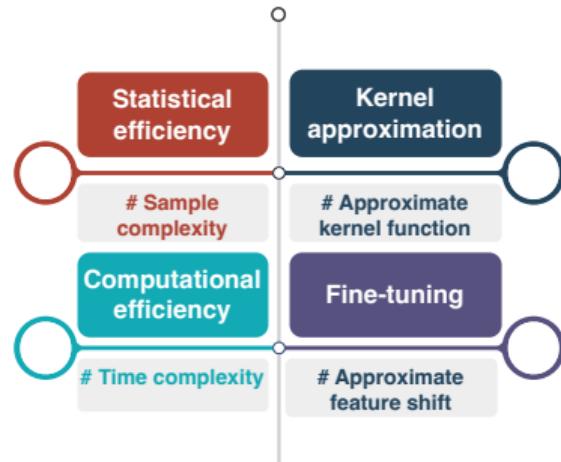
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Data



Model



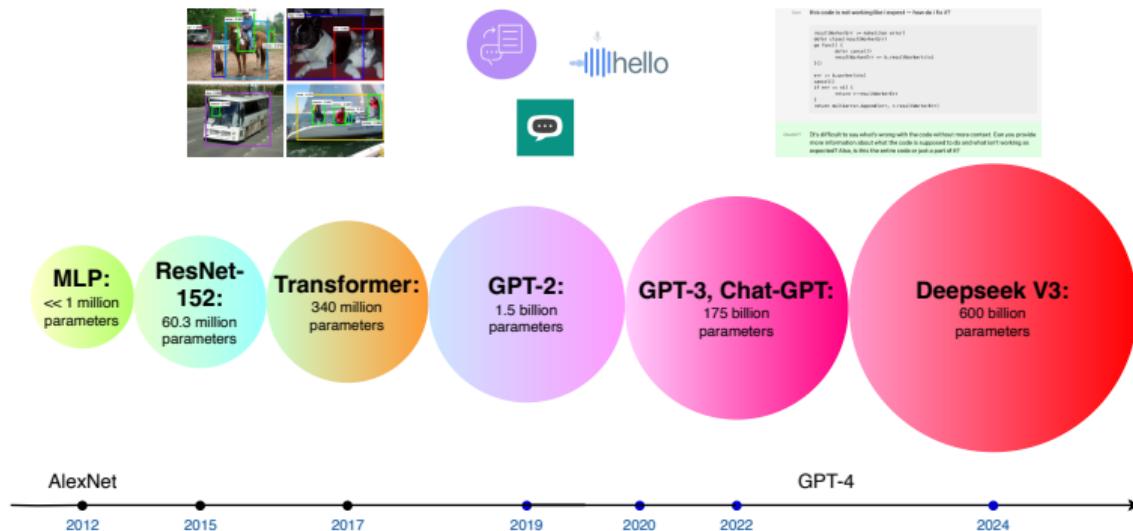
Algorithm



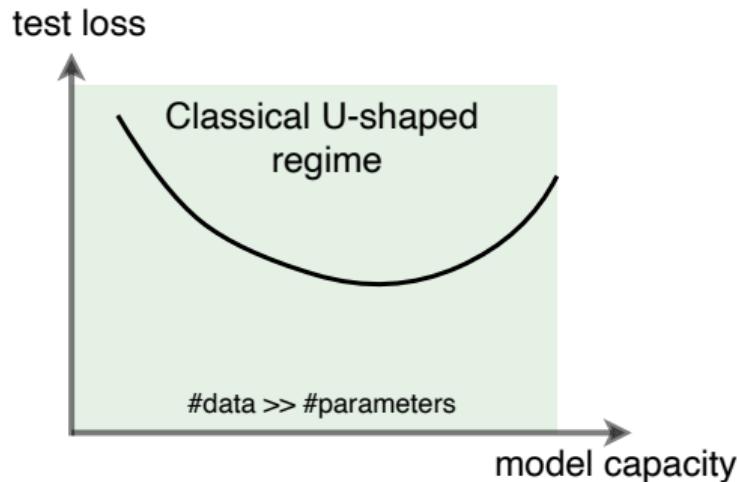
Compute

# In the era of machine learning

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

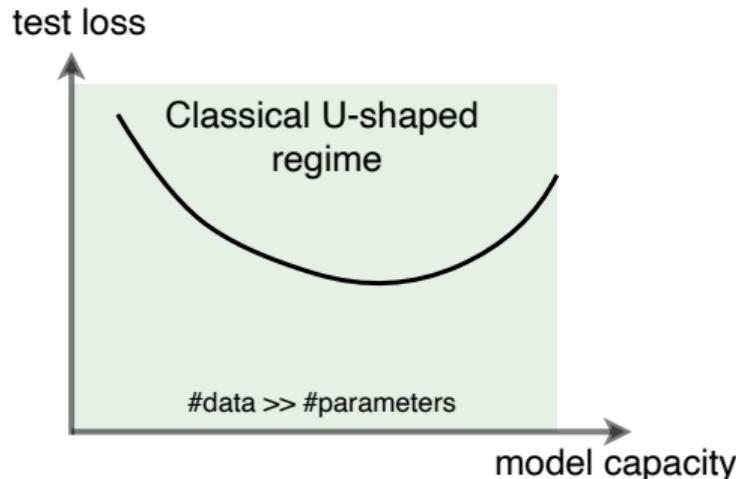


ML textbooks: Larger models tend to overfit!

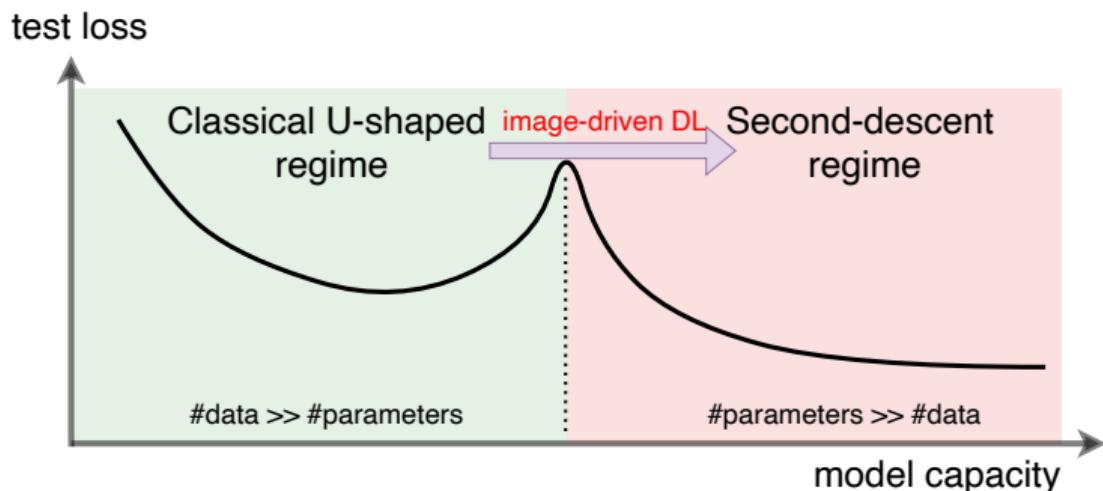


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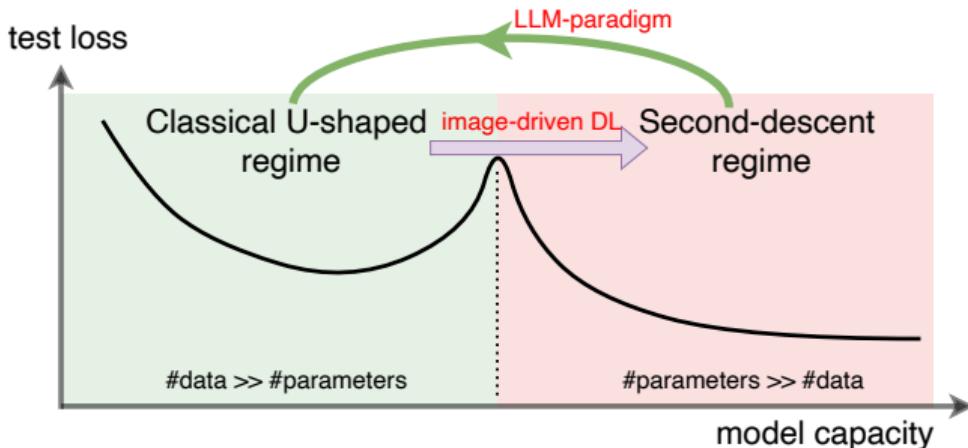


Practice of deep learning: bigger models perform better!



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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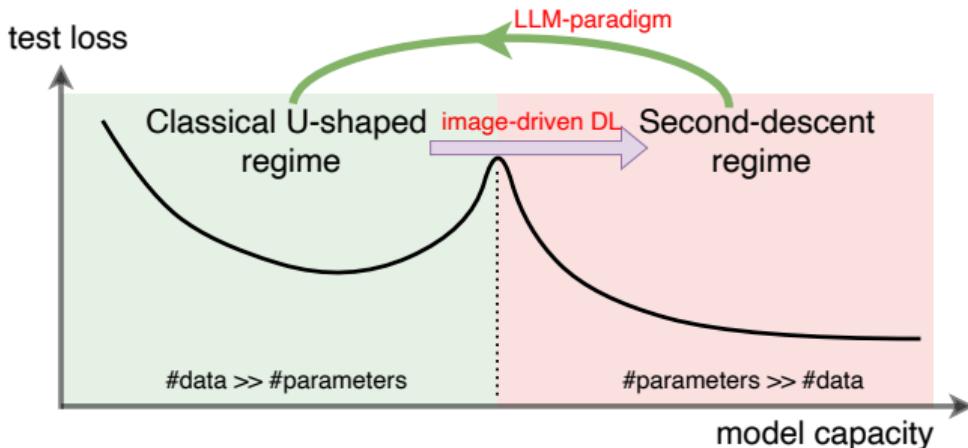


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# A fundamental concept in machine learning: model capacity

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](#))

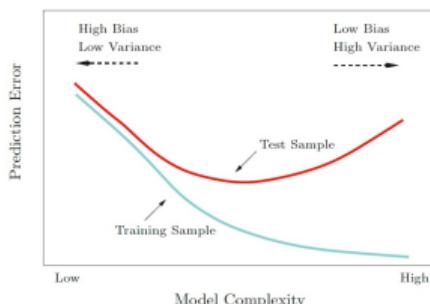
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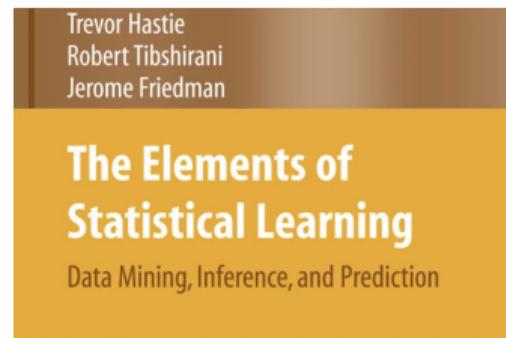
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## Bias-variance decomposition

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



([Hastie et al., 2009](#), Figure 2.11)



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## Bias-variance decomposition

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

"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.

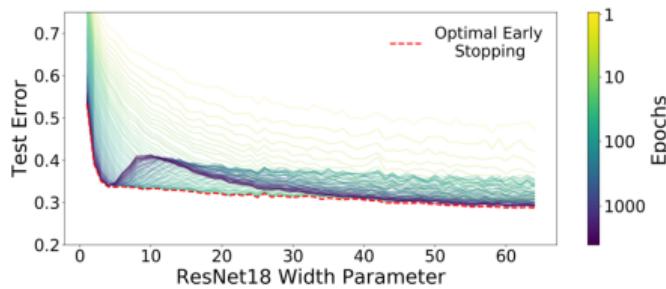
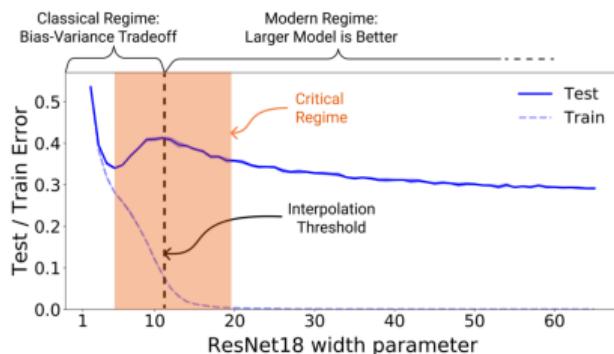
— Ben Recht, 2025

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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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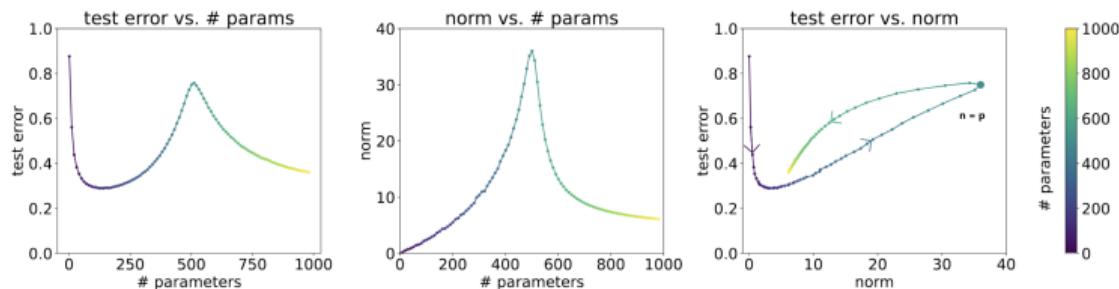


Figure 3: Stanford CS229 lecture notes ([Ng and Ma, 2023](#), Figure 8.12).

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

- 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. *Re-examining double descent and scaling laws under norm-based capacity via deterministic equivalence.* 2025. [arXiv](#)

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

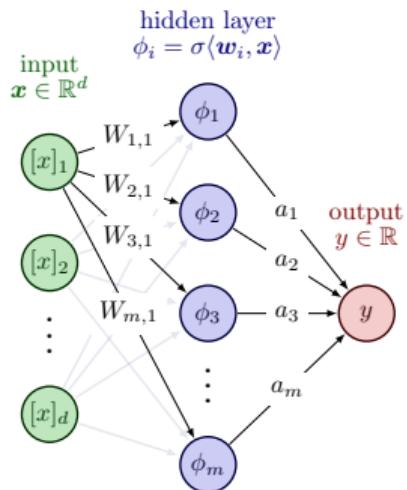
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- What is the induced function space and statistical/computational efficiency under norm-based capacity?
- Which function class can be **efficiently** learned by neural networks?
- Fanghui Liu, Leello Dadi, and Volkan Cevher. *Learning with norm constrained, over-parameterised, two-layer neural networks.* JMLR 2024.

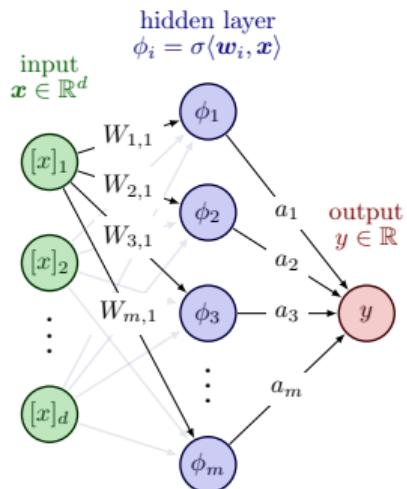
## Background: Random features model, two-layer neural networks



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

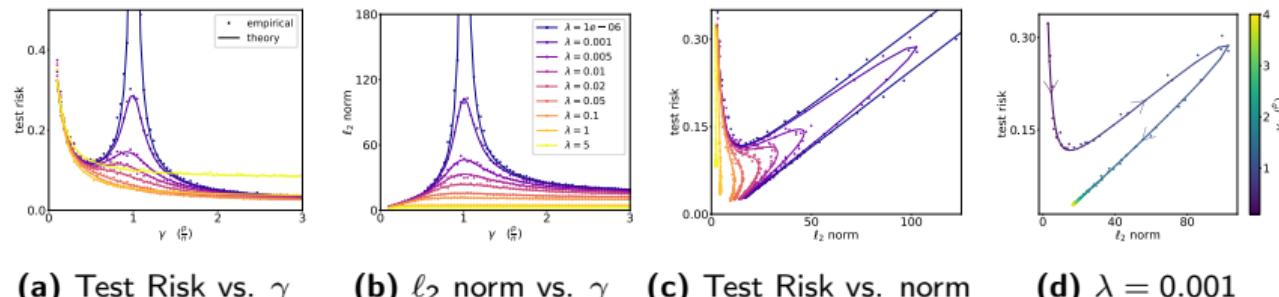
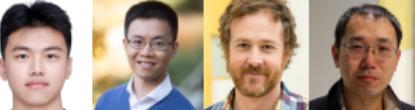
- $\phi : \mathcal{X} \times \mathcal{W} \rightarrow \mathbb{R}$ , e.g., ReLU:  
 $\phi(\mathbf{x}, \mathbf{w}) = \max(\langle \mathbf{x}, \mathbf{w} \rangle, 0)$
- Random features models (RFMs) Rahimi and Recht (2007):
  - $\{\mathbf{w}_i\}_{i=1}^m \stackrel{iid}{\sim} \mu$  for a given  $\mu \in \mathcal{P}(\mathcal{W})$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

## Background: Random features model, two-layer neural networks

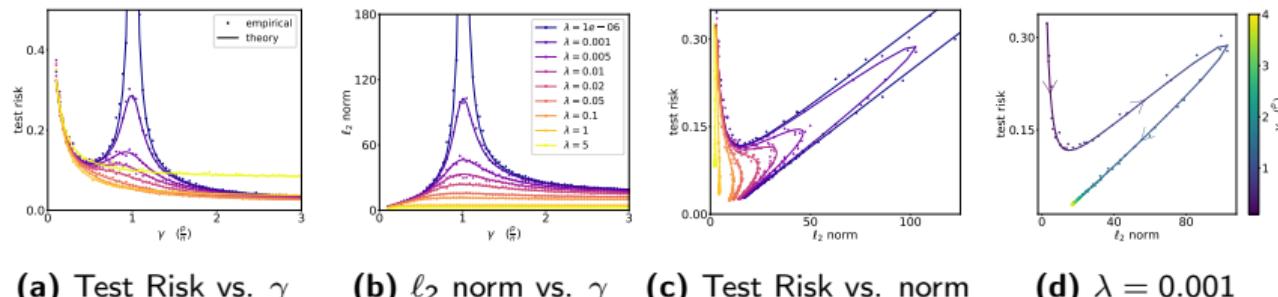
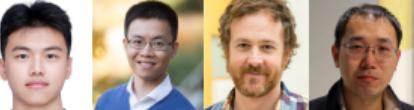


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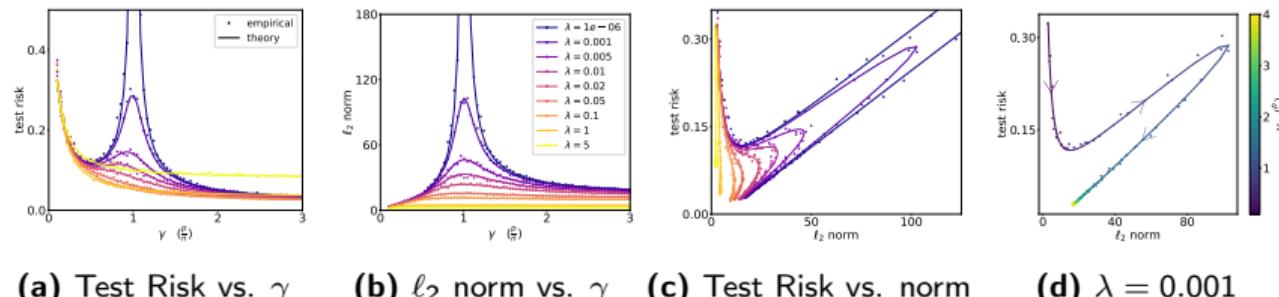
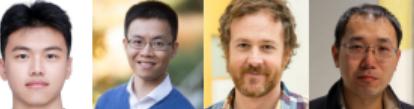
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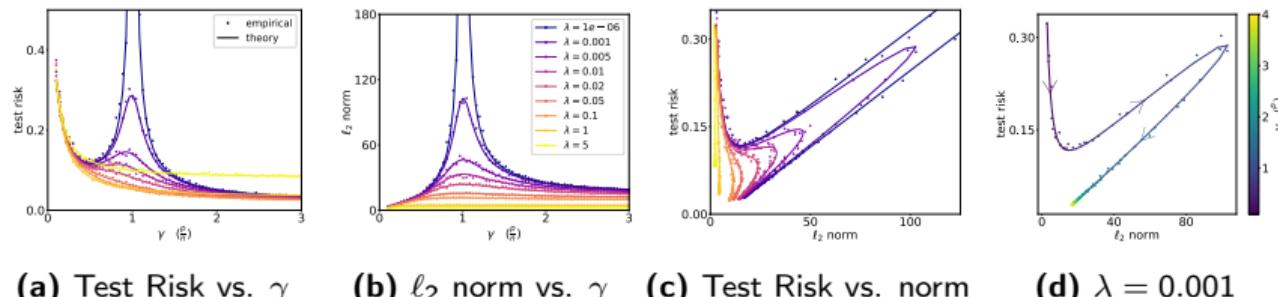
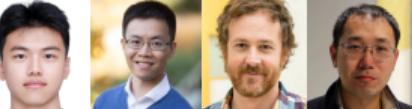
- $\gamma := p/n$ ,  $p$ : model size (width),  $n$ : data size
- Phase transition exists but double descent does not exist
- Reshape scaling-law:  
 $\text{test loss} = A \times \text{Data Size}^{-a} + B \times \text{Model Size}^{-b} + C$  with  $a, b > 0$   
 $\text{test loss} = A \times \text{Data Size}^{-a} \times \text{Norm Capacity}^{-b}$  with  $a > 0$  and  $b \in \mathbb{R}$
- Over-parameterization is still better than under-parameterization



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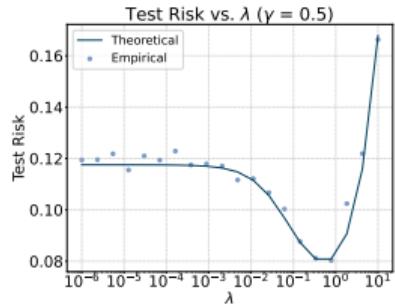


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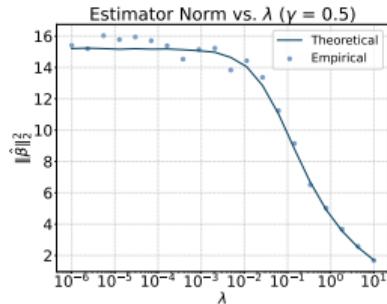


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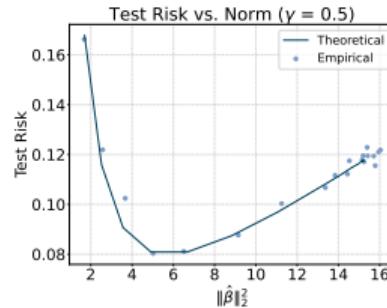
# Precise analysis: L-curve (Hansen, 1992)



(a) Test risk vs.  $\lambda$

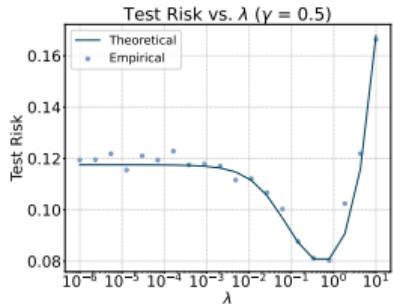


(b) Norm vs.  $\lambda$

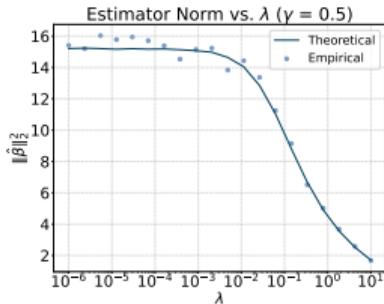


(c) Test risk vs. Norm

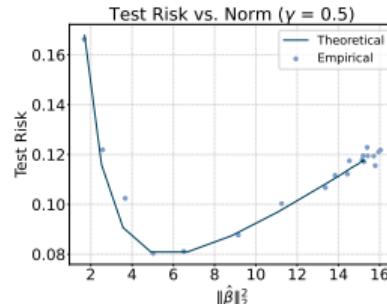
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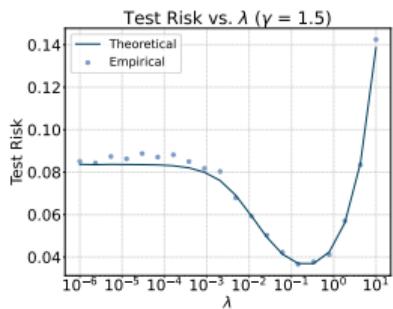
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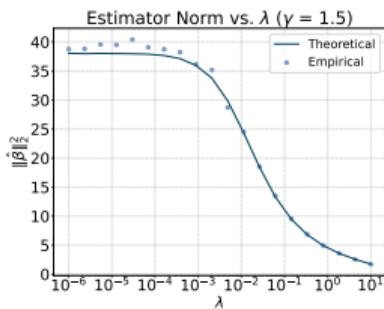
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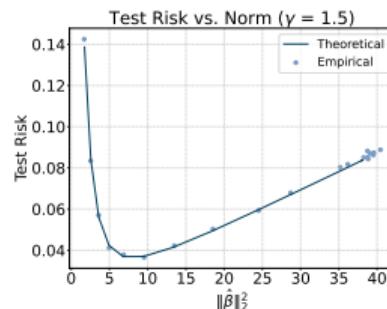
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(d) Test risk vs.  $\lambda$



(e) Norm vs.  $\lambda$



(f) Test risk vs. Norm

## 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](#)): law of large samples/dimensions in random matrix theory

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  
$$n - \frac{\lambda}{\lambda_*} = \text{Tr}(\Sigma (\Sigma + \lambda_*)^{-1}).$$

## Our results

### 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

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

$$\mathcal{V}_{\mathcal{N},\lambda} := \frac{\sigma^2 \text{Tr}(\Sigma(\Sigma + \lambda_*)^{-2})}{n - \text{Tr}(\Sigma^2(\Sigma + \lambda_*)^{-2})}.$$

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

- Norm-based capacity: ✓ ☺
- effective dimension-style  $\text{Tr}(\Sigma(\Sigma + \lambda I)^{-1})$ : ✗ ☺

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

- Norm-based capacity: ✓ ☺
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## Our results

### Theorem (Deterministic equivalence of estimator's norm)

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

- Test risk  $R_\lambda$  and norm  $N_\lambda$  formulates a cubic curve (complex but precise).
  - min-norm interpolator ( $\lambda = 0$ ):

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

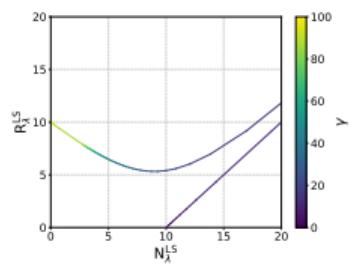
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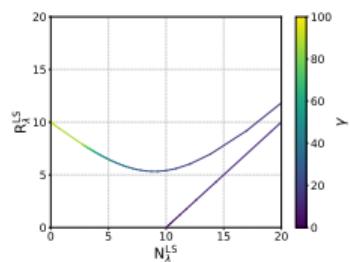
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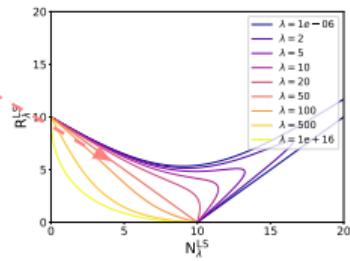
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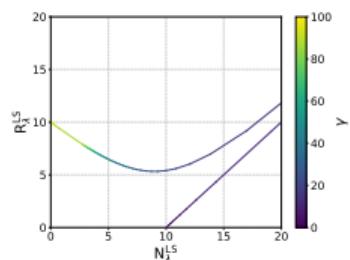
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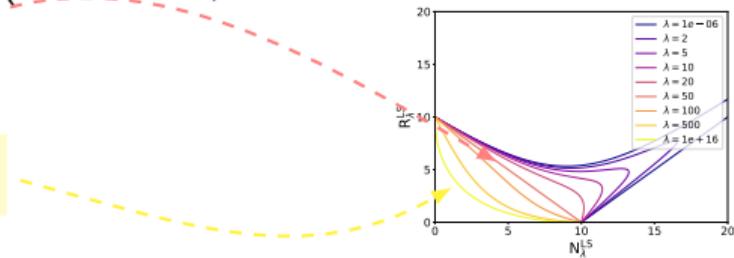
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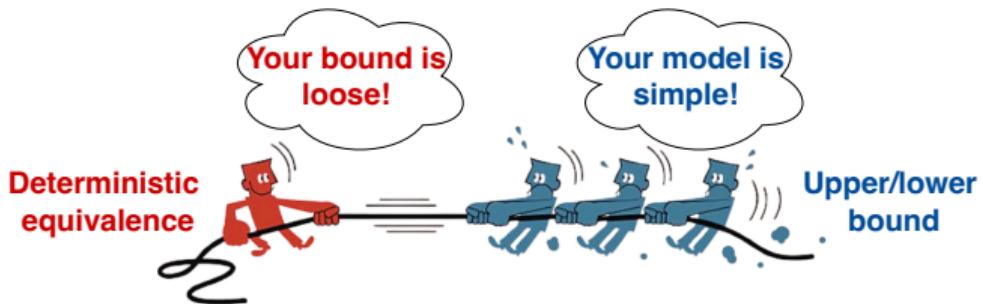


## Precise analysis via deterministic equivalence

- Precisely describe the learning curve.
  - phase transitions, (non-)monotonicity, etc.
- Enables *accurate comparison* between estimators/algorithms.
  - **Foundations of scaling law**: data or parameter under the same budget, 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
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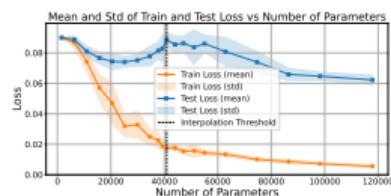
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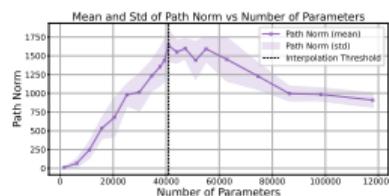
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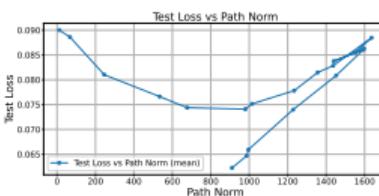
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(a) Test (training) Loss vs.  $p$



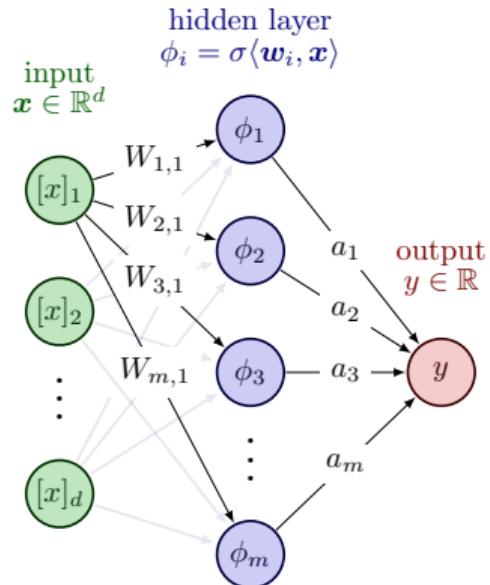
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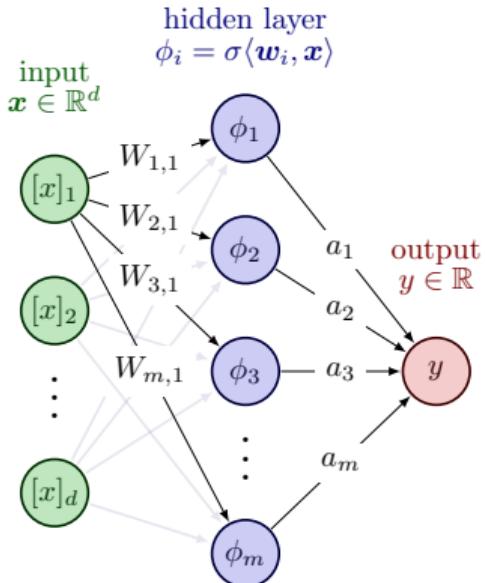
(c) Test Loss vs. Path-norm

**Figure 5:** Experiments on two-layer neural networks.

## Two-layer neural networks, path norm



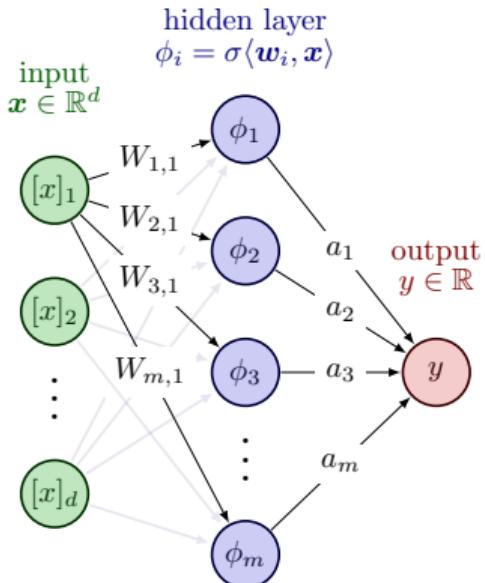
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$\ell_1$ -path norm (Neyshabur et al., 2015)

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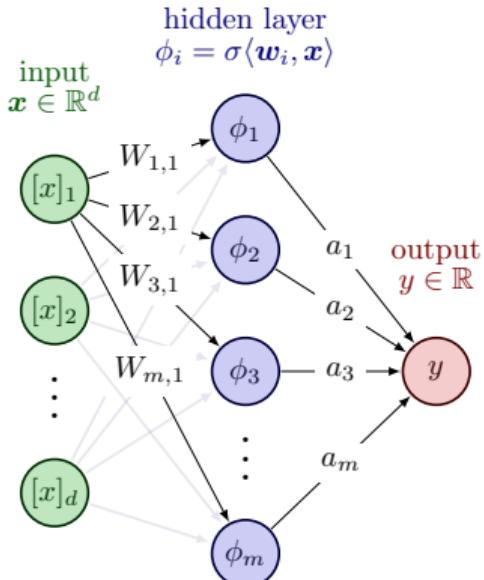
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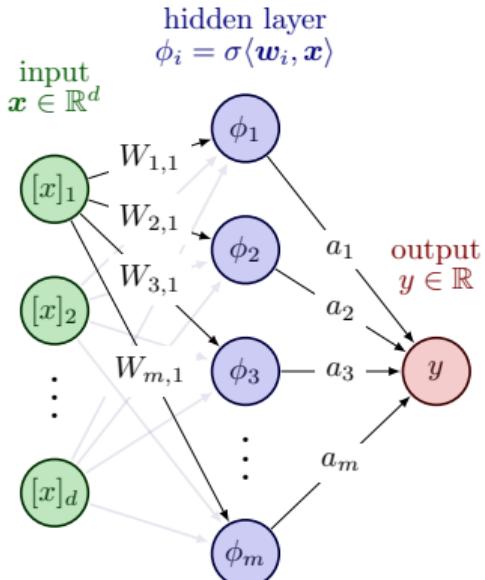
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Can neural networks identify this structure?



## 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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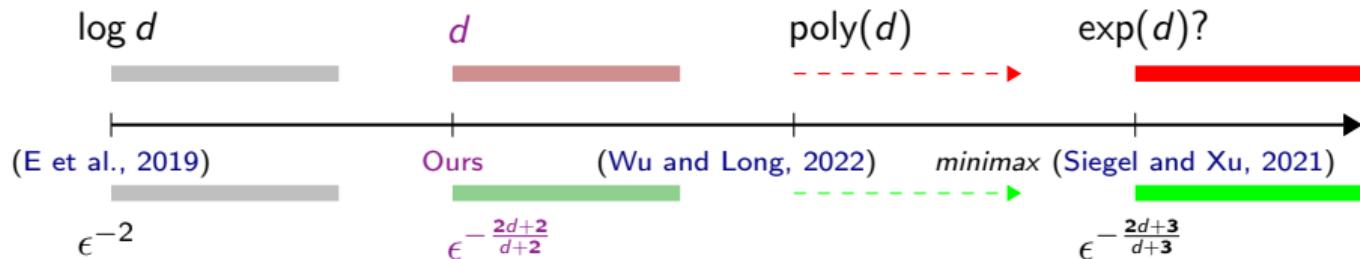
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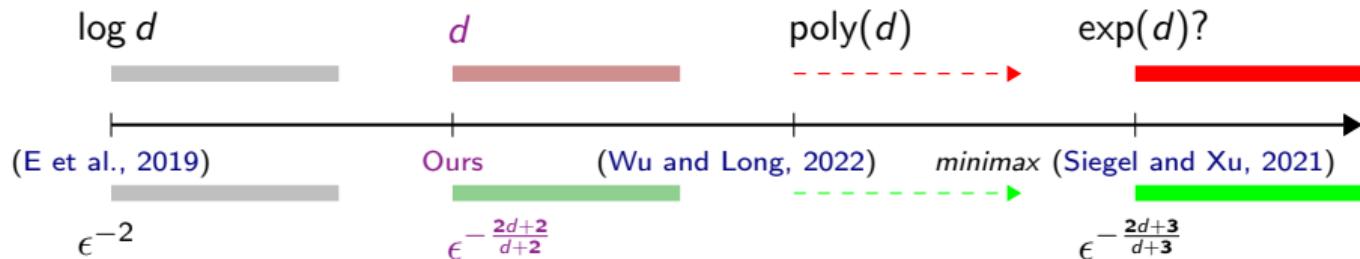
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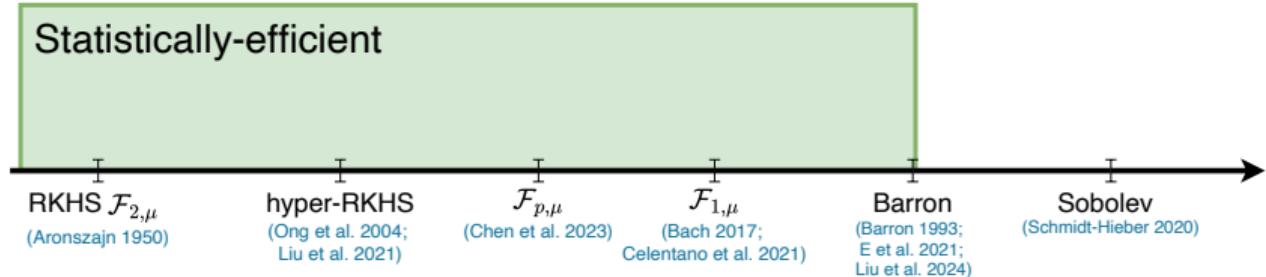
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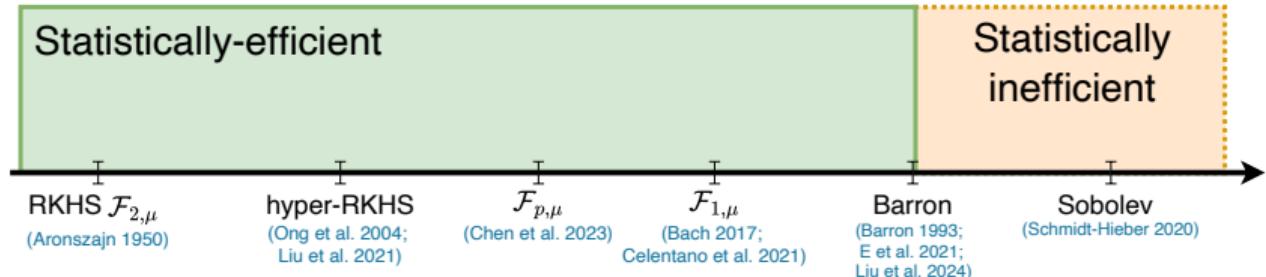


The “best” trade-off between  $\epsilon$  and  $d$ .

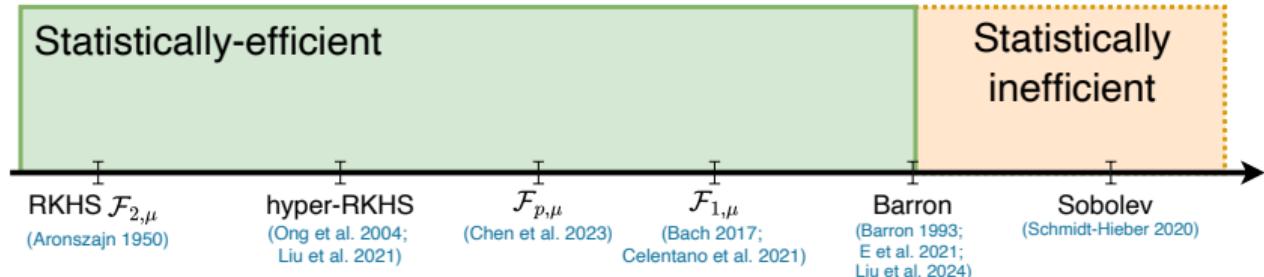
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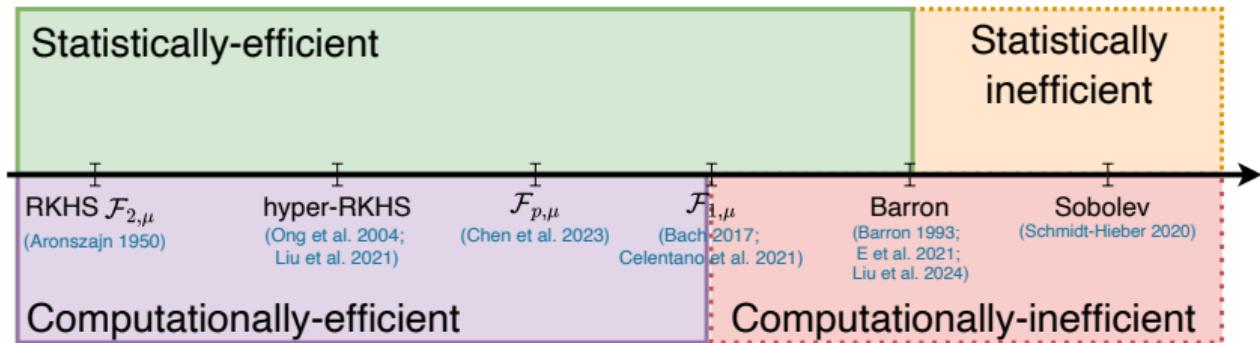


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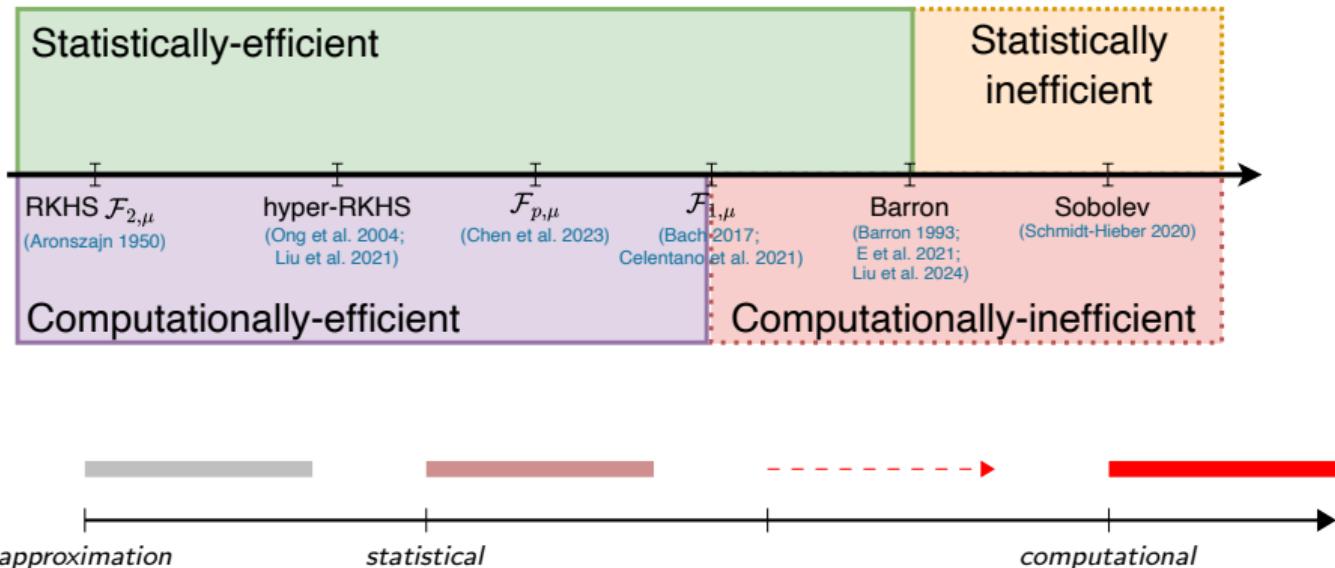


Optimization in Barron spaces is NP hard: curse of dimensionality!  
(Bach, 2017)

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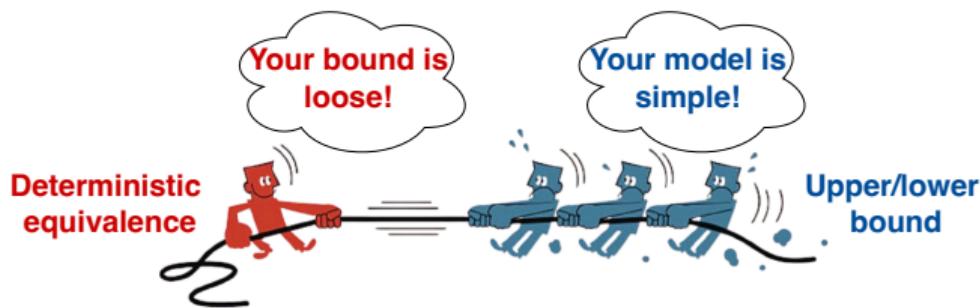


- ReLU neurons (Chen and Narayanan, 2023)
- Low-dimensional polynomials (Arous et al., 2021; Lee et al., 2024)

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

### Be aware of model capacity!

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

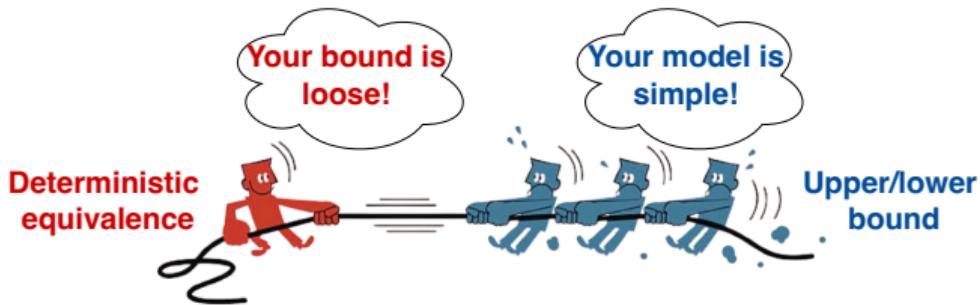


# Takeaway messages

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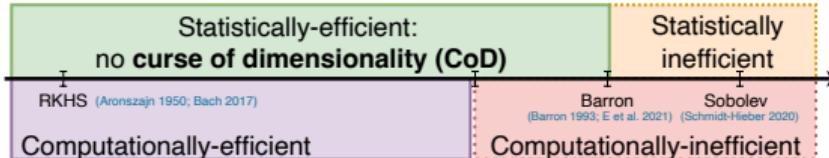
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### Which function class can be **efficiently** learned by neural networks?

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

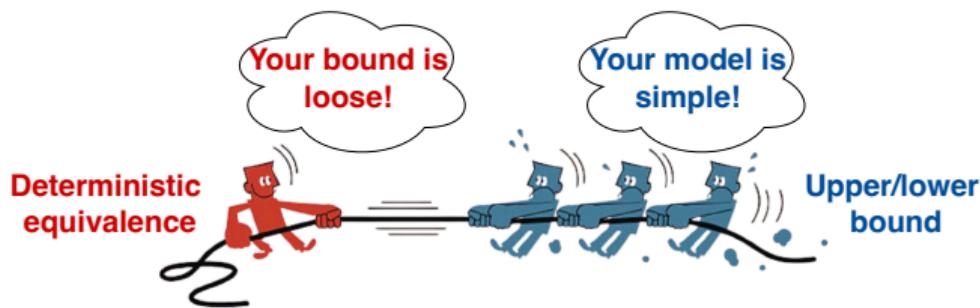


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### **Theoretical advances $\Rightarrow$ principled guidance in practical problems**

#### How does our theory contribute to practical fine-tuning problems?

- One-step full gradient can be sufficient! [\[GitHub\]](#)

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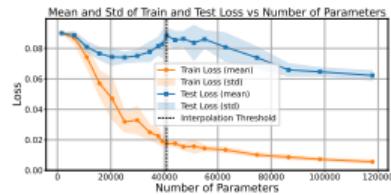
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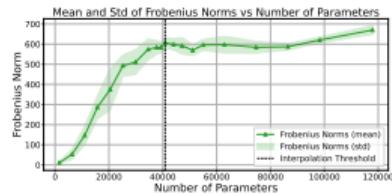
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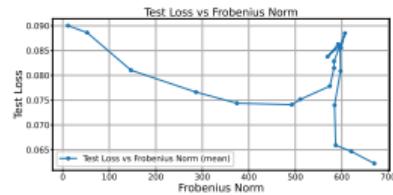
# Experimental results



(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

- $\{(\mathbf{x}_i, y_i)\}_{i=1}^n \stackrel{i.i.d.}{\sim} \mu, \mathbf{x}_i \in \mathbb{R}^d, y_i \in \mathbb{R}$ , 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

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

- $\mathcal{B}_{\mathcal{R}, \lambda}^{\text{LS}} = \lambda^2 \langle \boldsymbol{\beta}_*, (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \Sigma (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \boldsymbol{\beta}_* \rangle$
- $\mathcal{V}_{\mathcal{R}, \lambda}^{\text{LS}} = \sigma^2 \text{Tr}(\Sigma \mathbf{X}^\top \mathbf{X} (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-2})$
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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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## Proof of sketch on bias

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

◦ first term

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

◦ second term

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

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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  $p < 2$
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For any  $1 \leq p \leq \infty$ , define

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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  $\textcolor{red}{C}$

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

# Proof sketch: convex hull technique and its constant!

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