Neural Tangent Kernel and Double Descent

Jacob Steinhardt

Stat 240 Lecture 28

Tangent Kernel

Talked last time about random feature models and kernels, e.g. $k(x, y) = \mathbb{E}_\phi[\phi(x)\phi(y)]$

Neural networks (or any parameterized family) also look locally like kernels

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For neural nets, basically sum over all edges in network. Full rank as long as $p \gg n$.

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Jacot et al. (2018) take both limits at once and characterize the resulting kernel

- This was the first use of the phrase neural tangent kernel

Realistic Regimes

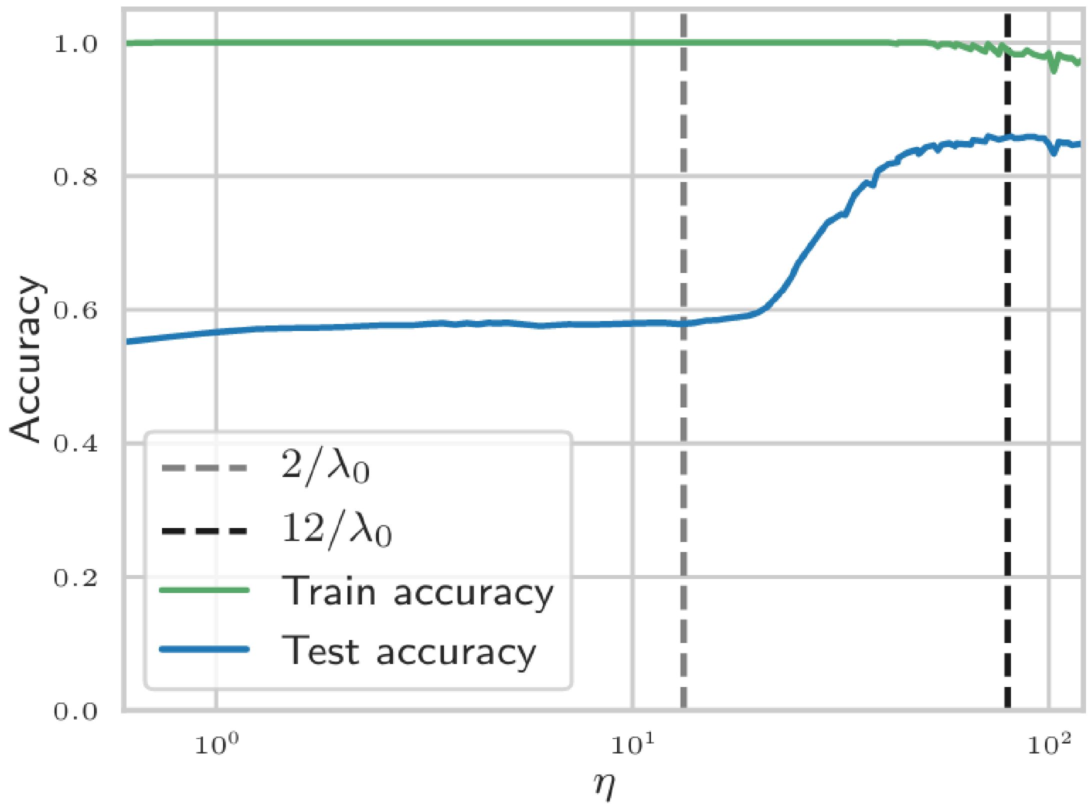
The infinite-width limit is reasonable: most networks have large width

Small learning rate is not: effectively implies that no feature learning happens (obviously false)

Lewkowycz et al. (2020) go beyond this: **catapult mechanism**

- Takes effect at intermediate learning rates (diverge at high learning rate)
- Removes high-curvature ($\approx$ high-variance) directions

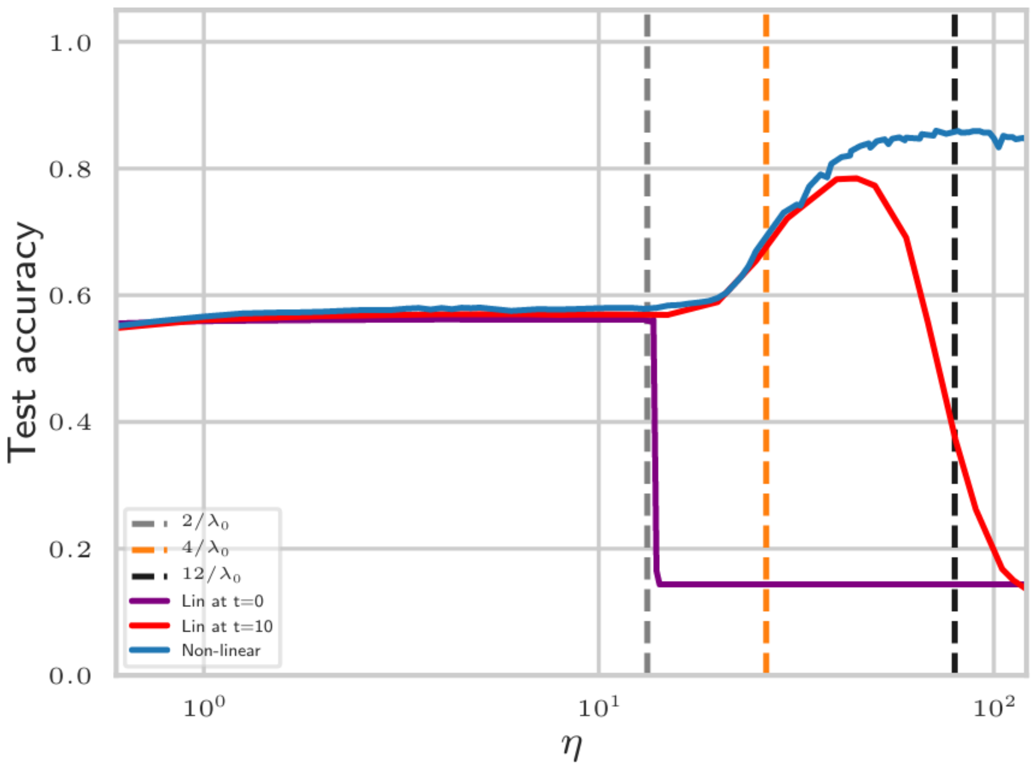
Evidence for Catapult Mechanism



Return to Linearity

Math also predicts good linear approximation after $\log(n)$ steps.

Supported empirically:



Bias-Variance Decomposition

Learned classifier $f(x)$ (depends on dataset $\mathcal{D}$), predict y

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Intuition: more complex models have lower bias but higher variance

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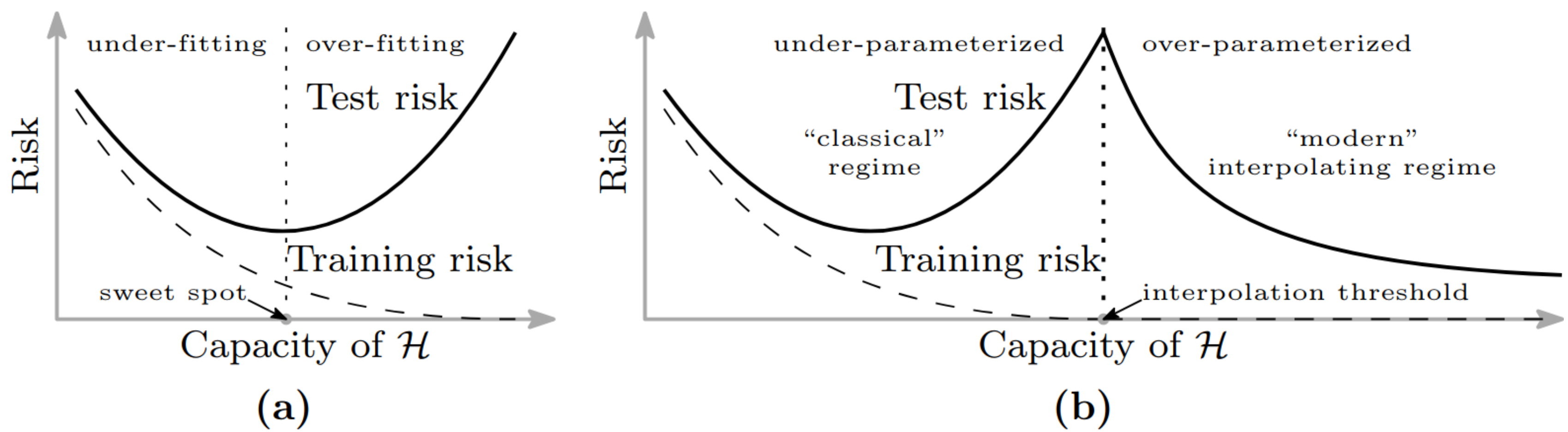
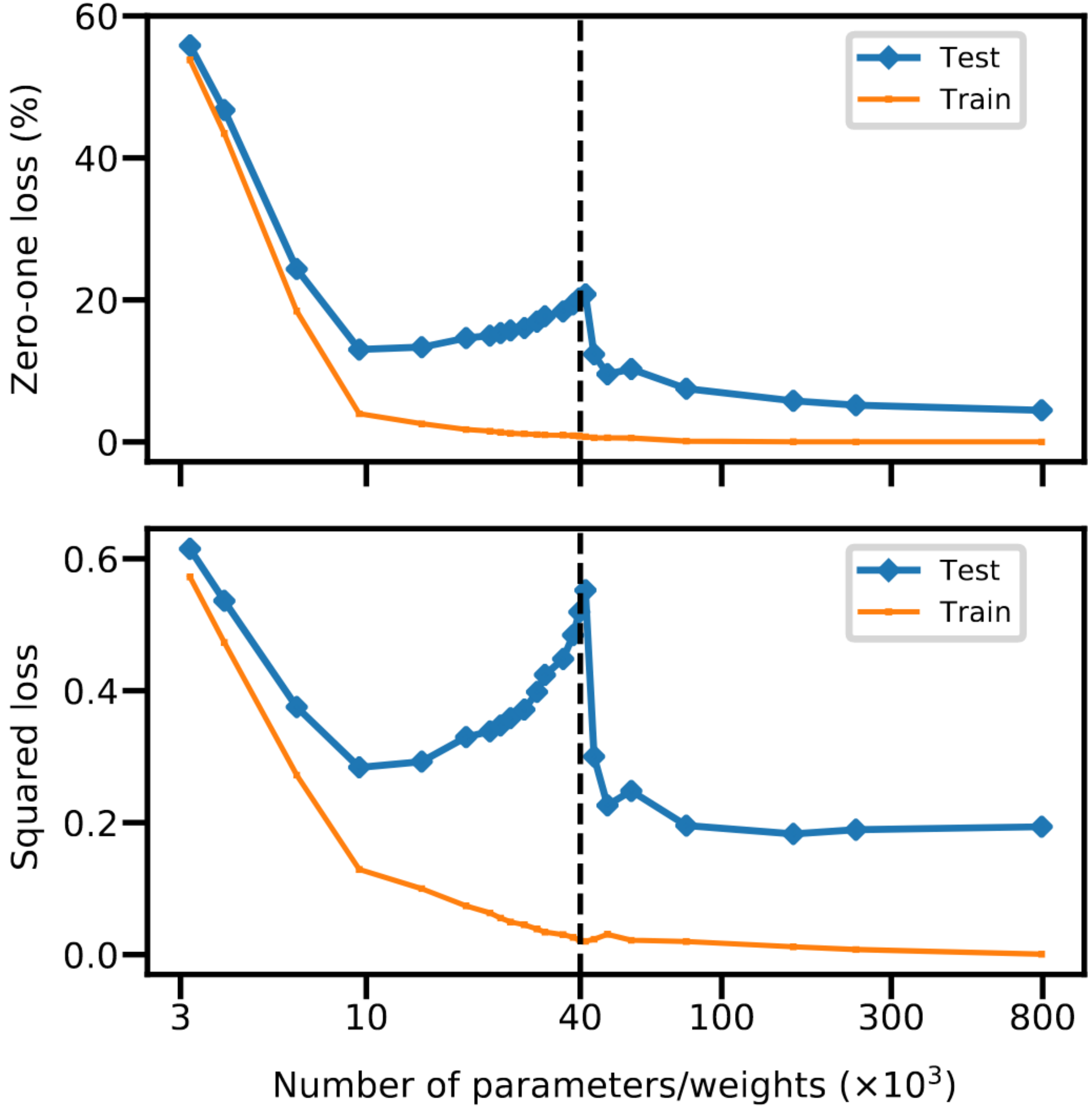
Proposed solution: double descent curve



Belkin et al., 2018

Double Descent on MNIST



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Requires lots of assumptions, so also consider **random design**

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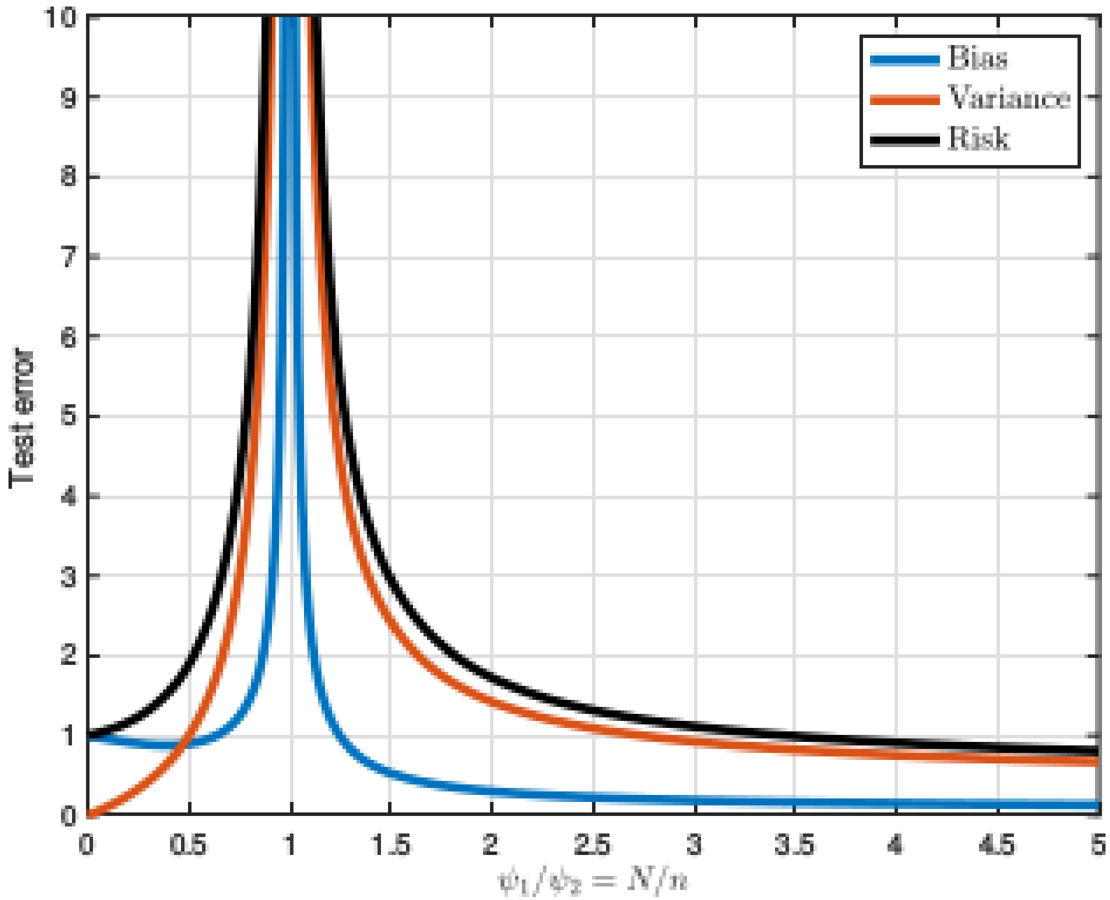
Compute bias via $\mathrm{Bias}^2 = \mathrm{MSE} - \mathrm{Variance}$

Theoretical Characterization (Fixed Design)



Mei and Montanari, 2019

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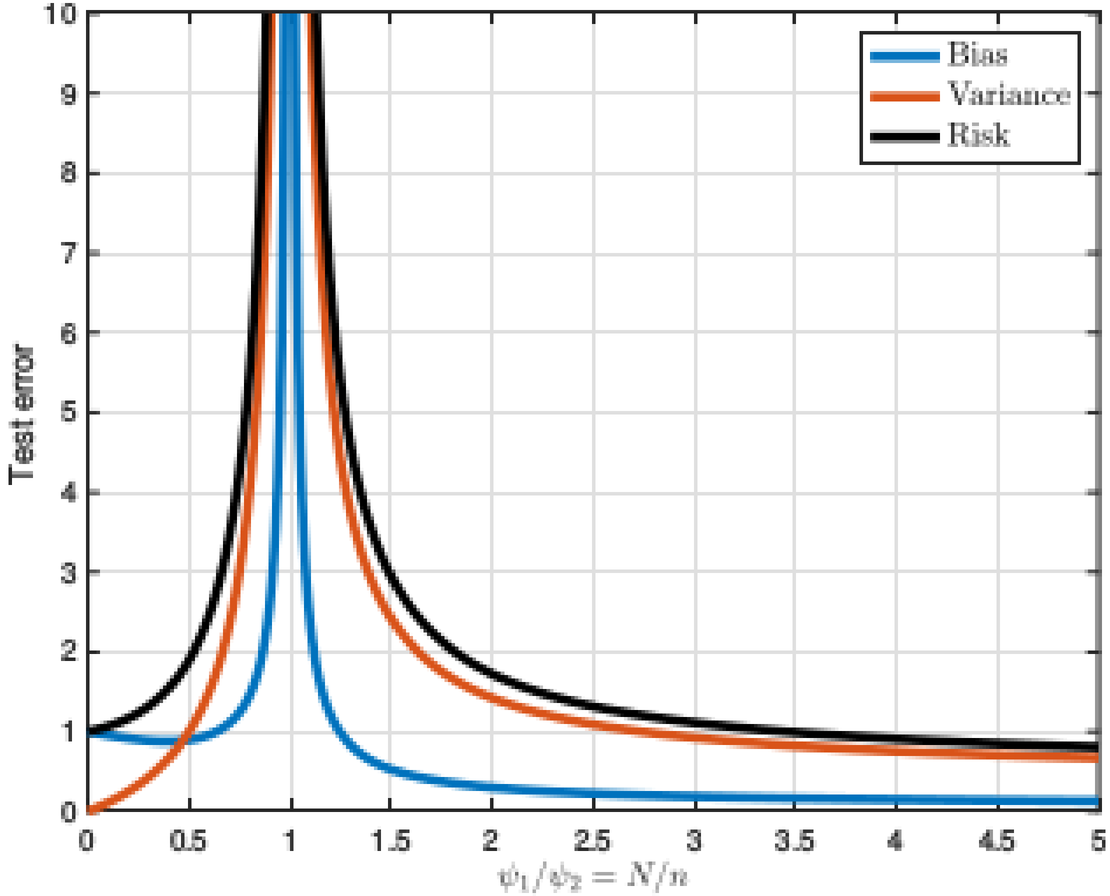

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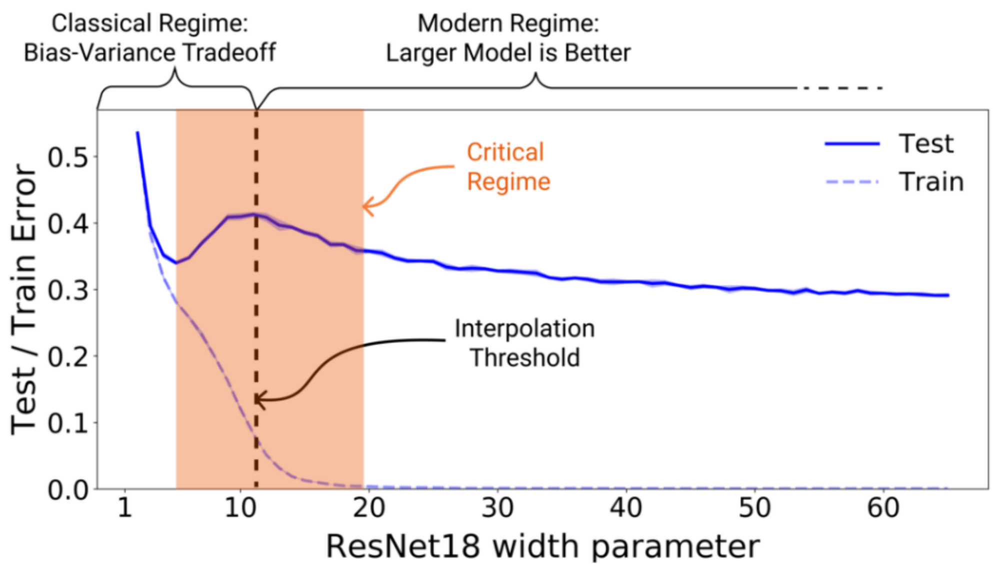
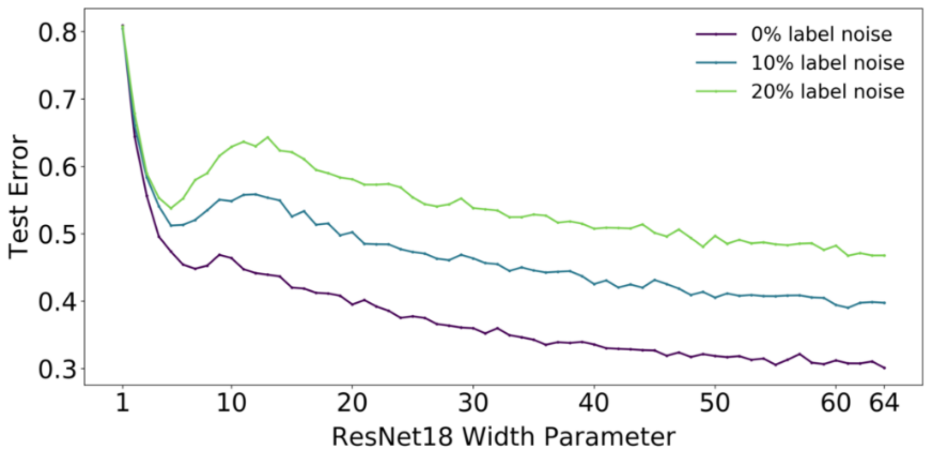
Fixed-design: attributes some **variance** to **bias**.

Double Descent on CIFAR



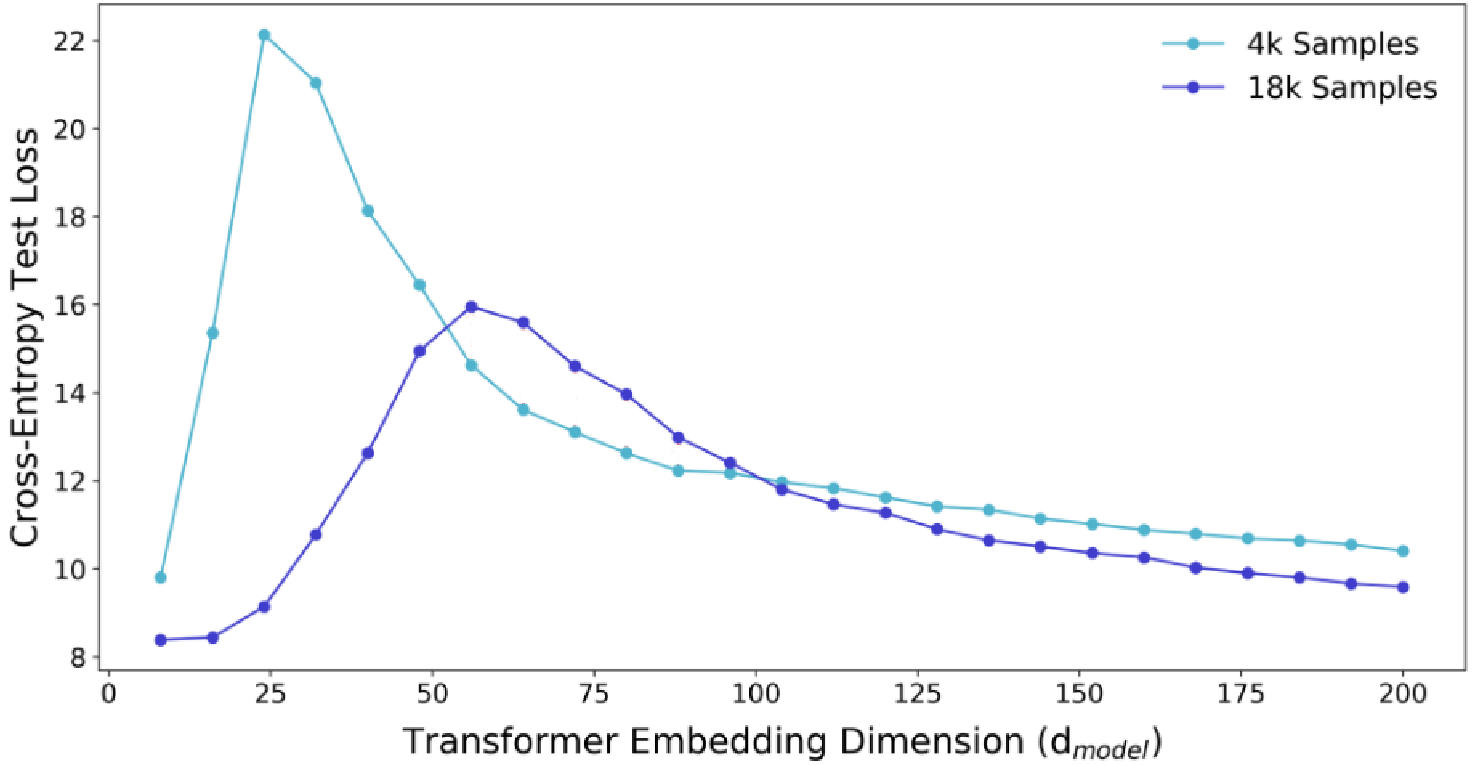
CIFAR-10.



CIFAR-100.

Nakkiran et al., 2019

Unimodal Risk in in NLP



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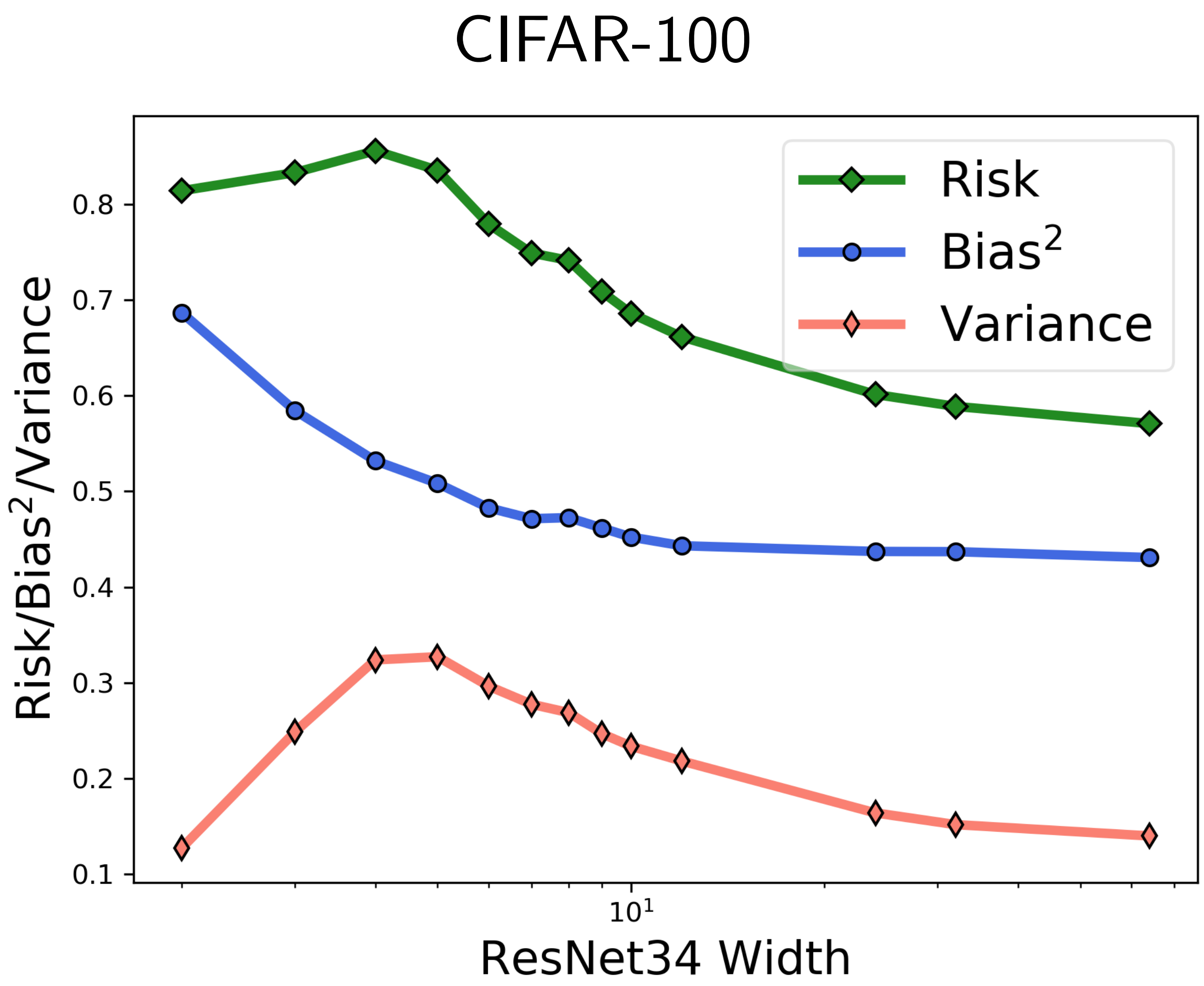
Is there a simpler underlying phenomenon?

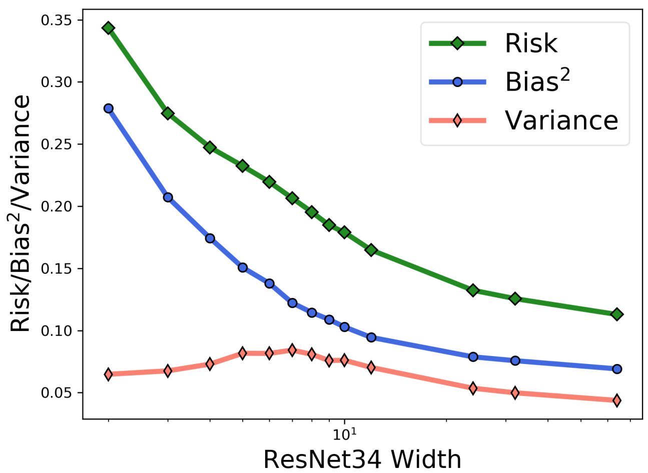
Explanation: Revisiting Bias-Variance



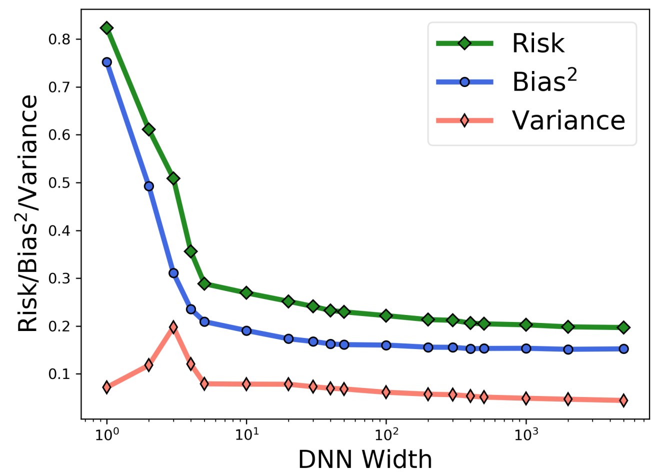
Phenomenon: monotonic bias + **unimodal** variance

Robustness of the Phenomenon

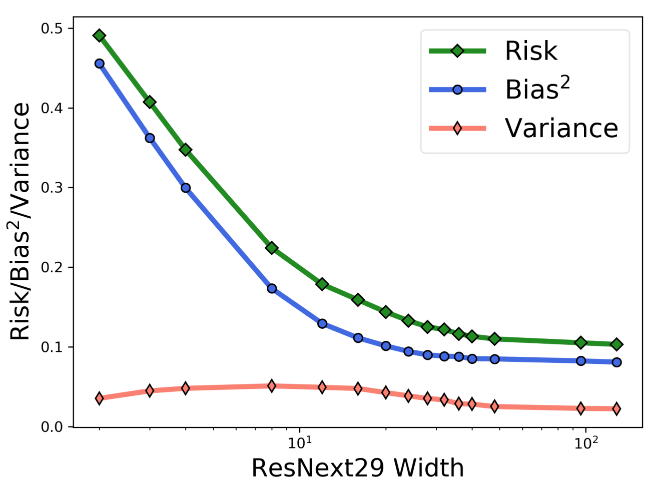
CIFAR-10



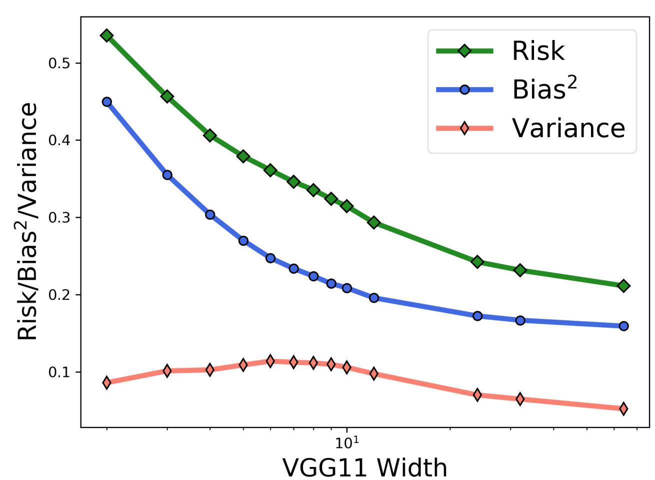
Fashion-MNIST



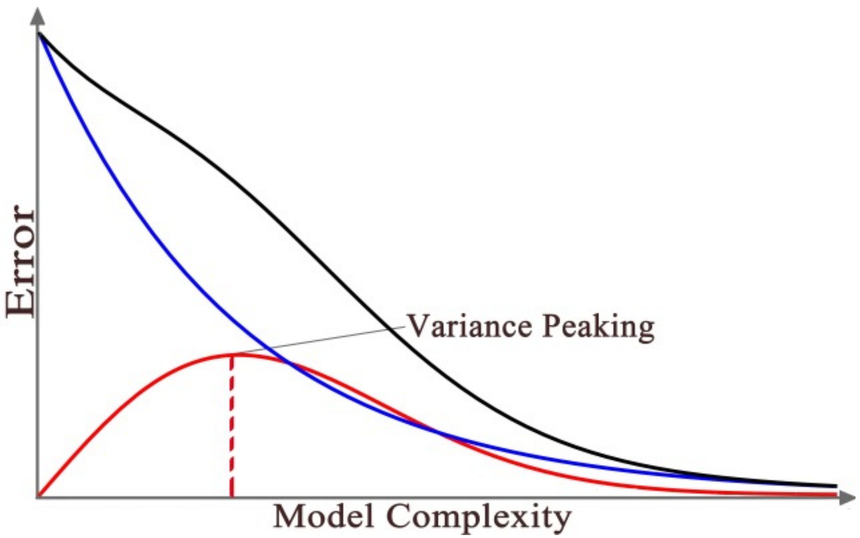
ResNext29

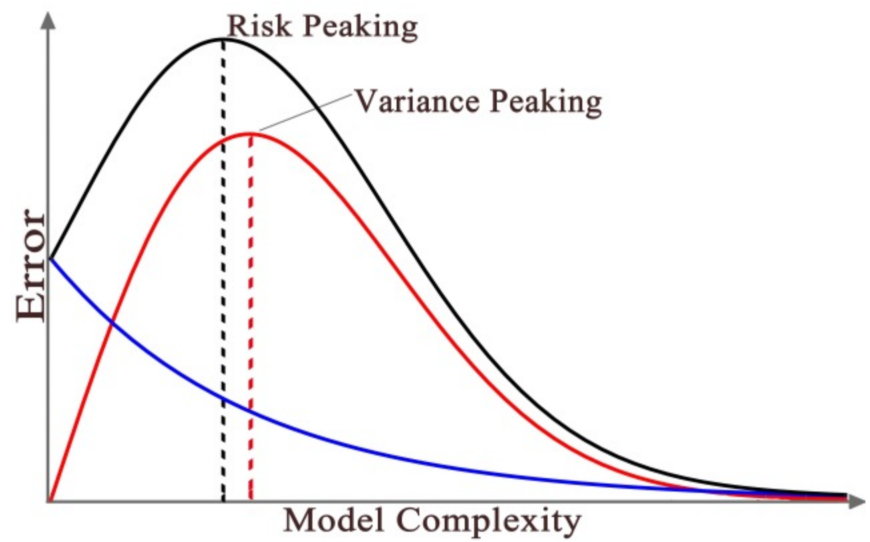


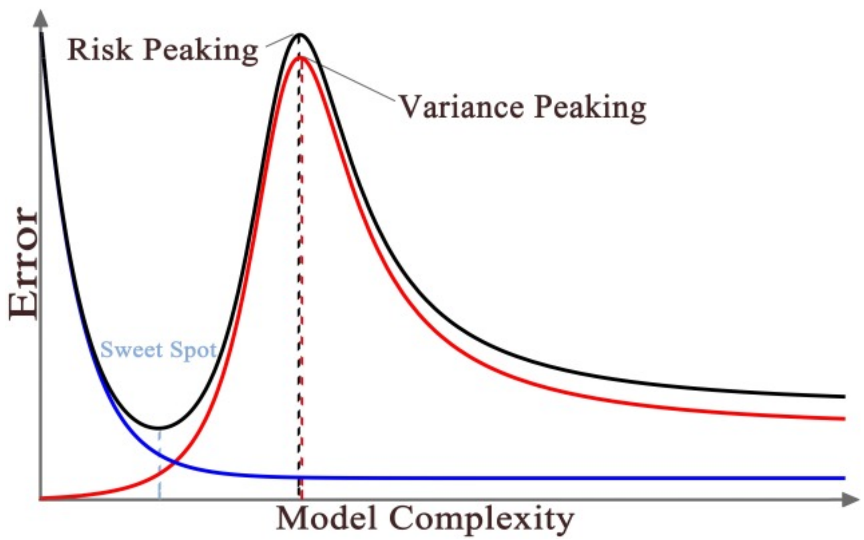
VGG11



Three Possible Behaviors







Bias-Variance for Cross-Entropy

Most networks trained with cross-entropy loss, not MSE

Generalized bias-variance decomposition for Bregman divergence

Pfau, 2013

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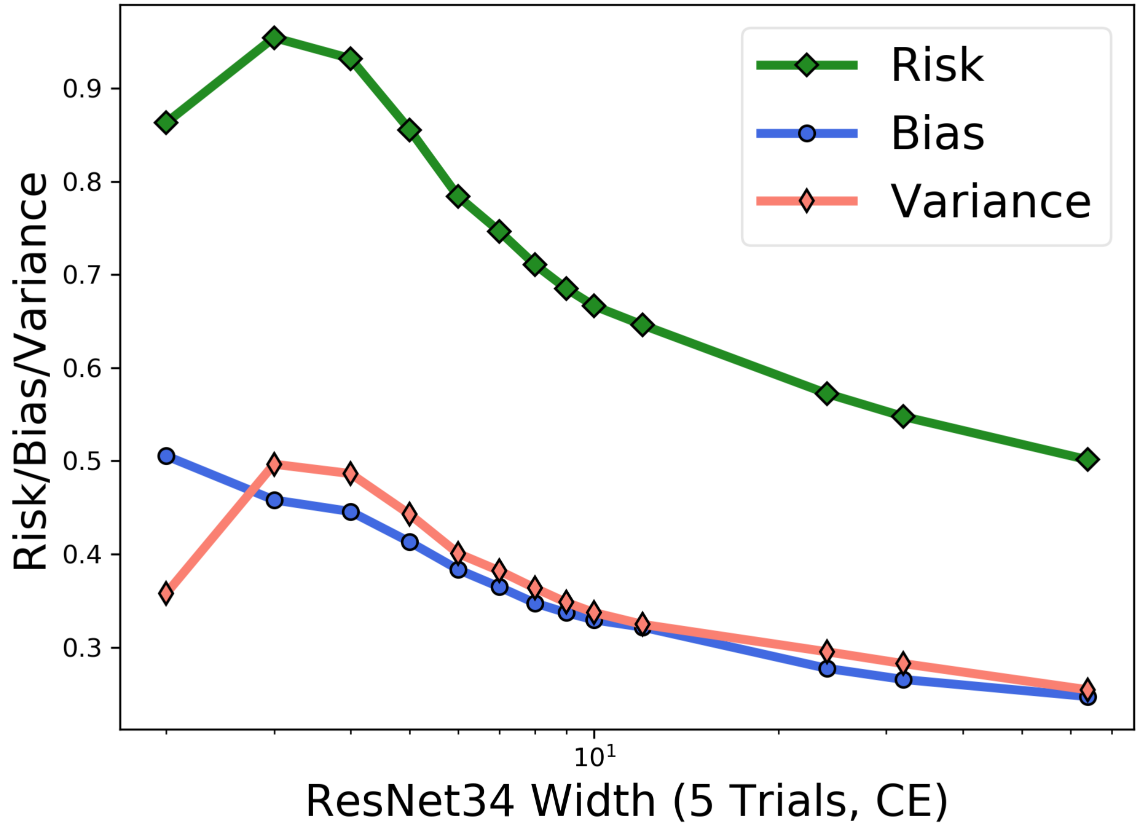

Characterizing Sources of Error

MSE: Get unbiased estimate, but how much finite-sample variability?

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Idea: replicate entire experiment on two halves of training data

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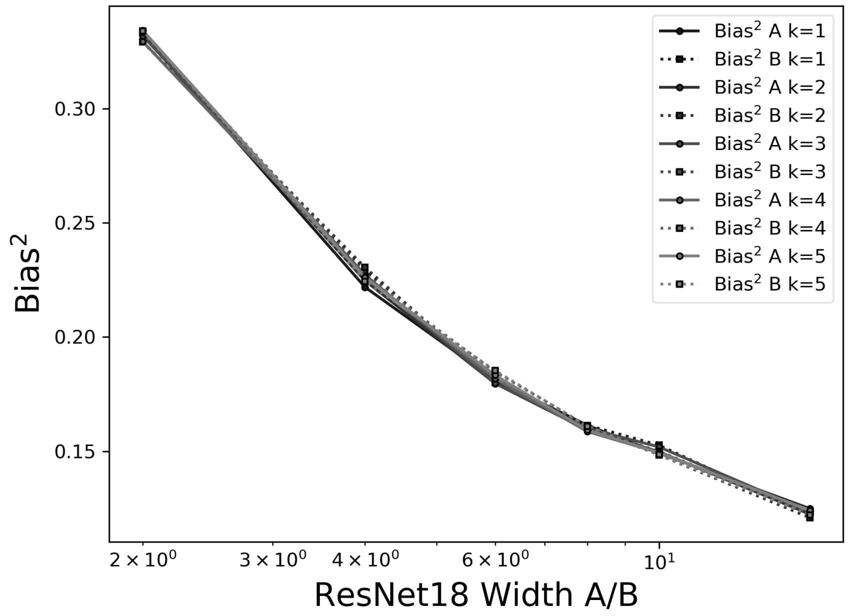

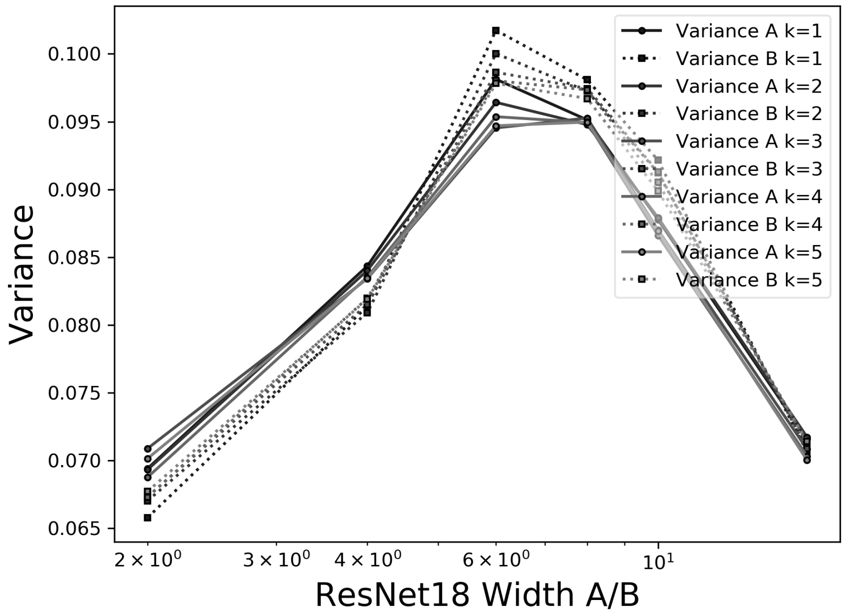

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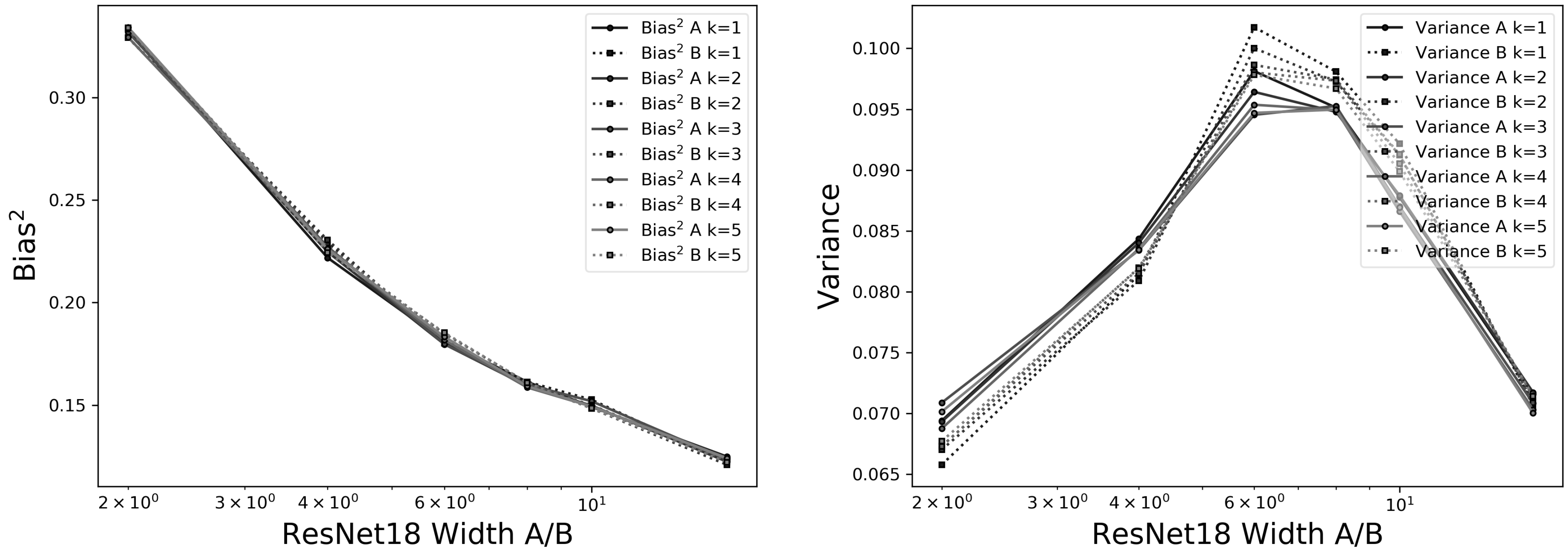
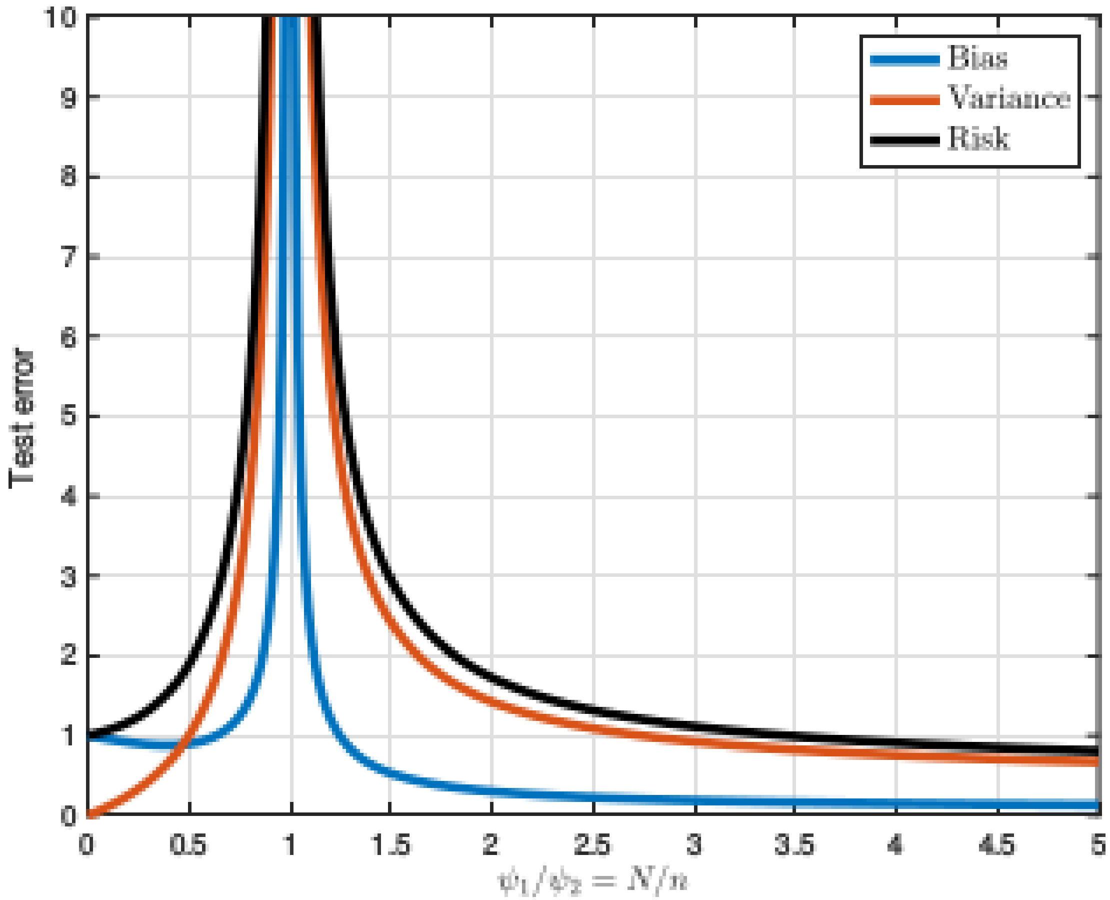


Cross-entropy: harder (no unbiased estimate)

Take-away

Use computer simulation to assess **all** sources of error

Revisiting Fixed-Design Case



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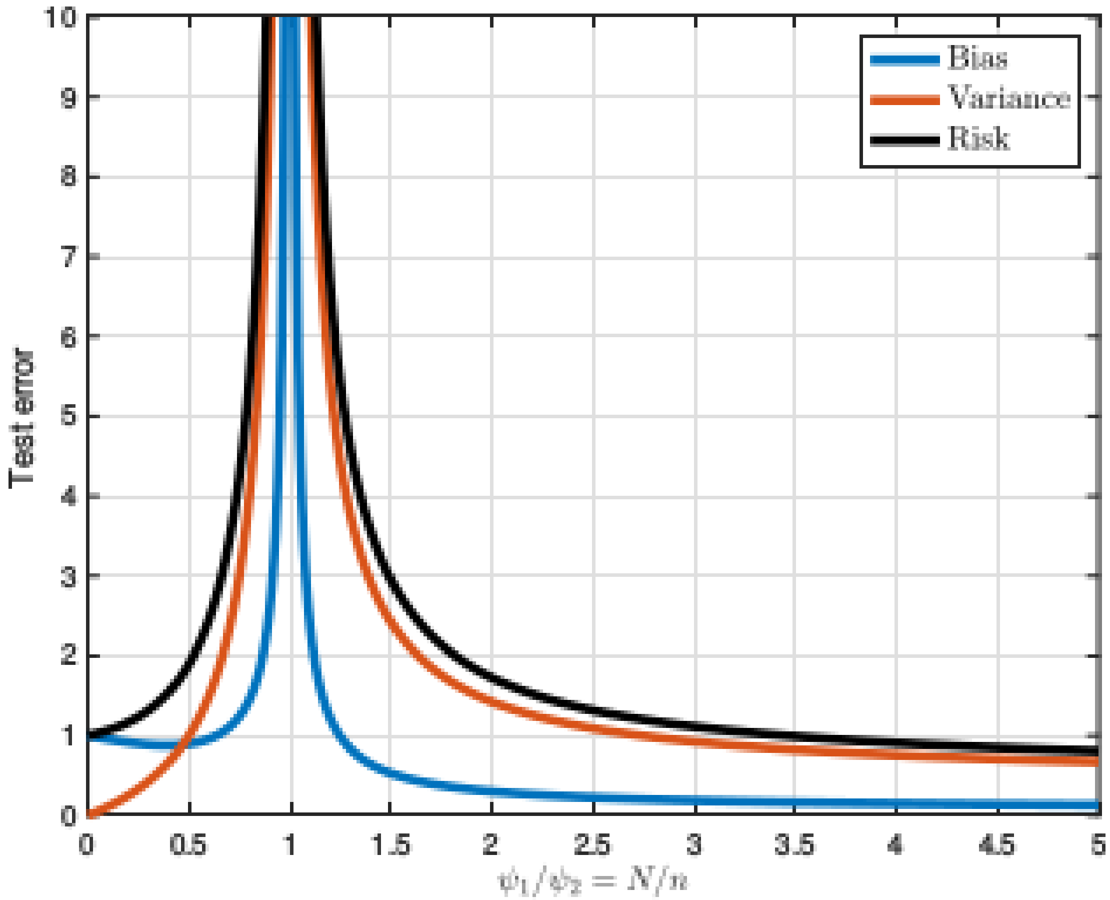

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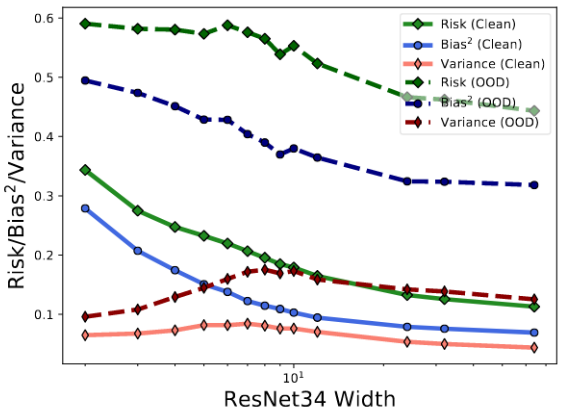
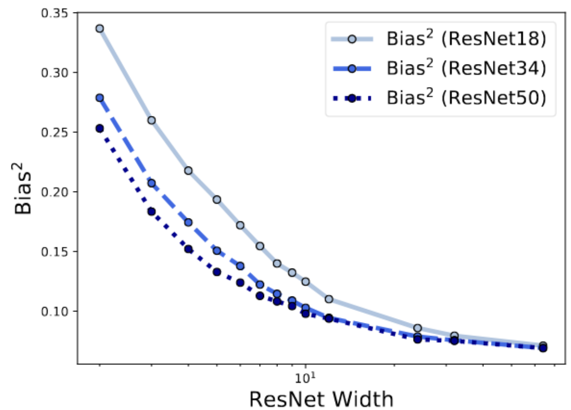
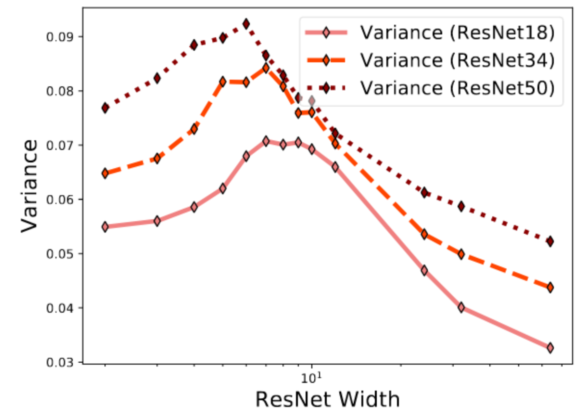
Effect of Depth



(a) OOD Example

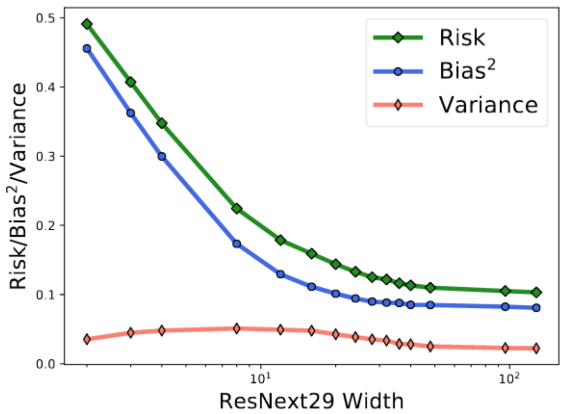


(b) Bias of model with different depth

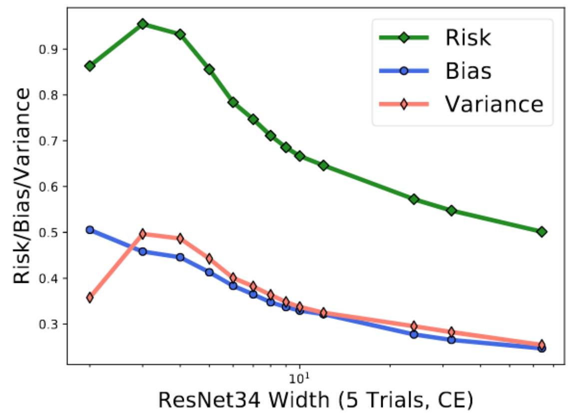


(c) Variance of model with different depth

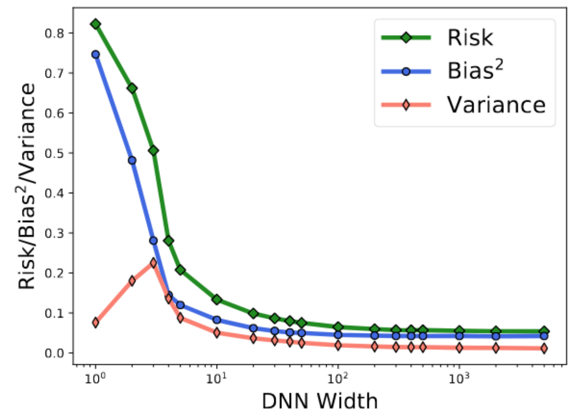
More Robustness Checks



(a) ResNext29, MSE loss, CIFAR10



(b) ResNet34, CE loss, CIFAR10



(c) DNN, MSE loss, MNIST

Ongoing Work

Extensions to classification (e.g. Montanari, Ruan, Sohn, Yan 2020)

Bias-variance for other settings (e.g. Yu, Yang, Dobriban, Steinhardt, Ma 2021)

Characterizing when more data hurts (e.g. Raghunathan, Xie, Yang, Duchi, Liang 2020)

Using random features models to explain scaling laws (e.g. Bahri, Dyer, Kaplan, Lee, Sharma 2021)