Reconciling modern machine-learning practice and the classical bias-variance trade-off

Benign Overfitting & Double Descent

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The Cornerstone: Bias-Variance Decomposition

Goal: Decompose the Expected Prediction Error

We want to analyze the expected squared error of our learned model $\hat{h}(x)$ on a new, unseen data point (x_0, y_0). The expectation is over different training sets $\mathcal{D}$.

$$\text{Error}(x_0) = E_{\mathcal{D},\varepsilon}\left[(y_0 - \hat{h}(x_0))^2\right]$$

where the true model is $y_0 = f(x_0) + \varepsilon$, with $E[\varepsilon] = 0$ and $Var(\varepsilon) = \sigma^2$.

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Step 1: Substitute the true model

$$\begin{aligned}
\text{Error}(x_0) &= E\left[(f(x_0) + \varepsilon - \hat{h}(x_0))^2\right] \\
&= E\left[(f(x_0) - \hat{h}(x_0))^2 + 2\varepsilon(f(x_0) - \hat{h}(x_0)) + \varepsilon^2\right] \\
&= E\left[(f(x_0) - \hat{h}(x_0))^2\right] + E[2\varepsilon(f(x_0) - \hat{h}(x_0))] + E[\varepsilon^2] \\
&= E\left[(f(x_0) - \hat{h}(x_0))^2\right] + \sigma^2 \quad \text{(Since } f, \hat{h} \text{ are independent of } \varepsilon \text{ and } E[\varepsilon] = 0\text{)}
\end{aligned}$$

Bias-Variance Decomposition (Cont.)

Step 2: Decompose the model error term

Now let's focus on the term $E\left[(f(x_0) - \hat{h}(x_0))^2\right]$. We add and subtract the mean prediction $E[\hat{h}(x_0)]$:

$$
\begin{aligned}
& E\left[(f(x_0) - E[\hat{h}(x_0)] + E[\hat{h}(x_0)] - \hat{h}(x_0))^2\right] \\
&= E\Big[(f(x_0) - E[\hat{h}(x_0)])^2 + (\hat{h}(x_0) - E[\hat{h}(x_0)])^2 \\
&\quad + 2(f(x_0) - E[\hat{h}(x_0)])(\hat{h}(x_0) - E[\hat{h}(x_0)])\Big]
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Step 3: Analyze the cross term

The expectation of the cross term is zero:

$$\begin{aligned} & E\left[2(f(x_0) - E[\hat{h}(x_0)])(\hat{h}(x_0) - E[\hat{h}(x_0)])\right] \\ &= 2(f(x_0) - E[\hat{h}(x_0)]) \cdot E\left[\hat{h}(x_0) - E[\hat{h}(x_0)]\right] \\ &= 2(f(x_0) - E[\hat{h}(x_0)]) \cdot (E[\hat{h}(x_0)] - E[\hat{h}(x_0)]) = 0 \end{aligned}$$

The Cornerstone: Bias-Variance Trade-off

Proposition

For a true model $y = f(x) + \varepsilon$, and our learned model $\hat{h}(x)$, the Expected Prediction Error at a point x_0 is:

$$\begin{aligned}
\text{EPE}(x_0) &= E\left[(y_0 - \hat{h}(x_0))^2\right] \\
&= \underbrace{\left(E[\hat{h}(x_0)] - f(x_0)\right)^2}_{\text{Bias}^2} + \underbrace{E\left[(\hat{h}(x_0) - E[\hat{h}(x_0)])^2\right]}_{\text{Variance}} + \underbrace{\sigma^2}_{\text{Irreducible Error}} \\
&= \text{Bias}^2 + \text{Variance} + \sigma^2
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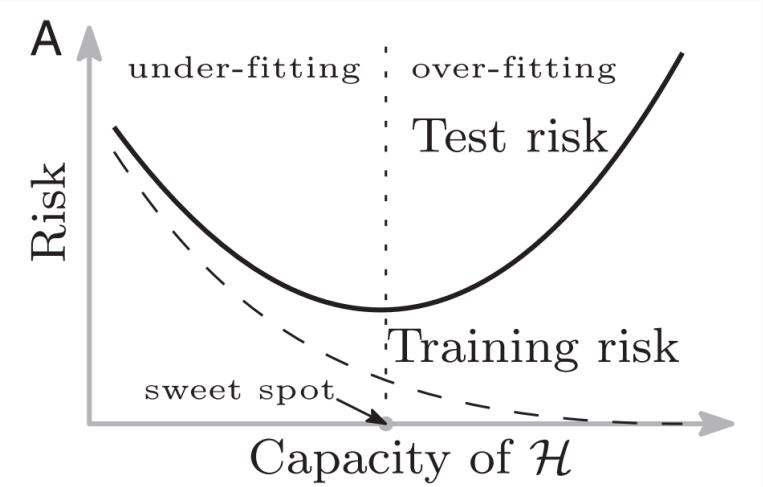
- **High Bias:** Simple models (e.g., linear) can't capture the true complexity.
- **High Variance:** Complex models (e.g., high-degree polynomial) are too sensitive to the training data.



The Great Divide: Theory vs. Reality

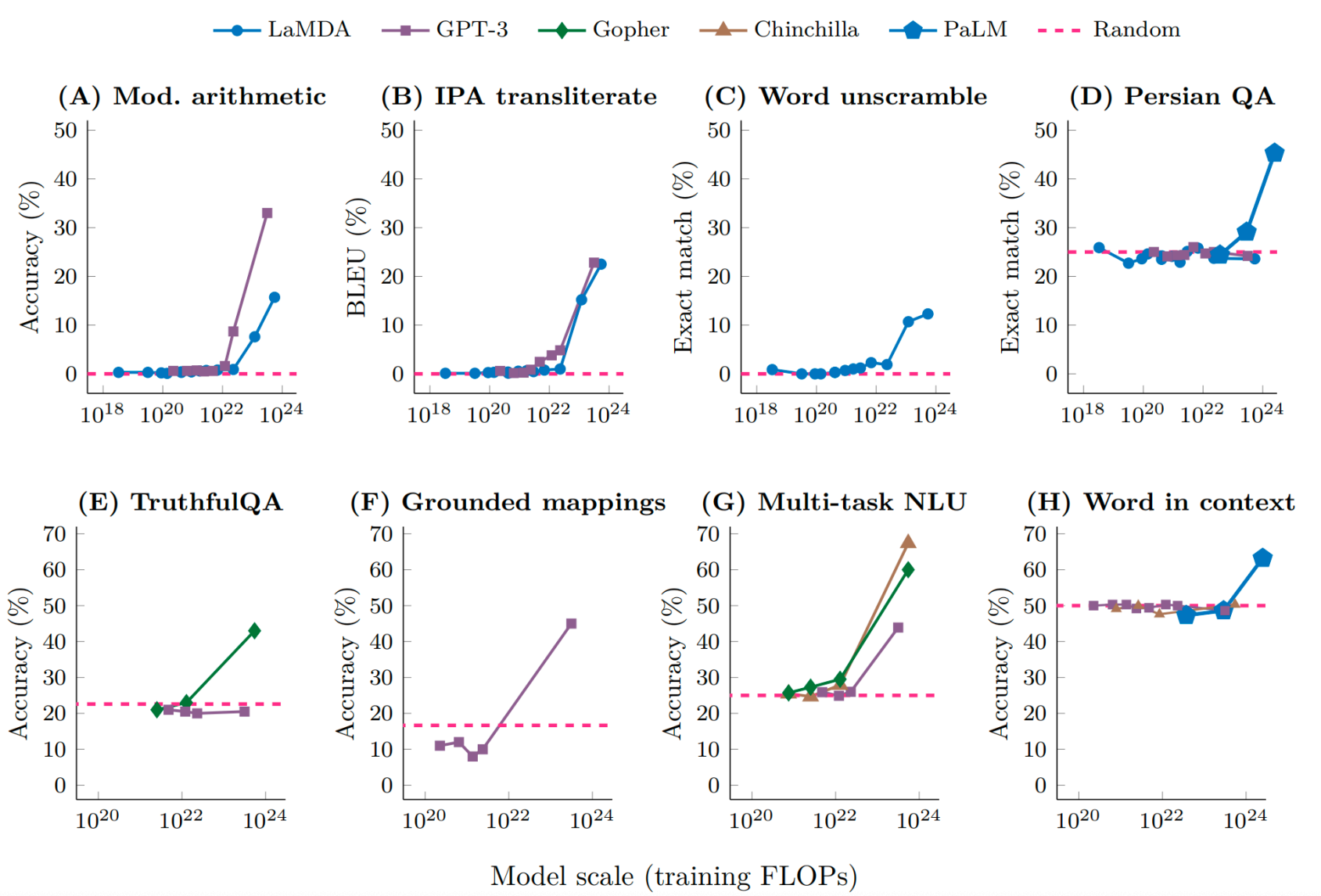


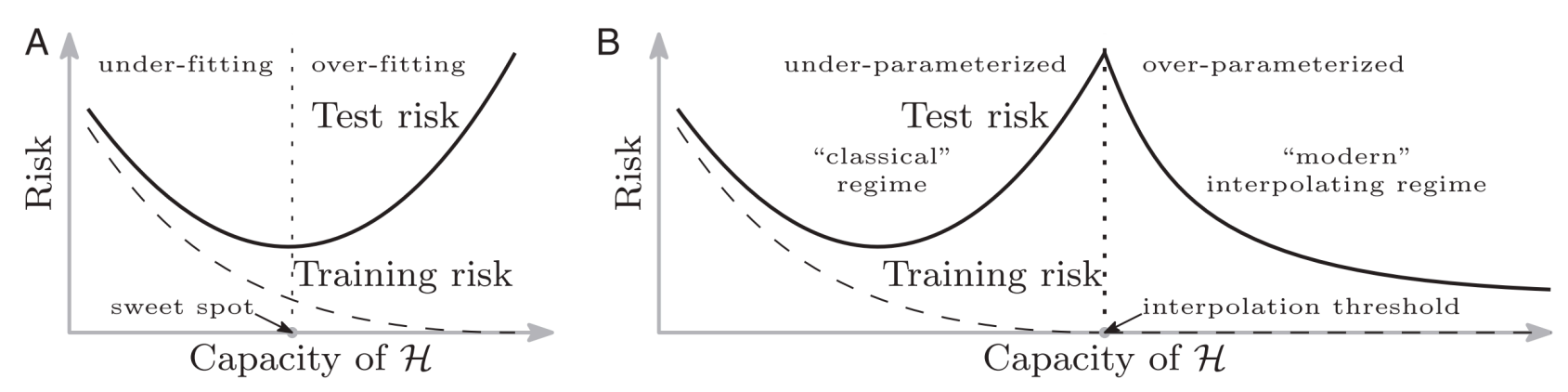
Figure 2: Source: Wei, Tay, Bommasani, et al. (2022), Figure 2.

The Core Question

Is our classical theory flawed?

Why is it that under extreme overparameterization, models not only don't collapse but become even more powerful?

A More Complete Picture: The Double Descent Curve



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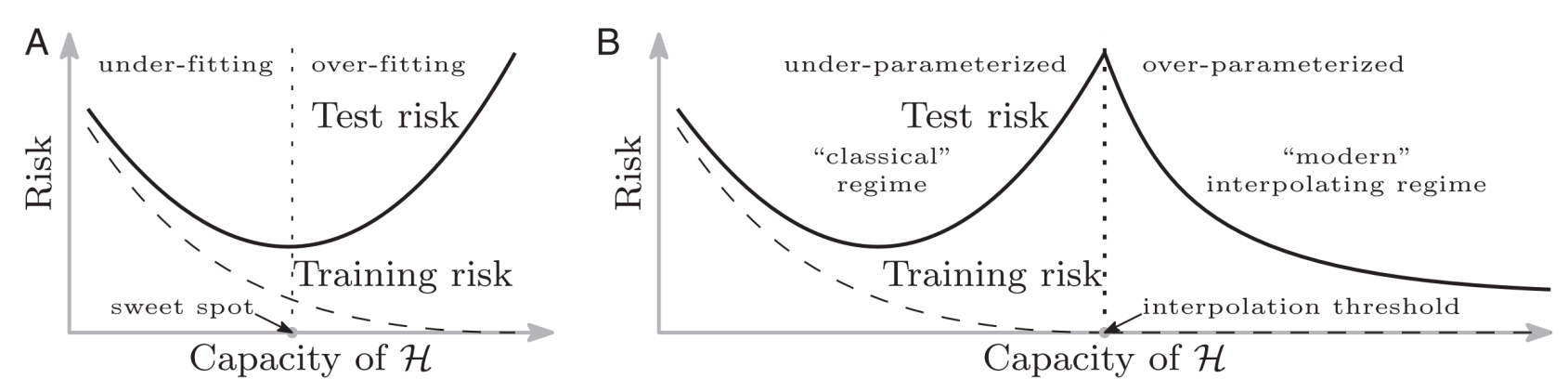

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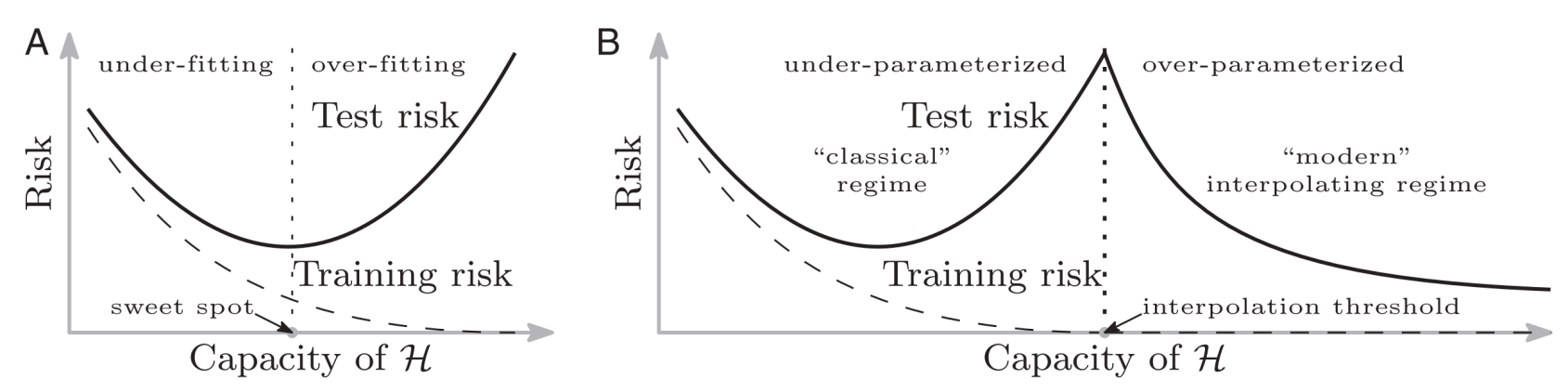

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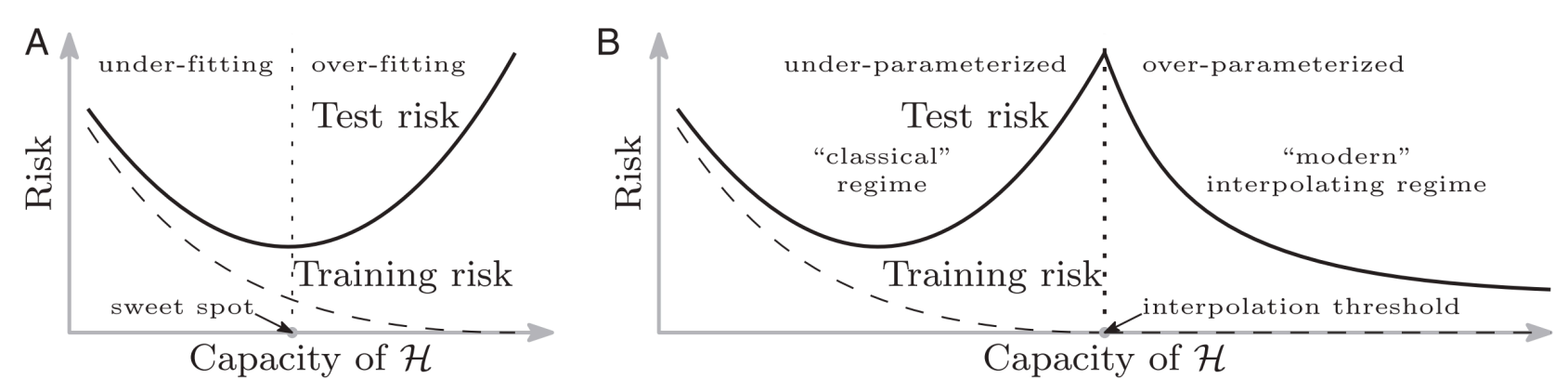

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  Critically parameterized. Test error peaks.
- **Overparameterized ($p > n$):**
  Modern regime. Test error descends again.

The Theoretical Underpinning

Approximation Theorem

In a noiseless setting, for **any** function $h \in \mathcal{H}_\infty$ that **interpolates** the data, its uniform error is bounded with high probability:

$$\sup_{x \in \Omega} |h(x) - h^*(x)| \leq A e^{-B(n/\log n)^{1/d}} (\|h^*\|_{\mathcal{H}_\infty} + \|h\|_{\mathcal{H}_\infty})$$

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The error bound is proportional to the sum of the norms $(\|h^*\| + \|h\|)$. To minimize the error bound, one should choose the interpolating solution h with the **minimum norm**.

Proof Sketch

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   - By the triangle inequality: $\|f\|_{\mathcal{H}} \leq \|h\|_{\mathcal{H}} + \|h^*\|_{\mathcal{H}}$.
3. **Apply a Known Theorem:** Thm. 11.22(Wendland, 2004) bounds the maximum of such a $f(x)$ using $\|f\|_{\mathcal{H}}$ and κ_n.

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Mathematical Form
The model function $h(x)$ is a linear combination of N random features:

$$h(x) = \sum_{k=1}^{N} \alpha_k \phi(x; v_k)$$

N : The number of features. The crucial knob to control **model capacity**.

v_k : The fixed, random vectors (e.g., from a Gaussian distribution).

α_k : The learnable coefficients.

The Experimental Setup

Setup Details

- **Dataset:** A subset of MNIST (10-class handwritten digits).
- **Training Size (n): 10,000** samples. This number is the key to locating the interpolation threshold.
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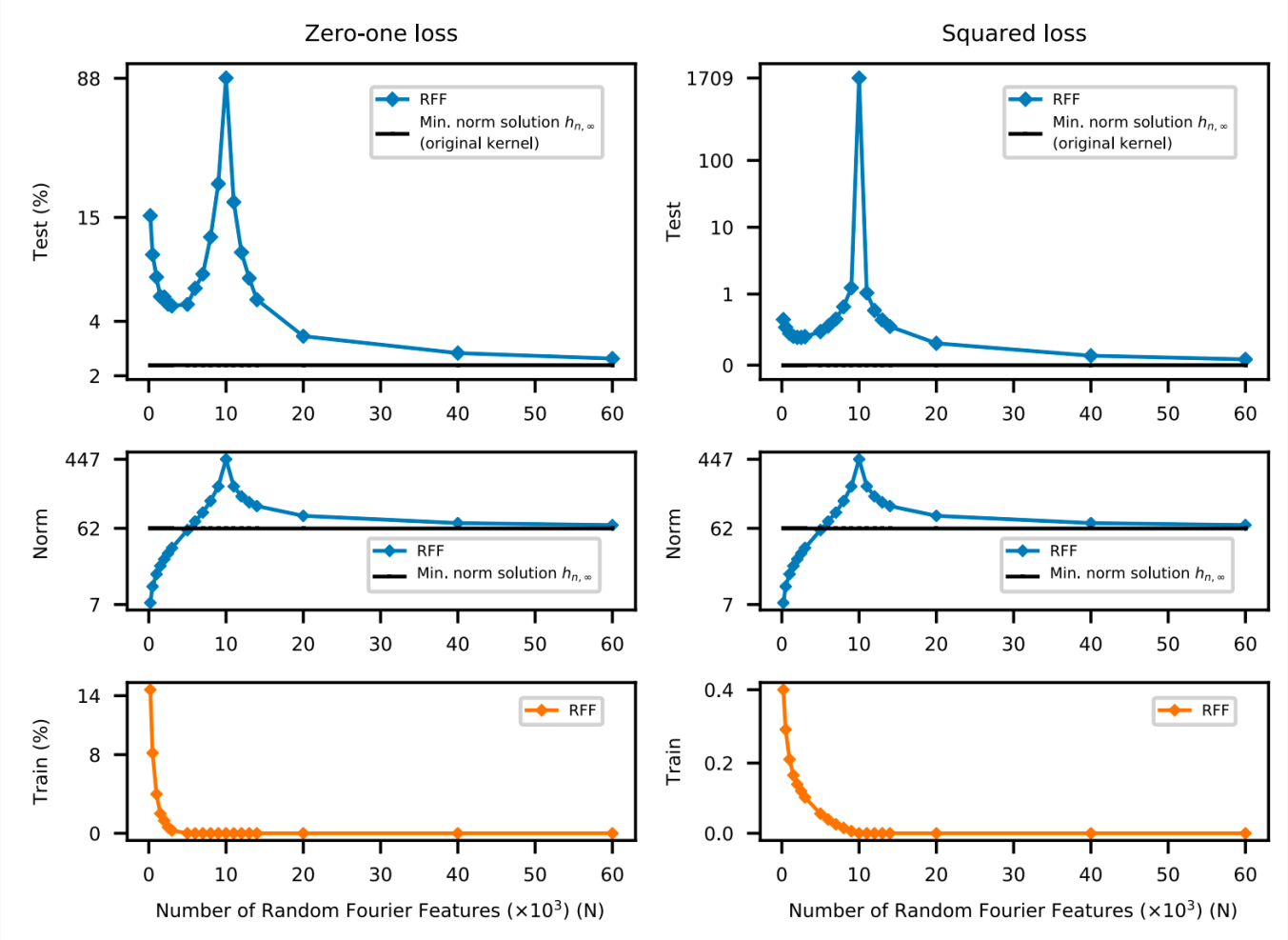
- When $N > n$, there are **infinite** interpolating solutions (solutions with zero training error).
- Which one to choose? The authors select the solution with the **minimum L2-norm** of the coefficients $\|\alpha\|_2$.
- This mimics an **implicit bias** of optimization algorithms (like gradient descent) towards "simpler" or "smoother" functions.

Results from RFF



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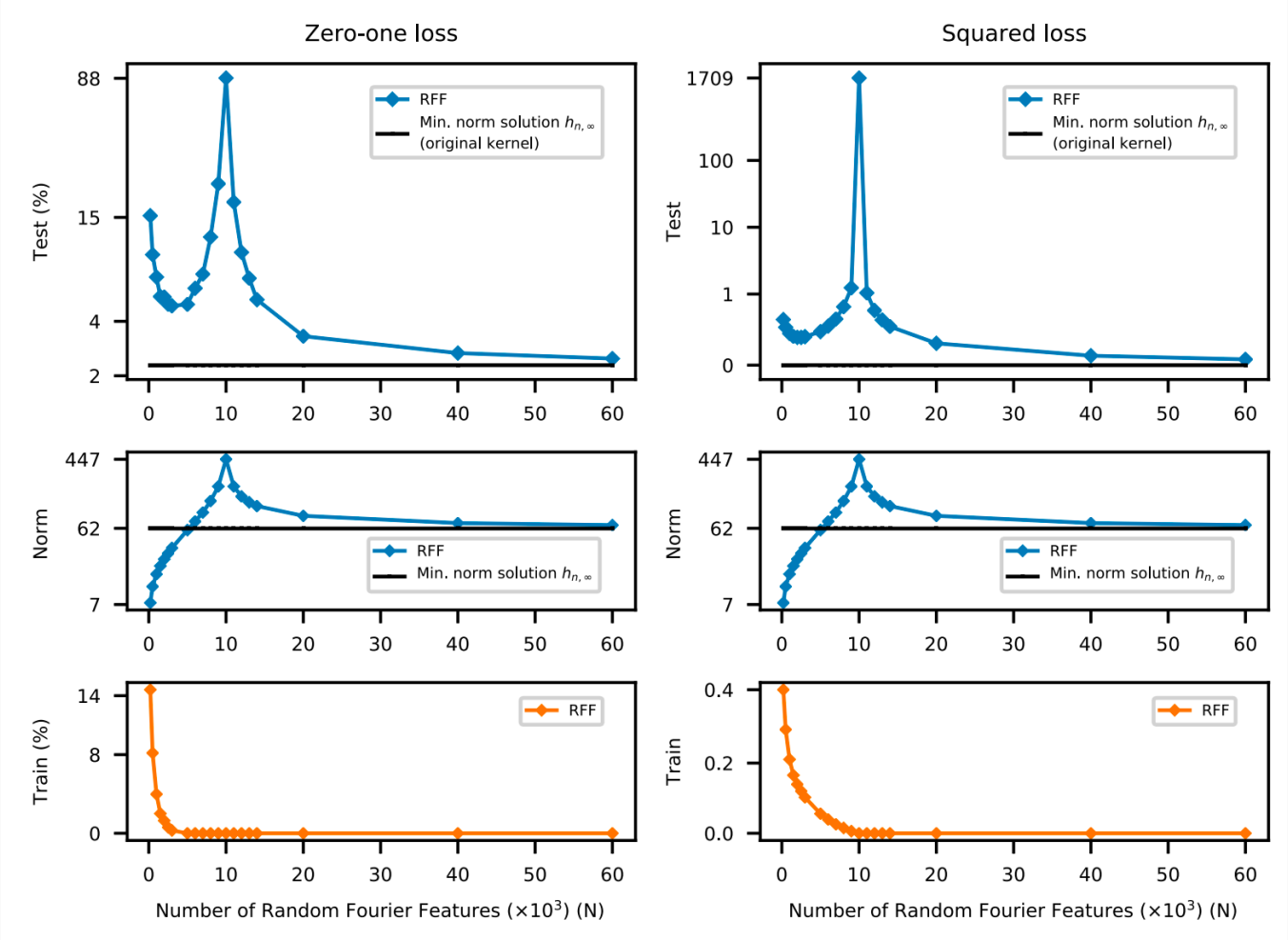

In the overparameterized regime, as model capacity increases, the norm of the learned solution **decreases**, correlating with lower test error. This points to an **implicit bias** towards simpler solutions.

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The answer lies in the **Inductive Bias** of the algorithm, which can be:

- **Explicit:** In models like **Kernel Machines**, the solution is mathematically defined to be the minimum norm interpolant in an RKHS.
- **Implicit:** In **Deep Neural Networks**, the bias comes from the **optimization algorithm** (e.g., SGD). While not fully understood, evidence points towards a preference for "simplicity":
  - SGD on linear models converges to the **max-margin** solution.
  - In deep networks, SGD often leads to **Neural Collapse** (Papyan et al., 2020), a highly structured and simple geometric configuration of features.
  - Minimum norm is just one well-studied instance of this broader principle.

Summary

1. The Classical Theory is Incomplete, Not Wrong

The U-shaped curve describes the underparameterized regime, not the whole story.

2. "Double Descent" Reveals a New "Bigger is Better" Paradigm

Increasing model capacity beyond the interpolation threshold can surprisingly improve generalization.

3. The Secret Sauce: Algorithm's Implicit Bias towards Simplicity

Overparameterization creates infinite solutions. The optimization algorithm's implicit bias (e.g., towards minimum norm) acts as an invisible regularizer, selecting the one that generalizes well.

The Grand Unifying Principle

Overparameterization + Implicit Bias = Benign Overfitting

Thank you.

Any questions?