Double Descent / Implicit Regularization + PAC-Bayes

CPSC 532S: Modern Statistical Learning Theory

30 March 2022

cs.ubc.ca/~dsuth/532S/22/

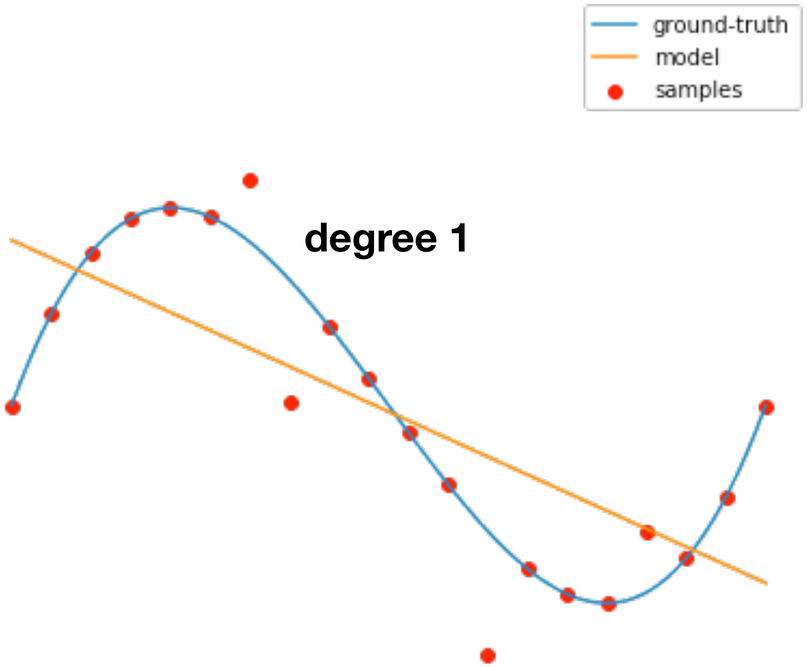
Admin

- A3 late-late deadline is tonight
- A4 out, due next Friday – late deadline Sunday, late-late deadline Tuesday

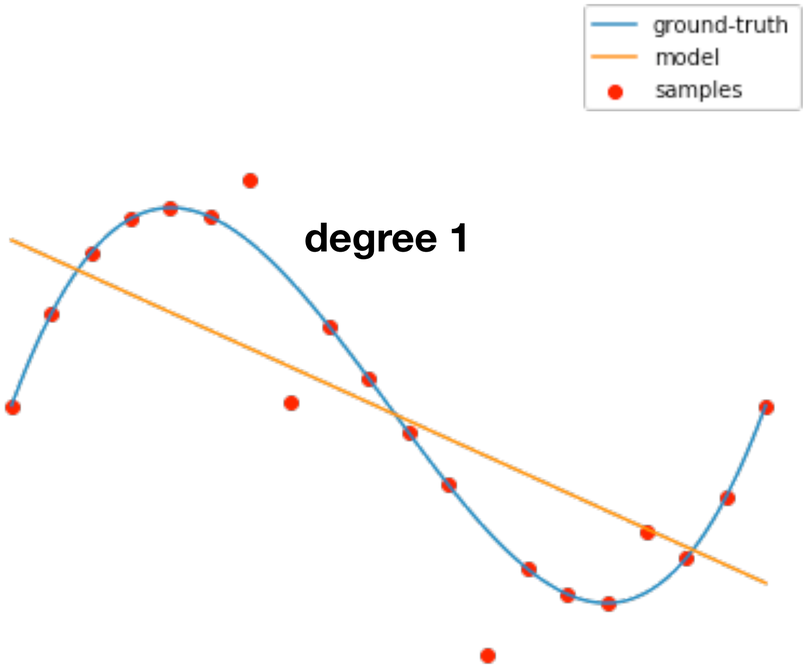
- Last regular class is Monday
  - Overview of online learning, privacy (~equivalent), connection to stability

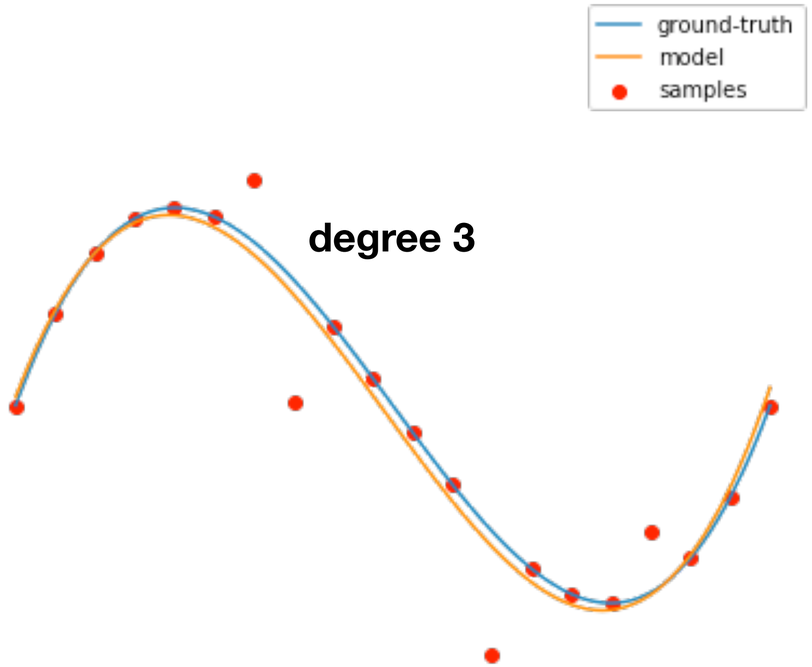
- Project presentations in class next Wednesday
  - Details were posted on Piazza a bit ago
  - Will post schedule tonight
- Project reports due next Friday – usual late policy (-5 Saturday, -10 Sunday)

- Final will be take-home, available over most of the finals period
  - Exact dates TBA – contact me if this really matters to you for whatever reason



Nakkiran et al. blog post's companion notebook





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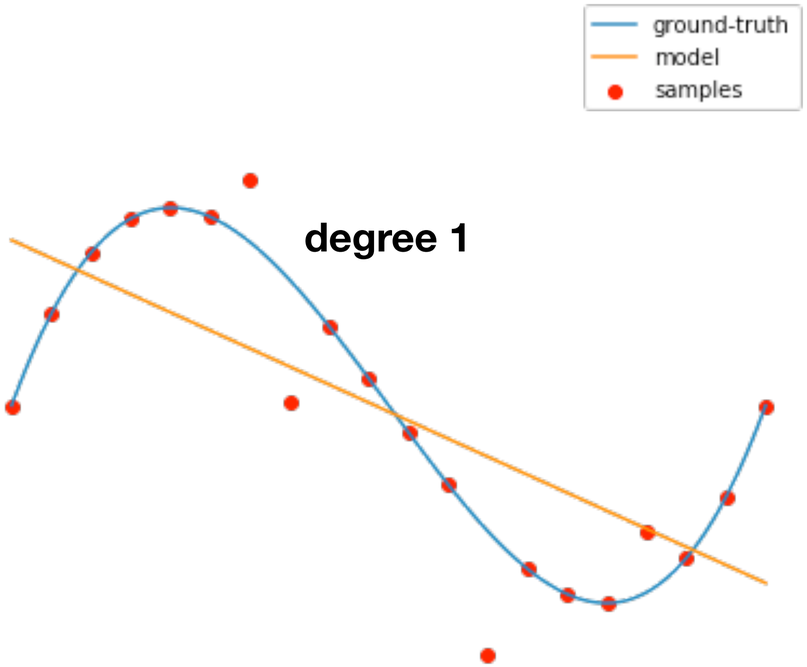

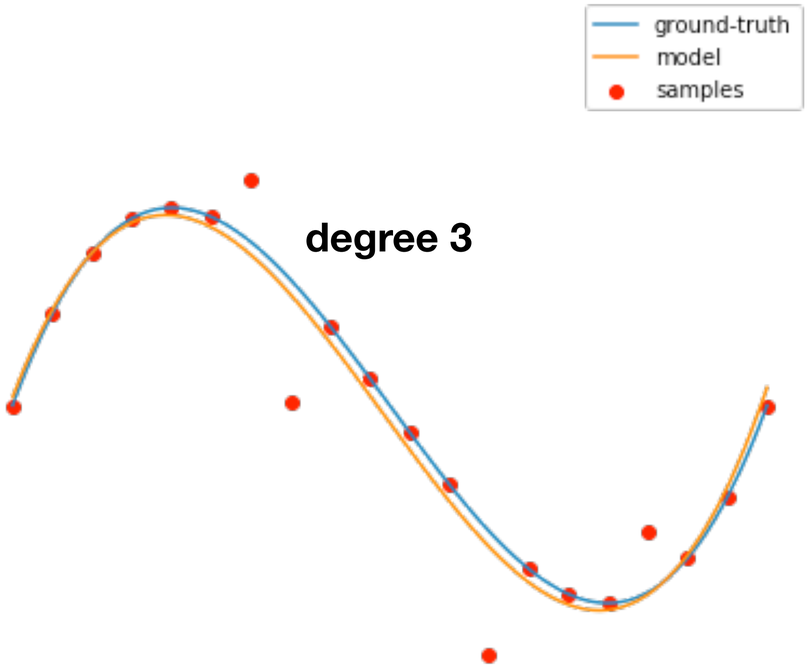

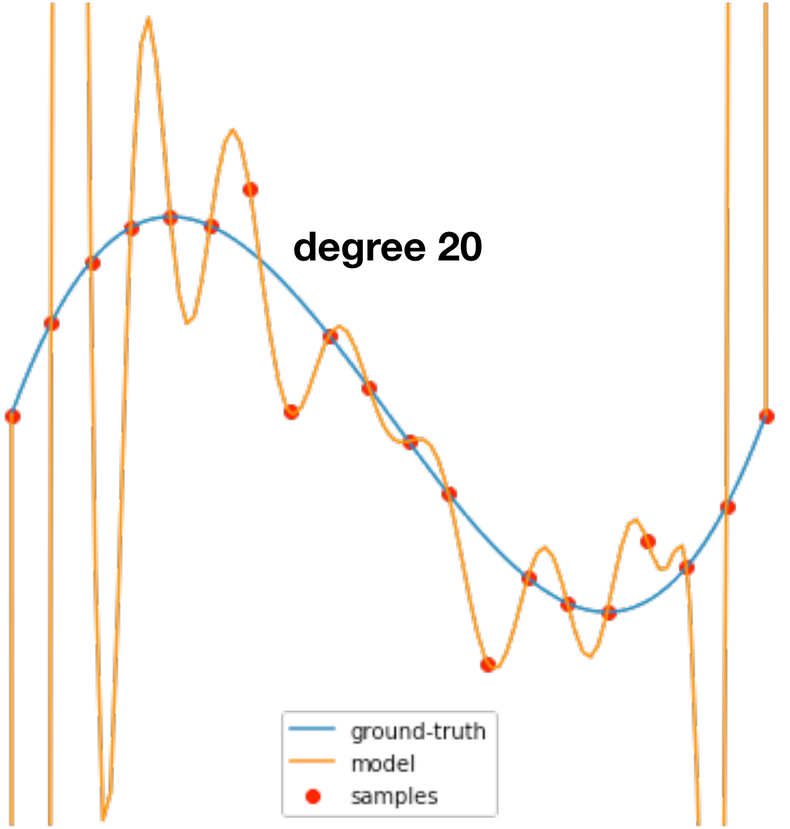

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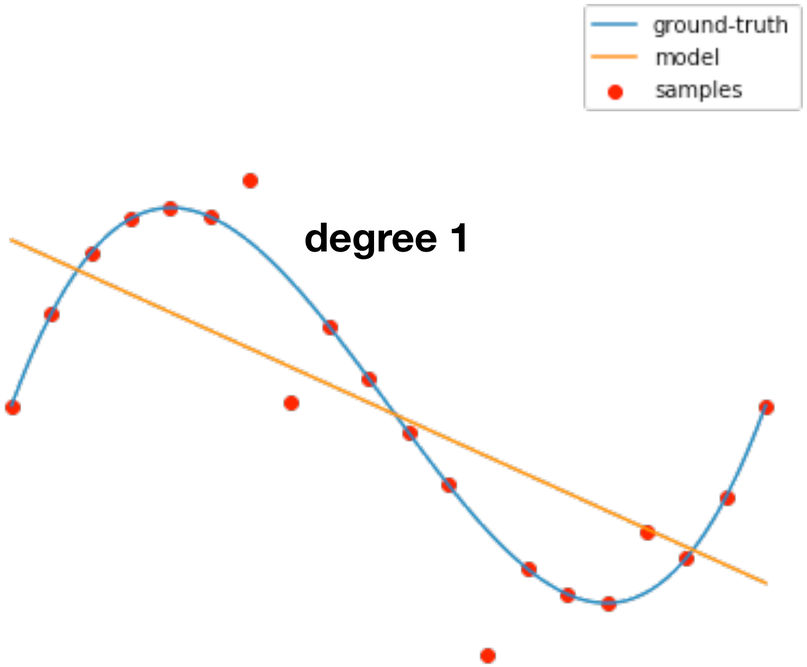

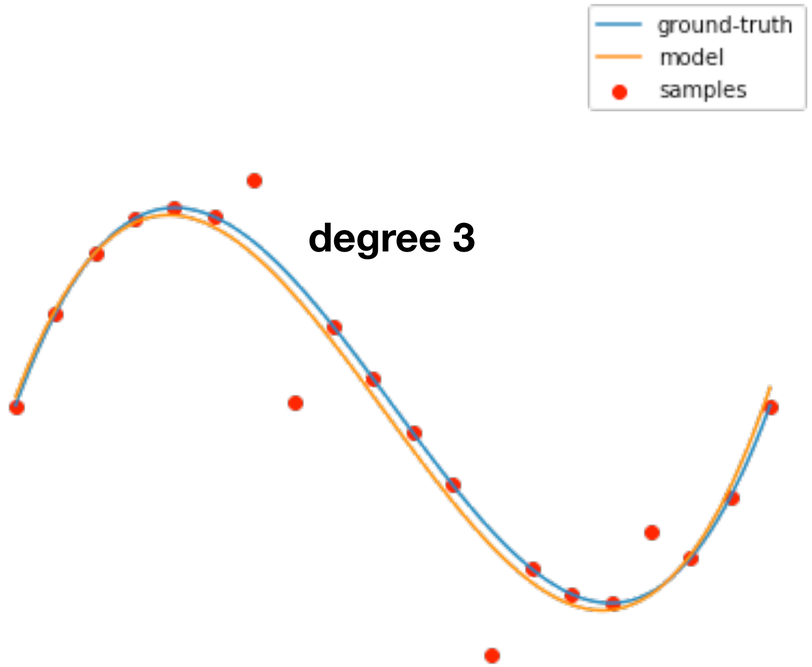

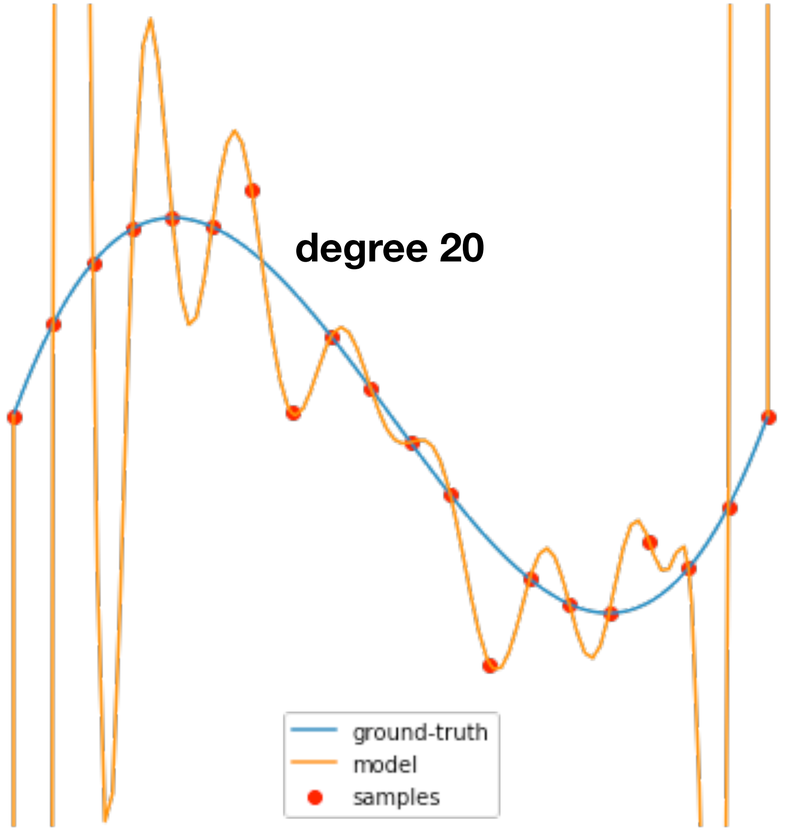

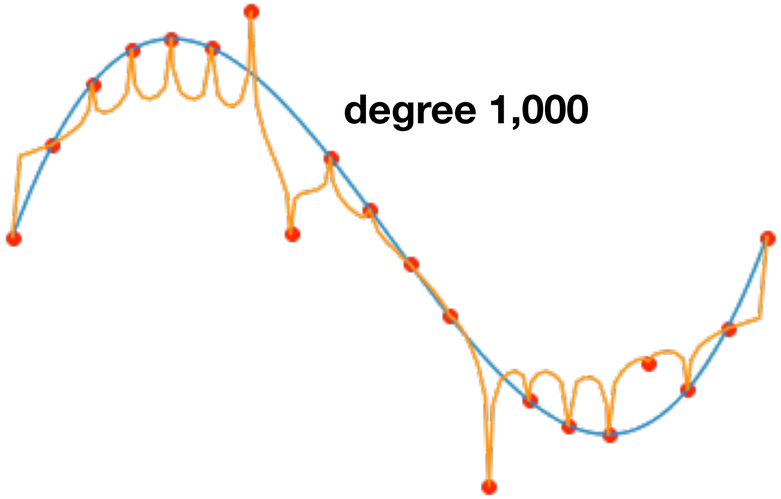

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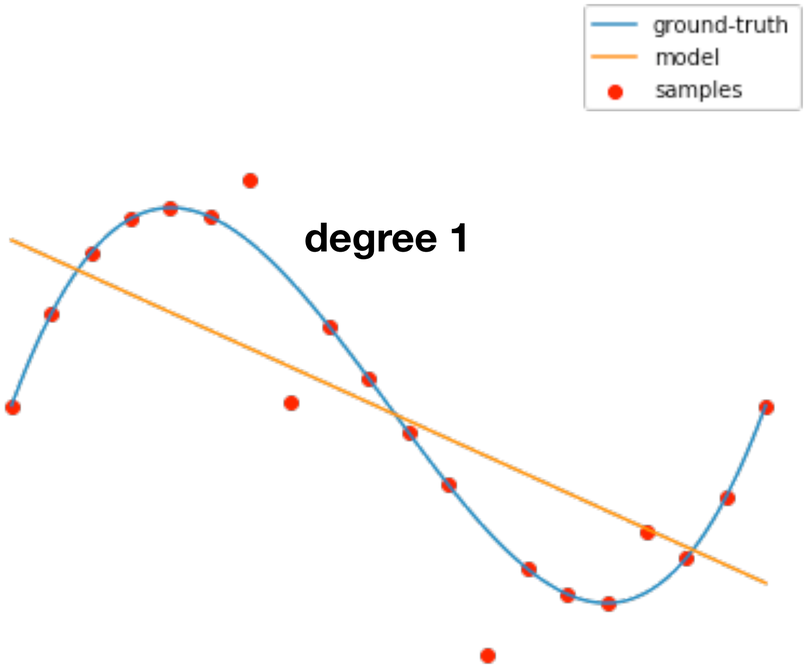

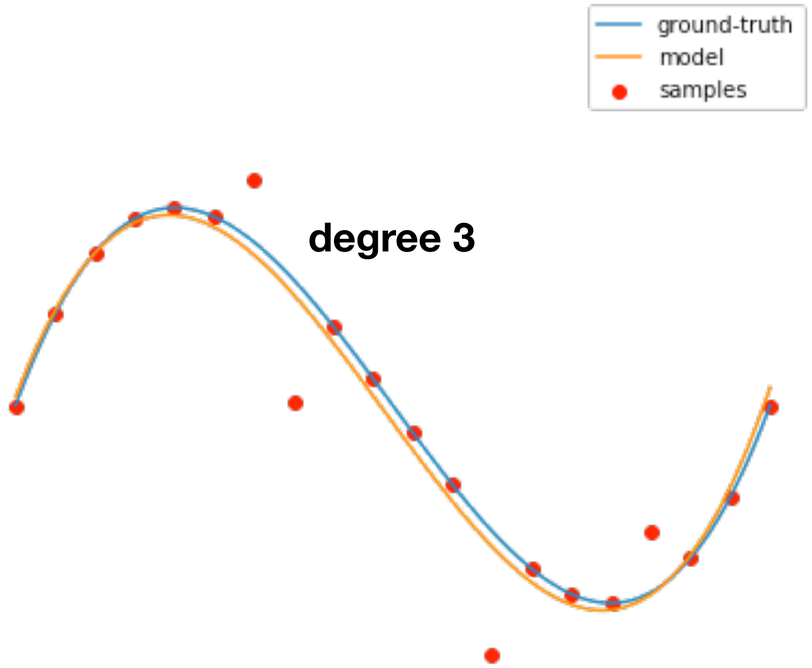

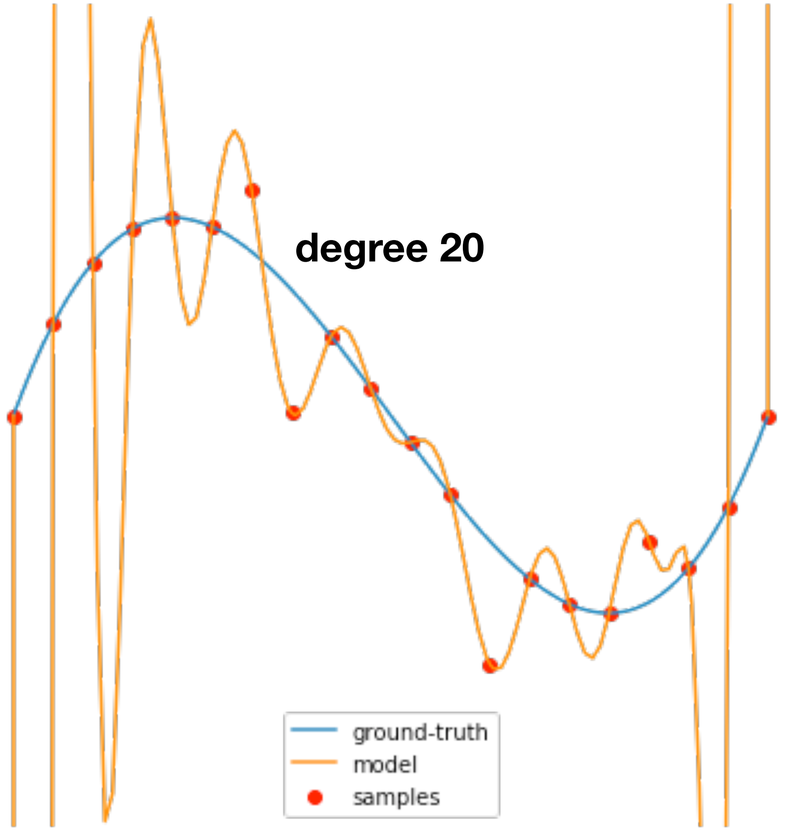

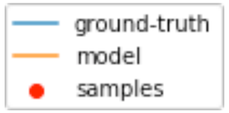

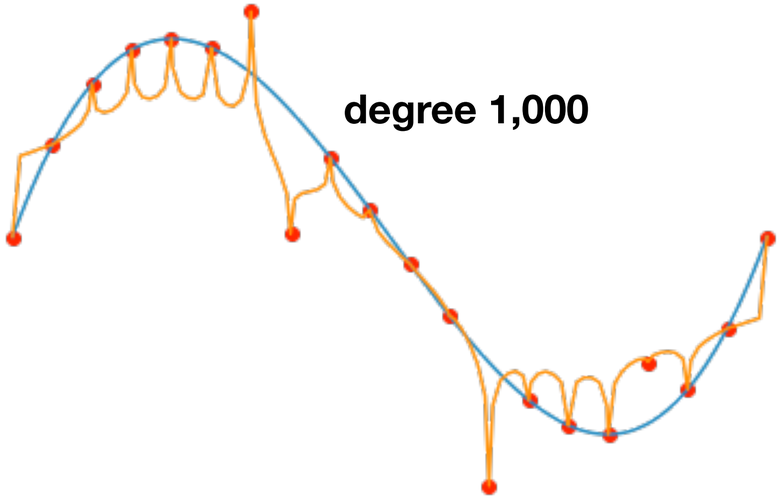

Important: this is the *minimum norm* solution!
(There are also terrible degree-1,000 ERMs)

Nakkiran et al. blog post's companion notebook

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Neumann series: $\sum_{\ell=0}^{\infty} A^\ell = (I - A)^{-1}$ when $\|A\|_{\text{op}} < 1$

$L_S(w) = \frac{1}{2n}\|Xw - y\|^2$ $X \in \mathbb{R}^{n\times d}$ with $n < d$, of rank n $\nabla L_S(w) = \frac{1}{n}X^\top(Xw - y)$ $w_0 = 0$

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Double descent

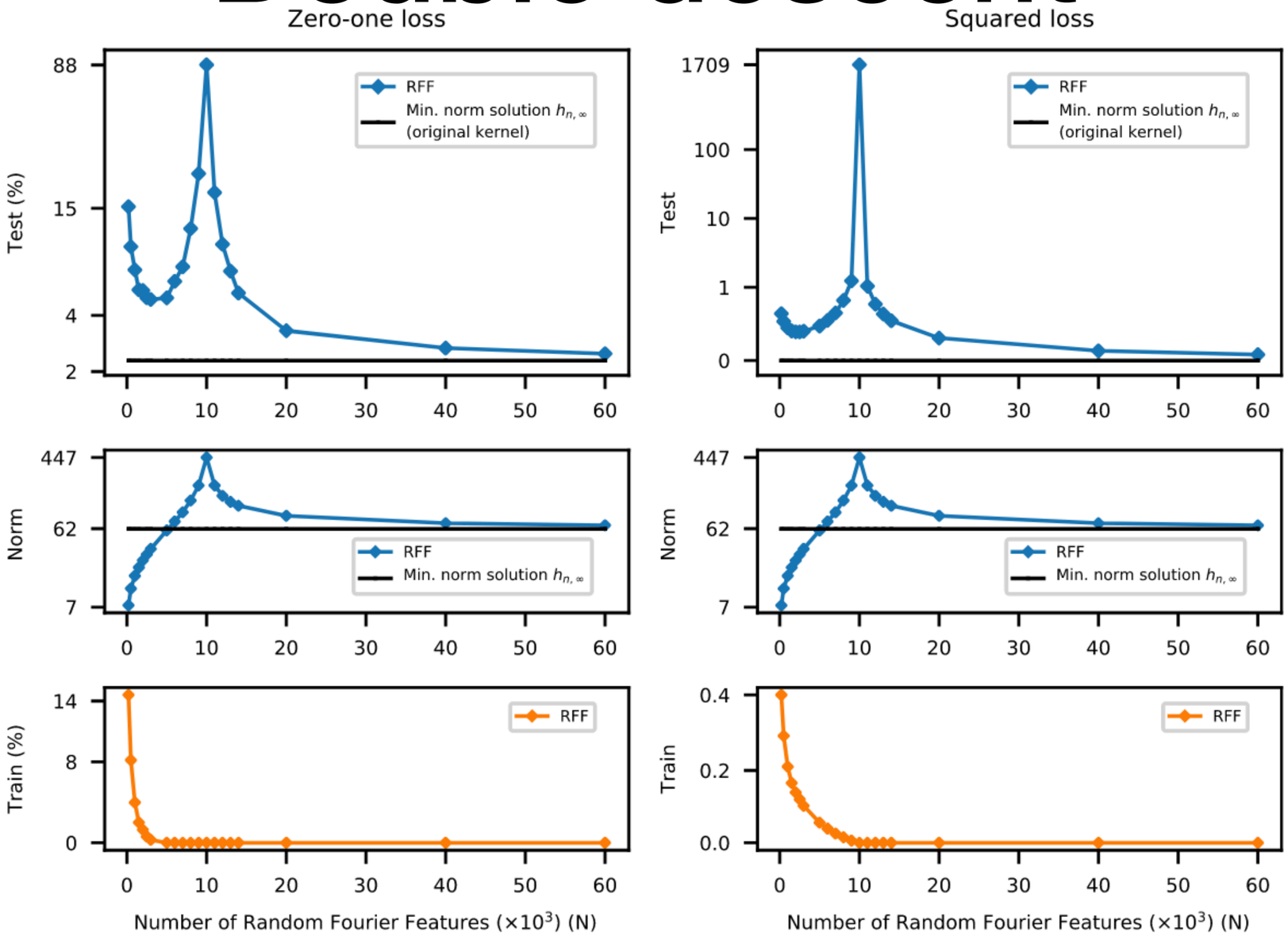
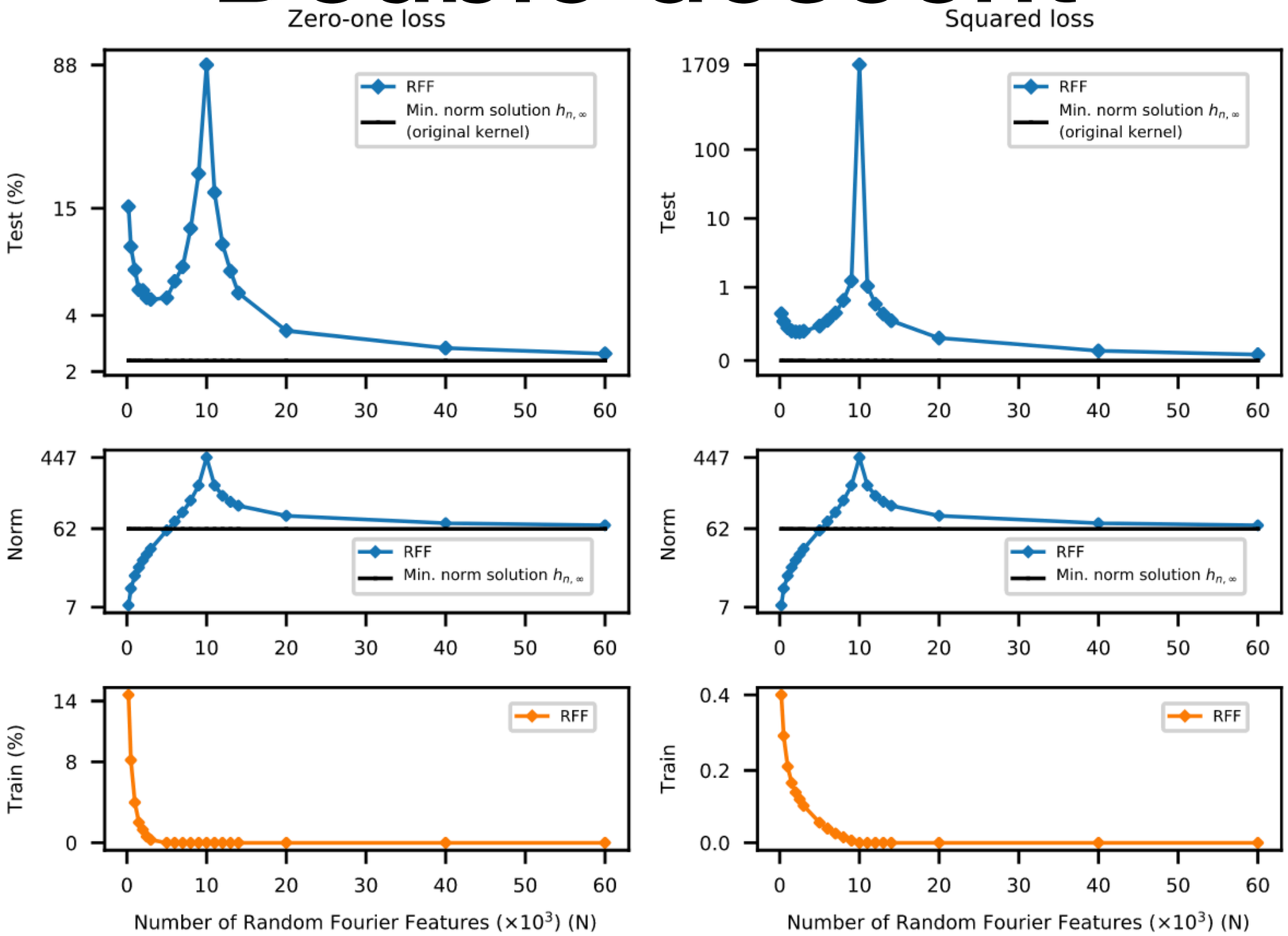


Fig. 2. Double-descent risk curve for the RFF model on MNIST. Shown are test risks (log scale), coefficient ℓ_2 norms (log scale), and training risks of the RFF model predictors $h_{n,N}$ learned on a subset of MNIST ($n = 10^4$, 10 classes). The interpolation threshold is achieved at $N = 10^4$.

Belkin/Hsu/Ma/Mandal, PNAS 2019

Double descent

Classical regime (left of peak): unique ERM



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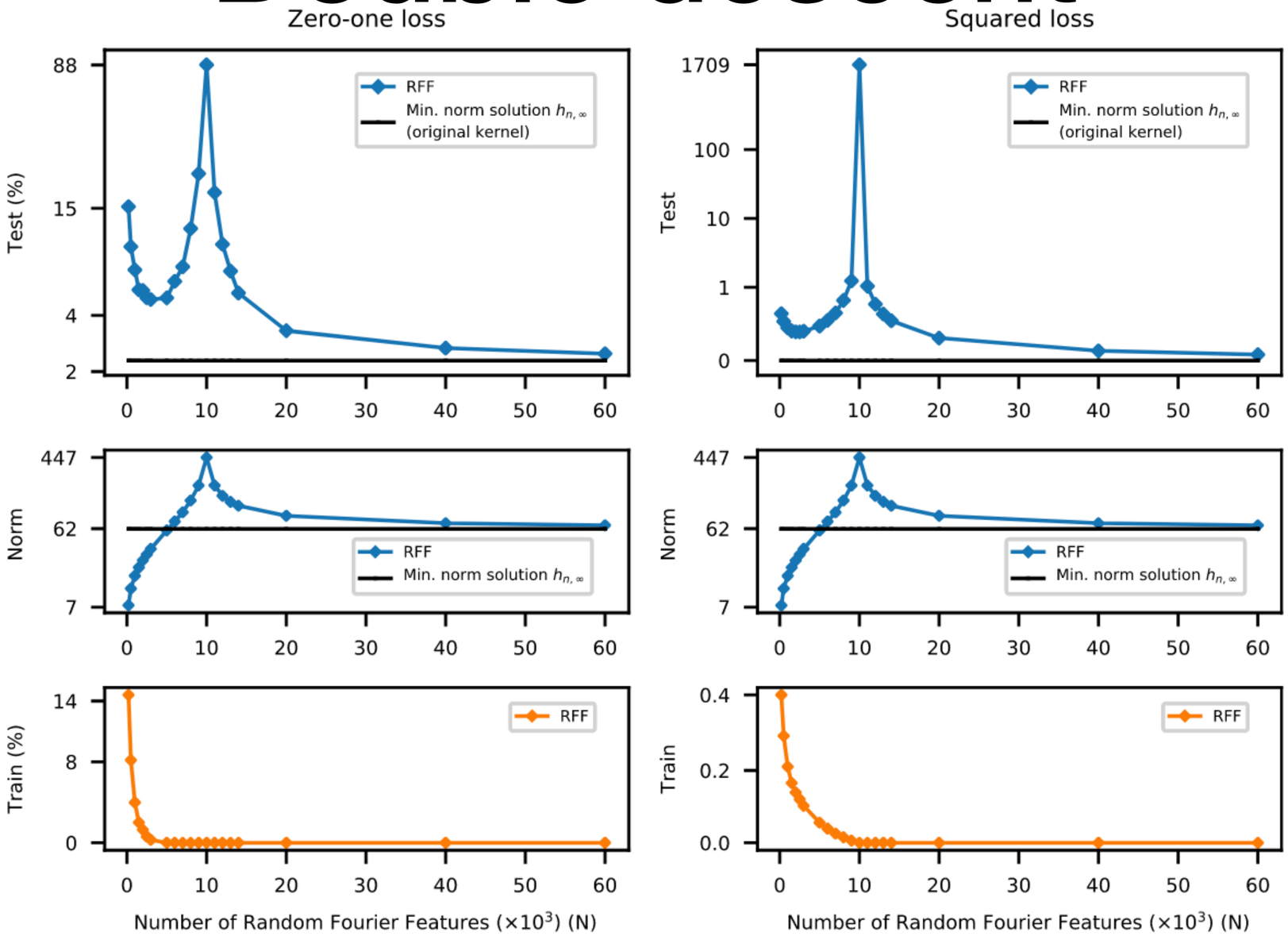

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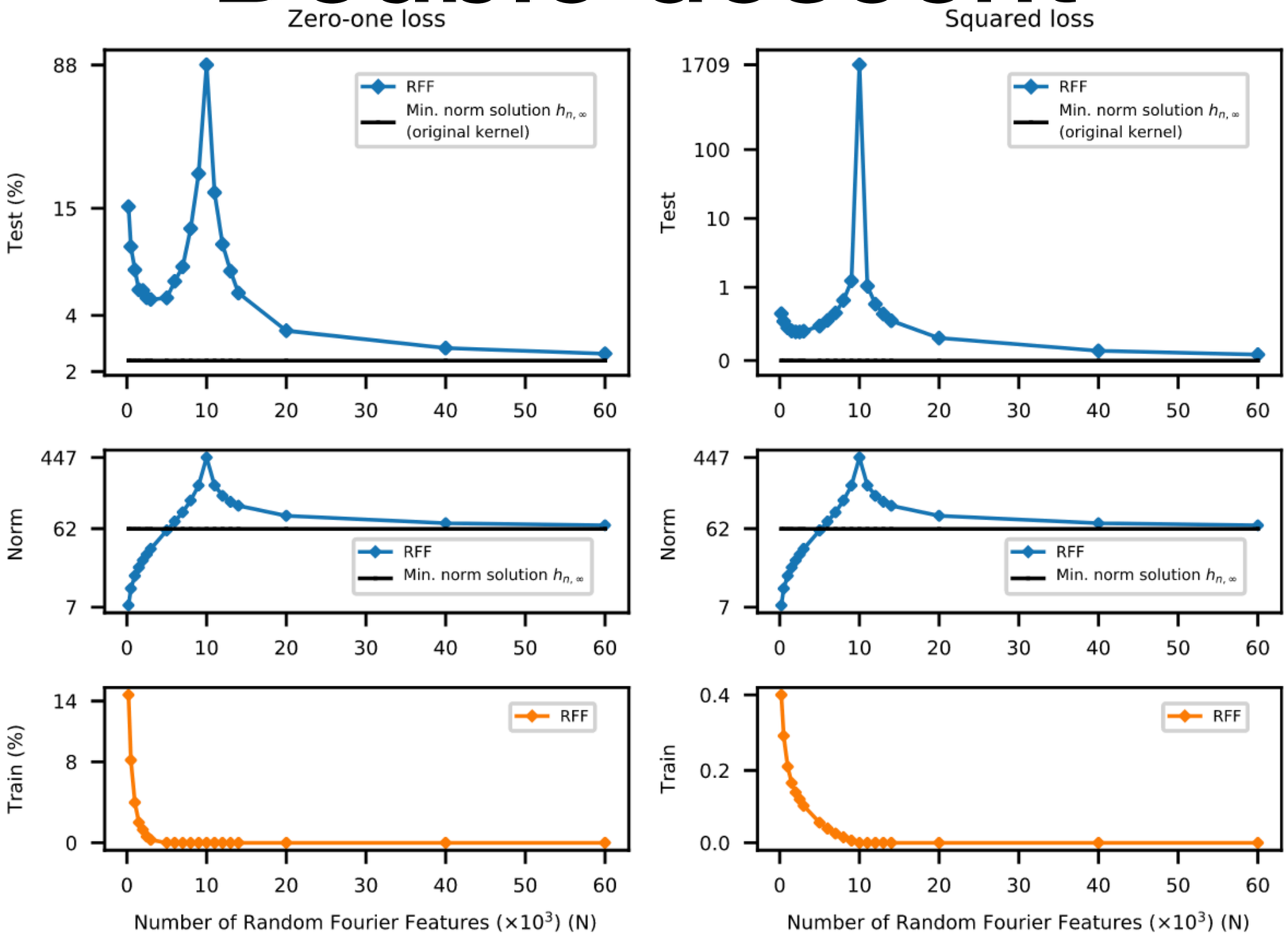

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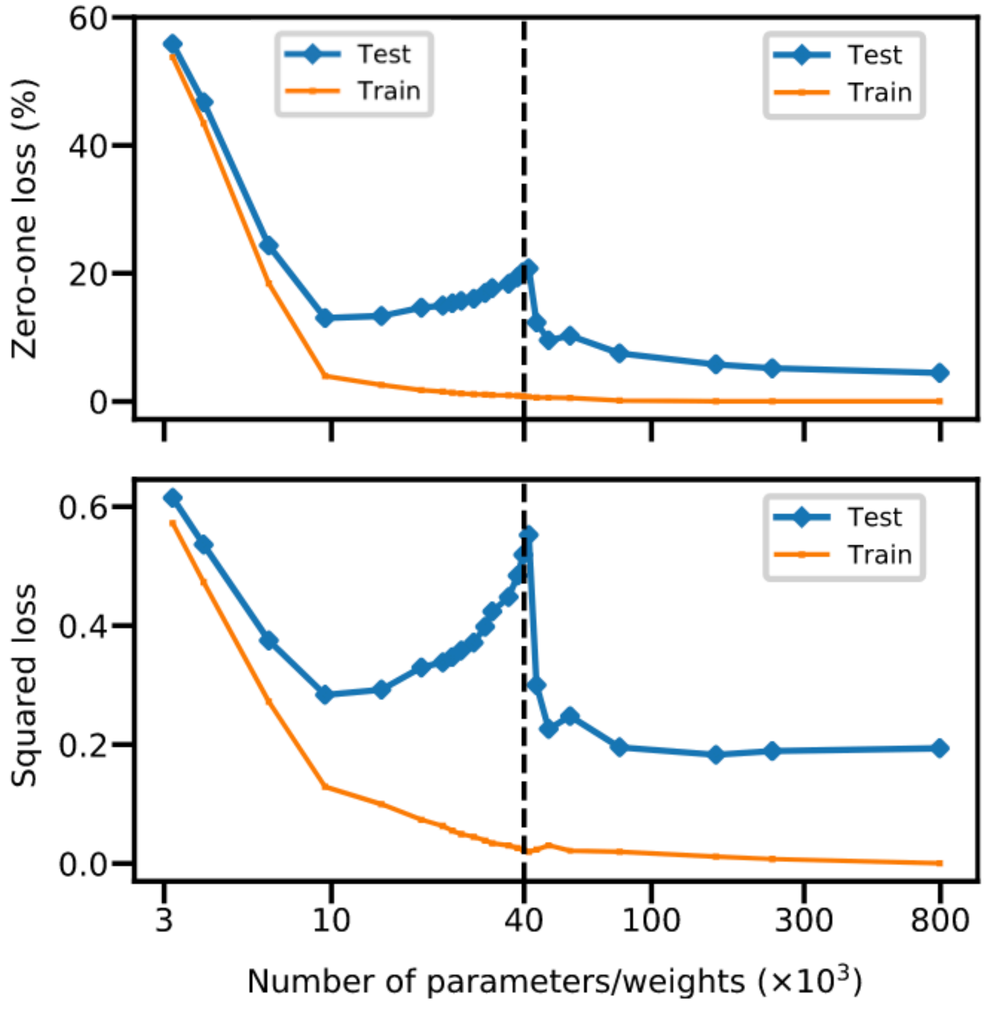


Fig. 3. Double-descent risk curve for a fully connected neural network on MNIST. Shown are training and test risks of a network with a single layer of H hidden units, learned on a subset of MNIST ($n = 4 \cdot 10^3$, $d = 784$, $K = 10$ classes). The number of parameters is $(d + 1) \cdot H + (H + 1) \cdot K$. The interpolation threshold (black dashed line) is observed at $n \cdot K$.

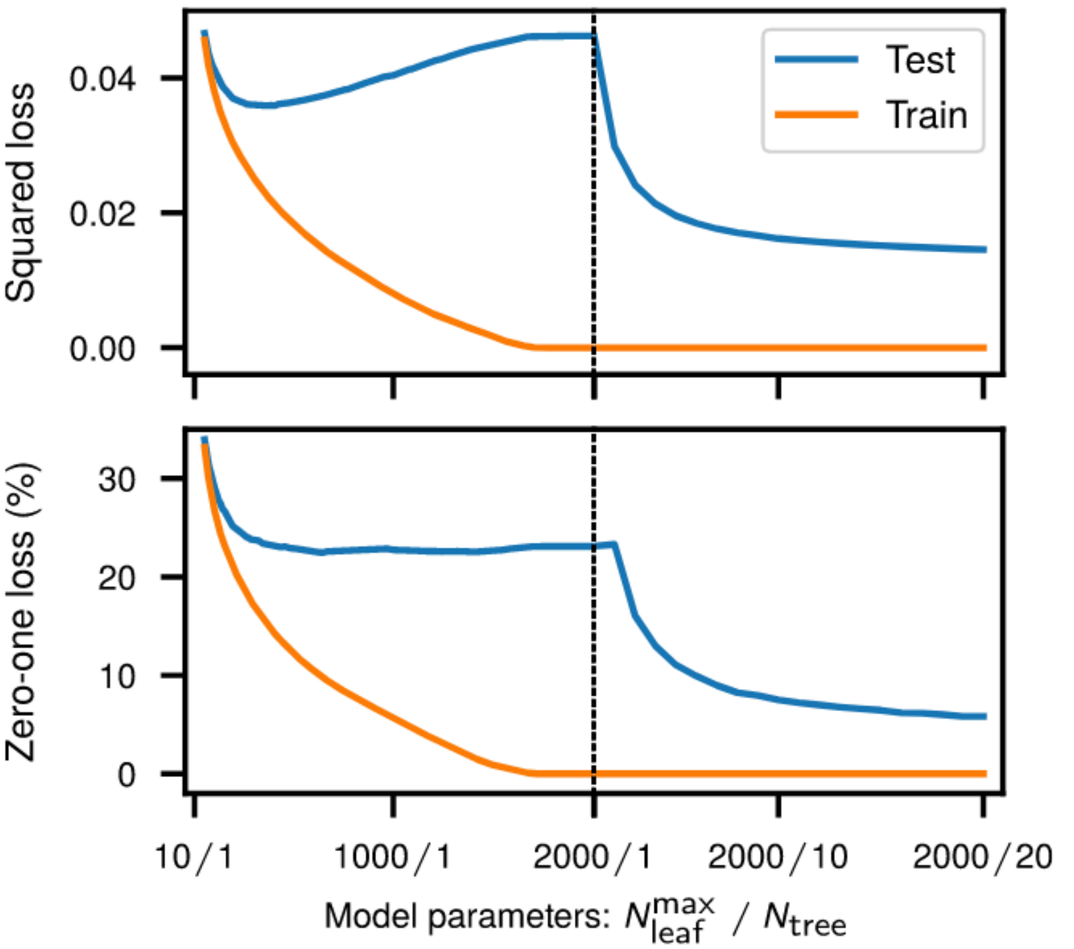
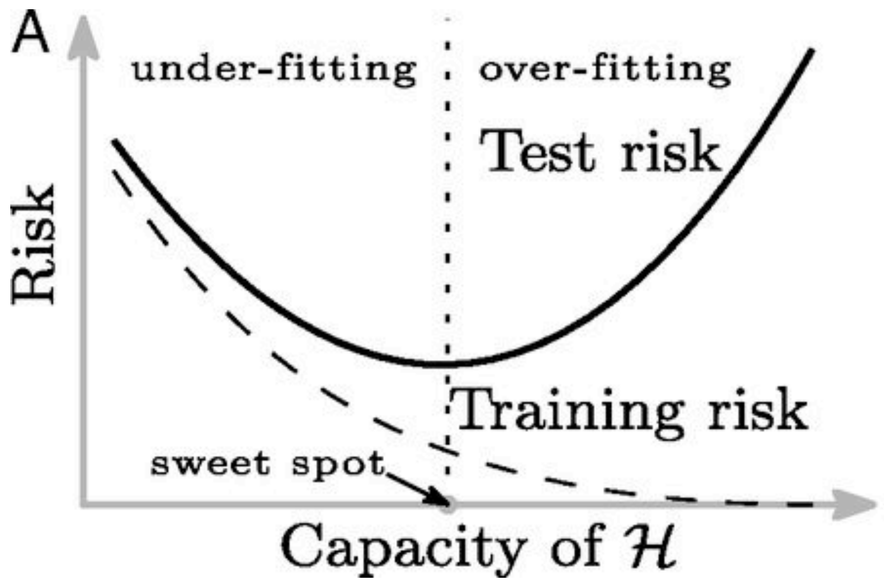
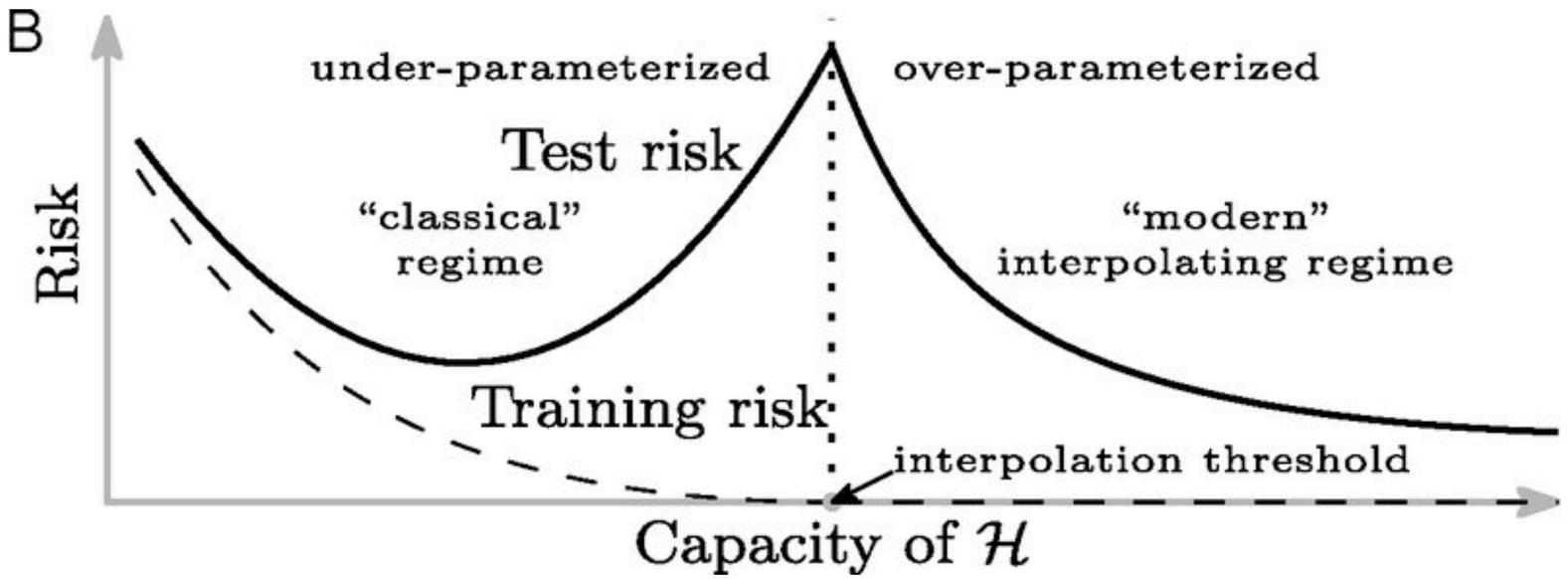


Fig. 4. Double-descent risk curve for random forests on MNIST. The double-descent risk curve is observed for random forests with increasing model complexity trained on a subset of MNIST ($n = 10^4$, 10 classes). Its complexity is controlled by the number of trees N_{tree} and the maximum number of leaves allowed for each tree $N_{\text{leaf}}^{\max}$.

Belkin/Hsu/Ma/Mandal, PNAS 2019





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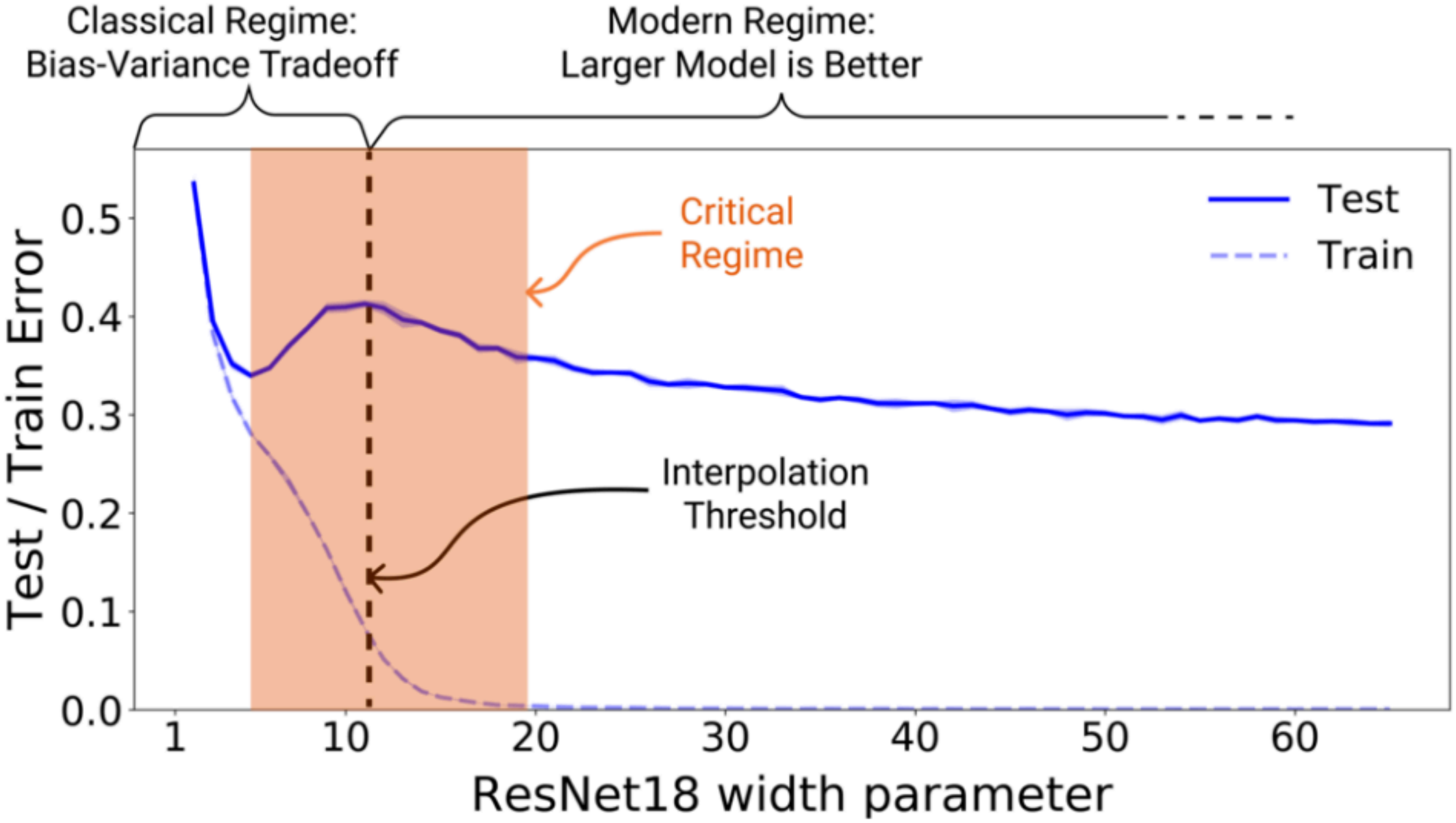
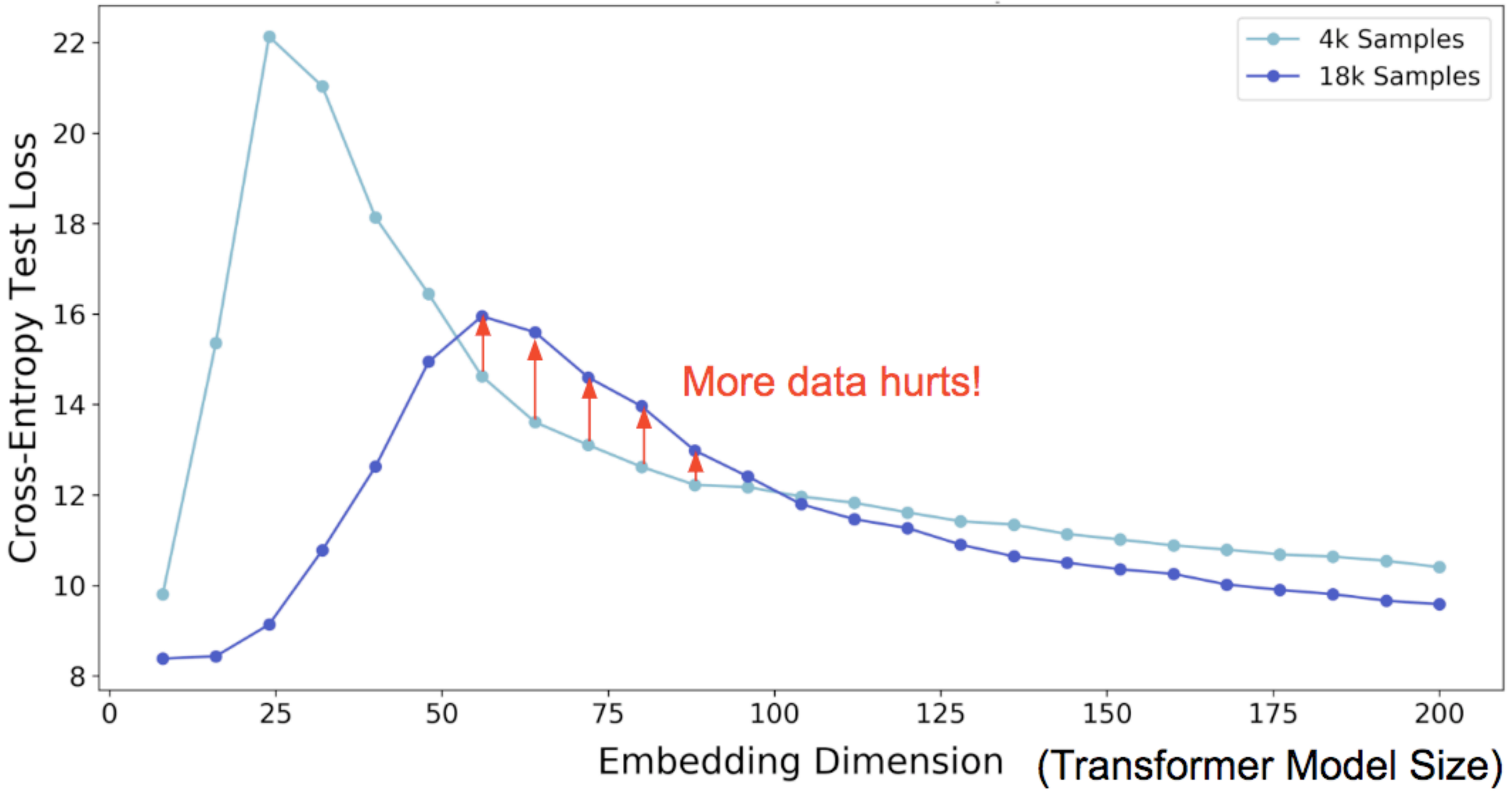


Nakkiran et al. ICLR-20



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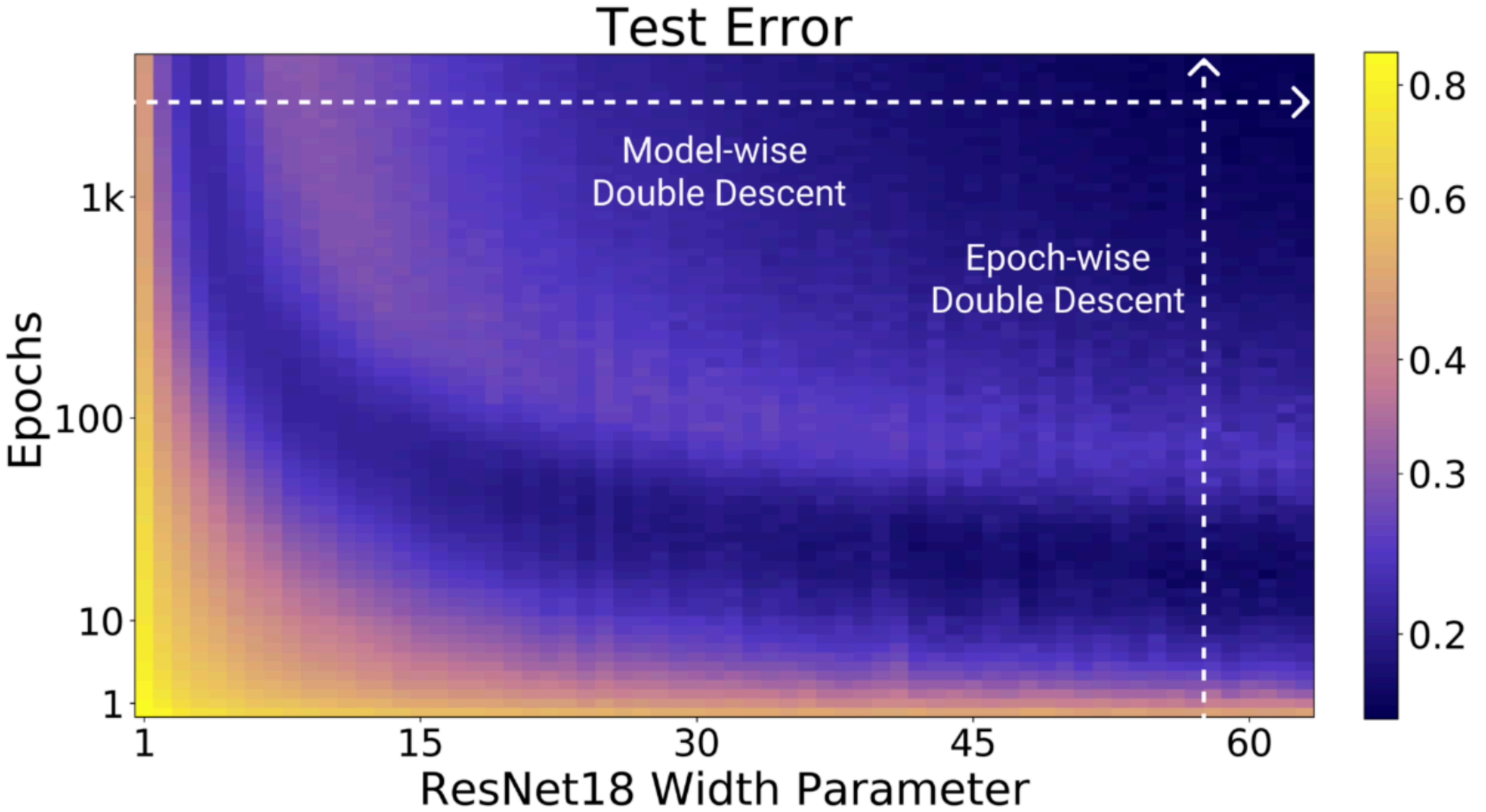

Nakkiran et al. ICLR-20

Definition 1 (Effective Model Complexity) *The* Effective Model Complexity *(EMC) of a training procedure $\mathcal{T}$, with respect to distribution $\mathcal{D}$ and parameter $\epsilon > 0$, is defined as:*

$$\mathrm{EMC}_{\mathcal{D},\epsilon}(\mathcal{T}) := \max\{n \mid \mathbb{E}_{S\sim\mathcal{D}^n}[\mathrm{Error}_S(\mathcal{T}(S))] \leq \epsilon\}$$

where $\mathrm{Error}_S(M)$ is the mean error of model M on train samples S.

Our main hypothesis can be informally stated as follows:

Hypothesis 1 (Generalized Double Descent hypothesis, informal) *For any natural data distribution $\mathcal{D}$, neural-network-based training procedure $\mathcal{T}$, and small $\epsilon > 0$, if we consider the task of predicting labels based on n samples from $\mathcal{D}$ then:*

Under-paremeterized regime. *If $\mathrm{EMC}_{\mathcal{D},\epsilon}(\mathcal{T})$ is sufficiently smaller than n, any perturbation of $\mathcal{T}$ that increases its effective complexity will decrease the test error.*

Over-parameterized regime. *If $\mathrm{EMC}_{\mathcal{D},\epsilon}(\mathcal{T})$ is sufficiently larger than n, any perturbation of $\mathcal{T}$ that increases its effective complexity will decrease the test error.*

Critically parameterized regime. *If $\mathrm{EMC}_{\mathcal{D},\epsilon}(\mathcal{T}) \approx n$, then a perturbation of $\mathcal{T}$ that increases its effective complexity might decrease* **or increase** *the test error.*

Nakkiran et al. ICLR-20

(pause)

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PAC-Bayes: McAllester bound

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  - Proved in SSBD chapter 31 (not bad at all)

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  - For instance: could learn a $\hat{h}$ with (S)GD and then add noise to it
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  - But note that if $\rho \to$ point mass and π continuous, $\mathrm{KL}(\rho\|\pi) \to \infty$

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  - …as long as we can still bound $\mathrm{KL}(\rho \| \pi)$

Other forms of PAC-Bayes bounds

- Linear bound: $L_{\mathscr{D}}(\rho) \leq \frac{1}{\beta} L_S(\rho) + \frac{\mathrm{KL}(\rho\|\pi) + \log\frac{1}{\delta}}{2\beta(1-\beta)n}$ for any $\beta \in (0,1)$

- Catoni bound: for $\alpha > 1$, $\Phi_\gamma^{-1}(x) = (1-\exp(-\gamma x))/(1-\exp(-\gamma))$,

  $$L_{\mathscr{D}}(\rho) \leq \inf_{\lambda>1} \Phi_{\lambda/n}^{-1}\left(L_S(\rho) + \frac{\alpha}{\lambda}\left[\mathrm{KL}(\rho\|\pi) - \log\varepsilon + 2\log\frac{\log(\alpha^2\lambda)}{\log\alpha}\right]\right)$$

  - Can be much tighter (unfortunately) if $\mathrm{KL}(\rho\|\pi)/n$ is big

- Also variants based on general f-divergences, Wasserstein, …

NON-VACUOUS GENERALIZATION BOUNDS AT THE IMAGENET SCALE: A PAC-BAYESIAN COMPRESSION APPROACH

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- Pre-pick a coding scheme to represent networks (e.g. compress the weights)
- Train a network with SGD, sparsify it/etc to $\hat{h}$, then add a little noise to weights

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Table 1: Summary of bounds obtained from compression

Dataset	Orig. size	Comp. size	Robust. Adj.	Eff. Size	Error Bound Top 1	Error Bound Top 5
MNIST	168.4 KiB	8.1 KiB	1.88 KiB	6.23 KiB	$< 46\,\%$	NA
ImageNet	5.93 MiB	452 KiB	102 KiB	350 KiB	$< 96.5\,\%$	$< 89\,\%$

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- But…these then become "two-sided" bounds
  - Subject to the Nagarajan/Kolter failure mode (their Appendix J)

Uniform convergence may be unable to explain generalization in deep learning

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Recap

- Double descent
  - Classical behaviour, then descend again after interpolation peak
  - Highly dependent on learning algorithm's implicit regularization

- PAC-Bayes
  - A Primer on PAC-Bayesian Learning (Guedj 2019)
  - Tightest bounds we know for deep learning (afaik)…but still not *that* tight
  - Still, significant practical issues, not always super explanatory
  - Lots of ongoing fancy variations