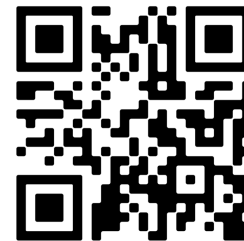


# Reconsidering Overfitting in the Age of Overparameterized Models



slides & refs

NeurIPS 2023 Tutorial, New Orleans

Speakers: Spencer Frei, Vidya Muthukumar, Fanny Yang, Moderator: Daniel Hsu



**UC DAVIS**  
UNIVERSITY OF CALIFORNIA

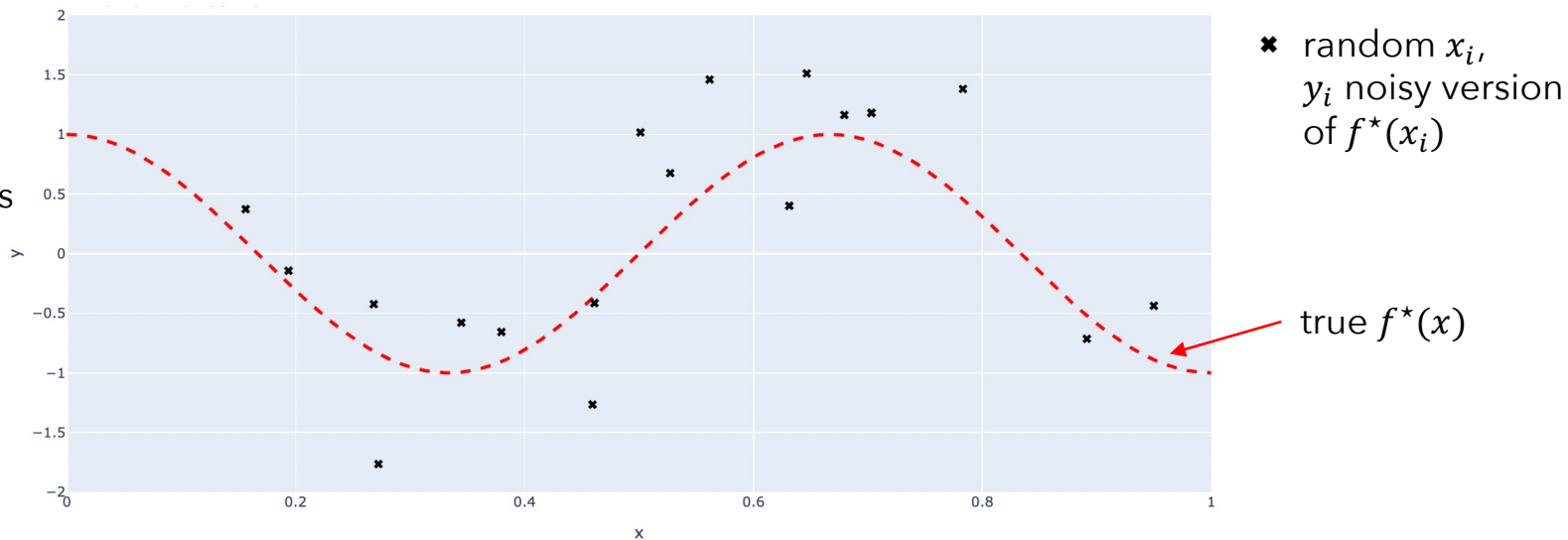
**GT** Georgia  
Tech.

**ETH** zürich

 **COLUMBIA**  
UNIVERSITY

# Textbook wisdom on overfitting

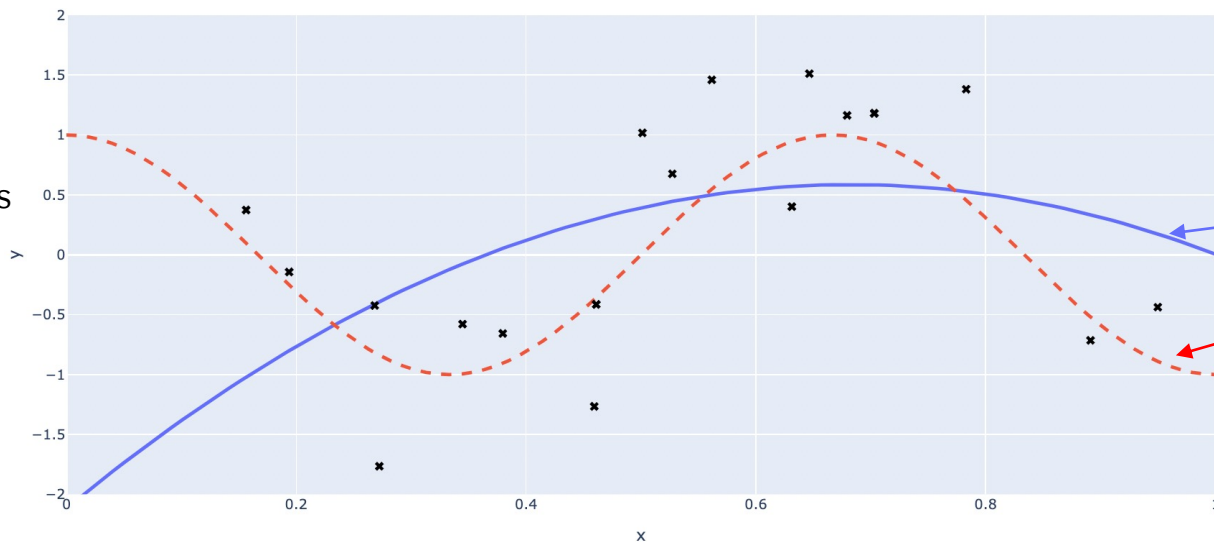
n = 20 samples



# Textbook wisdom on overfitting

$n = 20$  samples

polynomial fit  
degree  $d = 2$



\* random  $x_i$ ,  
 $y_i$  noisy version  
of  $f^*(x_i)$

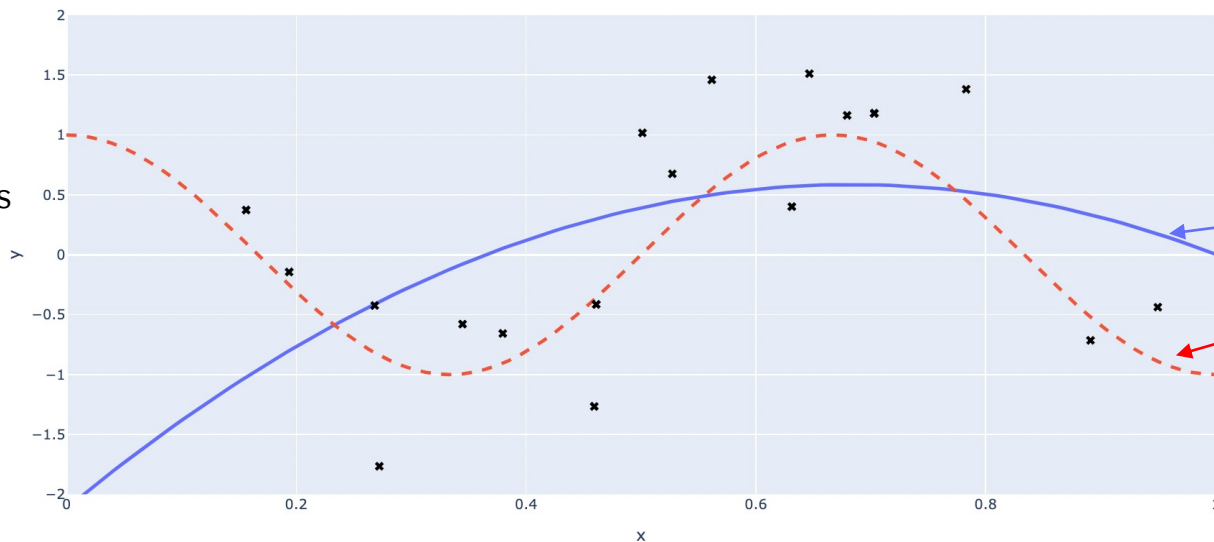
predicted  $\hat{f}(x)$

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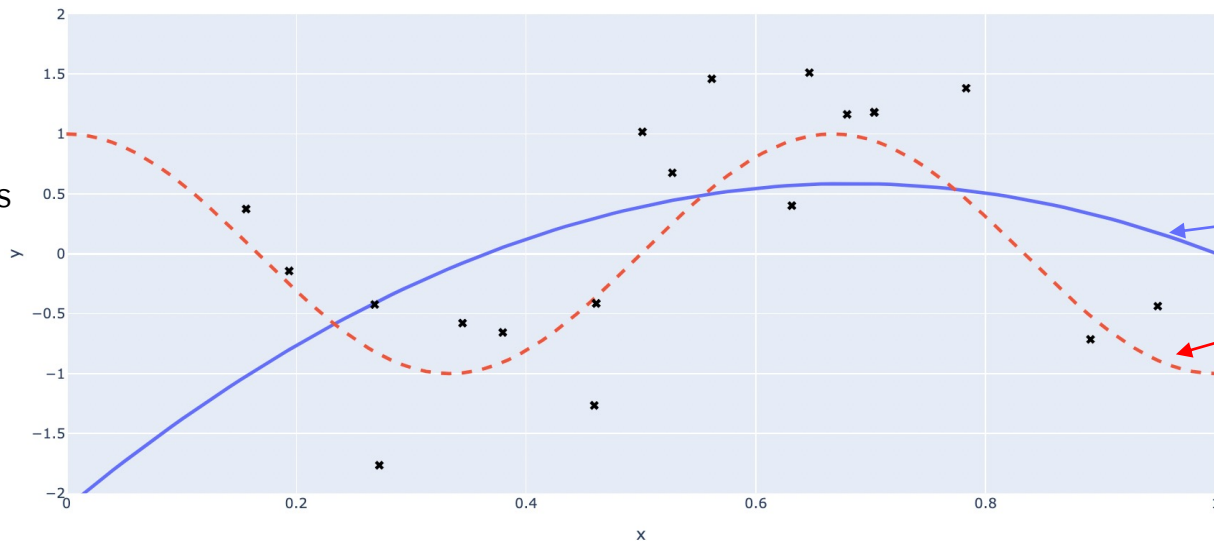
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Small models cannot fit perfectly: • cannot express function of interest (high statistical bias)

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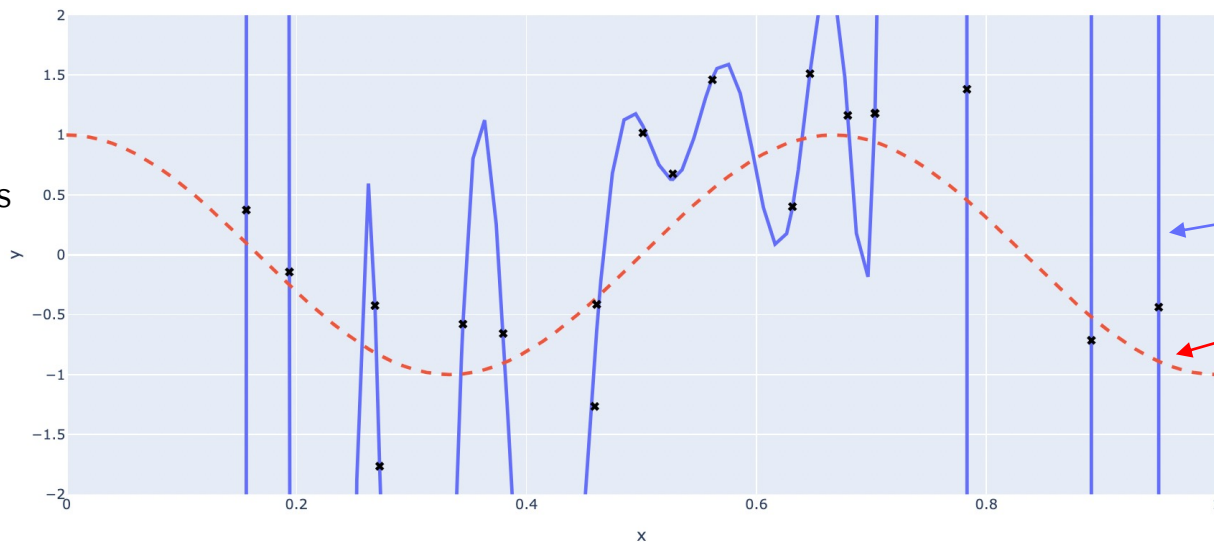
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- Small models cannot fit perfectly:
- cannot express function of interest (high statistical bias)
  - largely ignores noise  $\rightarrow$  does not fluctuate a lot (small variance)

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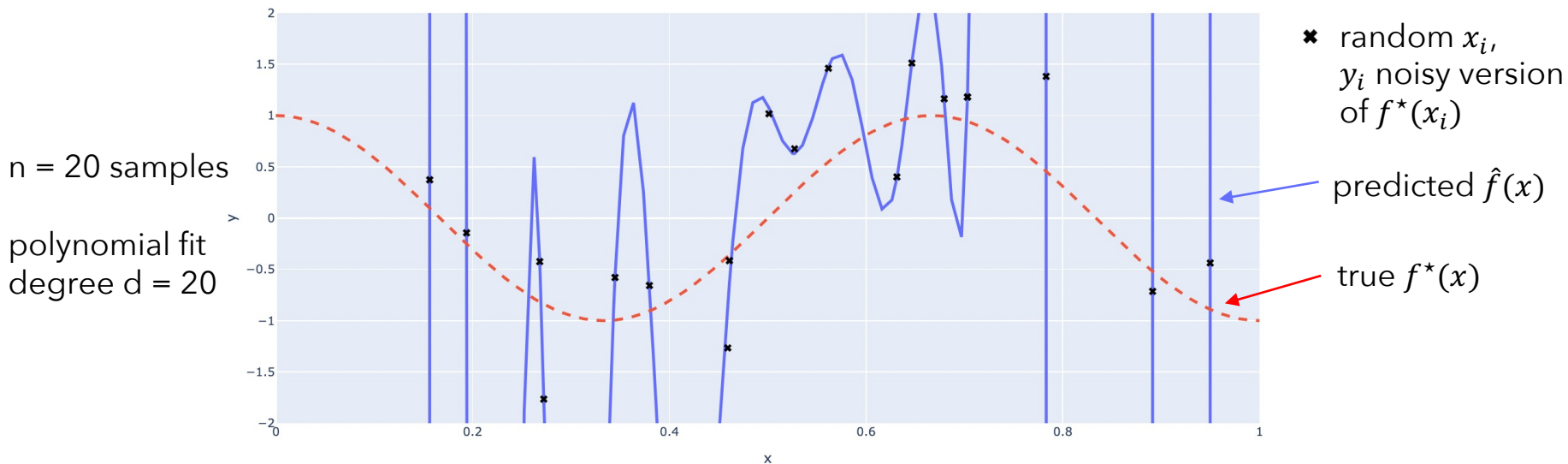


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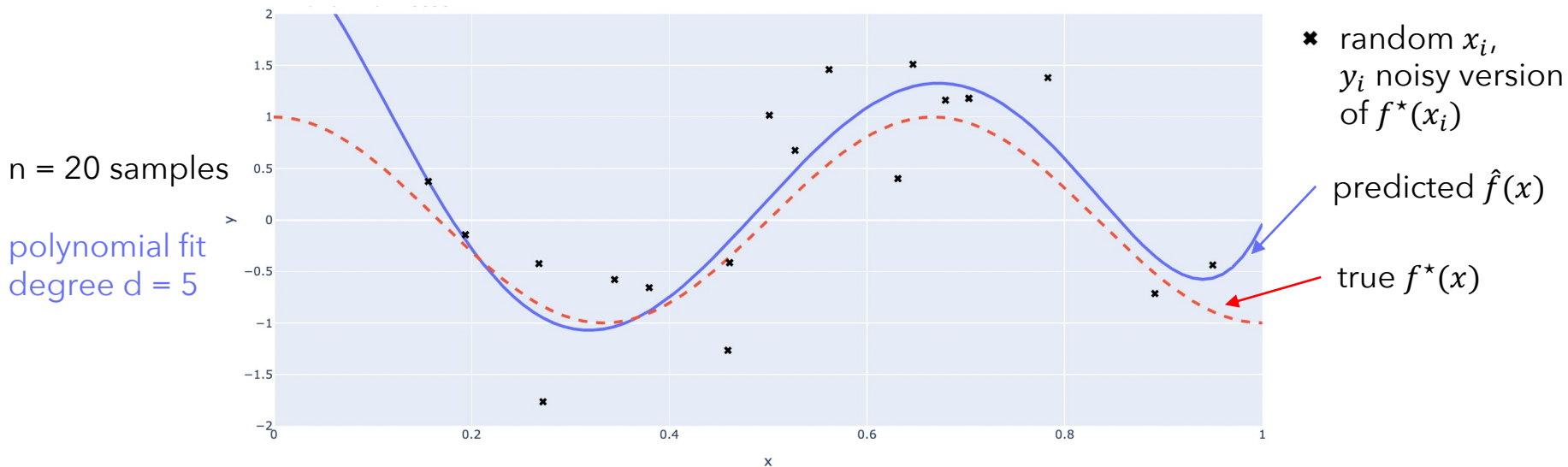
true  $f^*(x)$

# Textbook wisdom on overfitting



- Large models fit perfectly (overfit):
- flexible and can express function of interest (small bias)
  - fits too much of the noise (overfit)  $\rightarrow$  fluctuates a lot (high variance)

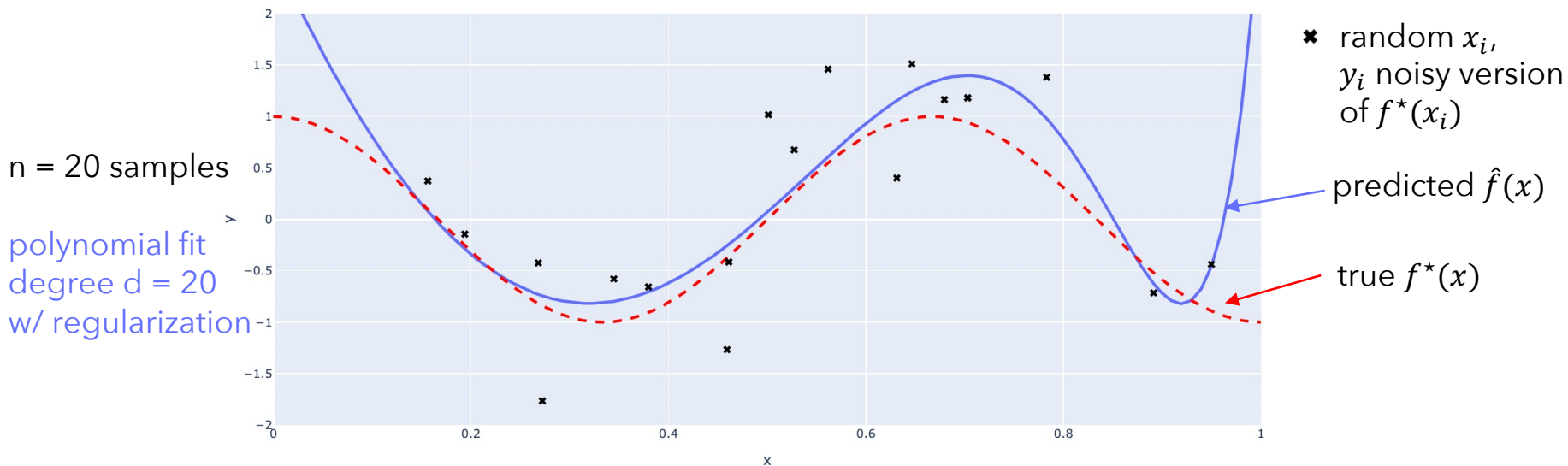
# Textbook wisdom: Avoid fitting noise



**Classical theory:** Improve generalization by optimizing expressivity via bias-variance trade-off

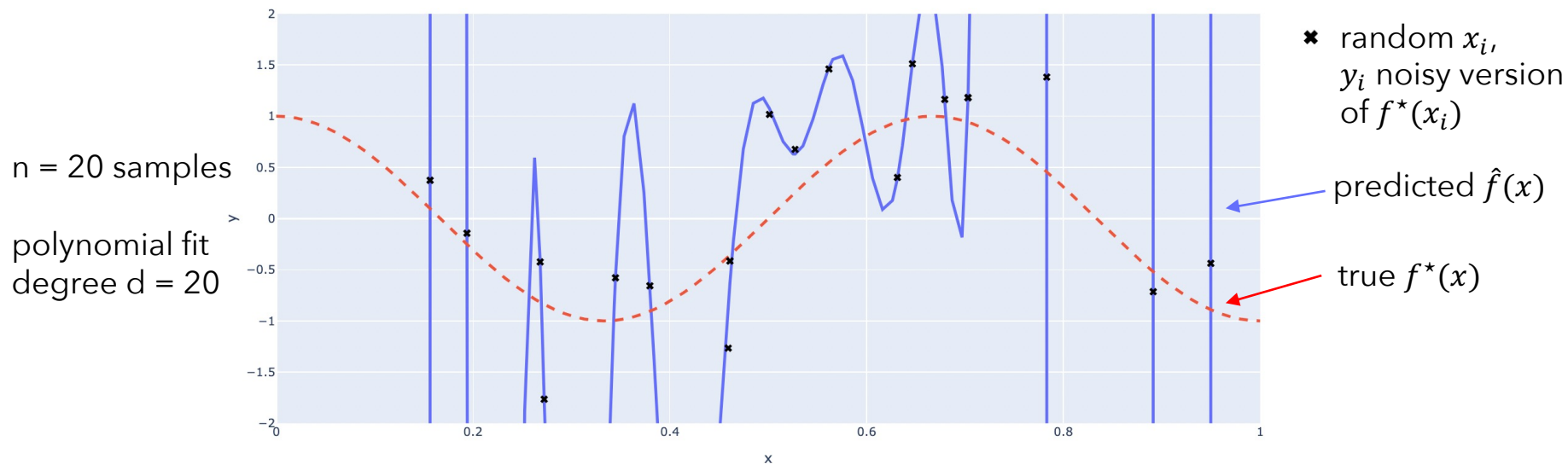


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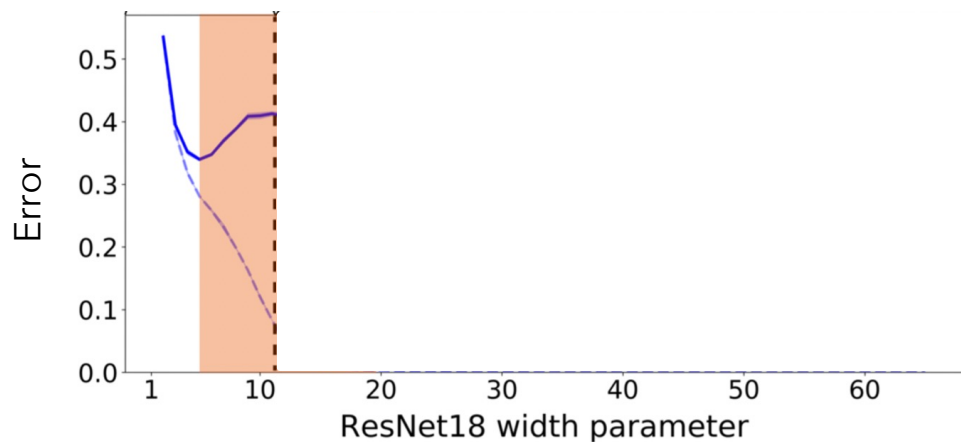
# Textbook wisdom on overfitting



What happens if we increase the polynomial degree even further without regularizing?

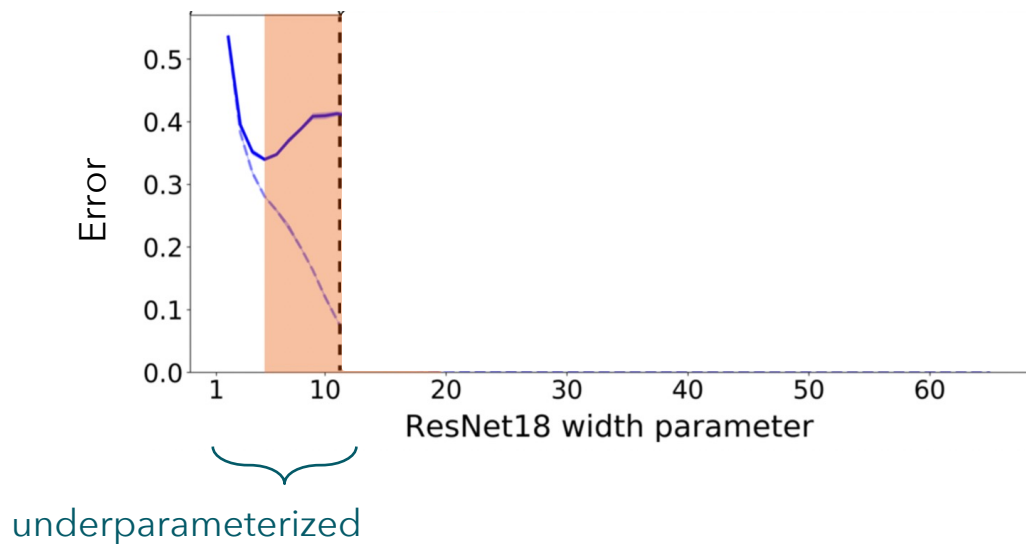
# Double descent on neural networks

Classification using neural networks and Adam on CIFAR-10 with 15% additional label noise



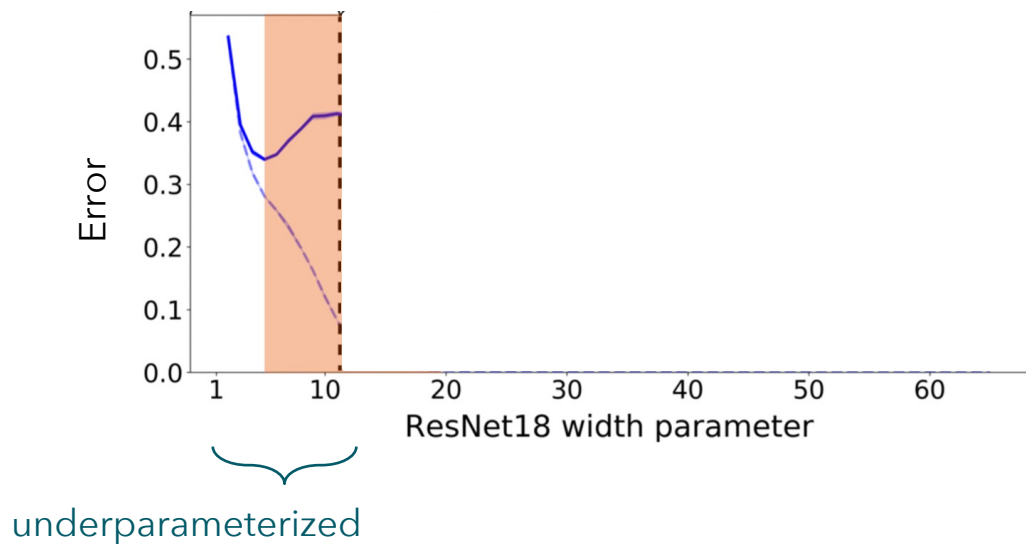
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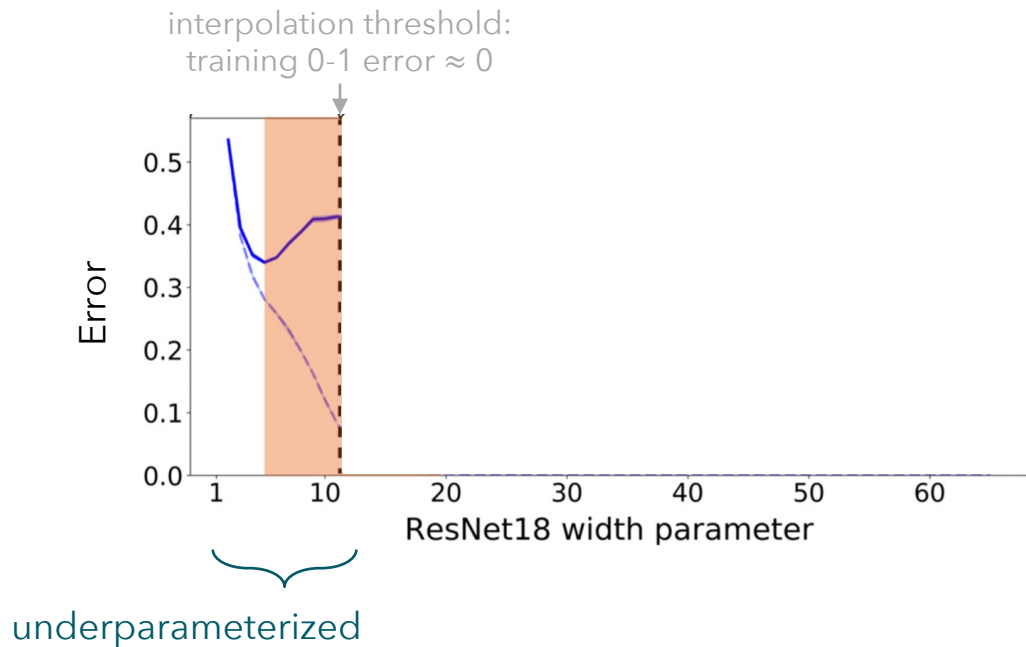
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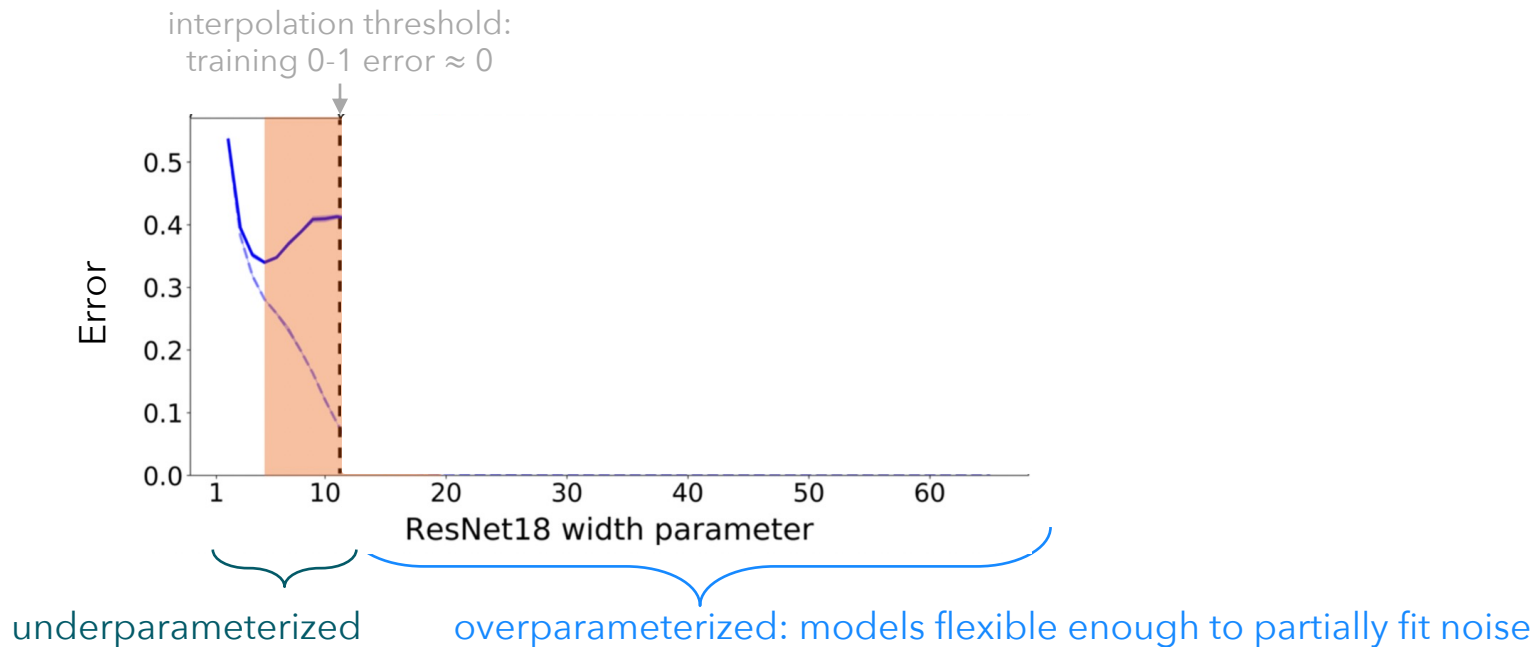
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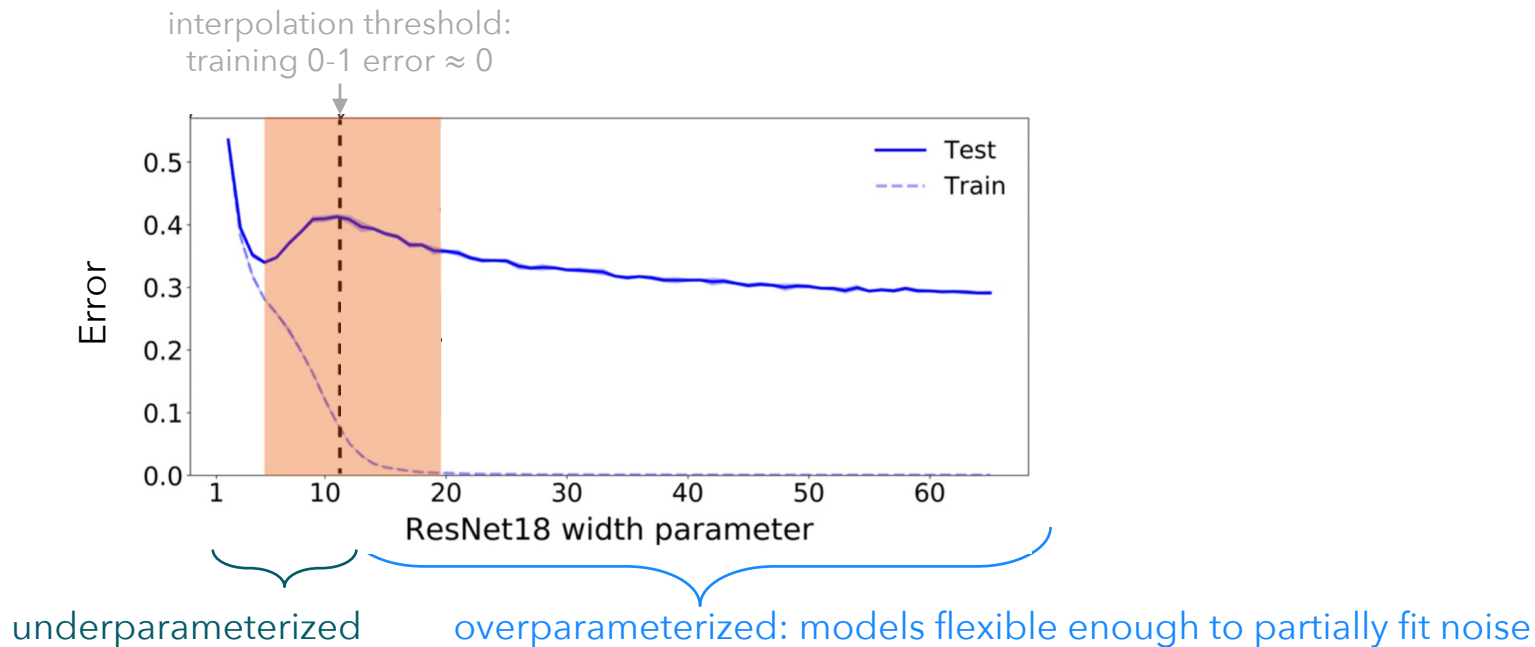
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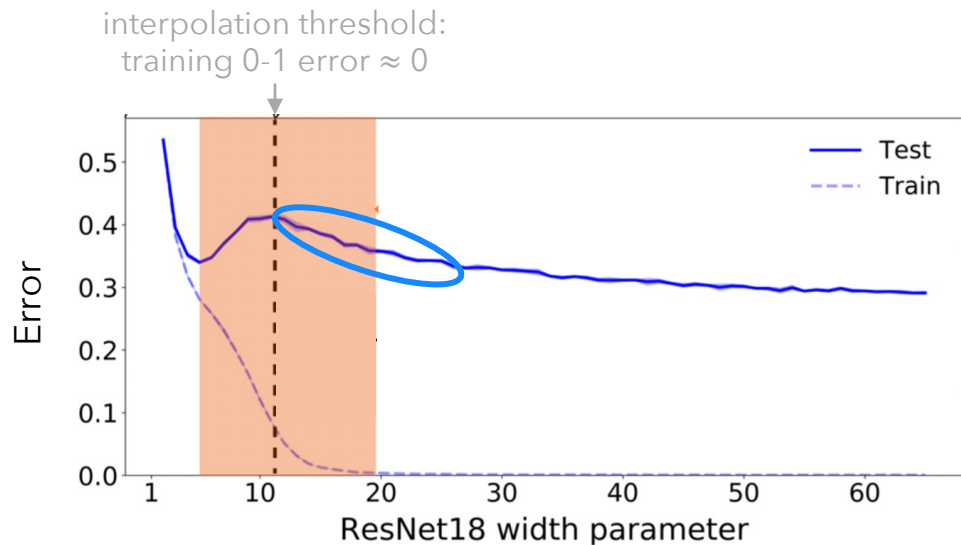
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# Obs. I: Second descent beyond interpolation

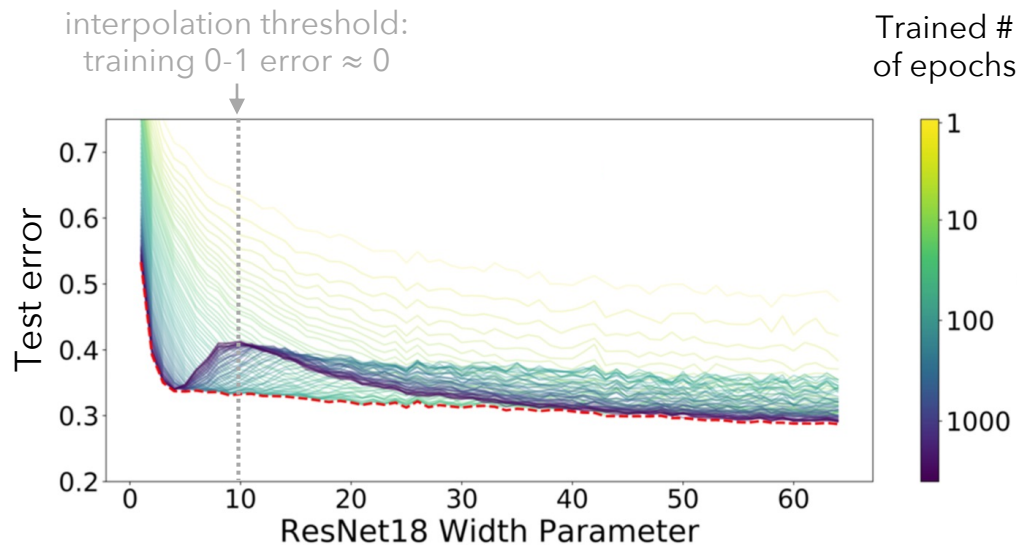
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1 After interpolation threshold, we have a [second "descent"](#) (double descent) for interpolators

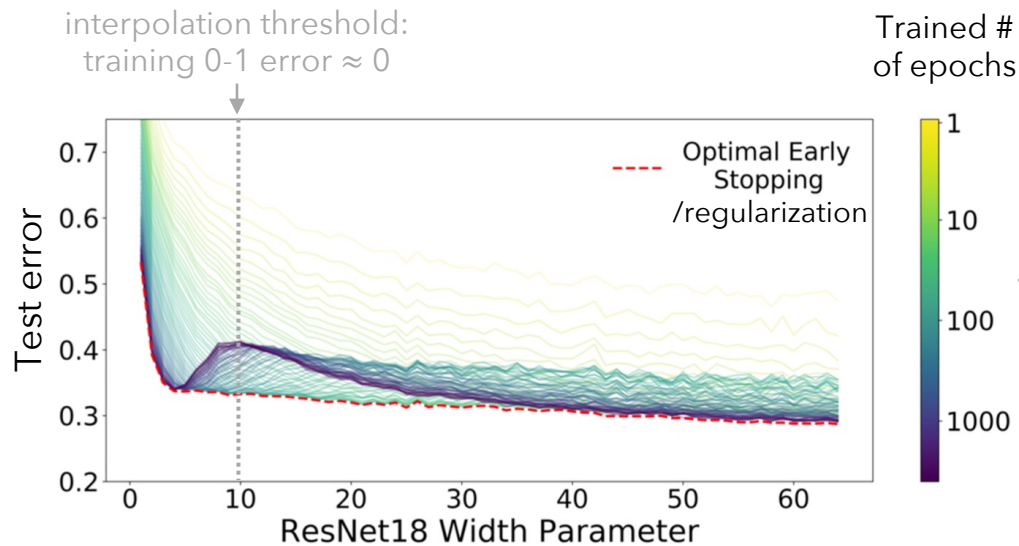
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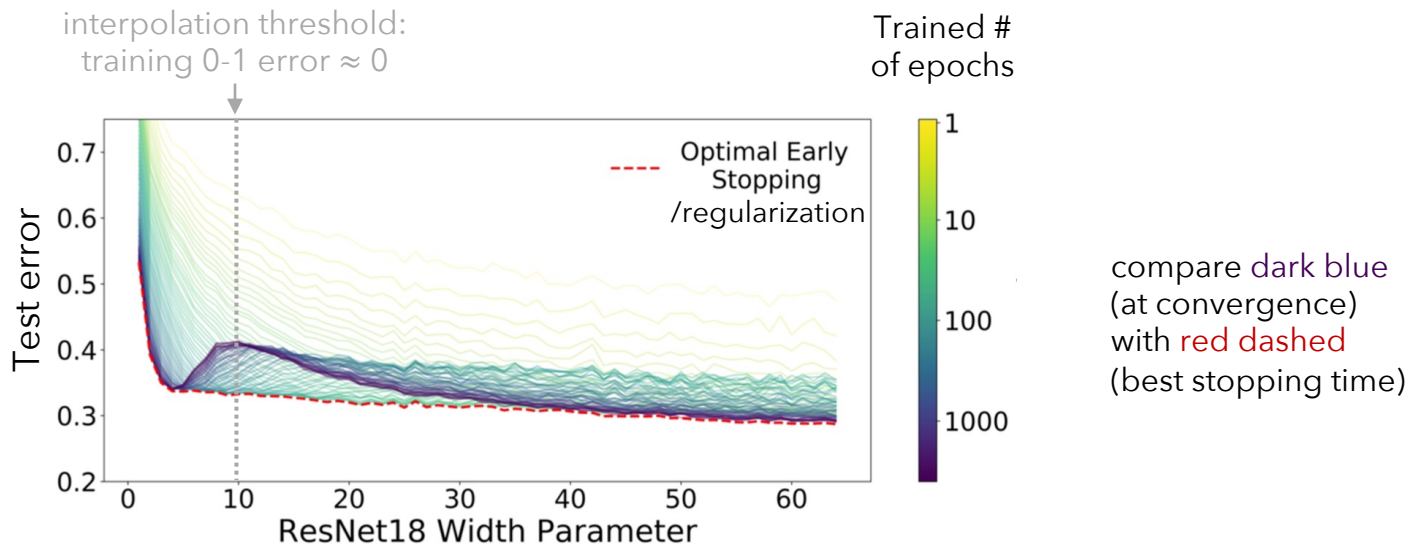
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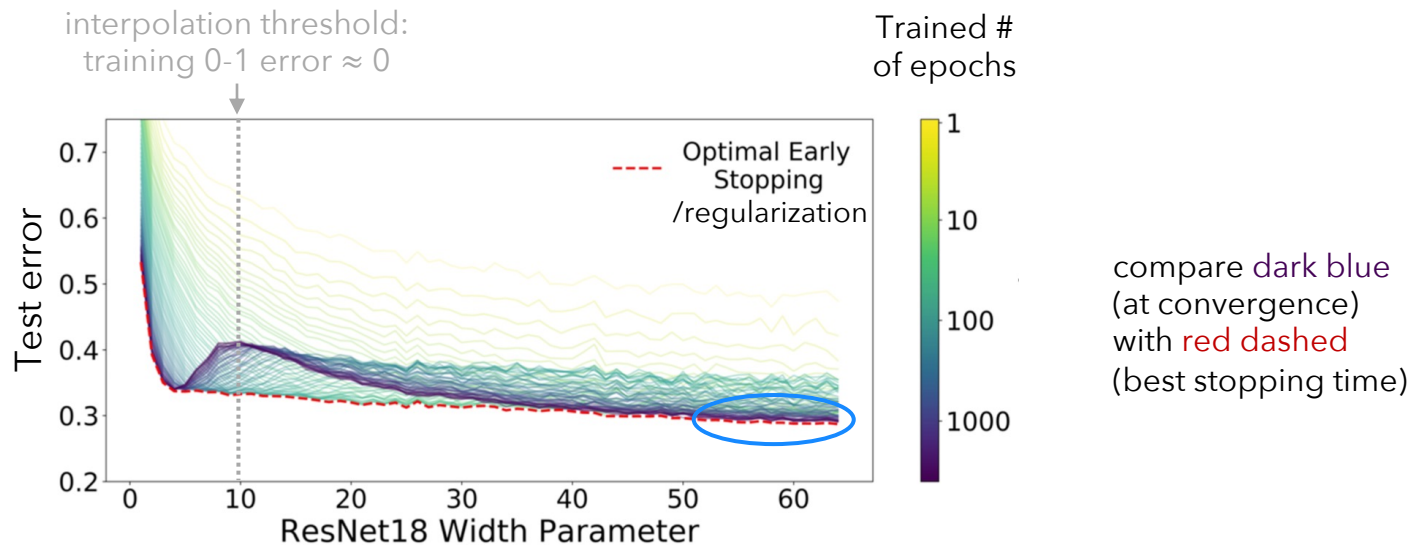
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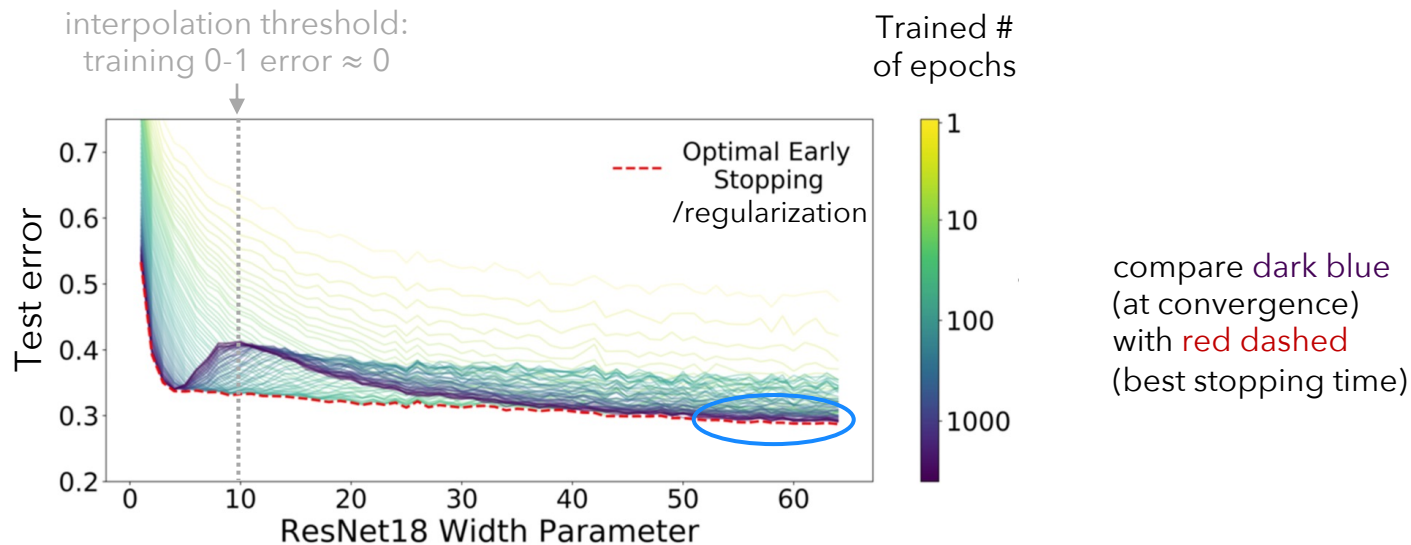
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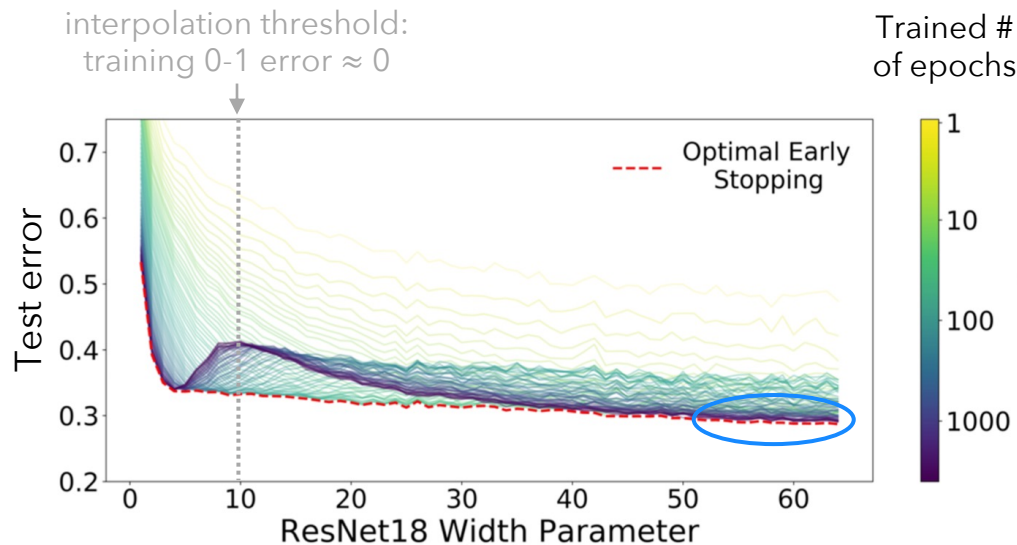
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2 For large models, interpolation is not worse than regularization ([harmless interpolation](#))

# Obs. III: Good generalization for large models

Classification using neural networks and Adam on CIFAR-10 with 15% additional label noise



3

For large models, we achieve reasonably good test accuracy

# Textbooks need an update...

uploaded 2016

DOI:10.1145/3446776



## Understanding Deep Learning (Still) Requires Rethinking Generalization

By Chiyuan Zhang, Samy Bengio, Moritz Hardt, Benjamin Recht, and Oriol Vinyals

Communications of the ACM, 2021

panelist today

\*and many more papers that expressed the need for “rethinking”



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# What the field set out to understand...

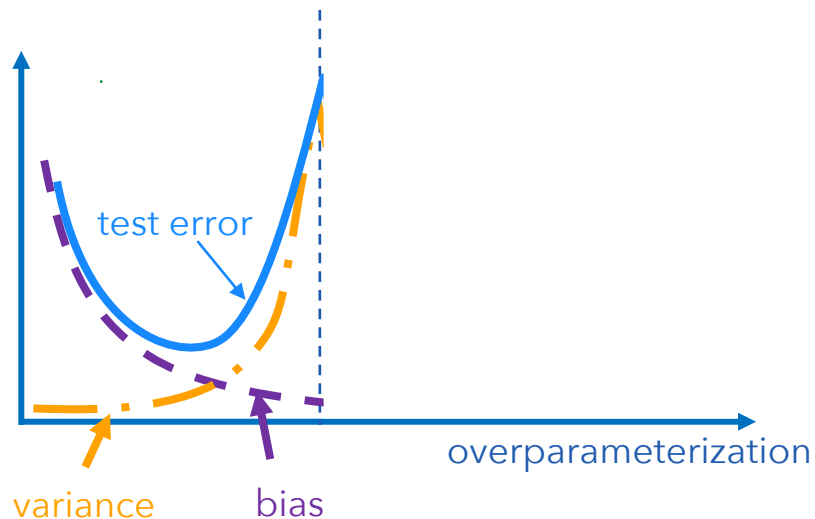
Try to understand **when** the following happens:

- 1 **Second “descent”** as model size grows grows beyond interpolation threshold
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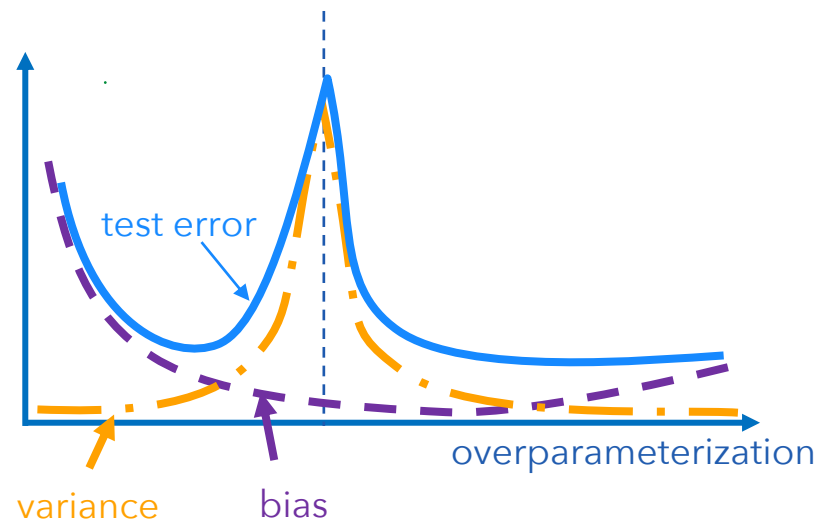
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variance decays



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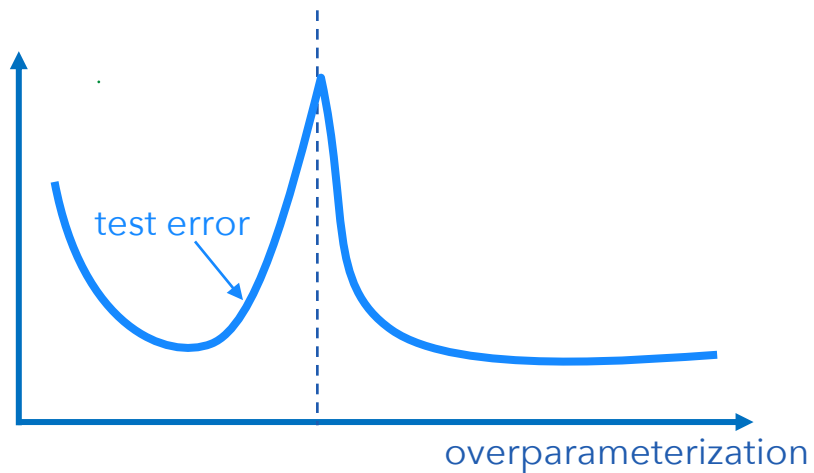
bias stays low

when is this the case?



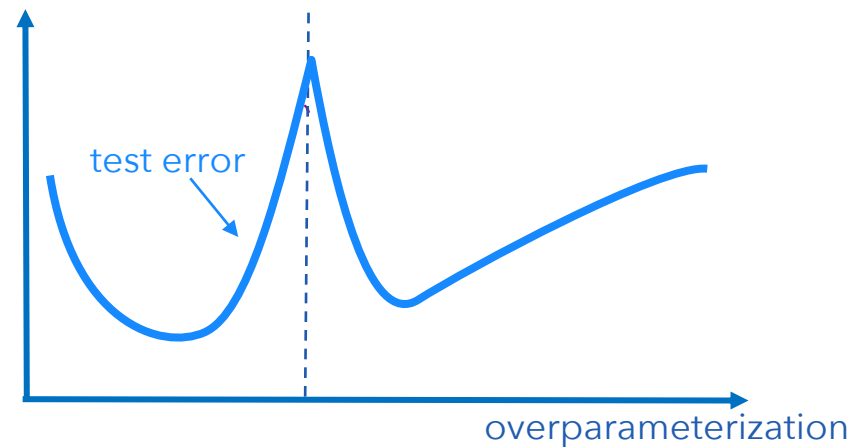
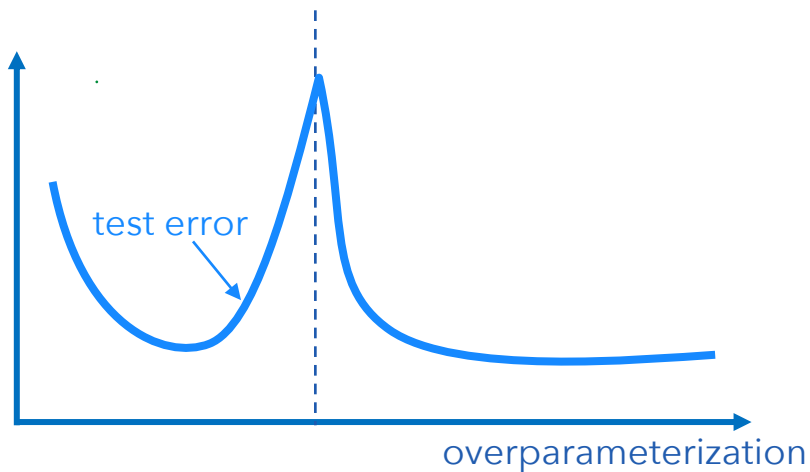
# Which factors govern...

when we have this picture...



# Which factors govern...

when we have this picture...



...rather than this picture





# Seeking answers using theoretical analysis...

## Neural network interpolators

- feature learning with [overparameterization](#)  $\triangleq$   
e.g. [width](#) of hidden layers
- found w/ 1st order methods to minimize **non-convex losses**





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Neural network interpolators  Kernel / random features

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complexity to analyze model

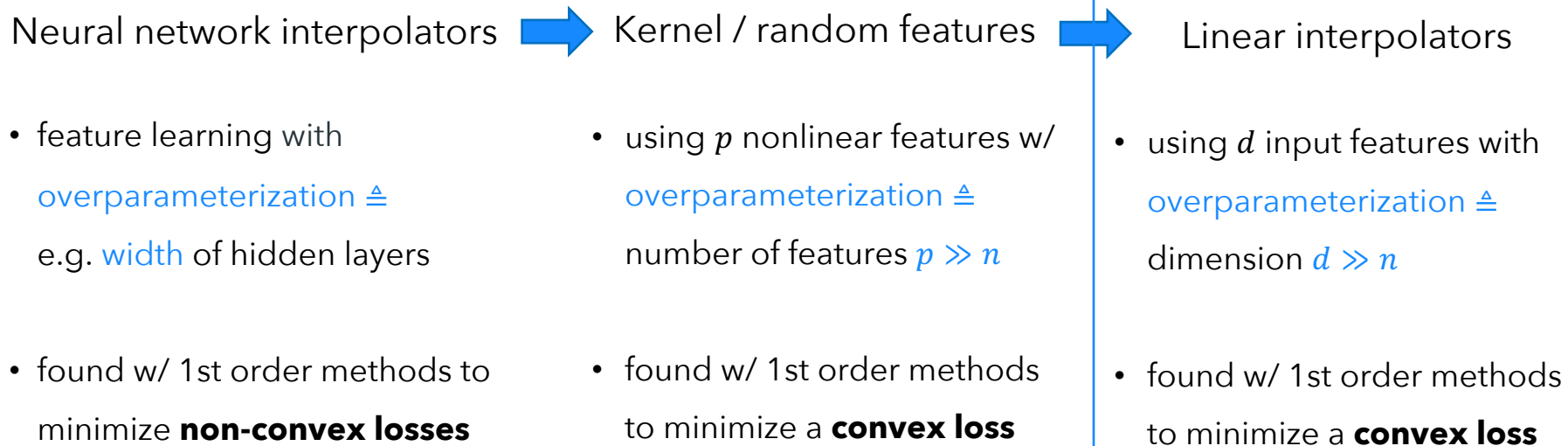
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## Linear interpolators

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**Part I:** For linear regression, we discuss how

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**Part II:** For classification, we discuss the

- effect of loss function choices
- implicit bias of optimization algorithms for neural networks
- generalization of neural networks on noisy, high-dimensional data



Goal is **not to find** better interpolators in practice  
but **to understand when** interpolation is benign

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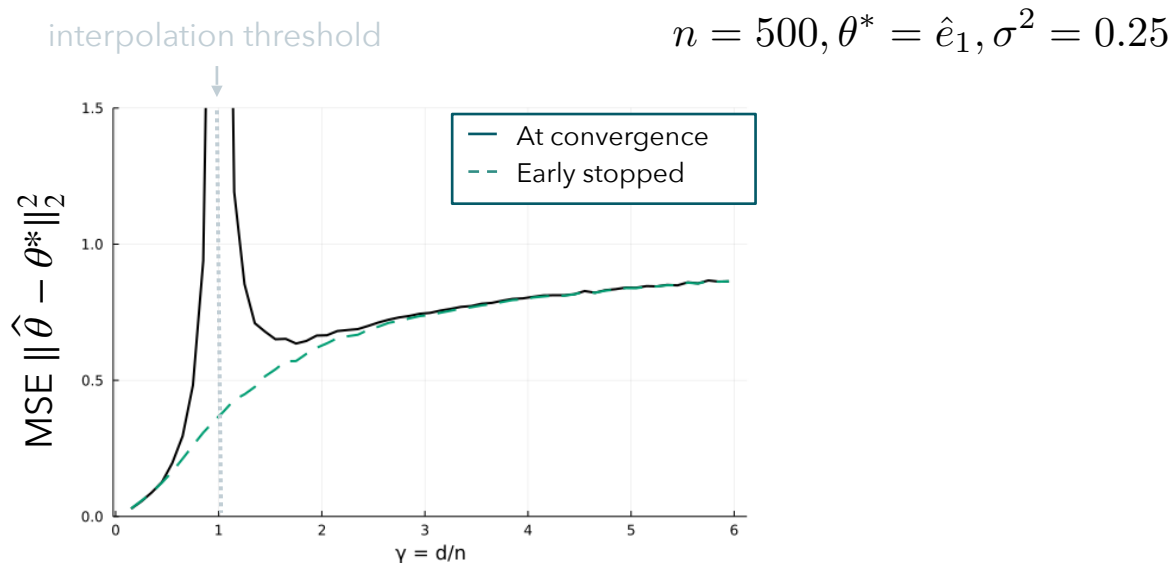
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## Benefits of overparameterization and interpolation in **linear models**

We run gradient descent on  $\|\mathbf{Y} - \mathbf{X}\theta\|_2^2$  at  $\theta_0 = 0$  for  $\mathbf{Y} = \mathbf{X}\theta^* + \mathbf{W}$   
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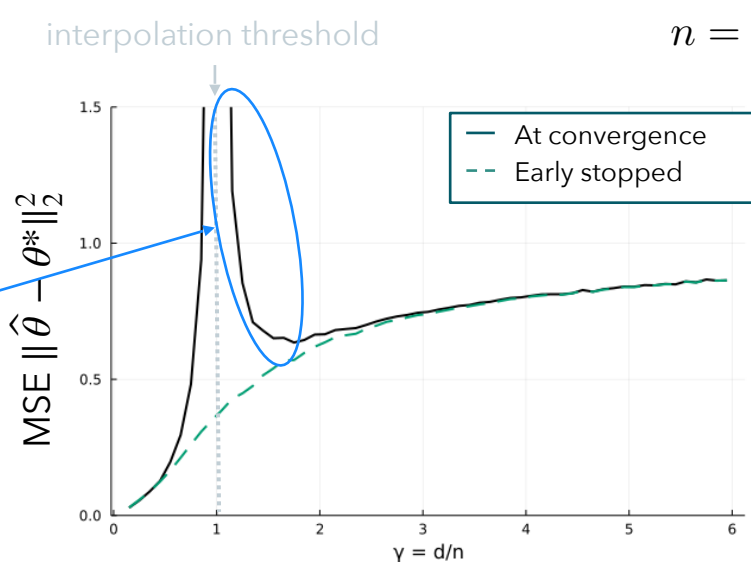


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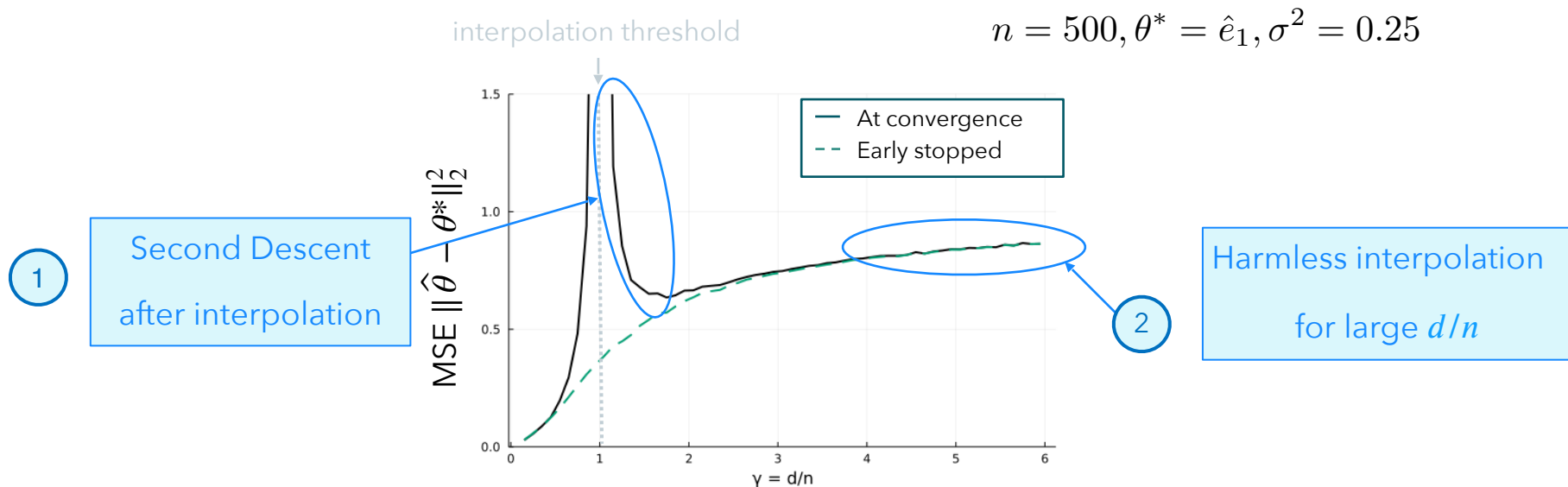
1

Second Descent  
after interpolation



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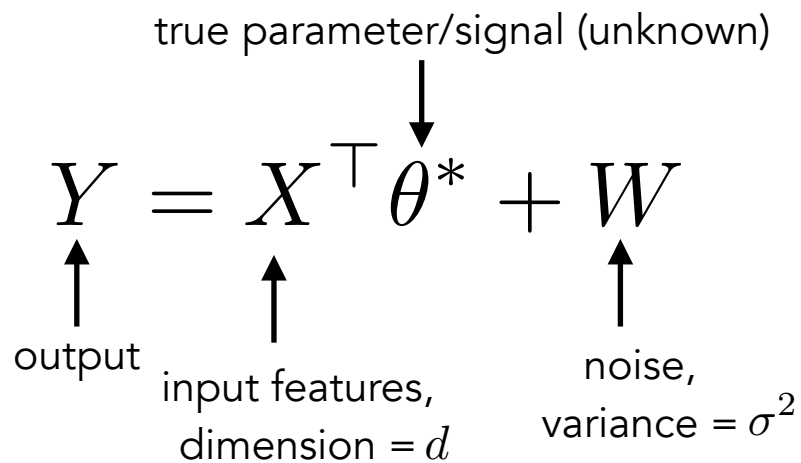
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Formal setup: overparameterized linear regression



## Formal setup: overparameterized linear regression

$$Y = X^T \theta^* + W$$


The diagram shows the equation  $Y = X^T \theta^* + W$  with three vertical arrows pointing upwards from labels to the variables  $Y$ ,  $X$ , and  $W$ . The label for  $Y$  is "output". The label for  $X$  is "input features, dimension =  $d$ ". The label for  $W$  is "noise, variance =  $\sigma^2$ ". Additionally, the text "true parameter/signal (unknown)" is positioned above the variable  $\theta^*$ , with a vertical arrow pointing downwards from it to  $\theta^*$ .

true parameter/signal (unknown)

output

input features,  
dimension =  $d$

noise,  
variance =  $\sigma^2$



# Formal setup: overparameterized linear regression

true parameter/signal (unknown)

$$Y = X^\top \theta^* + W$$

↑                    ↑                    ↑  
output                input features,        noise,  
                          dimension =  $d$                 variance =  $\sigma^2$

$$\mathbb{E}[X] = 0, \mathbb{E}[X X^\top] = \Sigma$$

(data covariance)

e.g. "isotropic covariance" means  $\Sigma = I$

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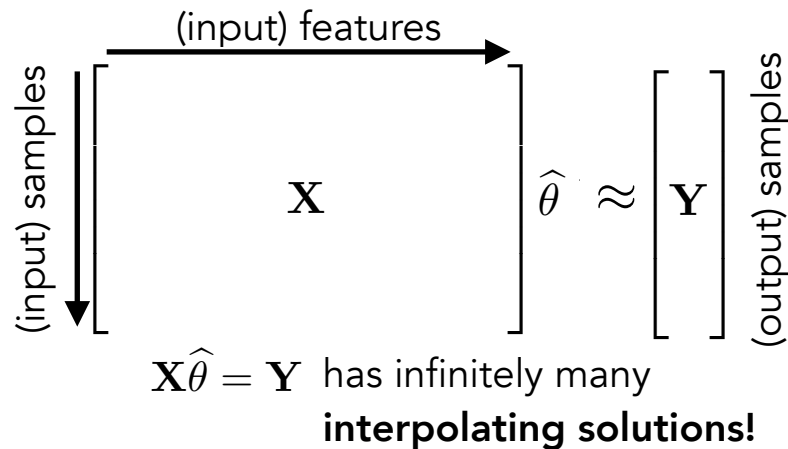
$$\begin{array}{c} \text{true parameter/signal (unknown)} \\ \downarrow \\ \mathbf{Y} = \mathbf{X}^\top \boldsymbol{\theta}^* + \mathbf{W} \\ \uparrow \quad \uparrow \quad \uparrow \\ \text{output} \quad \text{input features,} \quad \text{noise,} \\ \quad \quad \text{dimension} = d \quad \text{variance} = \sigma^2 \end{array}$$

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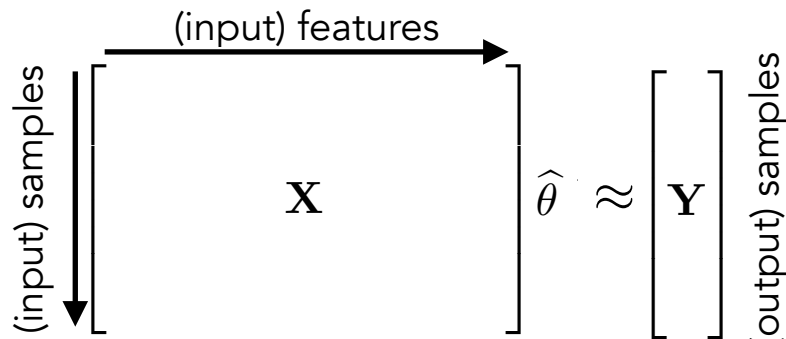
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$\mathbf{X}\hat{\boldsymbol{\theta}} = \mathbf{Y}$  has infinitely many  
**interpolating solutions!**

**Solutions of study today:**

The minimum- $l_p$ -norm interpolator

$$\hat{\boldsymbol{\theta}}_p = \arg \min \|\boldsymbol{\theta}\|_p \text{ subject to } \mathbf{X}\boldsymbol{\theta} = \mathbf{Y}.$$

(beginning with  $p = 2$ )

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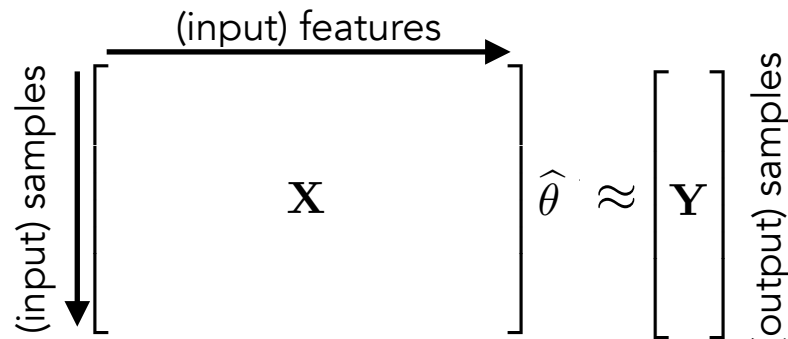
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Error metric is **mean-squared-error**:  $\mathcal{E}_{\text{MSE}} := \mathbb{E} \left[ (\mathbf{X}^\top (\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*))^2 \right]$

# Analysis framework

**Non-asymptotic:** we consider  $d = n^\beta, \beta > 1$  (or  $d \gg n$ ) and state results as:

- **Consistency:** goal is to have  $\mathcal{E}_{\text{MSE}} \rightarrow 0$  as  $n \rightarrow \infty$
- **Rates:** upper and lower bounds on  $\mathcal{E}_{\text{MSE}}$  as a function of  $n$  that match up to universal constants (not depending on  $n, d, \theta^*, \Sigma$ )

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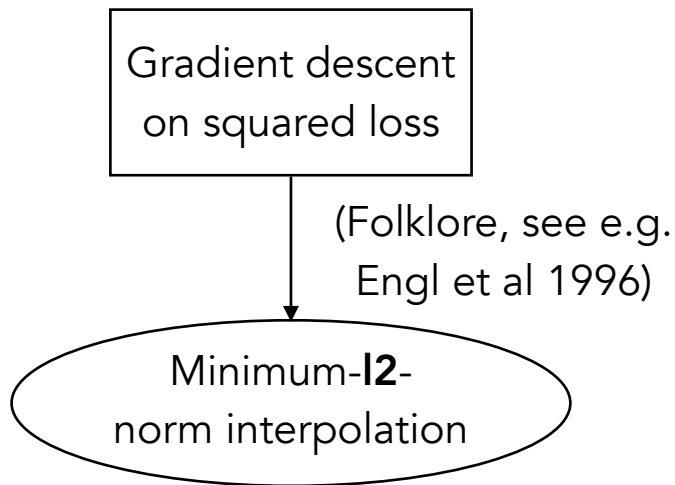
**An alternative asymptotic analysis framework (not the focus of this tutorial):**

Considers  $d \propto n, \frac{d}{n} = \gamma$ .

**Exact error expressions** derived as a function of  $\gamma$  as  $n, d \rightarrow \infty$  together.

# Why these types of “low-norm” interpolators?

**Popular optimization algorithms converge to “low-norm” solutions!**



$$\hat{\theta}_2 = \arg \min \|\theta\|_2$$

subject to

$$X_i^\top \theta = Y_i, i \in [n].$$

# Why these types of “low-norm” interpolators?

Popular optimization algorithms converge to “low-norm” solutions!

Mirror descent on squared loss,  
Potential =  $\|\cdot\|_p$

(Gunasekar et al,  
2018)

Minimum- **$l_p$** -  
norm interpolation

$$\hat{\theta}_p = \arg \min \|\theta\|_p$$

subject to

$$X_i^\top \theta = Y_i, i \in [n].$$

Coordinate descent/least-  
angle regression

(Efron et al, 2004)

Minimum- **$l_1$** -norm  
interpolation

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subject to

$$X_i^\top \theta = Y_i, i \in [n].$$



# Why these types of “low-norm” interpolators?

Popular optimization algorithms converge to “low-norm” solutions!

Mirror descent on squared loss,  
Potential =  $\|\cdot\|_p$

(Gunasekar et al,  
2018)

Minimum- **$l_p$** -  
norm interpolation

$$\hat{\theta}_p = \arg \min \|\theta\|_p$$

subject to

$$X_i^\top \theta = Y_i, i \in [n].$$

Coordinate descent/least-  
angle regression

(Efron et al, 2004)

Minimum- **$l_1$** -norm  
interpolation

$$\hat{\theta}_1 = \arg \min \|\theta\|_1$$

subject to

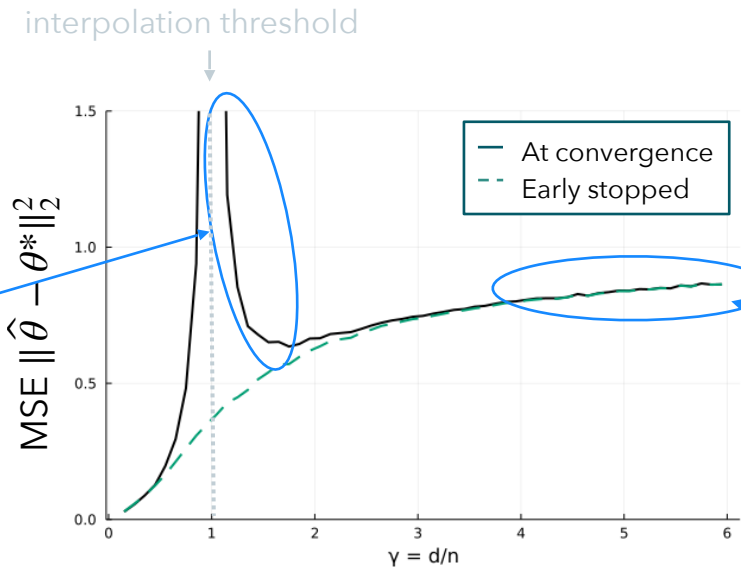
$$X_i^\top \theta = Y_i, i \in [n].$$

Implicit bias theory is a useful “sanity check” but not the full picture: do these solutions always generalize well?

# Recall: what was observed for min-l2-norm interpolator

1

Second Descent  
after interpolation

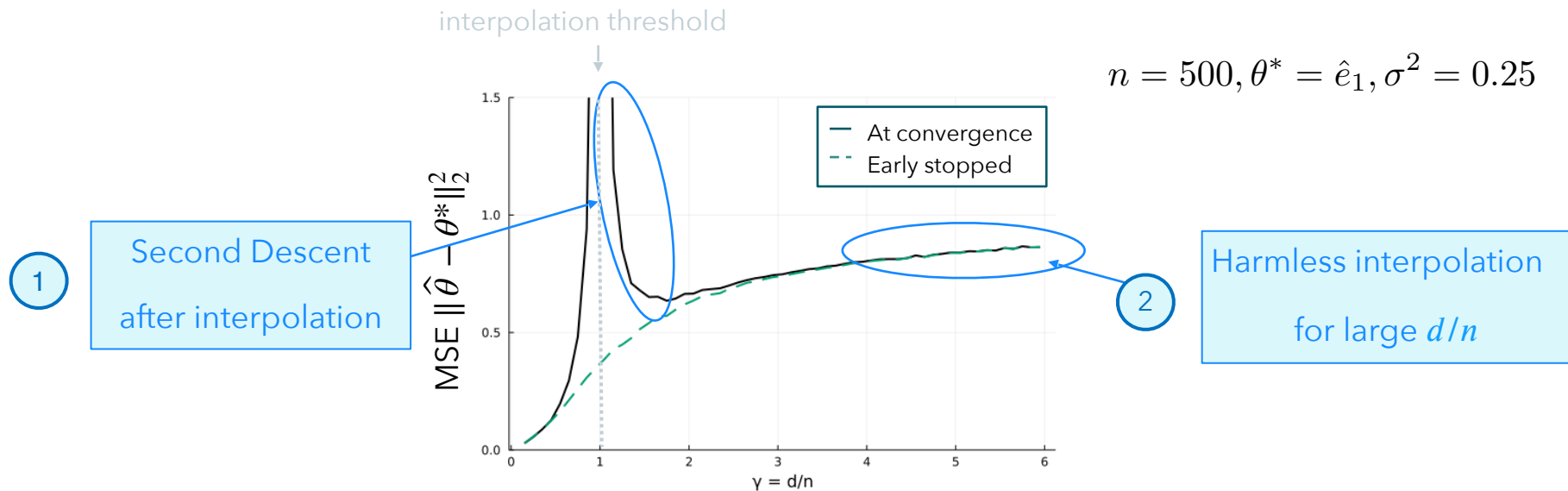


$$n = 500, \theta^* = \hat{e}_1, \sigma^2 = 0.25$$

2

Harmless interpolation  
for large  $d/n$

# Recall: what was observed for min-l2-norm interpolator



(1) and (2) are implied by **variance reduction with increased overparameterization!**

**Theorem (isotropic covariance)\*:** Variance term  $\asymp \frac{\sigma^2 n}{d}$ .

\*included in results of Hastie et al (2022), Bartlett et al (2020), Muthukumar et al (2020)

## Plan today...

**Part I:** For linear regression, we discuss how

- variance can decay as overparameterization increases (simple math)
- Two factors can govern variance decay vs. bias increase
  - For fixed interpolator, certain problem instances/distributions are more benign
  - For fixed problem instance, certain interpolators generalize better

**Part II:** For classification, we discuss the

- effect of loss function choices
- implicit bias of optimization algorithms for neural networks
- generalization of neural networks on noisy, high-dimensional data

## Variance reduction: main proof ideas

- **Step 1:** minimum-l2-norm interpolator can be expressed in closed form

$$\hat{\theta}_2 = \mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top)^{-1} \mathbf{Y} = \mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top)^{-1} \mathbf{X}\theta^* + \mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top)^{-1} \mathbf{W}$$

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- **Step 2:** variance term can also be expressed in closed form

$$\text{Variance} = \|\mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top)^{-1} \mathbf{W}\|_2^2 = \mathbf{W}^\top (\mathbf{X}\mathbf{X}^\top)^{-1} \mathbf{X}\mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top)^{-1} \mathbf{W}$$



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**Note:** this calculation is simplified for isotropic data covariance, but works more generally (Bartlett et al, 2020)

## Variance reduction: main proof ideas

- **Step 3:** data is **approximately orthogonal** when  $d \gg n$  (with high prob.)

$$\langle X_i, X_j \rangle \approx 0 \text{ for } i \neq j \text{ and } \|X_i\|_2^2 \approx d$$

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Total  
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Total  
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**Intuition:** noise energy is "spread out" along  $d$  feature dimensions, contributes more harmlessly as  $d$  increases

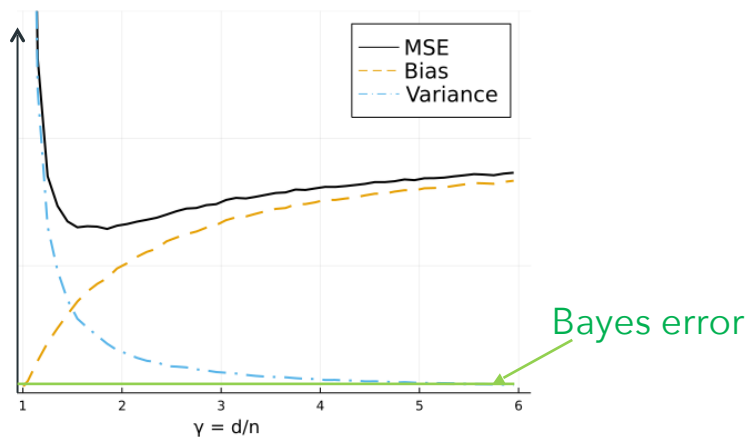
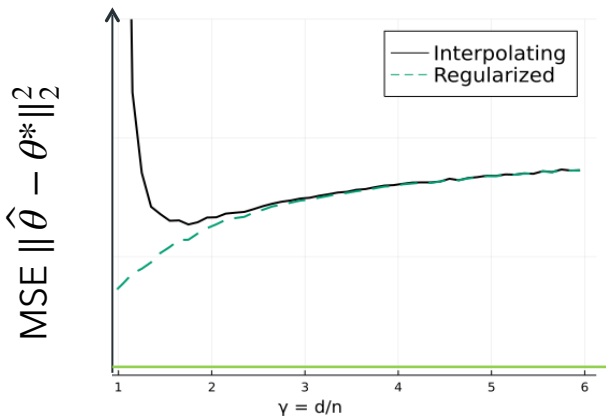
**Note:** can show corresponding **precise** results when  $d \propto n$ ,  $d, n \rightarrow \infty$  (Hastie et al, 2022)

# So is min- $\ell_2$ -norm interpolation *always* a good idea?

Interpolator  $\hat{\theta}_2 = \arg \min \|\theta\|_2$  subject to  $\mathbf{X}\theta = \mathbf{Y}$  vs.

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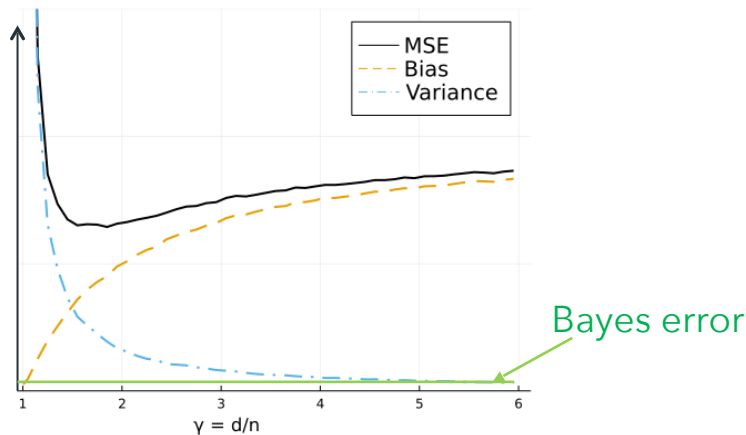
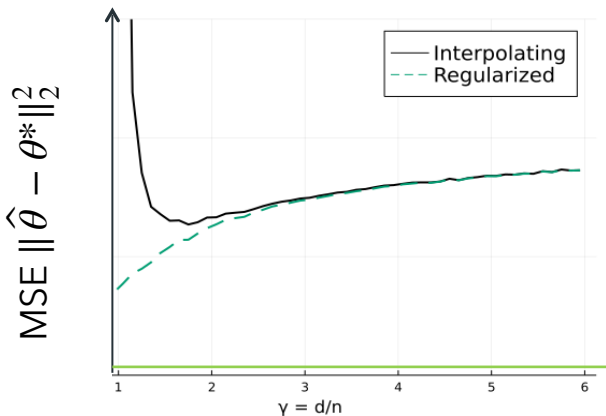


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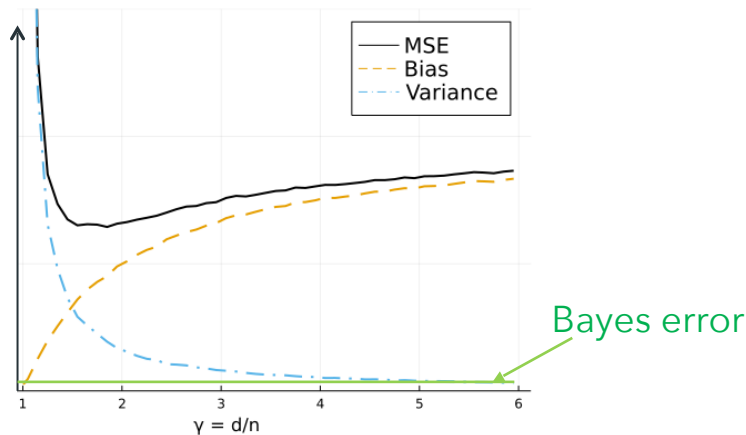
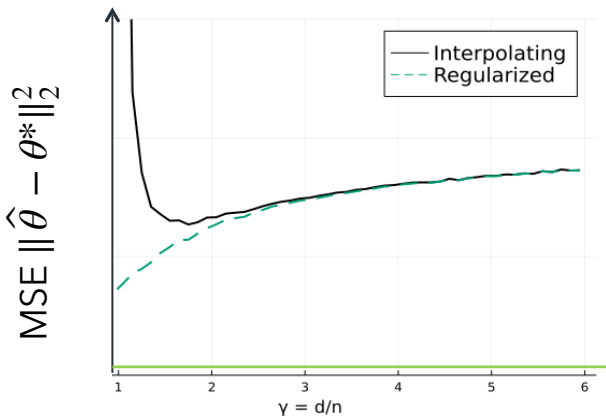


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Core issue: **bias increases with  $d$** , eventually dominates

## Issues with isotropy and min-l2 inductive bias

**Recall:** minimum-l2-norm interpolator can be expressed in closed form

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## Isotropy and min-l2-norm bias visualized at feature-by-feature level

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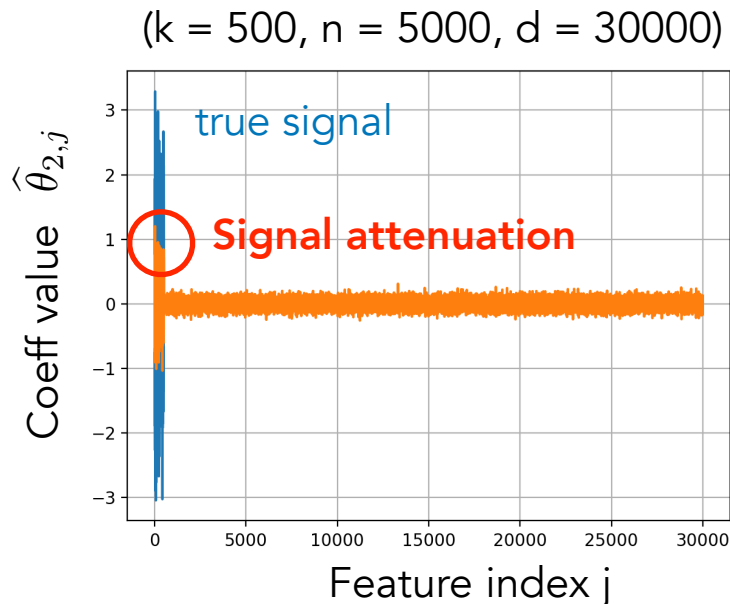
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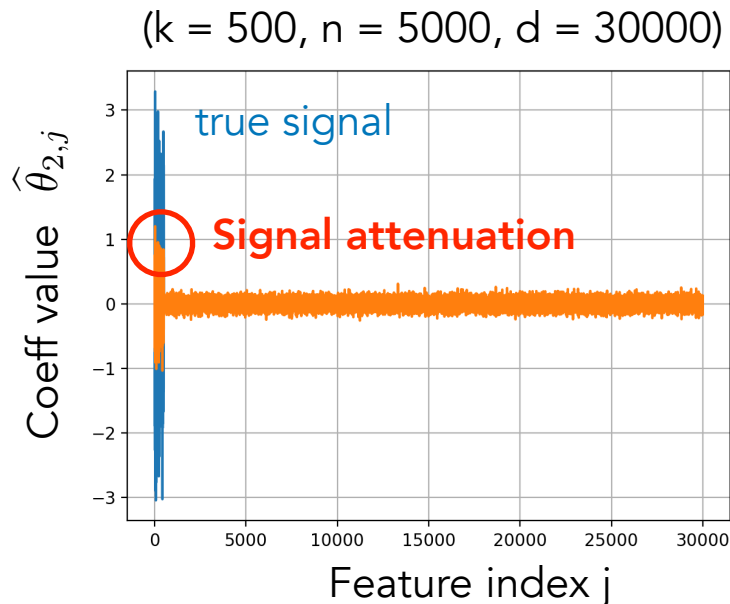
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**Core issue for bias:**  $|\hat{\theta}_j| \ll |\theta_j^*|$  for all  $j \in [k]$ !



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**Part I:** For linear regression, we discuss how

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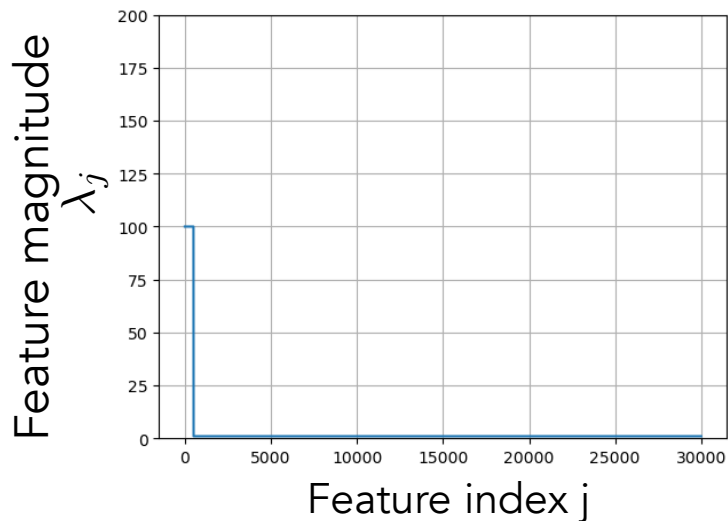
## Anisotropy to the rescue: “upweighting” features aligned with signal

- A special case  $\Sigma = \begin{bmatrix} R\mathbf{I}_k & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{d-k} \end{bmatrix}, R \gg 1$  (spiked-covariance)

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Effective “upweighting” on top k features

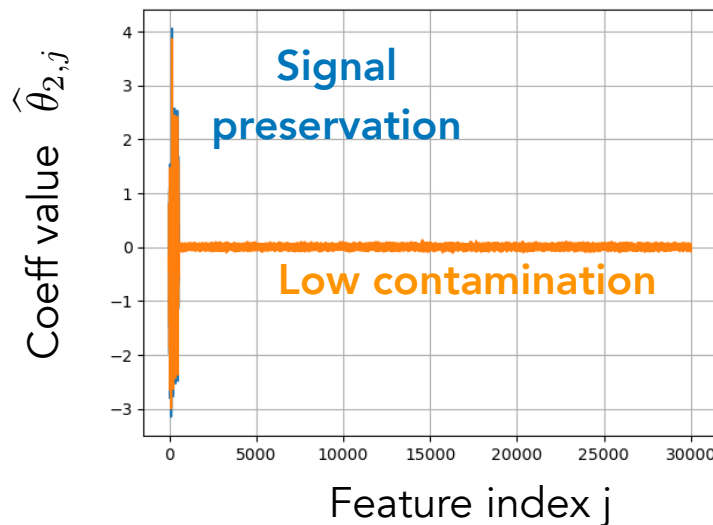
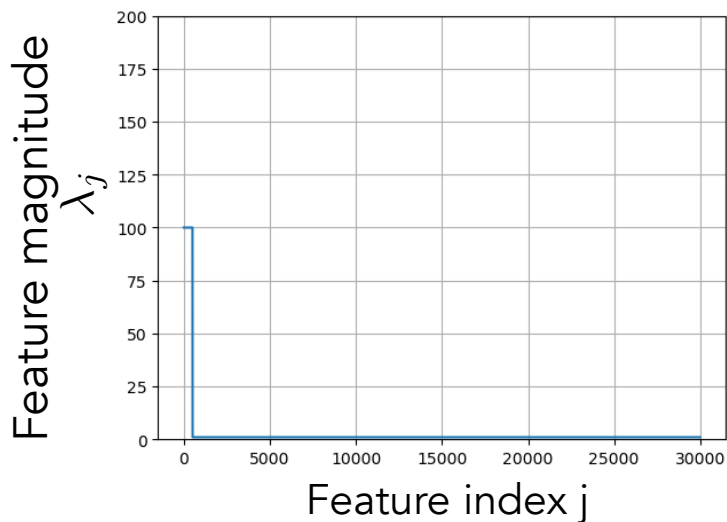


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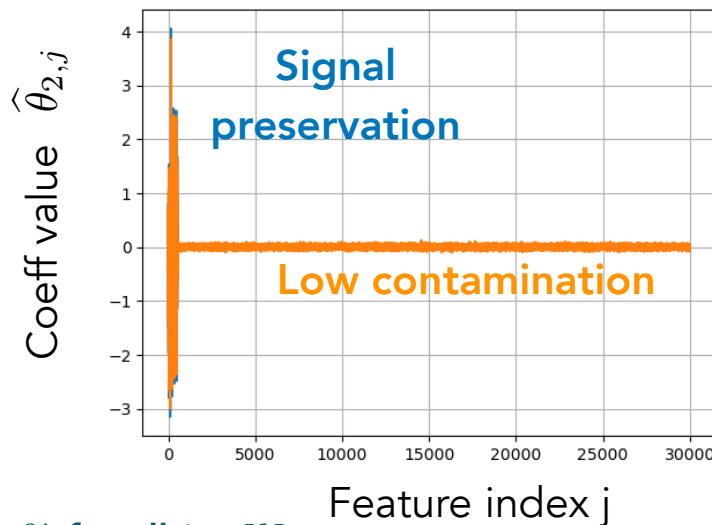
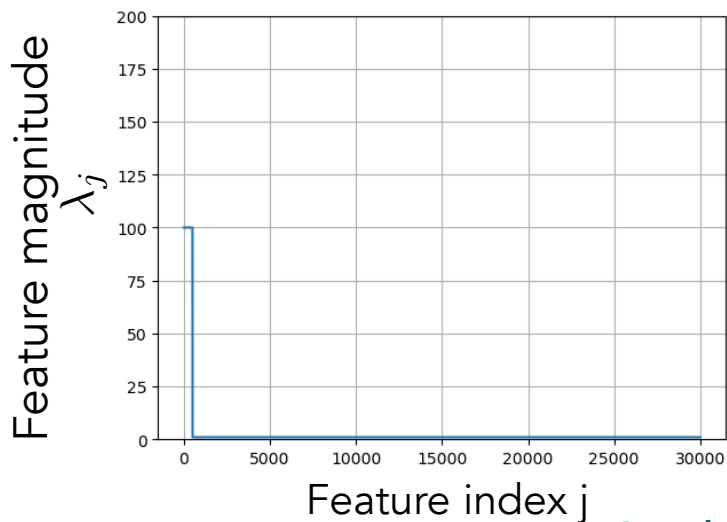


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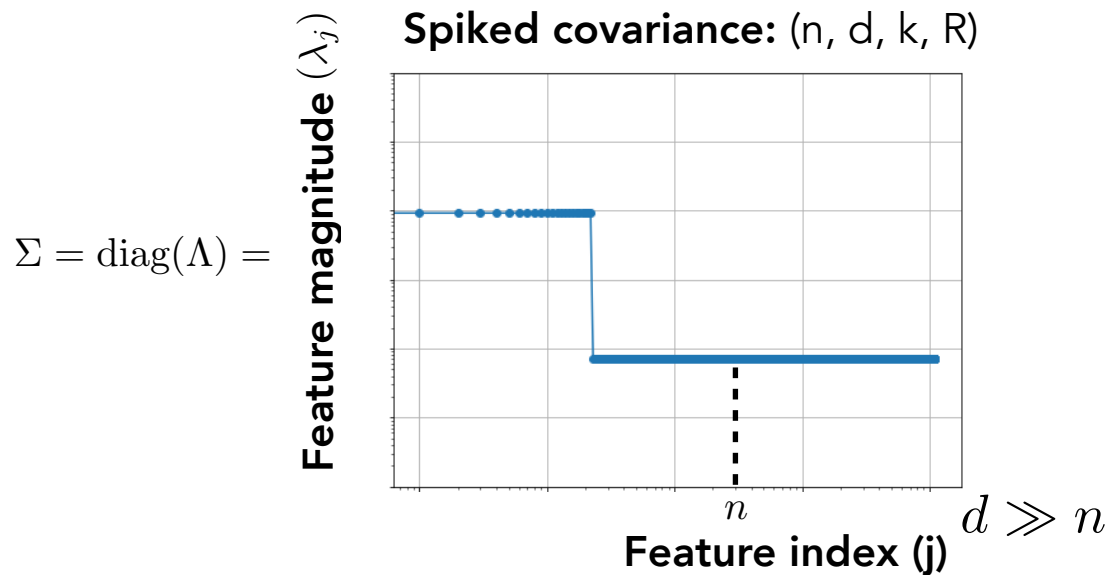
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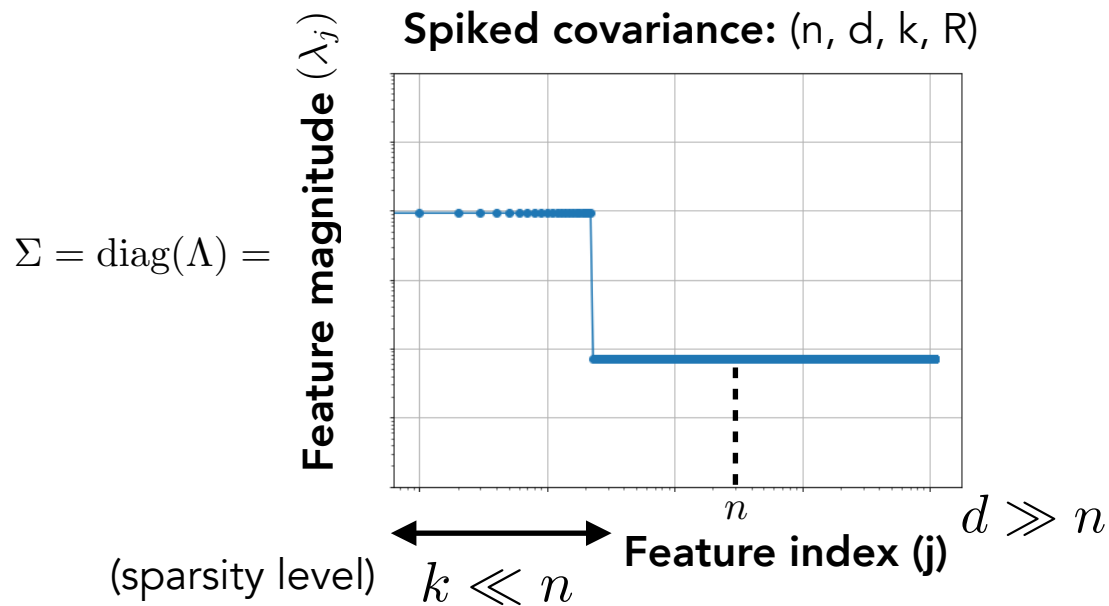
Low bias iff  $\hat{\theta}_j \approx \theta_j^*$  for all  $j \in [k]$

**Intuition:** under near-orthogonality,  $\hat{\theta}_j \propto \sum_{i=1}^n y_i x_{i,j}$  - attenuation mitigated for larger  $R$  as  $x_{i,j} \sim \mathcal{N}(0, R)$  for  $j \in [k]$

# A sensible model for l2: the **spiked-covariance** ensemble

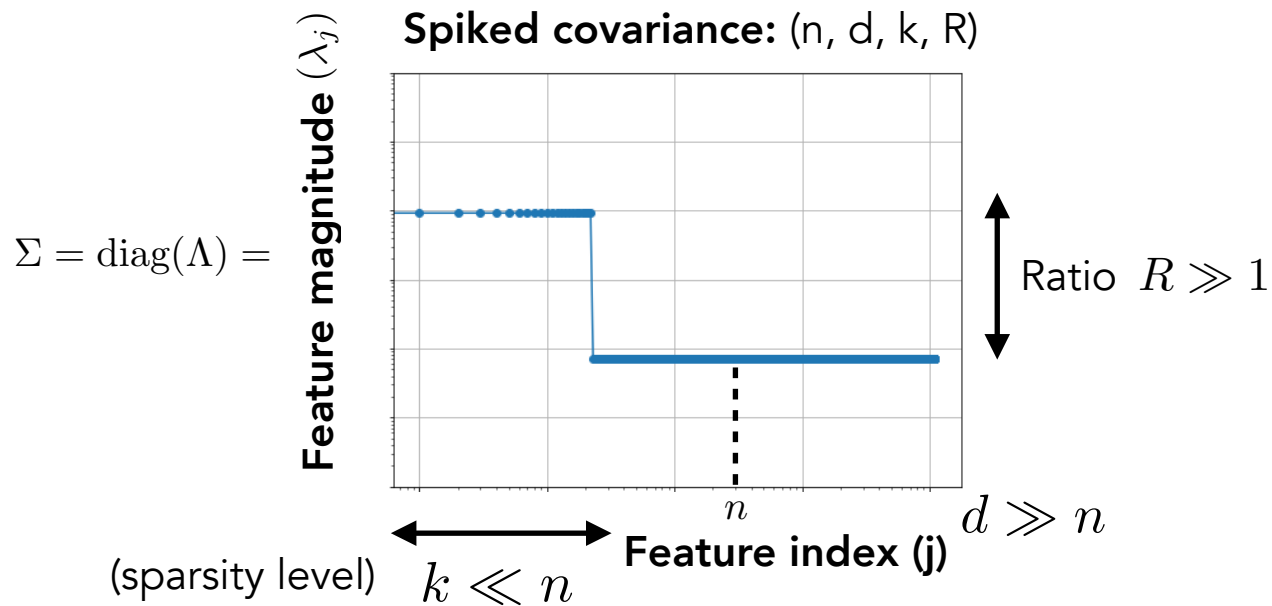


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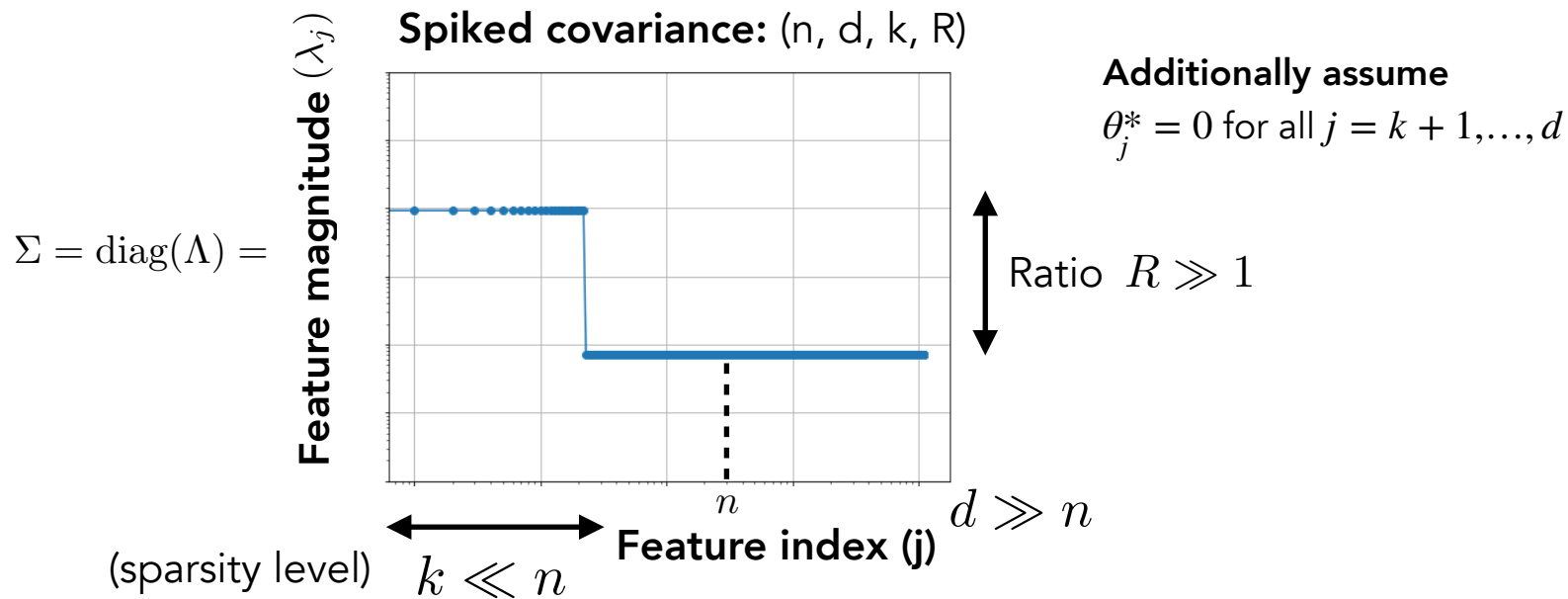




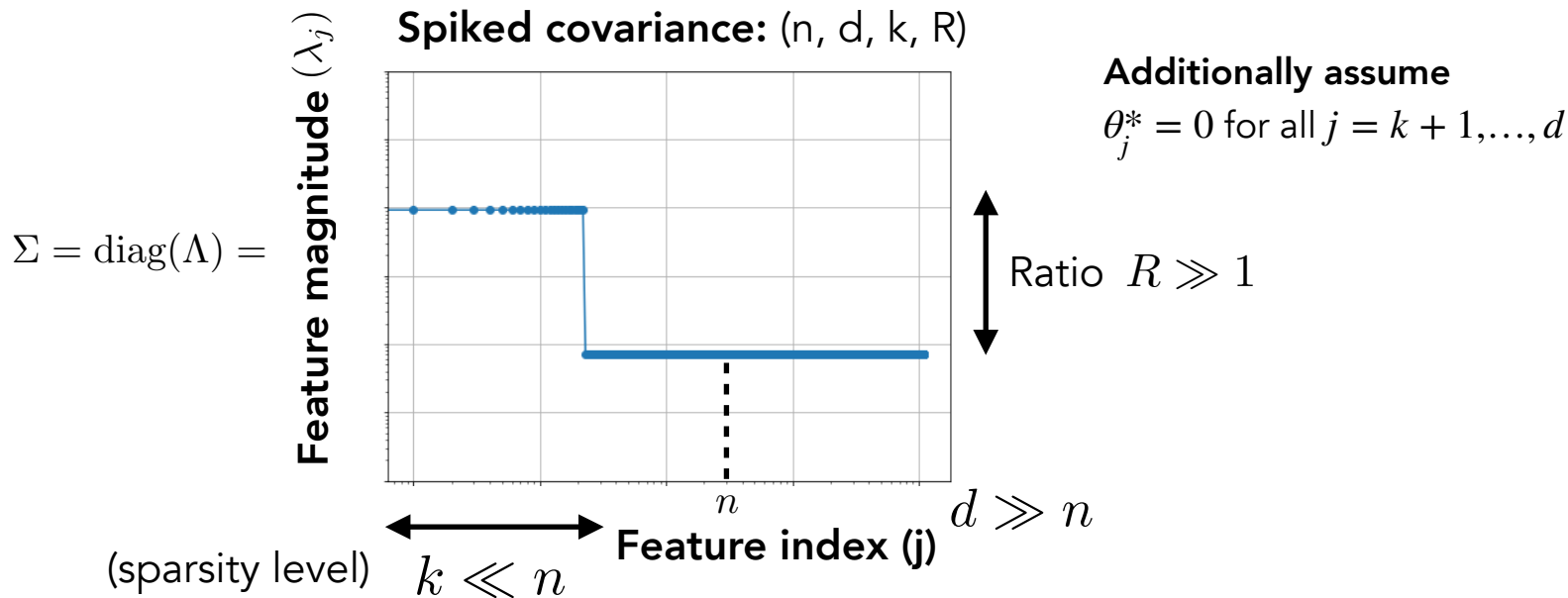
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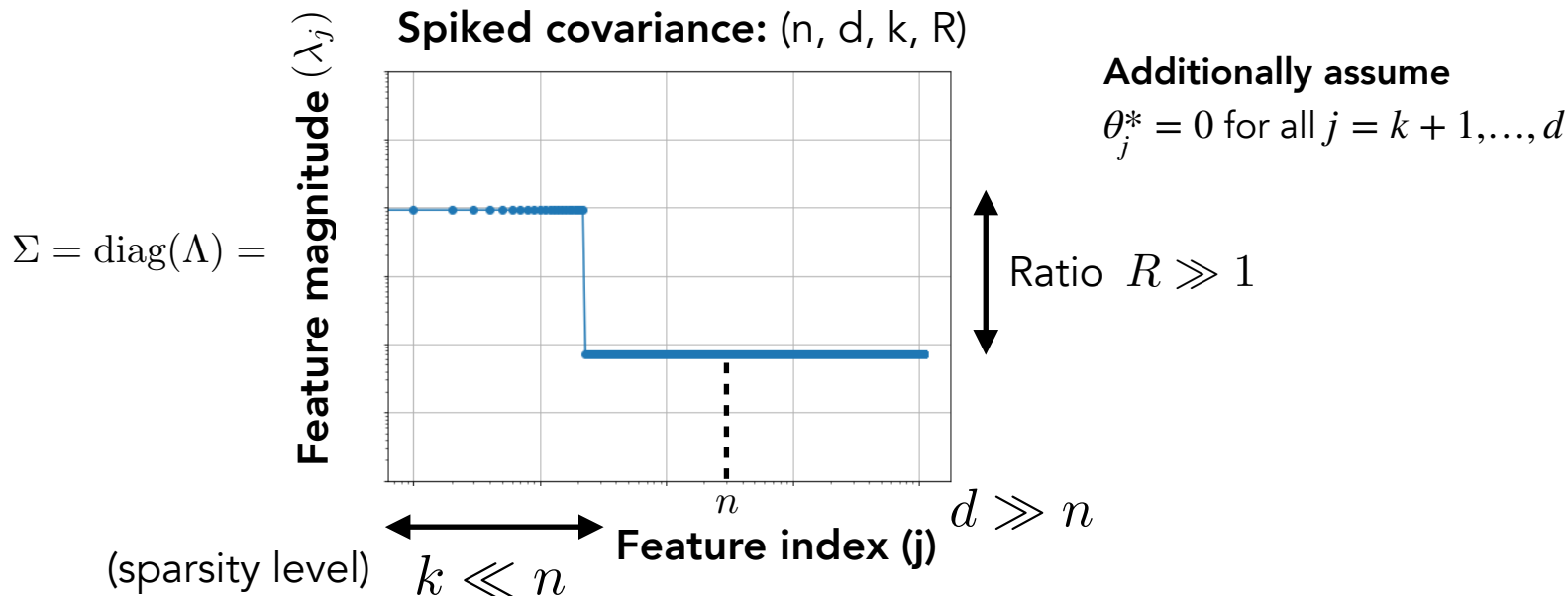


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Will **always** achieve  
Variance  $\rightarrow 0$  as  $n, d \rightarrow \infty$ :  
Noise hidden along  $(d-k)$  directions!

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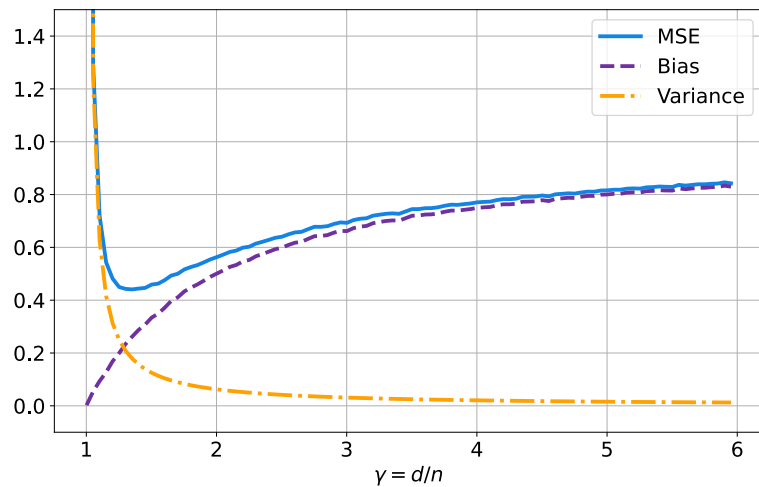


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Also achieves Bias  $\rightarrow 0$  as  $n, d \rightarrow \infty$   
 provided that  $R \gg \frac{d}{n}$

## Summary: Uniform benefits of overparameterization with spiked covariance

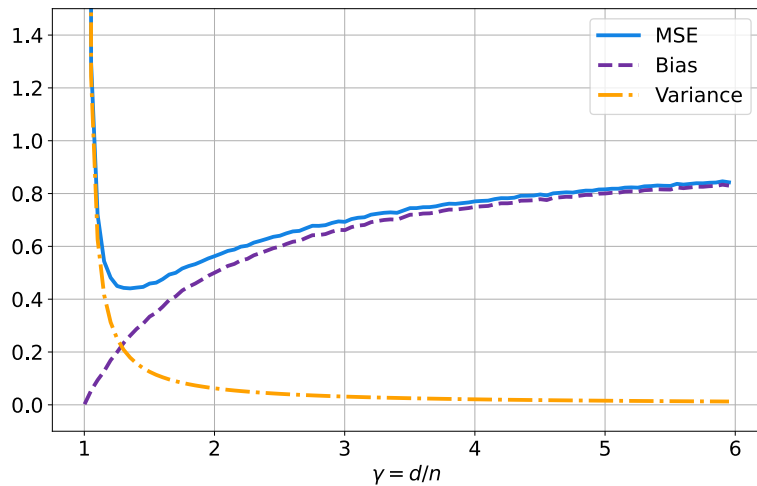
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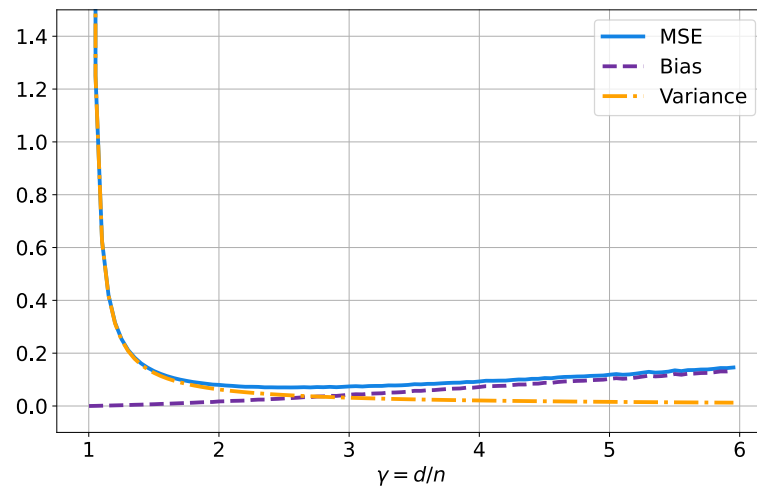
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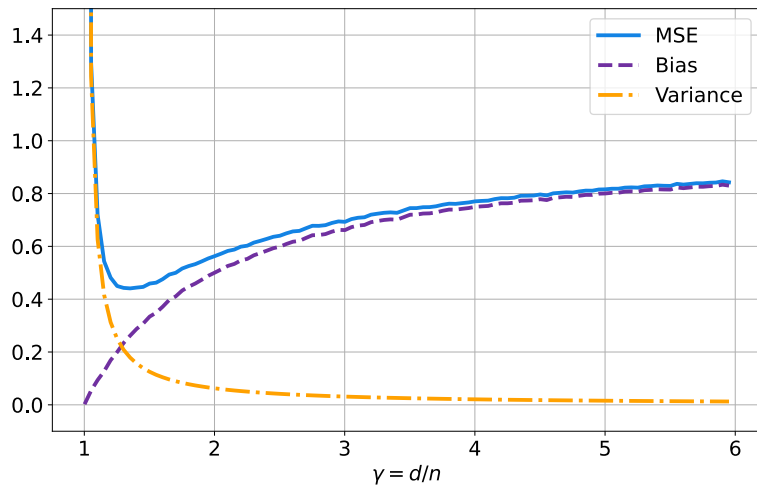
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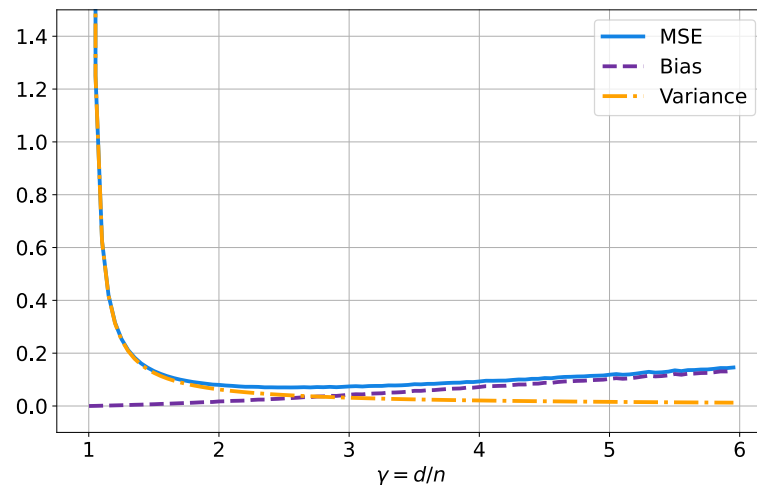
Spiked covariance,  $R = 10$

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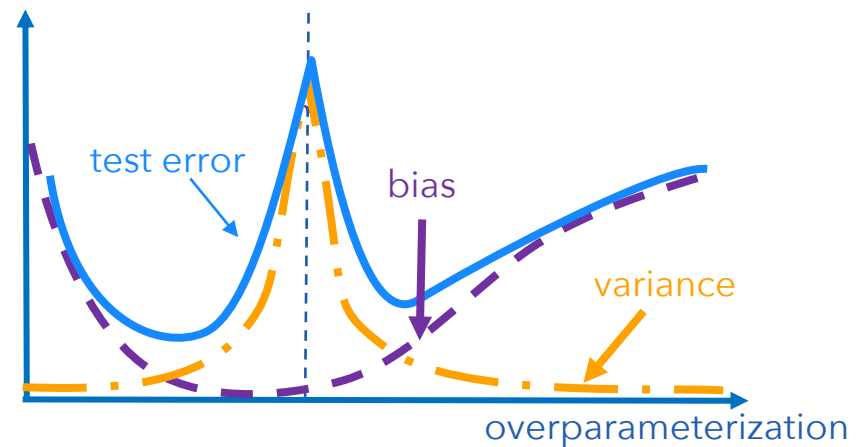
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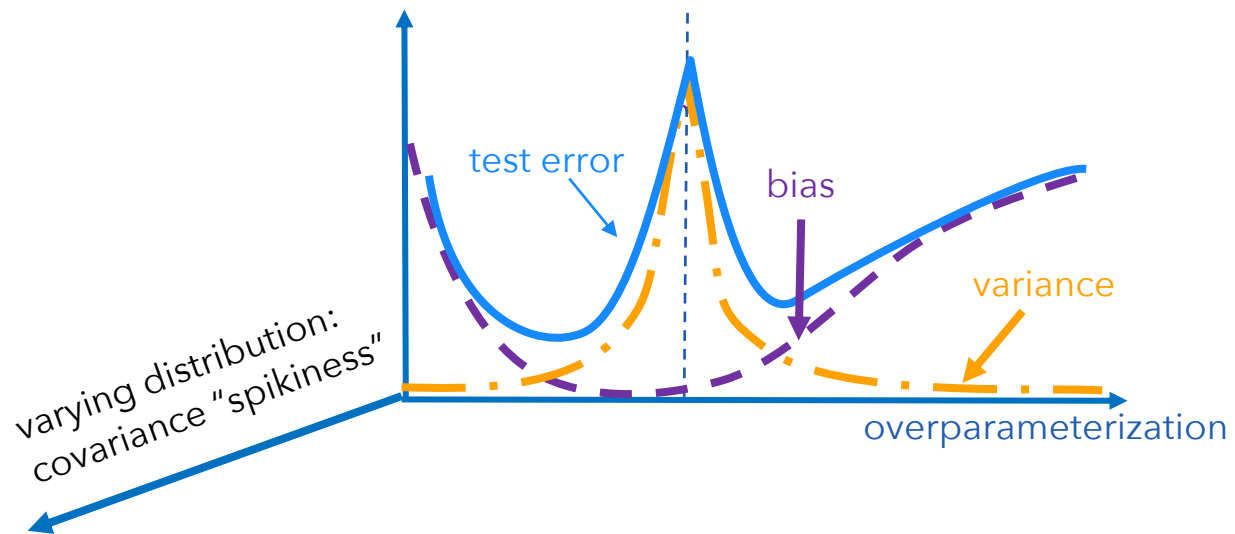
For spiked covariance: ① second descent ✓ ② harmless interpolation ✓ ③ good generalization ✓

For fixed interpolator...

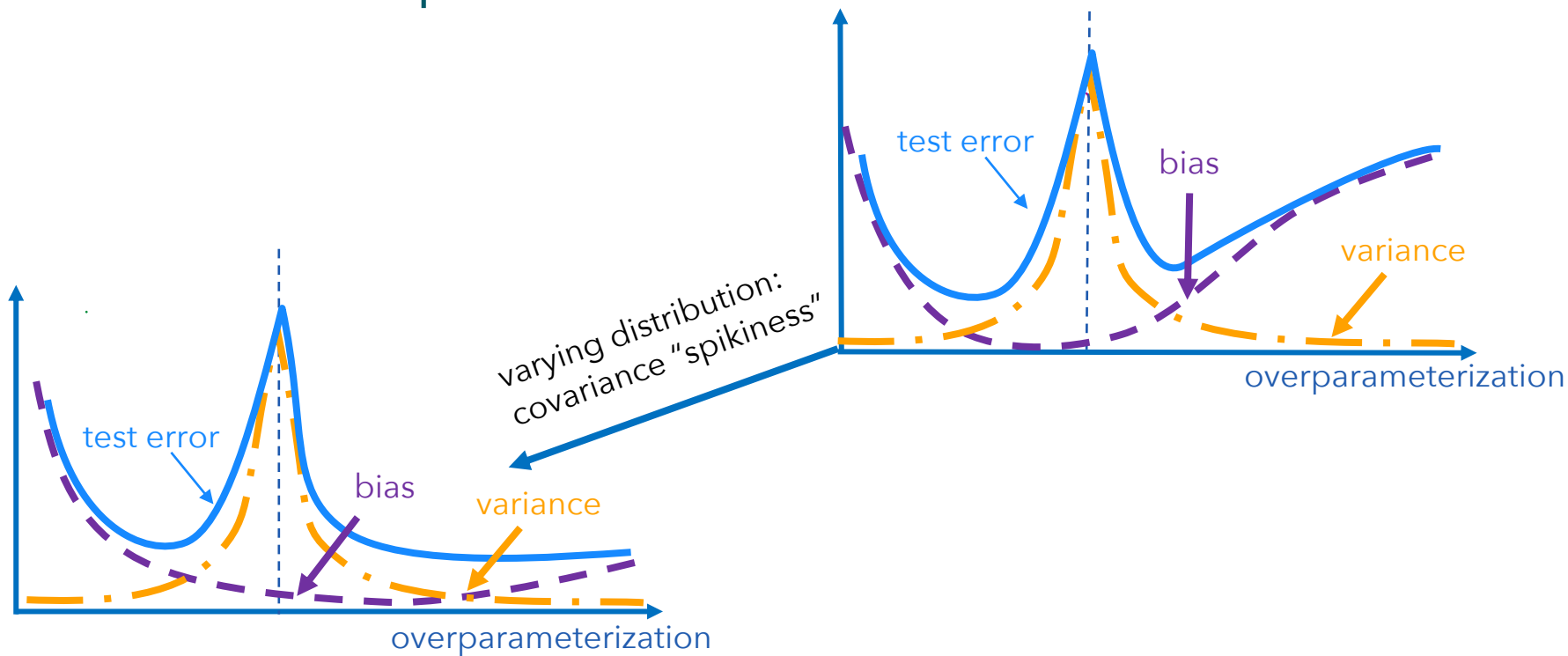




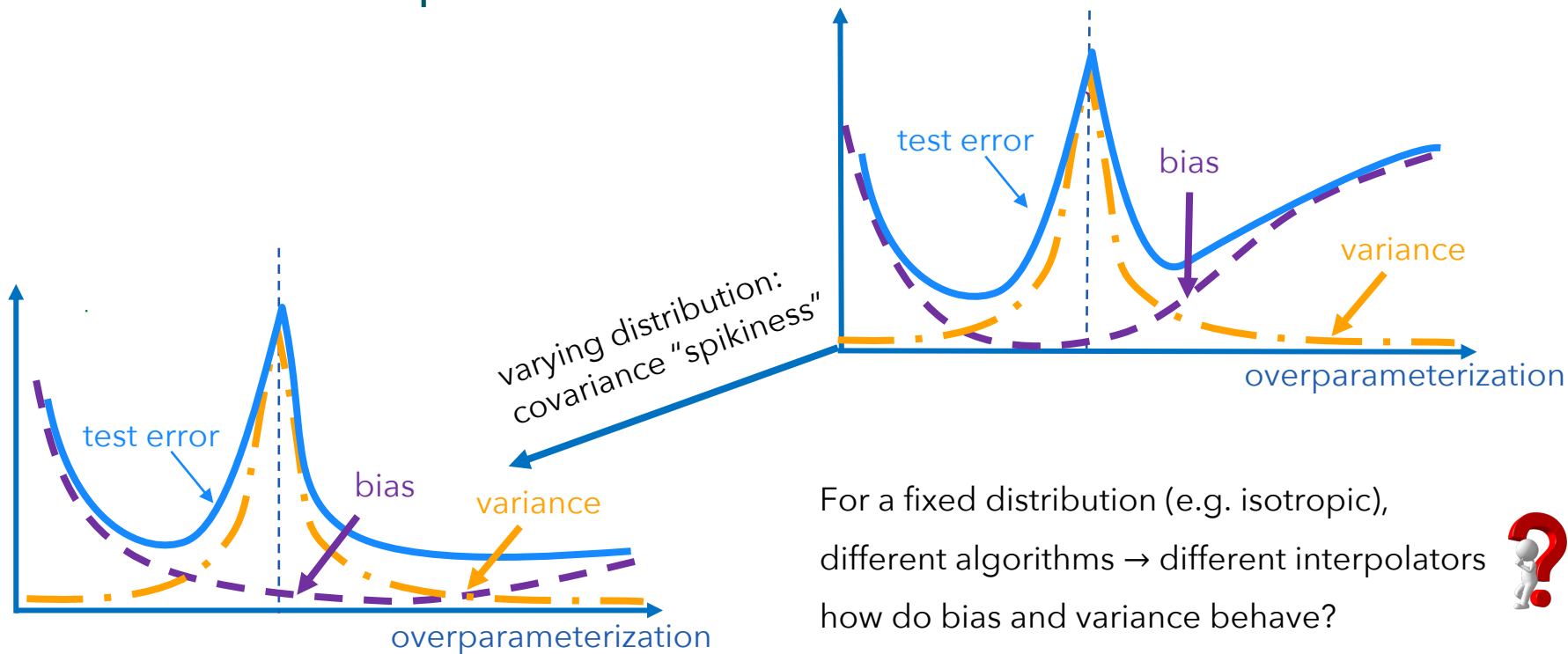
For fixed interpolator...



For fixed interpolator...



# For fixed interpolator...



For a fixed distribution (e.g. isotropic),  
different algorithms  $\rightarrow$  different interpolators  
how do bias and variance behave?



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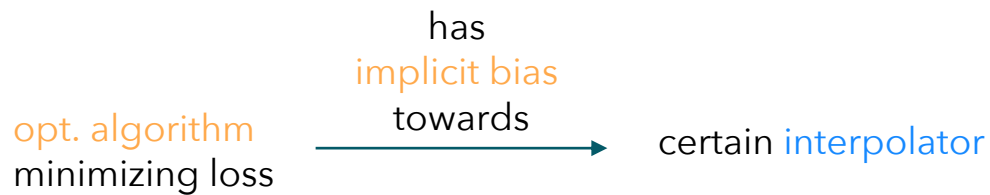
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# Implicit bias $\rightarrow$ inductive bias

opt. algorithm  
minimizing loss

# Implicit bias $\rightarrow$ inductive bias



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minimizing loss  $\xrightarrow[\text{towards}]{\text{has implicit bias}}$  certain interpolator

e.g. 1st order method

on  $\|y - Xw\|_2^2$

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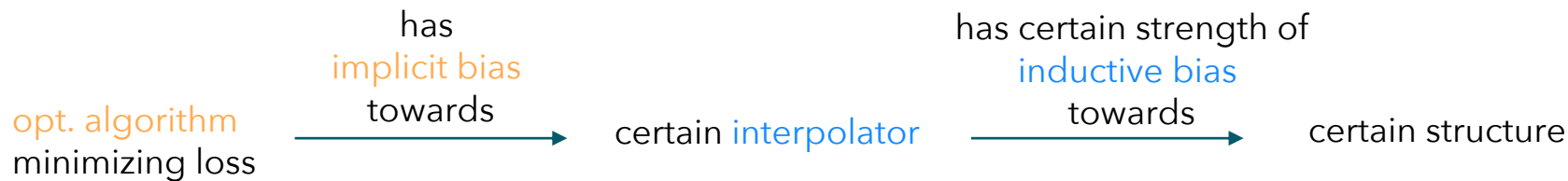
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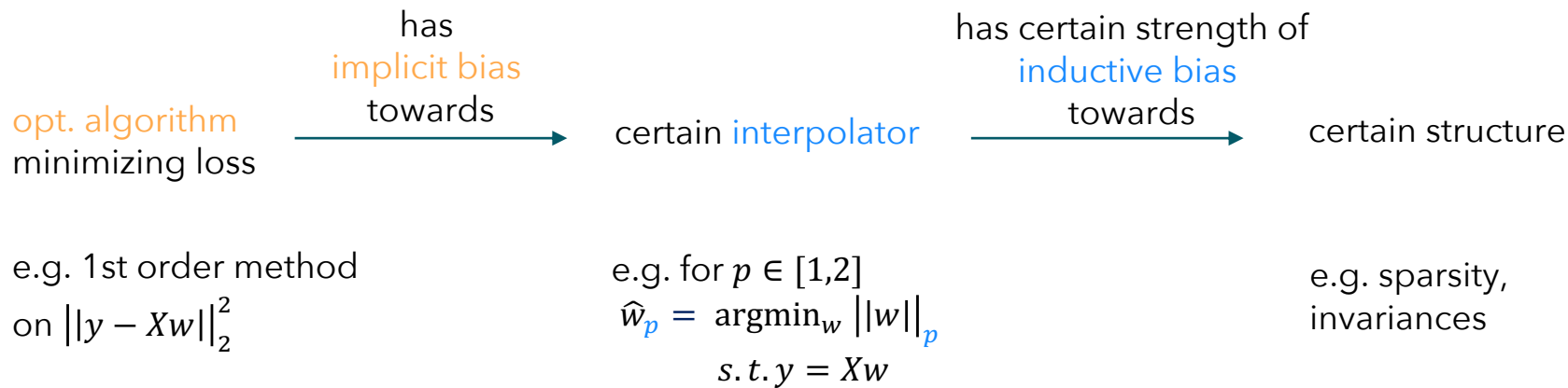
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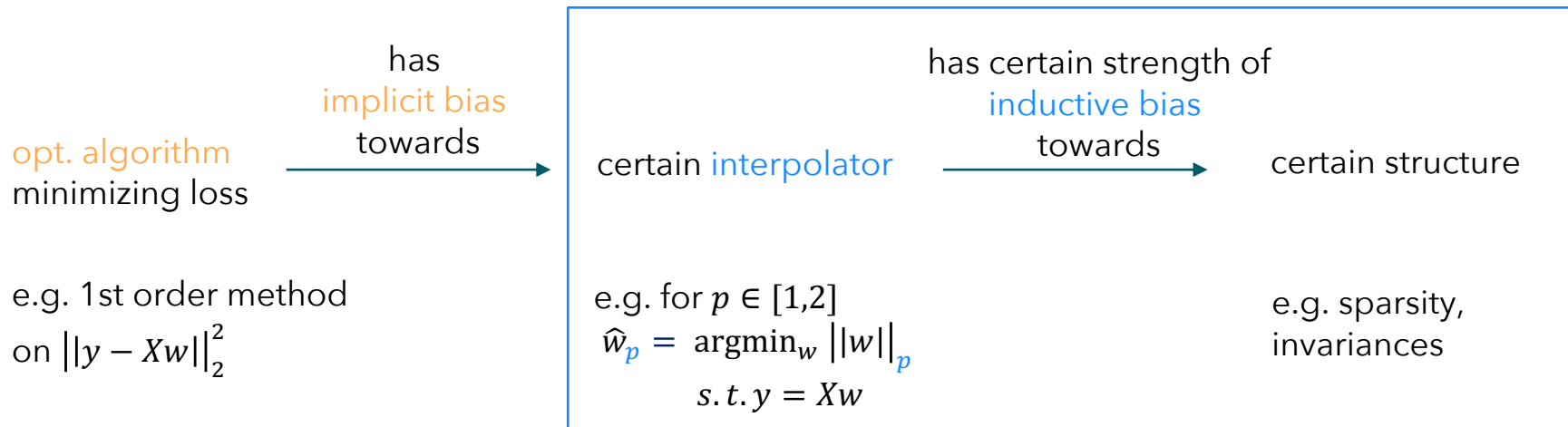
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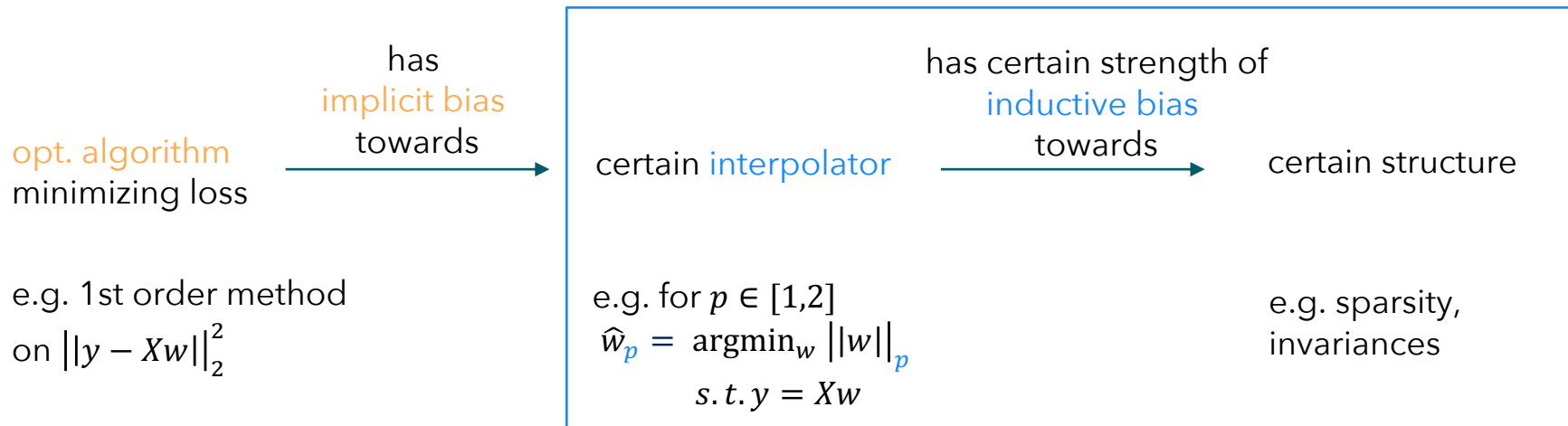
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Next: Recall how as  $p \rightarrow 1$  has an inductive bias towards sparse solutions

# Recall: Inductive bias for sparse linear models

Fixed distribution:  $y_i = \langle w^*, x_i \rangle + \xi_i$  with **sparse**  $w^*$ , i.e.  $\|w\|_0 = k \ll d$ , i.i.d. noise  $\xi_i$  and  $x_i \sim N(0, I)$

isotropic



•  $w^*$

• 0

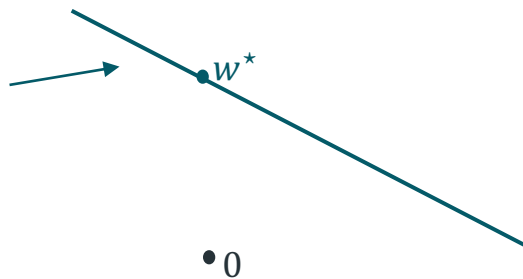
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for noiseless  $\xi_i = 0$



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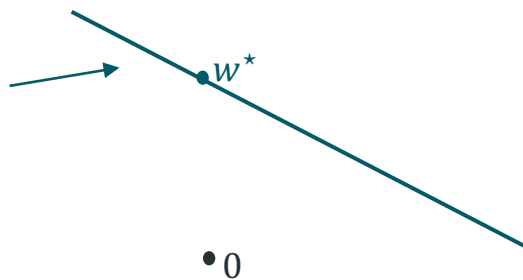
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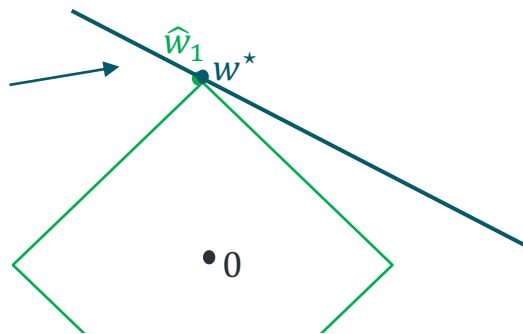
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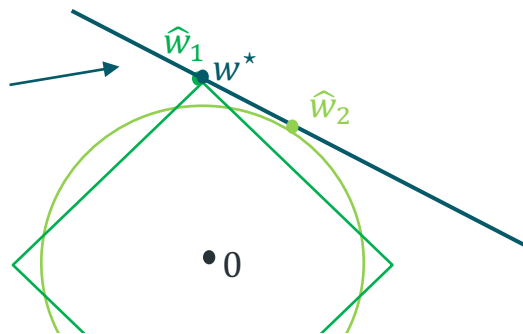
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when observations are noisy

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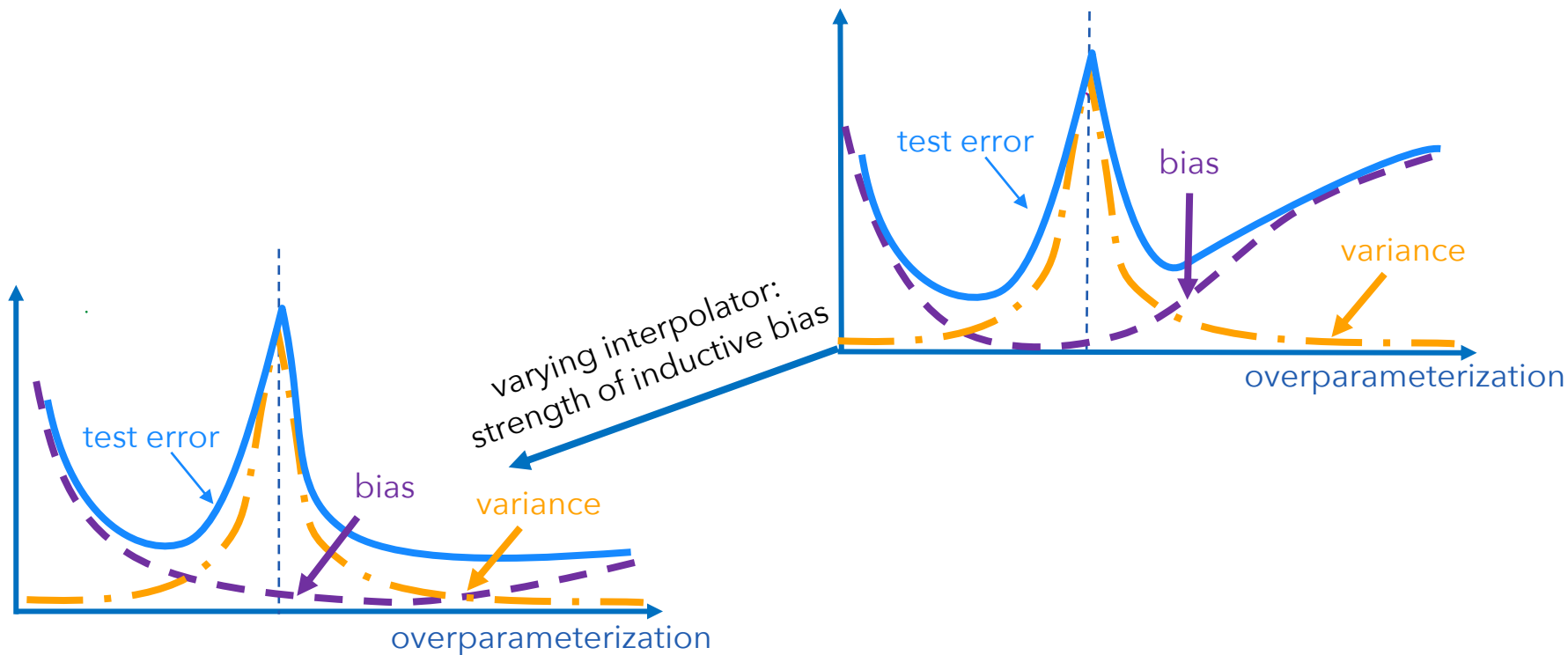
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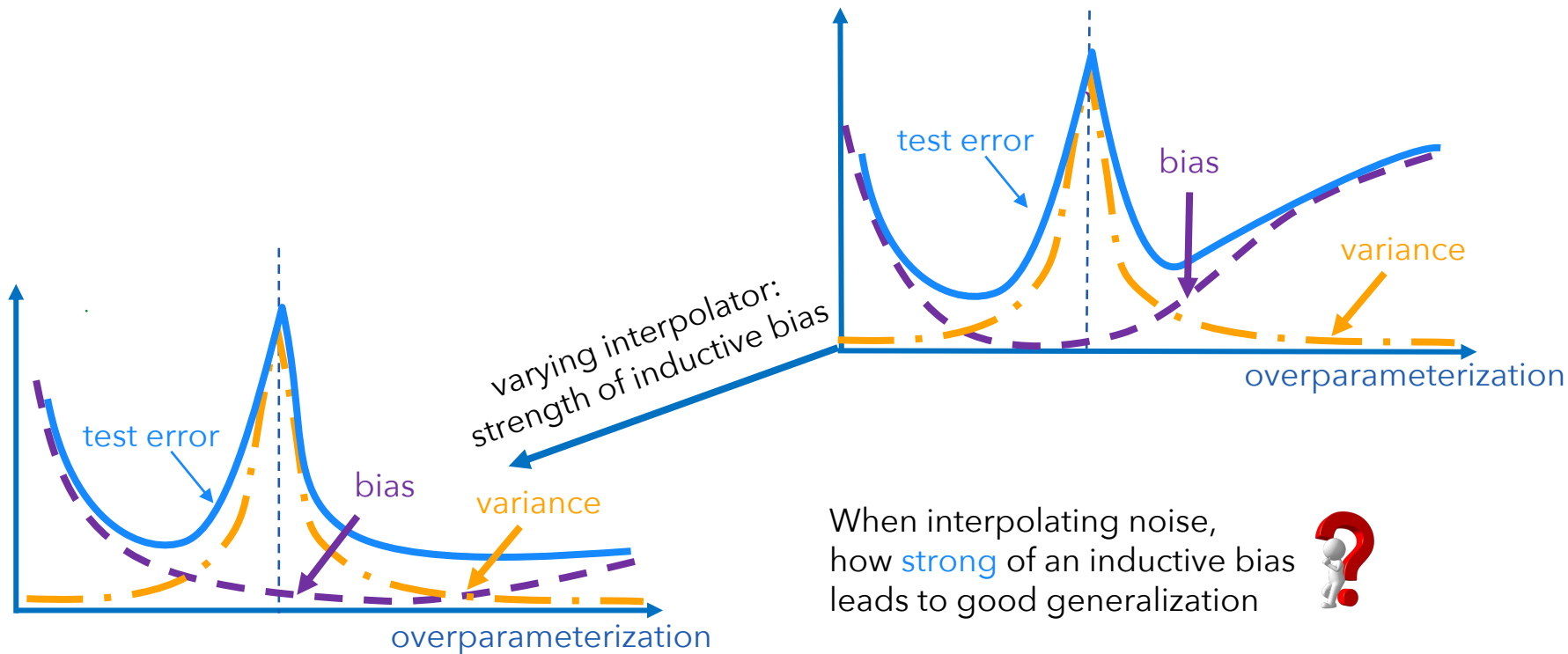
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Previously unknown: prediction/estimation error of min- $\ell_1$  interpolation for **noisy data**

For fixed distribution...



# For fixed distribution...



When interpolating noise, how **strong** of an inductive bias leads to good generalization





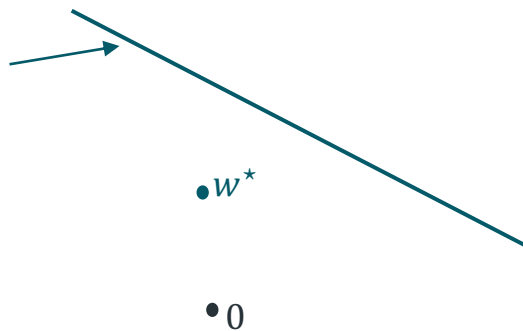
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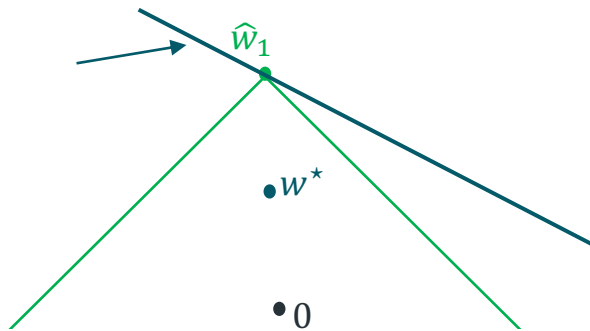
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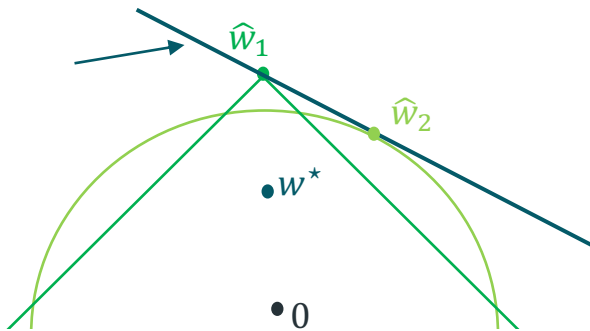
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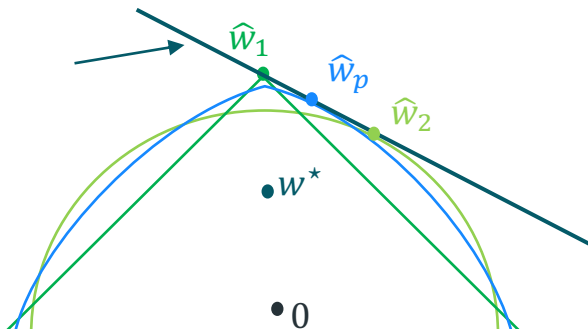
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strong inductive bias  
towards sparsity



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# Strong inductive bias: $p = 1$



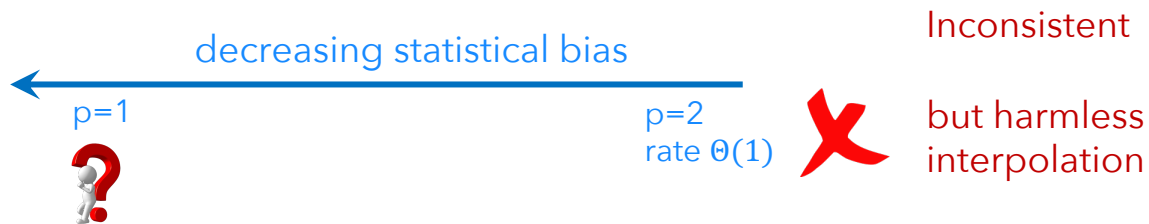
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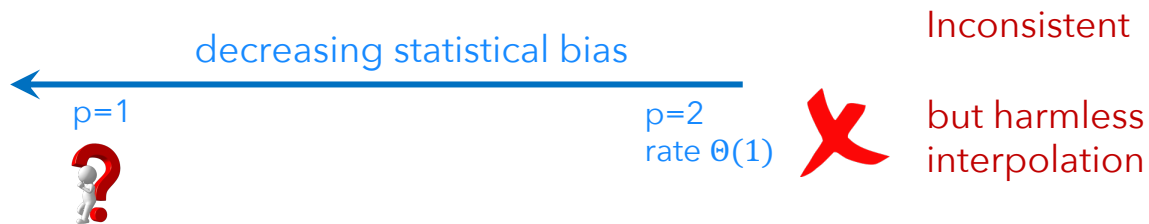


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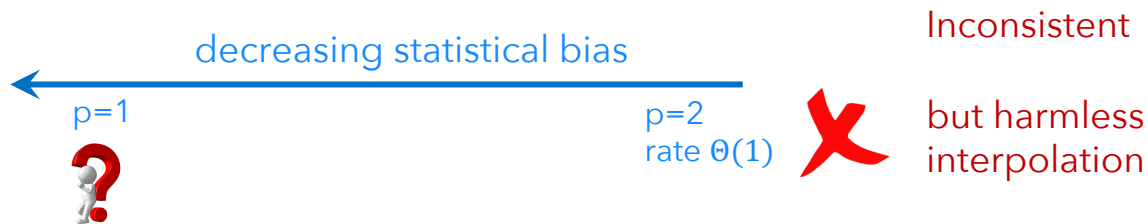
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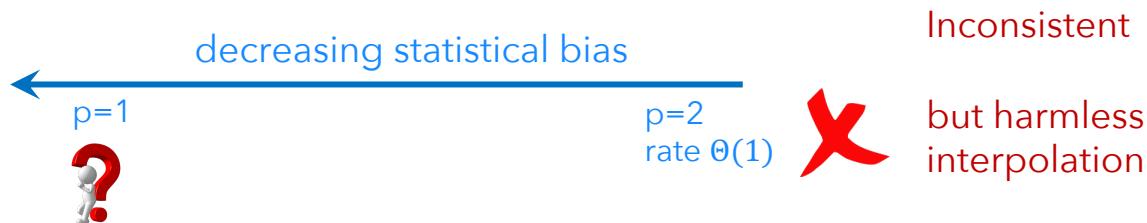
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Consistent

but harmful interpolation:  
opt. regularized  $O\left(\frac{k \log n}{n}\right)$



$p=1$

rate  $\Theta\left(\frac{1}{\log n}\right) = \tilde{\Theta}(1)$

decreasing statistical bias

$p=2$

rate  $\Theta(1)$



Inconsistent

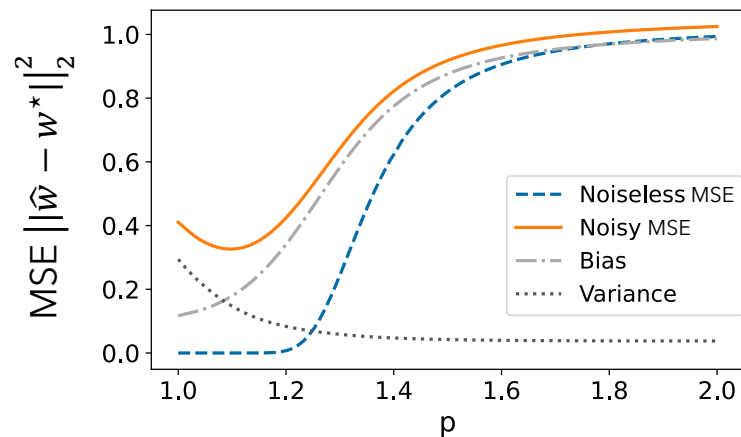
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# The problem of $p = 1$ lies in the variance...

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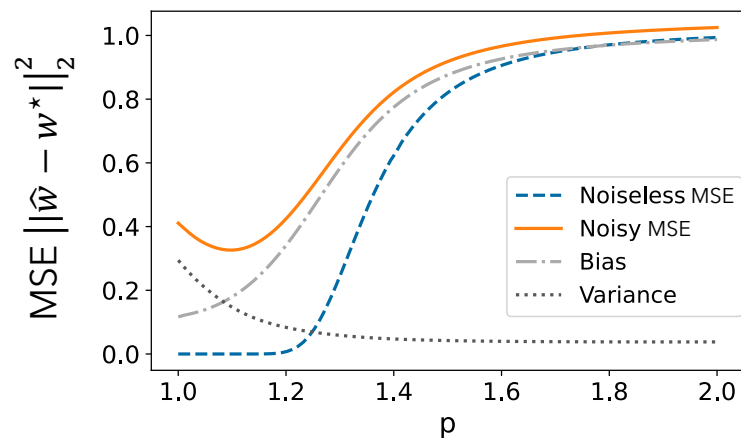
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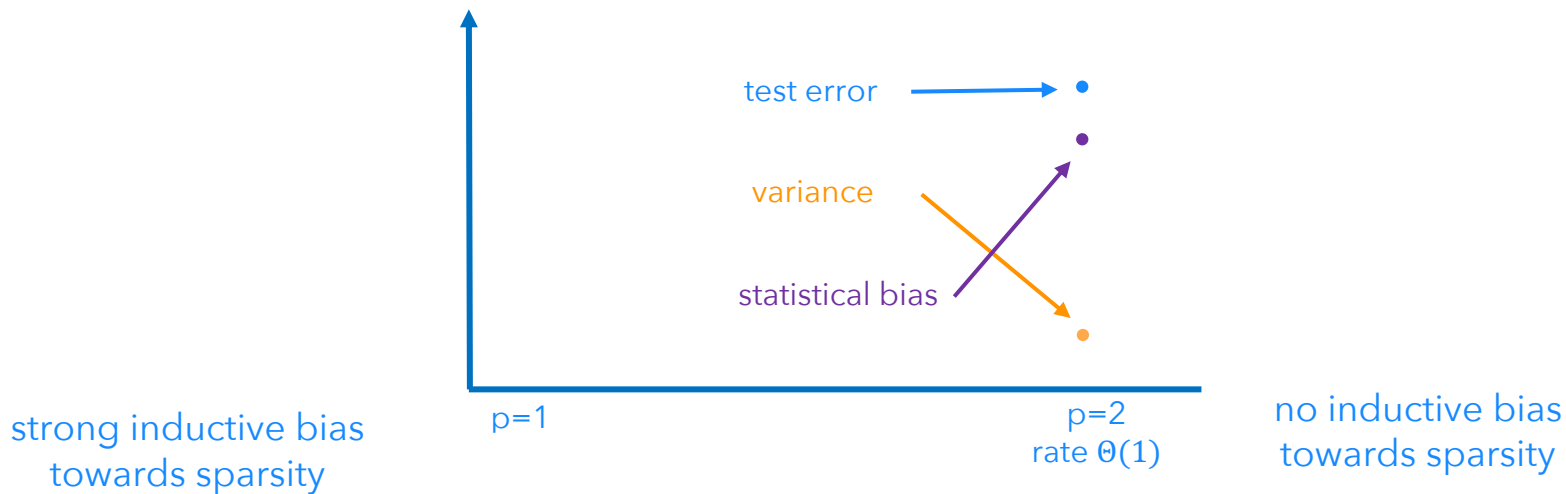


as overparameterization increases, variance decay is slower for  $p = 1$  than for  $p = 2$ !



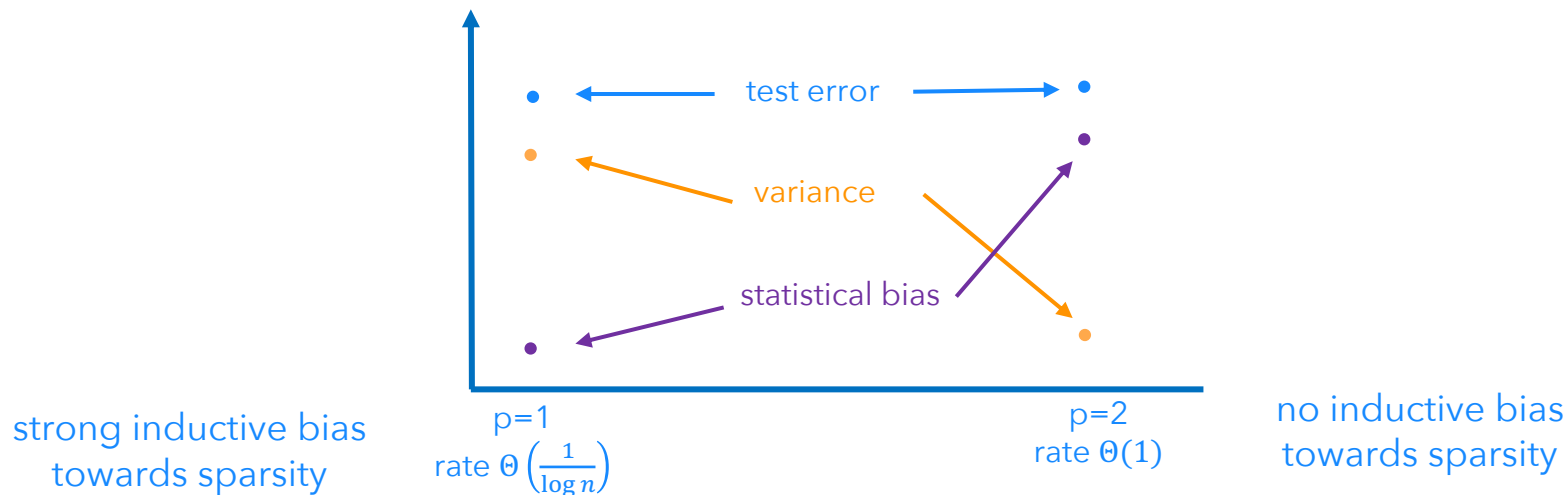
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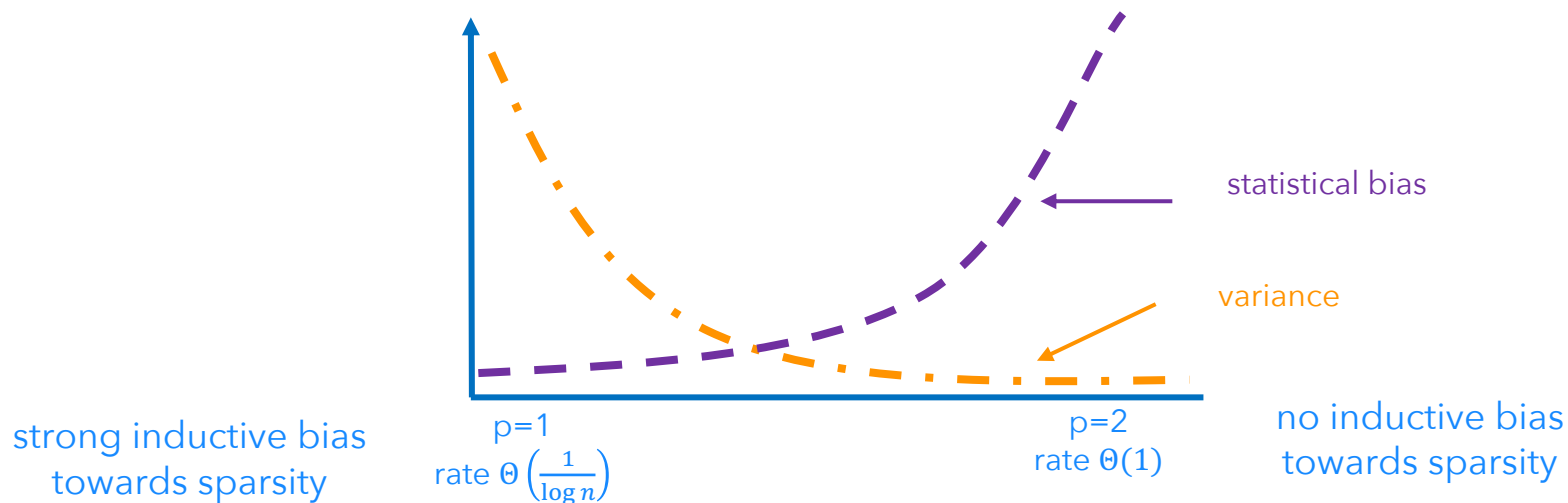
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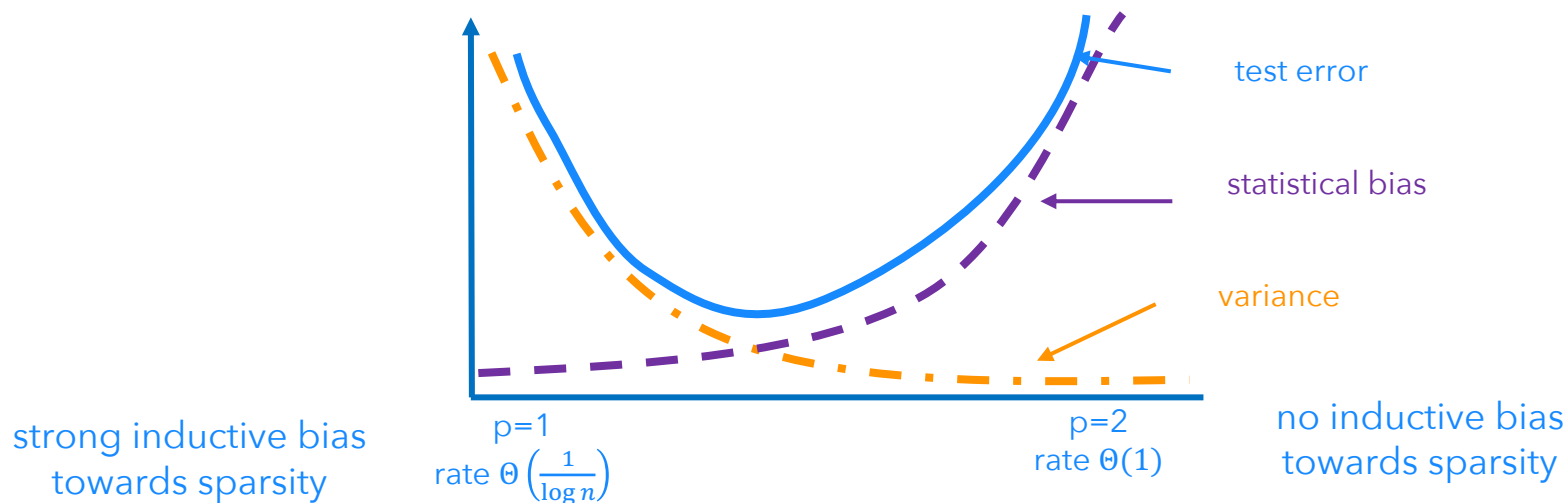
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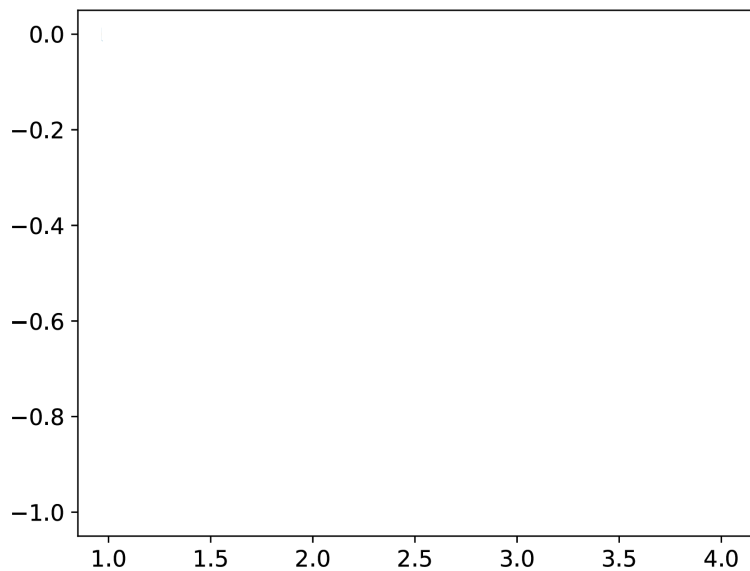
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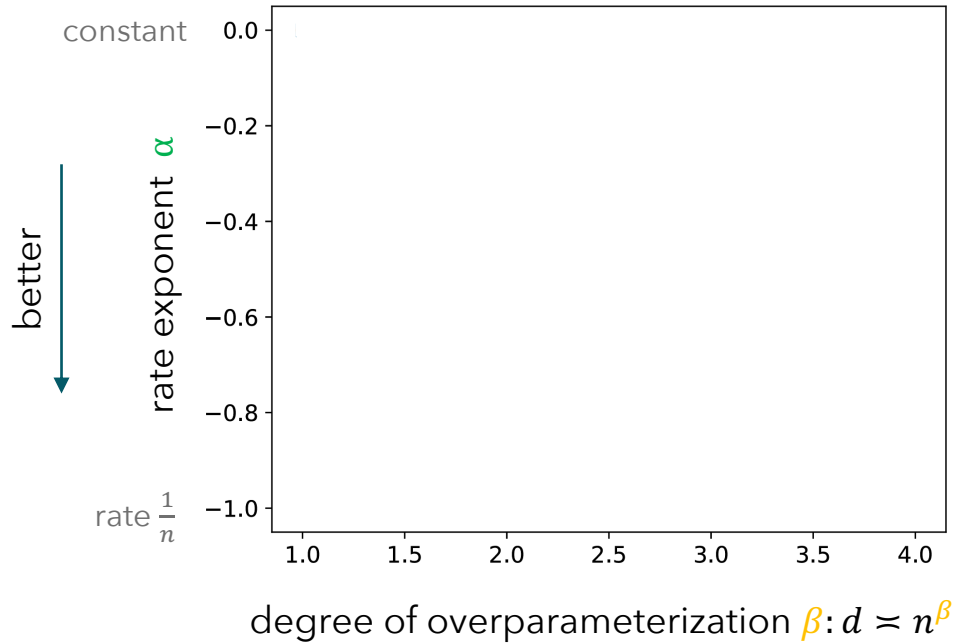
# Tight bounds for $p \in [1, 2]$



degree of overparameterization  $\beta: d \asymp n^\beta$

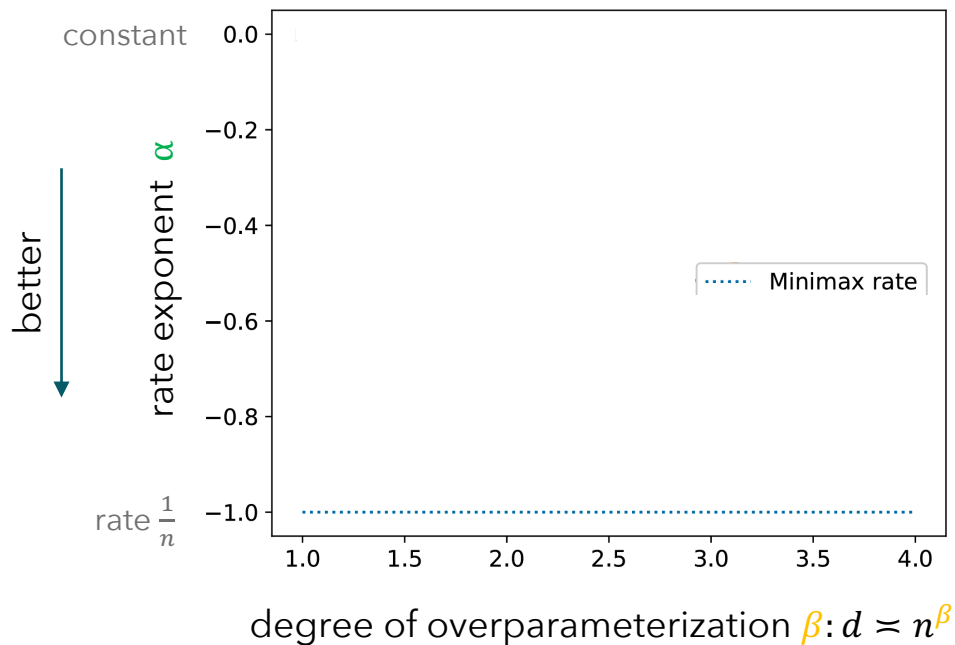
We plot  $\alpha$  where  $\|\widehat{w}_p - w^*\|^2 = \widetilde{\Theta}(n^\alpha)$  w.h.p.

## Tight bounds for $p \in [1, 2]$



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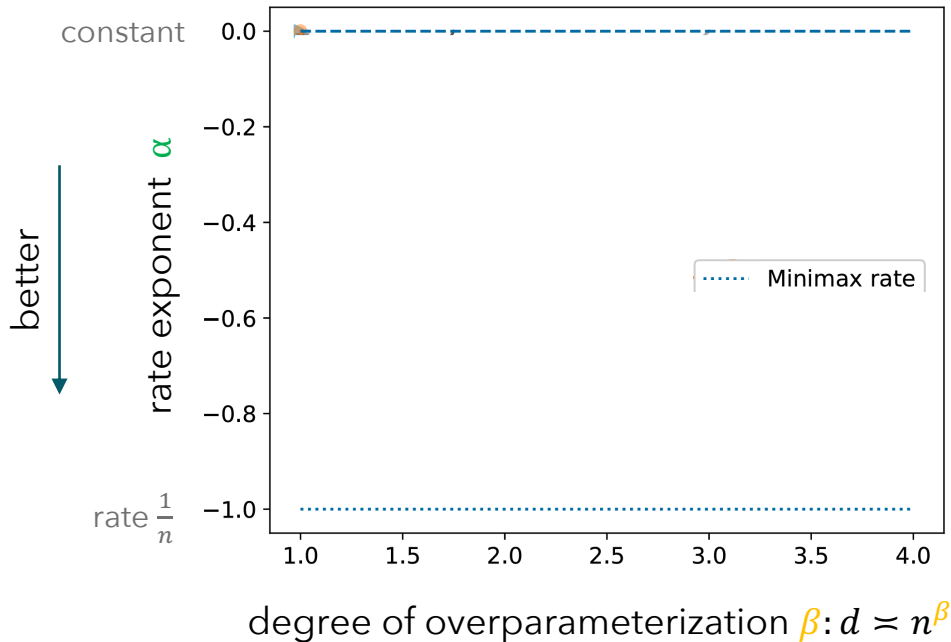


- minimax optimal rate, e.g. for (best) regularized estimator with  $p = 1$  (LASSO)  
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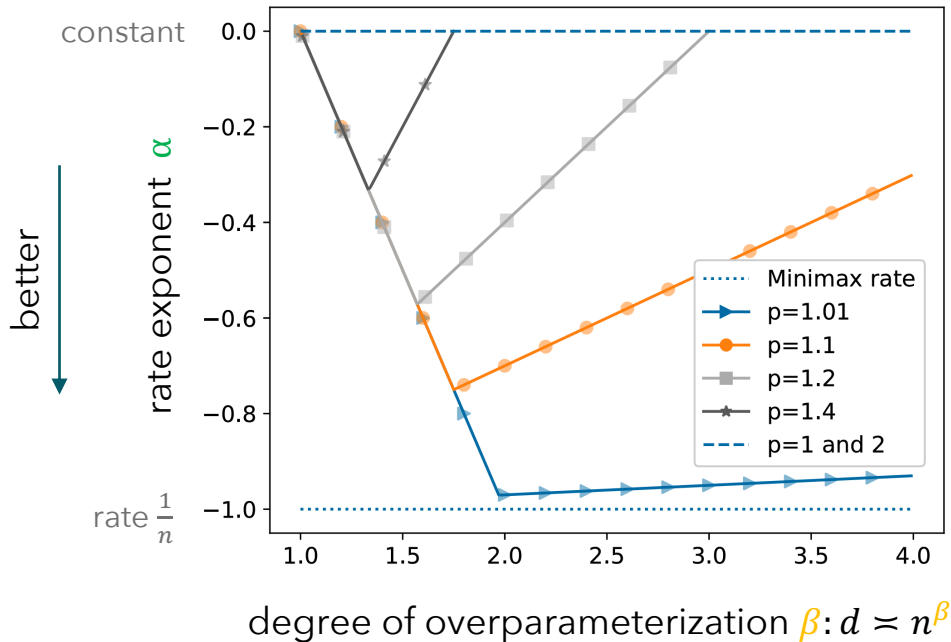


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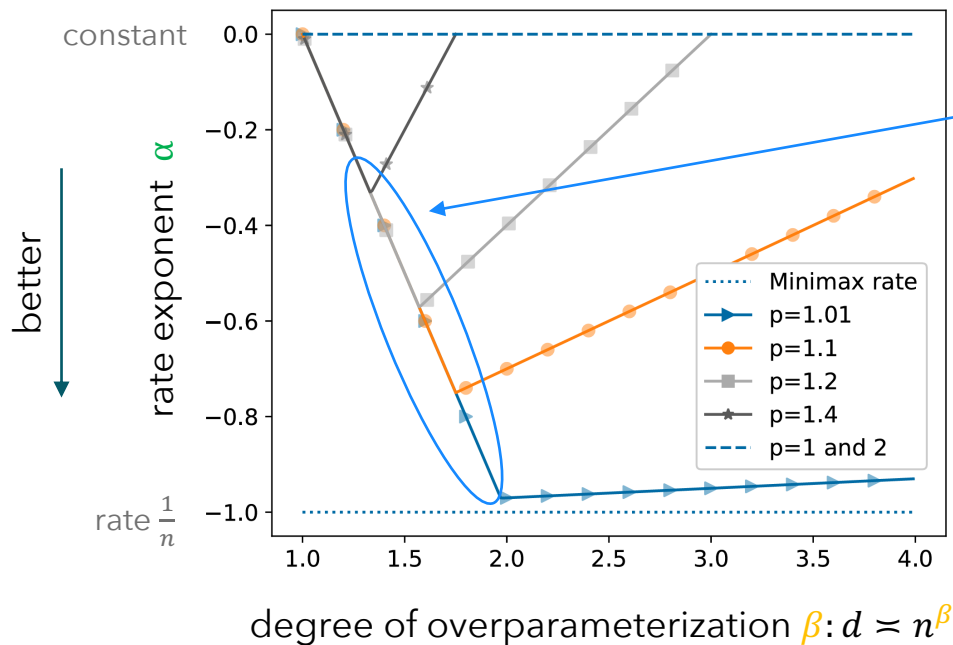
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- Interpolators for  $p \in (1, 2)$ :

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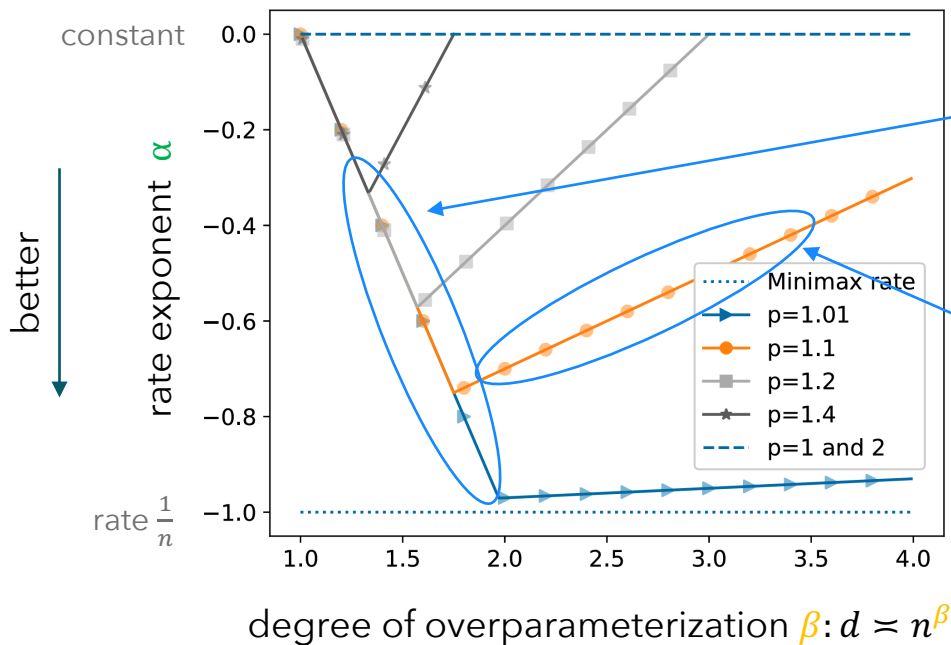
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“second” descent:  
decrease due to  
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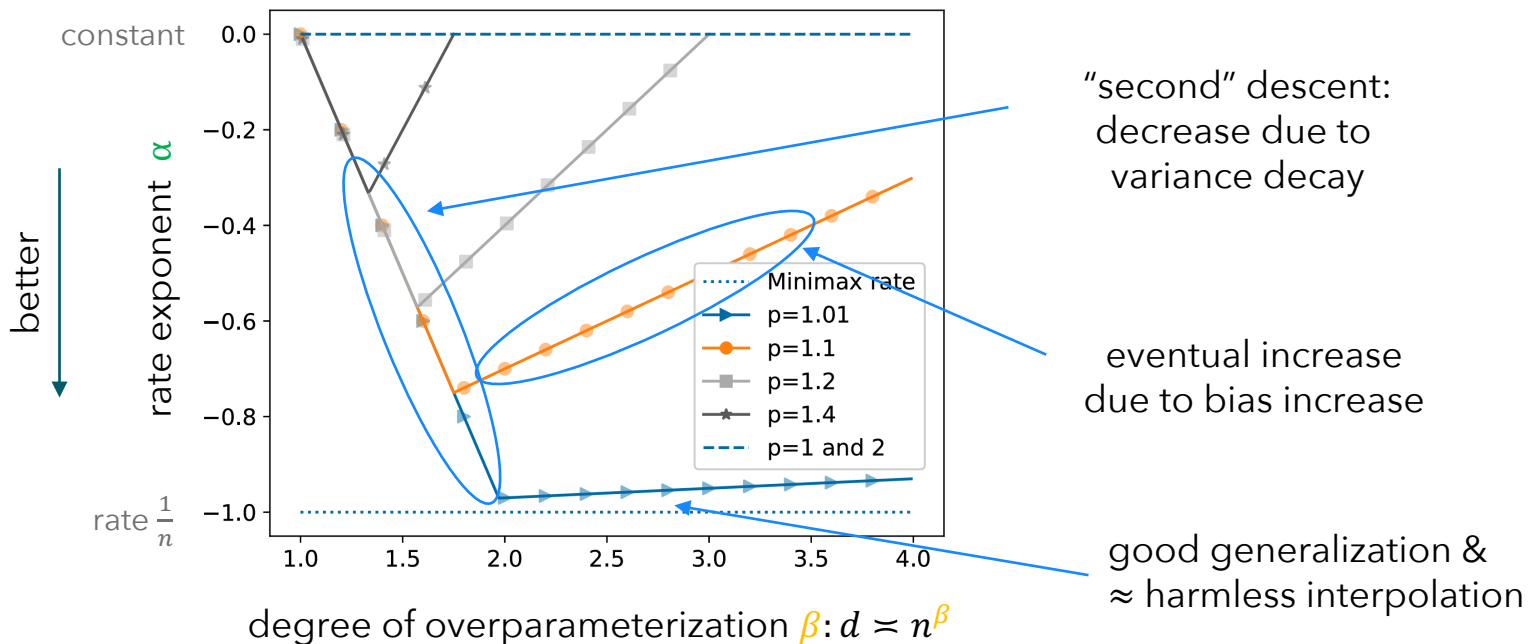


"second" descent:  
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eventual increase  
due to bias increase

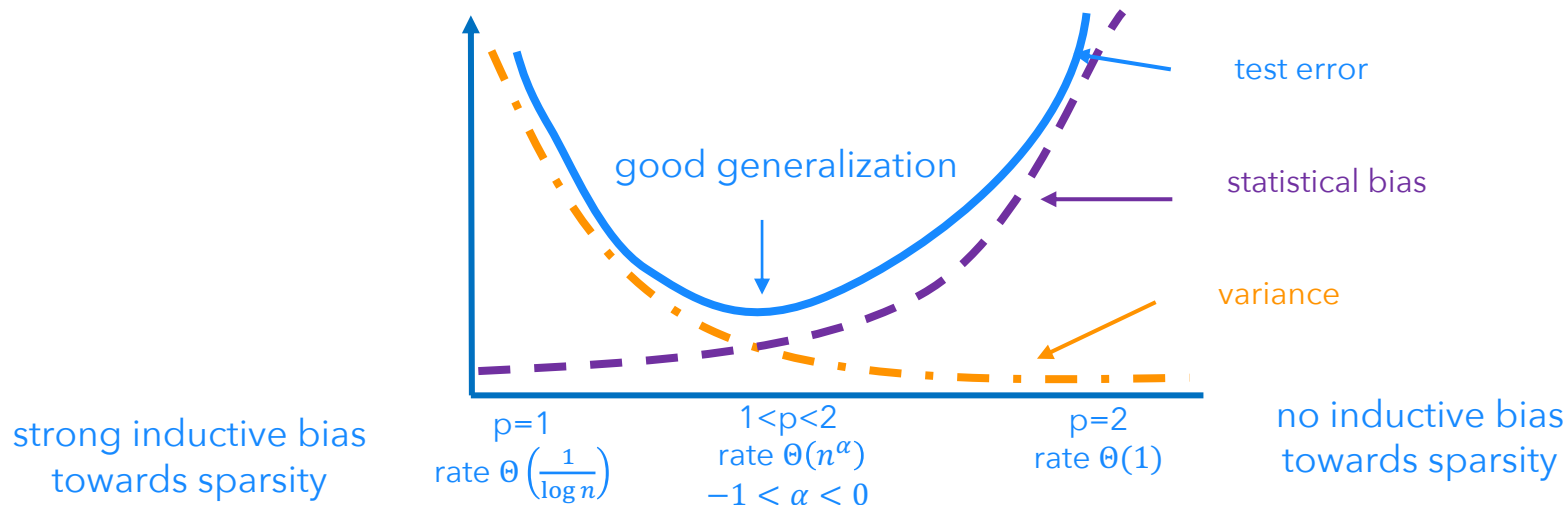
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# A new bias-variance trade-off for interpolators

$$\text{Min-}\ell_p\text{-norm interpolation } \hat{w}_p = \operatorname{argmin}_w \|w\|_p \text{ s.t. } y = Xw$$



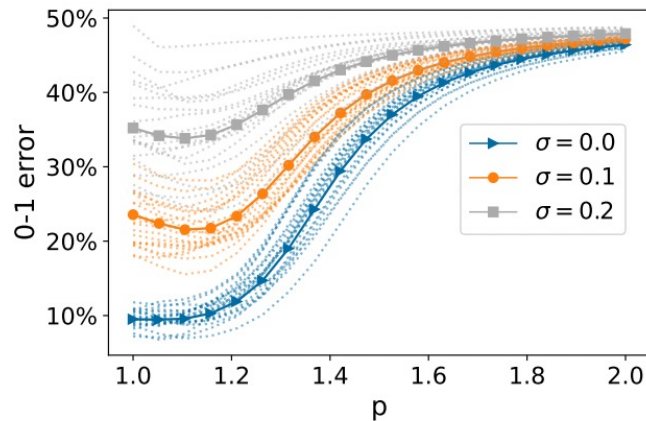
Take-away: medium strength of inductive bias is best when interpolating noise

# How transferable is this “new” intuition?

- Proof technique using Convex Gaussian Minmax Theorem [Thrampoulidis, Oymak, Hassibi '15] with localized convergence [Koehler, Zhou, Sutherland, Srebro '21] carries over to lin. classification

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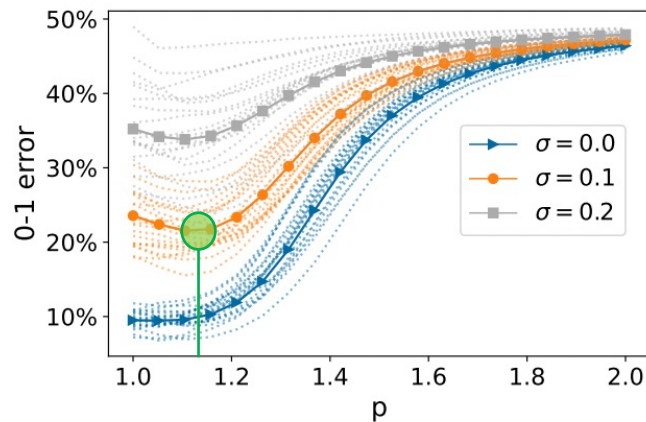


Synthetic experiment:  
Isotropic Gaussians with  $d \sim 5000, n \sim 100$



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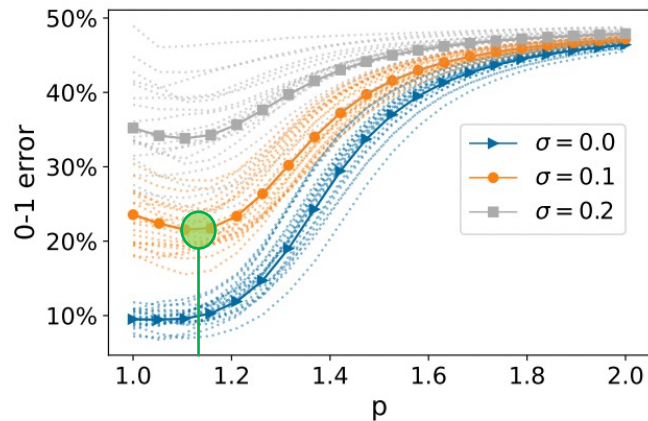
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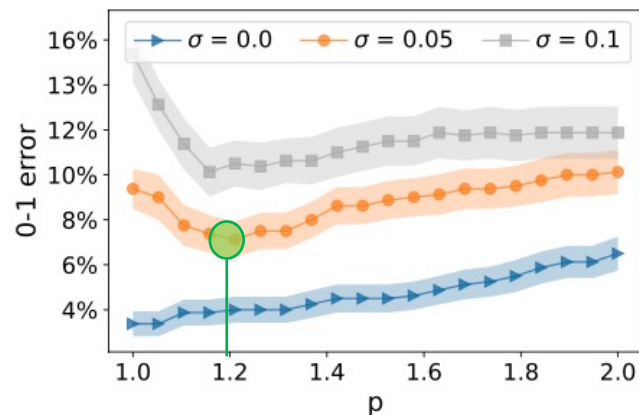
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Isotropic Gaussians with  $d \sim 5000, n \sim 100$



Real-world experiment:  
Leukemia dataset with  $d \sim 7000, n \sim 70$

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- Preliminary experiments for neural networks also suggest this behavior for rotational invariance and filter size...

# Nonlinear structure: Rotational invariance for WideResNet

- Satellite images (EuroSAT) to be classified in terms of type of land usage



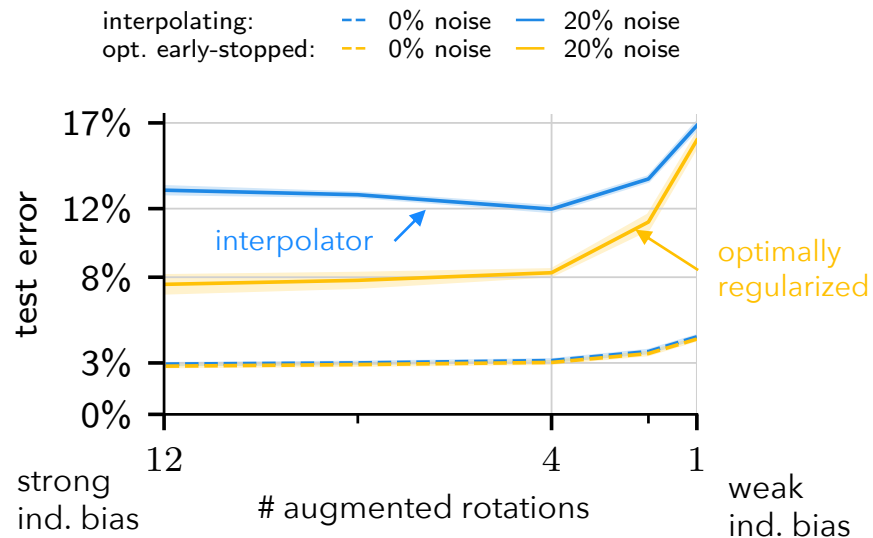
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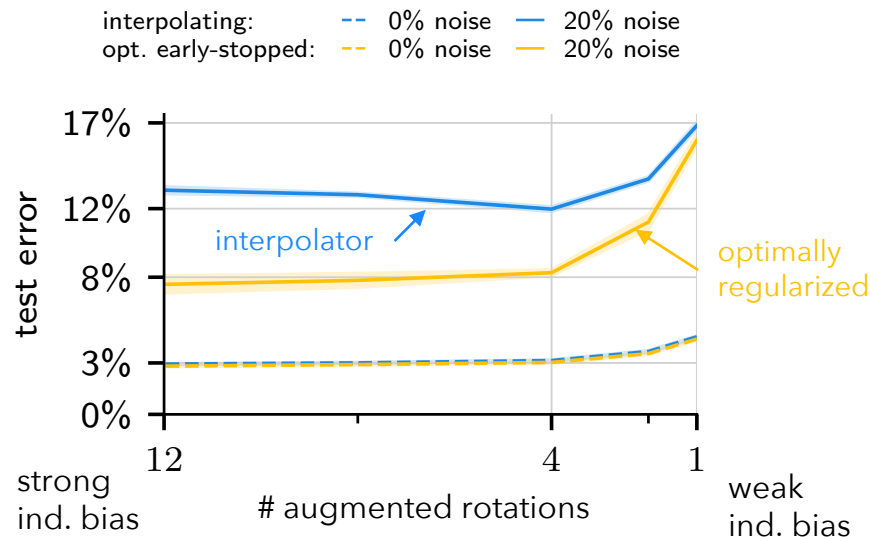


# Nonlinear structure: Rotational invariance for WideResNet

- Satellite images (EuroSAT) to be classified in terms of type of land usage



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Confirmed: medium strength of inductive bias is best when interpolating noise



# Open: How transferable is this “new” intuition?

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- Intuition carries over to high-dimensional kernel learning with convolutional kernels where bias and variance vary with inductive bias [Aerni, Milanta, Donhauser, Yang '23]
- Preliminary experiments for neural networks also suggest this behavior for rotational invariance and filter size

open: comprehensive experimental NN study!

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**Part I:** For linear regression, we discuss how

- variance can decay as overparameterization increases (simple math)
- Two factors can govern variance decay vs. bias increase
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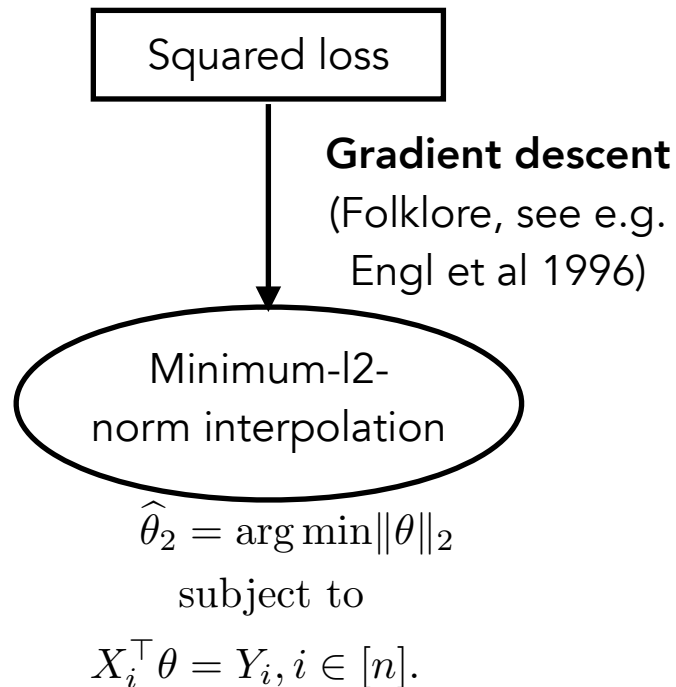
## Classification-vs-regression: A tale of two loss functions

	0-1 loss	Squared loss
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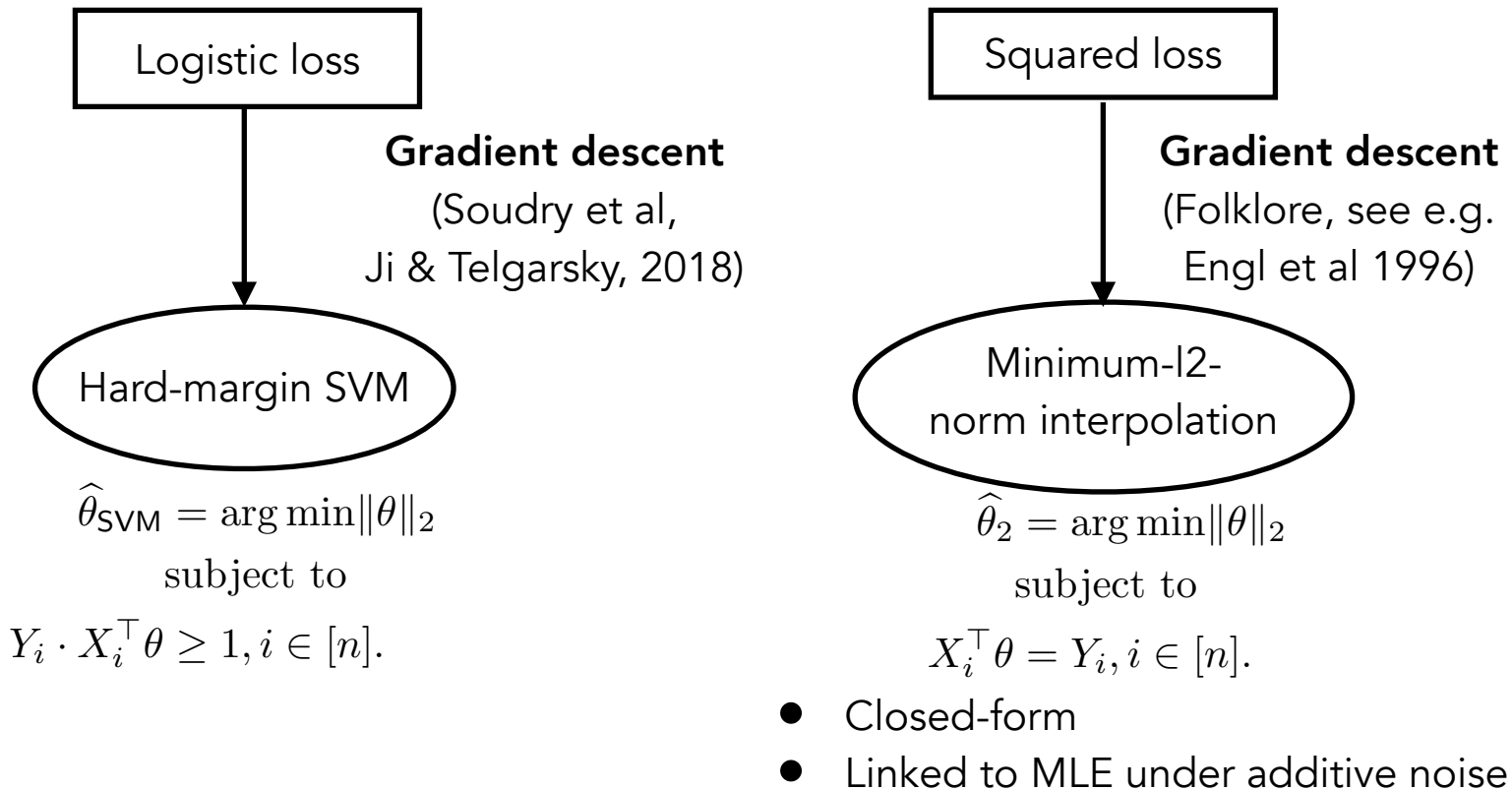
	0-1 loss	Squared loss
Logistic loss	Classification, most popular	
Squared loss	Classification, less popular	Regression

# Differences in training loss functions

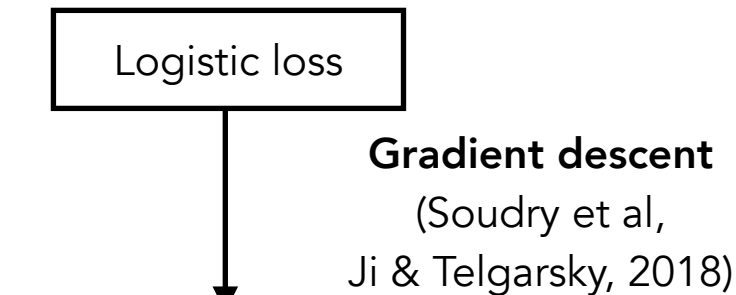


- Closed-form
- Linked to MLE under additive noise

## Differences in training loss functions



# Differences in training loss functions



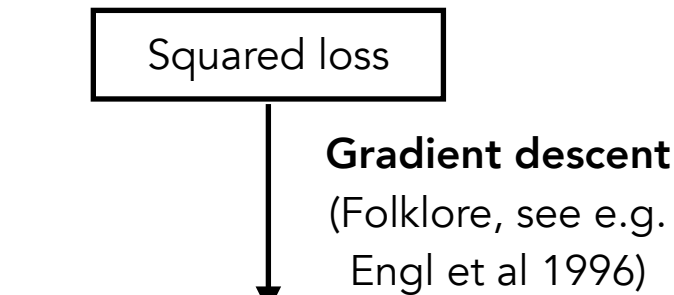
Hard-margin SVM

$$\hat{\theta}_{\text{SVM}} = \arg \min \|\theta\|_2$$

subject to

$$Y_i \cdot X_i^\top \theta \geq 1, i \in [n].$$

- Not closed-form
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Minimum-l2-  
norm interpolation

$$\hat{\theta}_2 = \arg \min \|\theta\|_2$$

subject to

$$X_i^\top \theta = Y_i, i \in [n].$$

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## Differences in test loss functions

### Regression: Test MSE

$$\mathcal{E}_{\text{MSE}} = \mathbb{E} \left[ (X^\top (\hat{\theta} - \theta^*))^2 \right]$$

### Classification: Test 0-1 error

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### Two core challenges when analyzing classification:

1. Hard-margin SVM does not have a closed-form solution, unlike minimum- $\ell_2$ -norm interpolation
2. 0-1 error metric challenging to sharply analyze as compared to MSE

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# One analysis path for l2, step 1: showing that **SVM = interpolation**

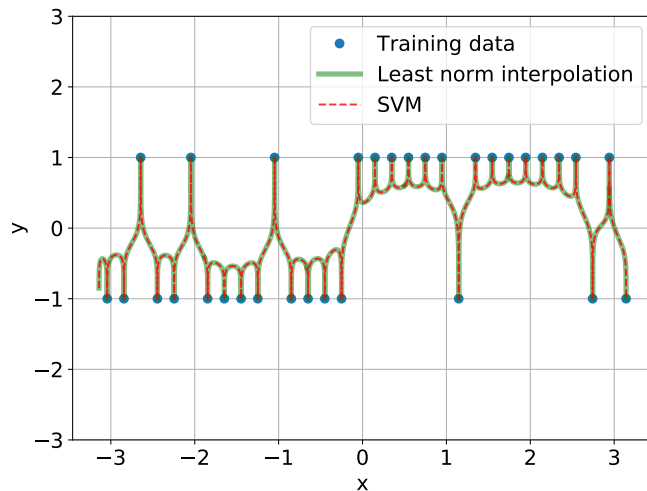
Fourier features  
on 1-dimensional data,  
isotropic covariance



$n = 32,$   
 $d = 1000$

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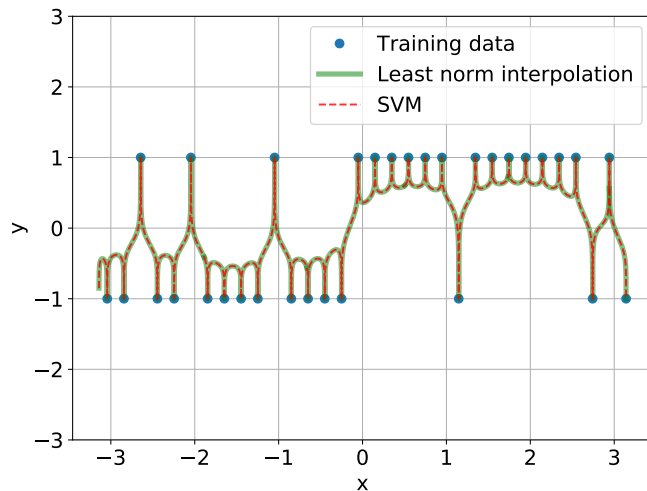


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**Result** (Hsu, Muthukumar and Xu 2021): **hard margin SVM = minimum-l2-norm interpolation on binary labels** in spiked covariance ensemble if  $d \gg n \log n$  and  $R \ll \frac{d}{n}$

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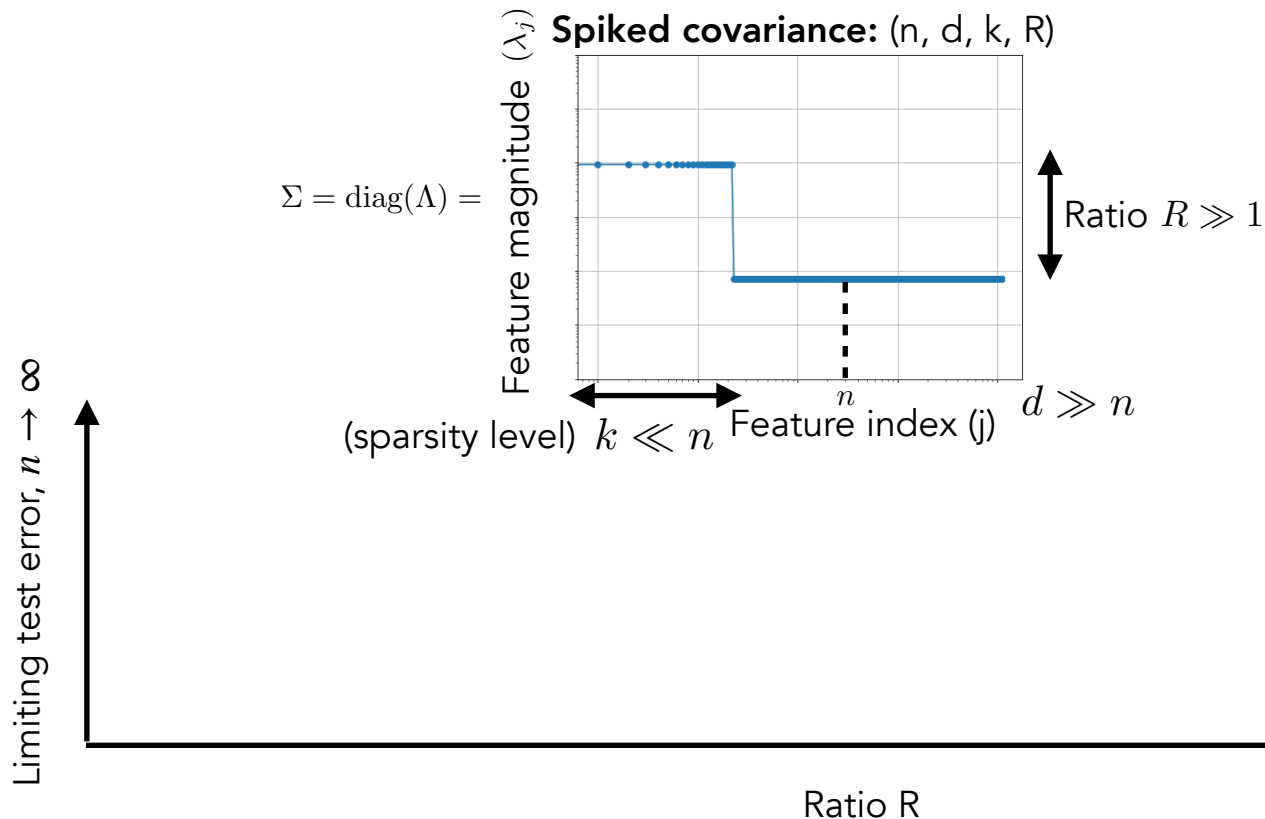


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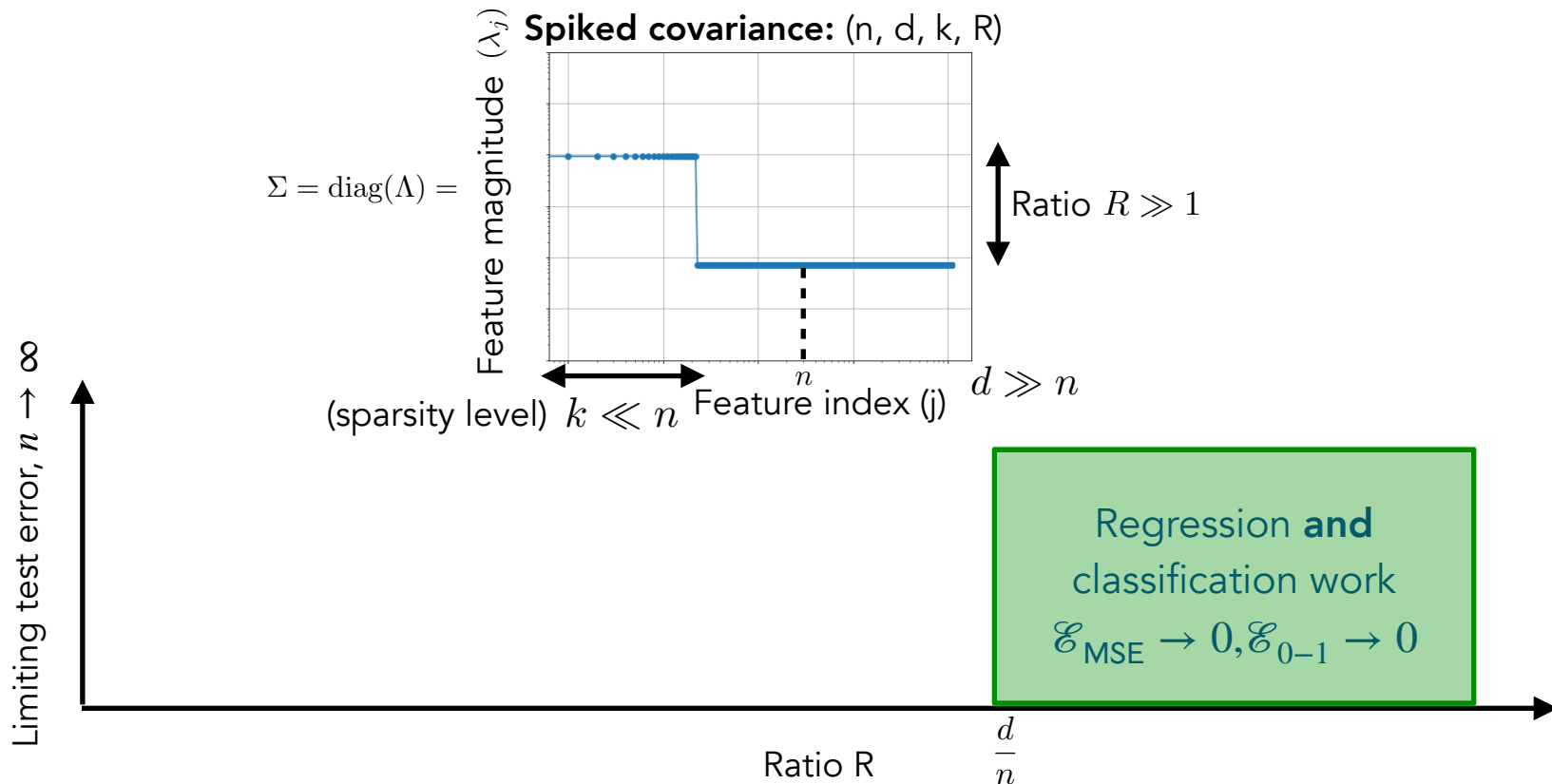
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**Implication:** SVM has a closed-form expression, can be more easily analyzed!

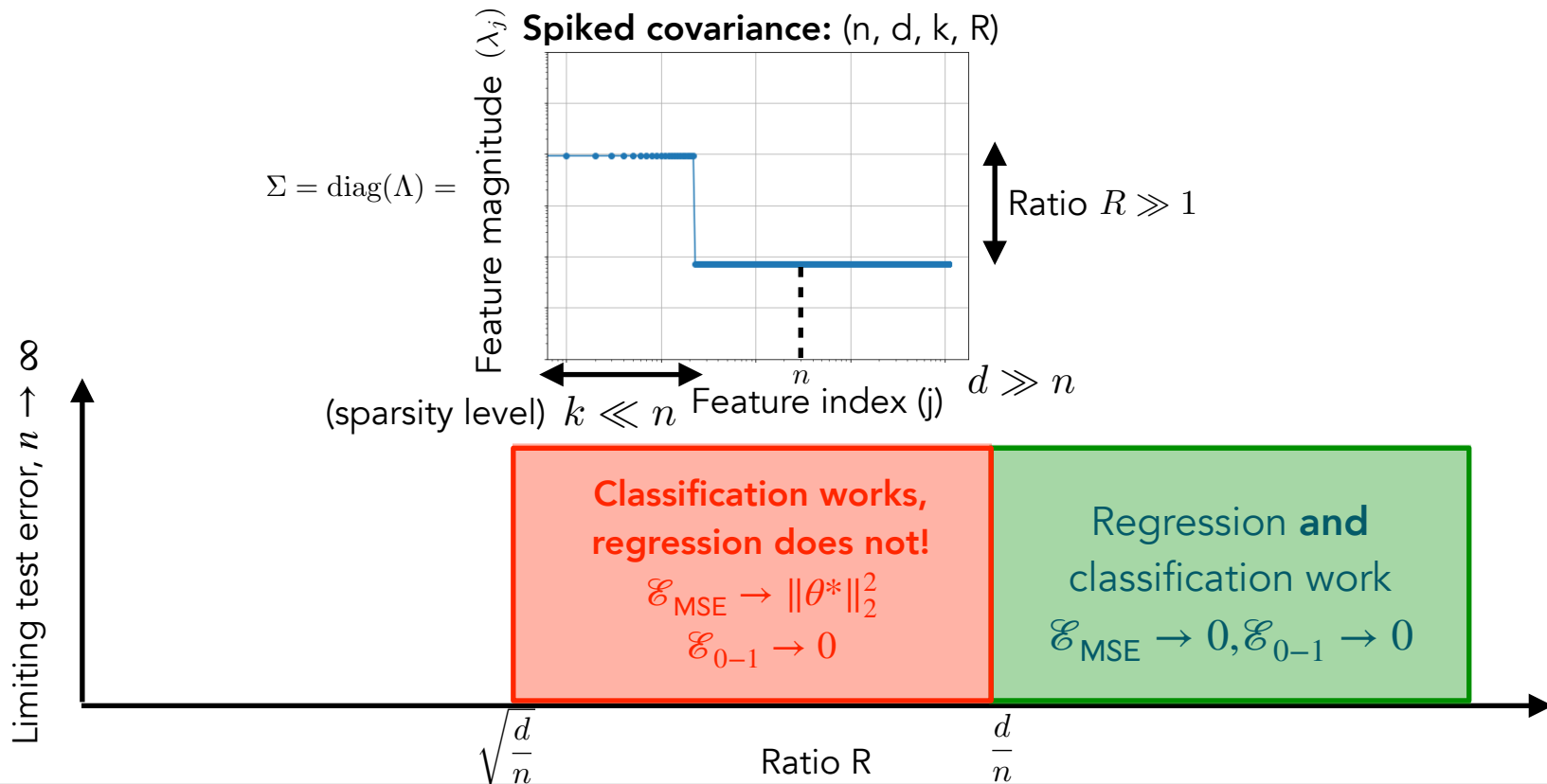
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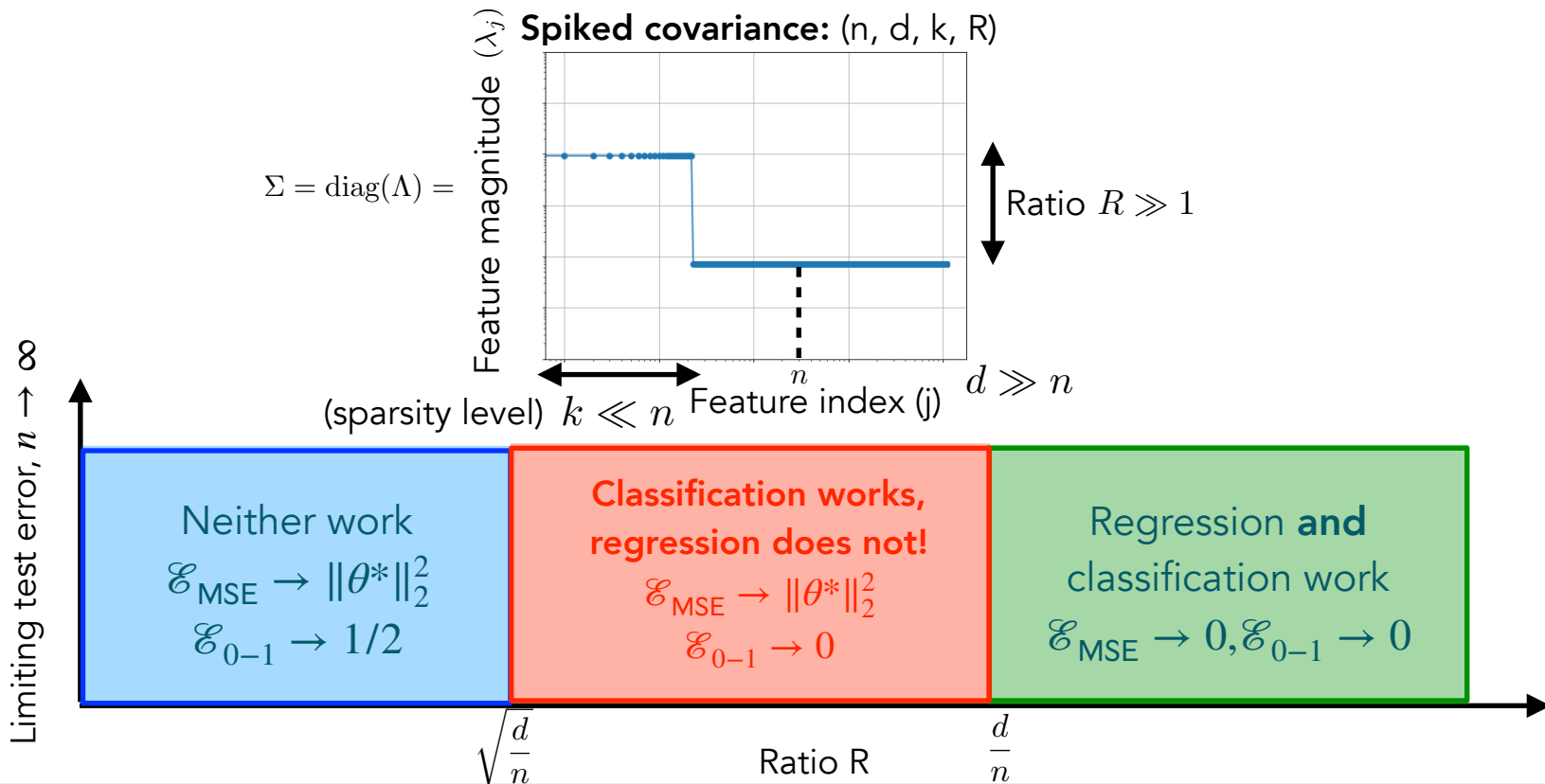


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- Different **training loss functions** could yield **similar or even identical solutions**
- Classification 0-1 test loss is **much more benign than regression MSE**; so  $l_2$ -inductive bias could work better for classification tasks

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- Most theoretical works on benign overfitting focus on linear/kernel setting.
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- We'll discuss recent works in neural networks and open questions.
- Notably: all results on benign overfitting in neural nets require ambient dimension  $d \gg n$
- Very unsatisfying: neural nets can be overparameterized in  $d \ll n$  regime, when is overfitting benign in this setting?

## Which estimators do we care about?

Model	Algorithm	Setting	Estimator
Linear	Gradient descent	Classification	$\ell_2$ max-margin
Linear	Gradient descent	Regression	$\ell_2$ min-norm interpolator
Linear	Adaboost	Classification	$\ell_1$ max-margin
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Neural nets	Gradient descent	Classification	?
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- Next: implicit bias of GD in neural net classification.
- After: “trajectory analysis”, directly analyzing properties of neural nets trained by GD



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## Theorem

For large class of neural nets, if GD/GF  $\theta(t)$  reaches a small enough loss, then  $\theta(t)$  converges in direction to a first-order stationary point (KKT point) of the  $\ell^2$ -max margin problem,

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- KKT point does not imply even local optimality in general.
- In general, very little is known about KKT points of (1).

## Implicit bias in neural networks

- A setting where we understand KKT points of max-margin: two-layer leaky ReLU nets with nearly-orthogonal data. ( $\phi(q) = \max(\gamma q, q)$ )

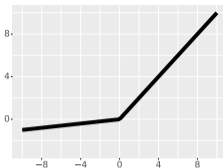
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- Satisfied in many settings w.h.p. when  $d \gg n^2$  and  $(x_i, y_i) \stackrel{\text{i.i.d.}}{\sim} \mathcal{P}$  (e.g.,  $x \sim \mathcal{N}(0, I_d)$ )

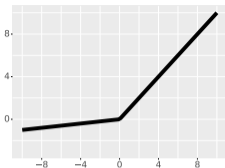


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## Theorem

Suppose data is **nearly orthogonal**. If  $\theta$  satisfies KKT conditions for  $\ell^2$ -max-margin, then  $\exists s_i > 0$  s.t.

$$\text{for any } x \in \mathbb{R}^d, \quad \text{sgn}(f(x; \theta)) = \text{sgn}\left(\left\langle \sum_{i=1}^n s_i y_i x_i, x \right\rangle\right),$$

where  $s_i > 0$  satisfy  $\max_{i,j} s_i/s_j = O(1)$ .

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Suppose data satisfies  $\|x_i\|^2 \gg n \max_{k \neq j} |\langle x_j, x_k \rangle|$ . If  $\theta$  satisfies KKT conditions for  $\ell^2$ -max-margin for 2-layer leaky nets, then  $\exists s_i > 0$  s.t.

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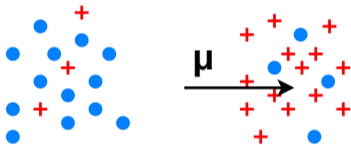
- Although two-layer nets are universal approximators, KKT points for margin maximization have linear decision boundaries under near-orthogonality.
- Decision boundary is very simple,  $\approx$  uniform average of data.
- Linear model can capture behavior of nonlinear net, trained beyond NTK.

## Benign overfitting of neural nets in mixture model

- KKT points for 2-layer leaky nets  $\approx \sum_{i=1}^n y_i x_i$ , when training data is nearly-orthogonal  $(\|x_i\|^2 \gg n \max_{k \neq j} |\langle x_j, x_k \rangle|)$ .

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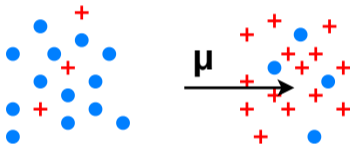
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- Following results will only hold in this low-SNR, high-dimensional regime
  - We'll see consistency is still possible in this setting

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- $\exp(-\Omega(n\|\mu\|^4/d))$  is minimax-optimal!

## Benign overfitting of neural nets in mixture model

Recall  $\text{sgn}(f(x; \theta)) = \text{sgn}(\langle \sum_{i=1}^n y_i x_i, x \rangle)$ . What does this estimator look like? Since  $x_i = \tilde{y}_i \mu + z_i$ ,

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Overfitting component helps interpolation, signal helps generalization:

Training data: classify  $(x_i, y_i)$  correctly

Test data: classify  $(x, \tilde{y})$  correctly

$\langle y_i x_i, \sum_{i=1}^n \tilde{y}_i z_i \rangle$  is large, positive,  
 $\langle y_i x_i, n\mu \rangle$  is small, noisy labels make  $\pm$ .

$\langle \tilde{y} x, \sum_{i=1}^n \tilde{y}_i z_i \rangle$  is small, random  $\pm$ ,  
 $\langle \tilde{y} x, n\mu \rangle$  is (optimally) large, positive.

- Signal and overfitting component balanced to allow both interpolation + generalization

# Other approaches for benign overfitting in neural nets

- Analysis of implicit bias (KKT conditions, minimum norm interpolation, ...)

Frei-Vardi-Bartlett-Srebro'23; Kornowski-Yehudai-Shamir'23; Kou-Chen-Gu'23; ...

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  - "Trajectory analysis": directly track the weights of neural net trained by GD/GF from random initialization on noisy data, show that it achieves small train and test error
- Frei-Chatterji-Bartlett'22; Xu-Gu'23; Kou-Chen-Chen-Gu ICML'23; Xu-Wang-Frei-Vardi-Hu'23; Meng-Zou-Cao'23; ...
- Characterizes finite time performance
  - More narrow, less clear "why" benign overfitting happens



## Benign overfitting from trajectory analysis

- Directly examine inductive bias of training by GD/GF, e.g. in 2 layer nets

$$f(x; \theta) = \sum_{j=1}^m a_j \phi(\langle \theta_j, x \rangle), \quad \hat{L}(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(f(x_i; \theta)),$$
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  - These two must be very different for benign overfitting to occur

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- Same generalization bound as KKT analysis, but now holds throughout GD trajectory.
  - Only tolerates  $p = O(1)$ , rather than  $p < 1/2$  from KKT analysis.



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- Known proofs all rely on nearly-orthogonal data ( $d \gg n$ ) to show this

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- $d/n \rightarrow \infty$  necessary for benign overfitting in linear models, but unknown if necessary for neural networks.

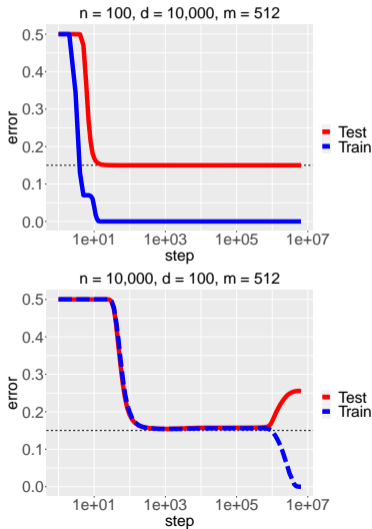
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- Learning dynamics different in  $n > d$  setting; overfitting less ‘benign’  
→ “Blessing of dimensionality”? See also:

[Kornowski-Yehudai-Shamir’23]





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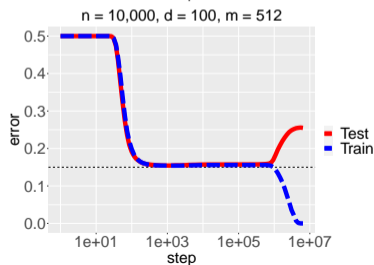
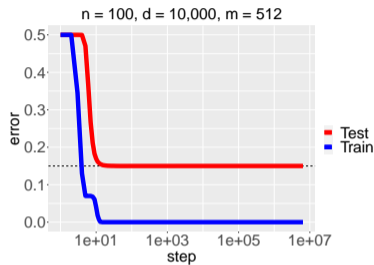
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- Neural net trained on high-dimensional mixture model: (provably) benign; low-dimensional: tempered?



## Open questions

- Is benign overfitting in neural nets possible in low dimensions ( $n \gg d$ )?
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  - Overparameterization through wider nets could help, but does it? When? Why?
- Which neural net interpolators do we care about in regression?
- Necessary and sufficient conditions for benign overfitting in linear classification?
  - Fairly complete picture of min- $\ell^2$  linear regression, but mostly sufficiency guarantees in classification.
  - Dream: data-dependent, signal-dependent, tight guarantees.

Thanks!