Learning From Data

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Lecture 8: Bias-Variance Tradeoff

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Outline

- Bias and Variance

- Learning Curves

Approximation-generalization tradeoff

Small E_{out}: good approximation of f out of sample.

More complex $\mathcal{H} \implies$ better chance of **approximating** f

Less complex $\mathcal{H} \implies$ better chance of **generalizing** out of sample

Ideal $\mathcal{H} = \{f\}$ winning lottery ticket ☺

Quantifying the tradeoff

VC analysis was one approach: $E_{\text{out}} \leq E_{\text{in}} + \Omega$

Bias-variance analysis is another: decomposing E_{out} into

1. How well $\mathcal{H}$ can approximate f

2. How well we can zoom in on a good $h \in \mathcal{H}$

Applies to **real-valued targets** and uses **squared error**

Start with E_{out}

$$E_{\text{out}}(g^{(\mathcal{D})}) = \mathbb{E}_{\mathbf{x}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]$$

$$\begin{aligned}\mathbb{E}_{\mathcal{D}}\left[E_{\text{out}}(g^{(\mathcal{D})})\right] &= \mathbb{E}_{\mathcal{D}}\left[\mathbb{E}_{\mathbf{x}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]\right] \\ &= \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]\right]\end{aligned}$$

Now, let us focus on:

$$\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]$$

The average hypothesis

To evaluate $\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]$

we define the 'average' hypothesis $\bar{g}(\mathbf{x})$:

$$\bar{g}(\mathbf{x}) = \mathbb{E}_{\mathcal{D}}\left[g^{(\mathcal{D})}(\mathbf{x})\right]$$

Imagine **many** data sets $\mathcal{D}_1, \mathcal{D}_2, \cdots, \mathcal{D}_K$

$$\bar{g}(\mathbf{x}) \approx \frac{1}{K}\sum_{k=1}^{K} g^{(\mathcal{D}_k)}(\mathbf{x})$$

Using $\bar{g}(\mathbf{x})$

$$\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right] = \mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x}) + \bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]$$

$$= \mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2 + \left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2\right.$$

$$\left. + \; 2\;\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)\;\left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)\right]$$

$$= \mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2\right] + \left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2$$

Bias and variance

$$\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right] = \underbrace{\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2\right]}_{\textsf{var}(\mathbf{x})} + \underbrace{\left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2}_{\textsf{bias}(\mathbf{x})}$$

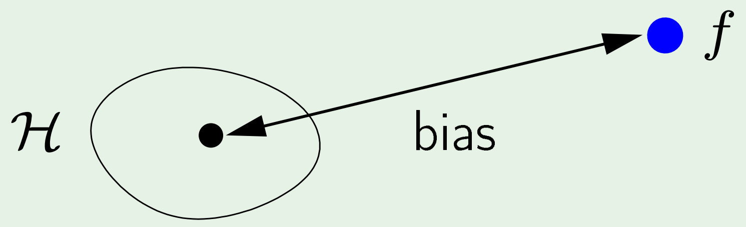
Therefore, $\mathbb{E}_{\mathcal{D}}\left[E_{\text{out}}(g^{(\mathcal{D})})\right] = \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]\right]$

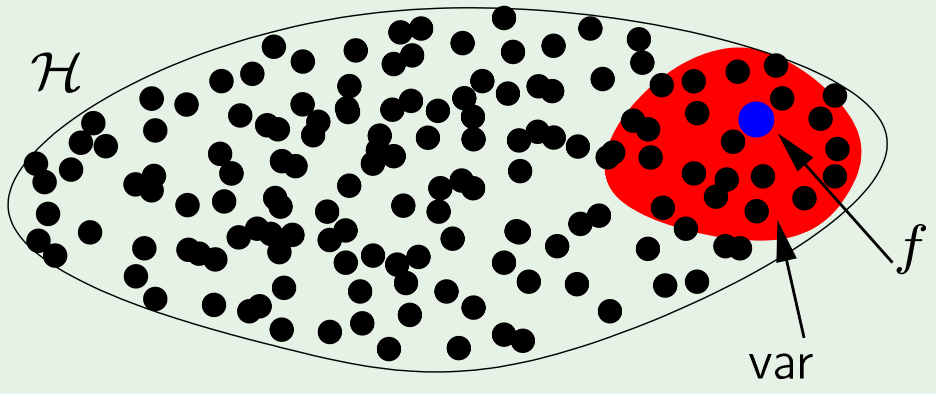
$$= \mathbb{E}_{\mathbf{x}}[\textsf{bias}(\mathbf{x}) + \textsf{var}(\mathbf{x})]$$

$$= \quad \textsf{bias} \quad + \quad \textsf{var}$$

The tradeoff

$$\text{bias} = \mathbb{E}_{\mathbf{x}}\left[\left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2\right] \qquad \text{var} = \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2\right]\right]$$





$$\downarrow \qquad \mathcal{H}\uparrow \qquad \uparrow$$

Example: sine target

$f : [-1, 1] \rightarrow \mathbb{R} \qquad f(x) = \sin(\pi x)$

Only two training examples! $\qquad N = 2$

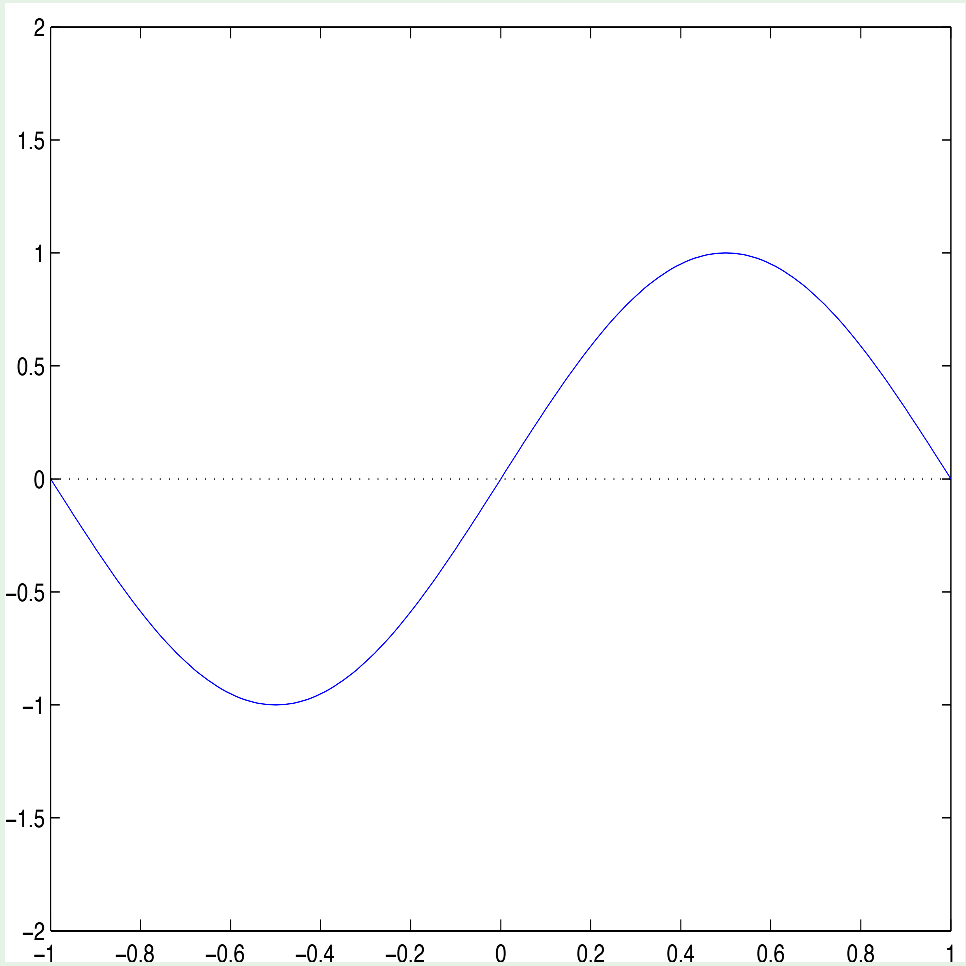
Two models used for learning:

$$\mathcal{H}_0: \quad h(x) = b$$

$$\mathcal{H}_1: \quad h(x) = ax + b$$

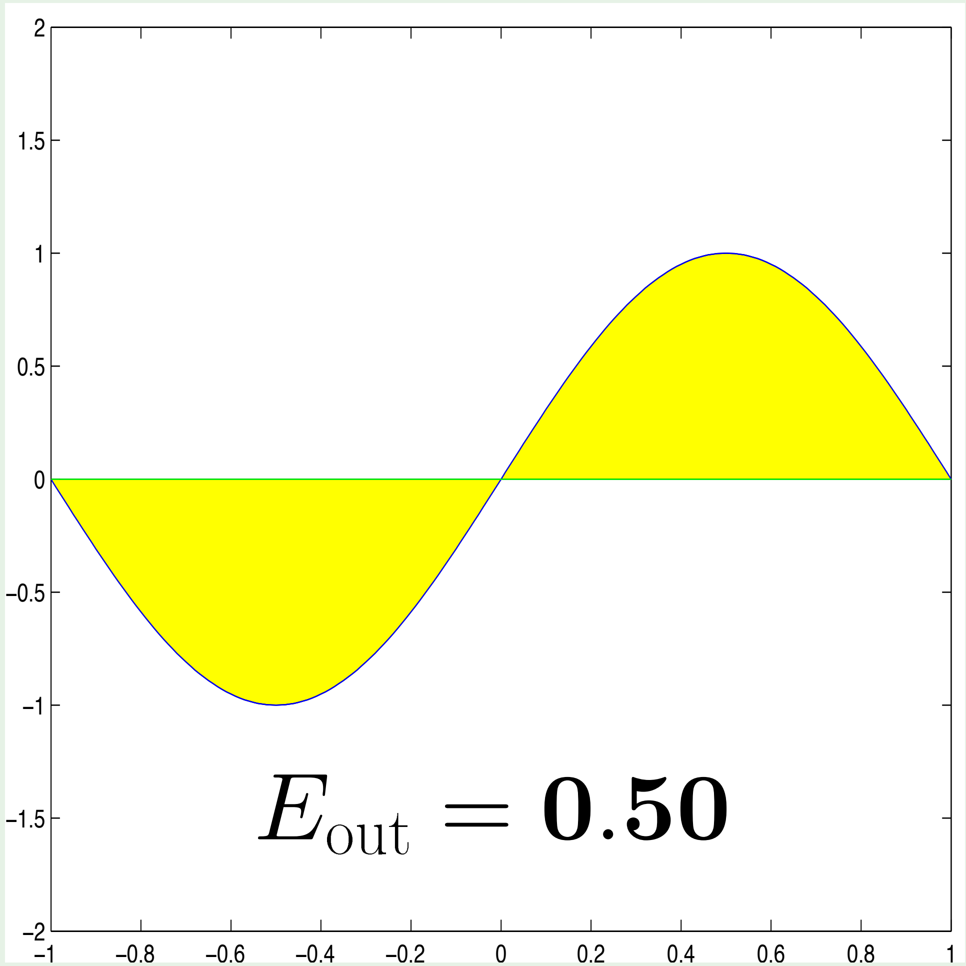
Which is better, $\mathcal{H}_0$ or $\mathcal{H}_1$?

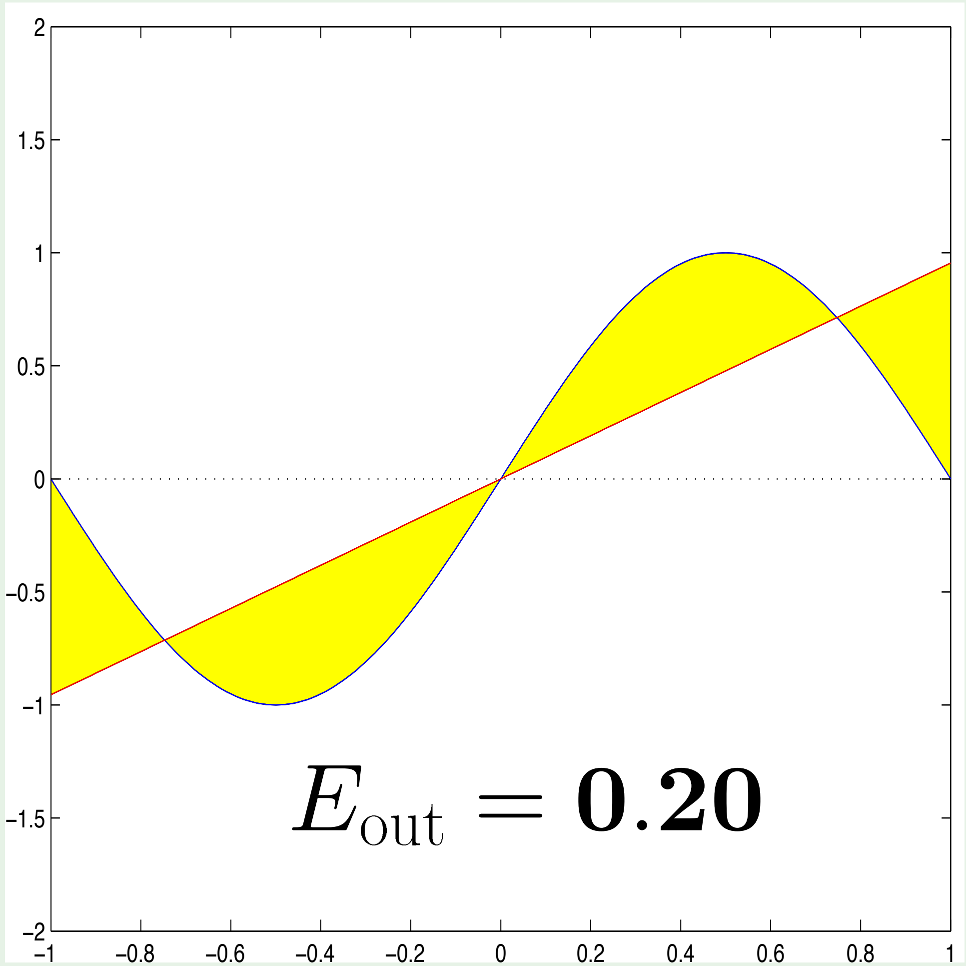
f



Approximation - $\mathcal{H}_0$ versus $\mathcal{H}_1$

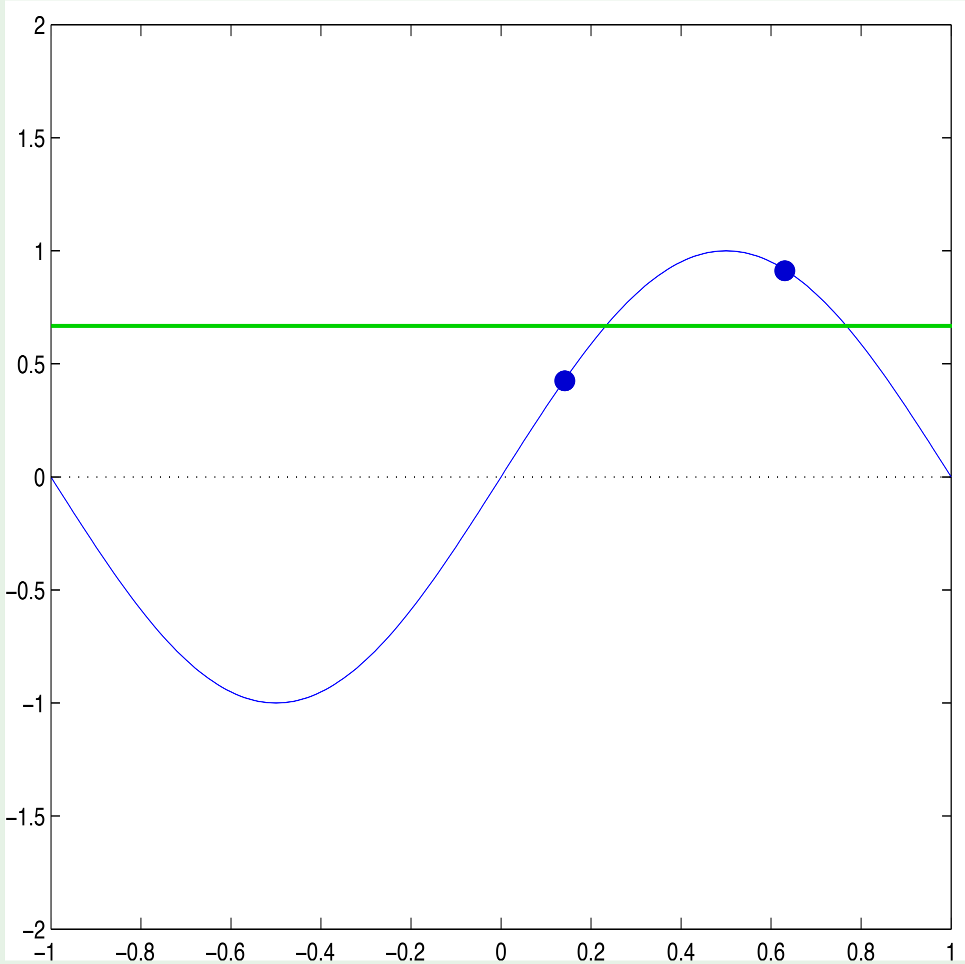
$\mathcal{H}_0$ $\qquad\qquad$ $\mathcal{H}_1$



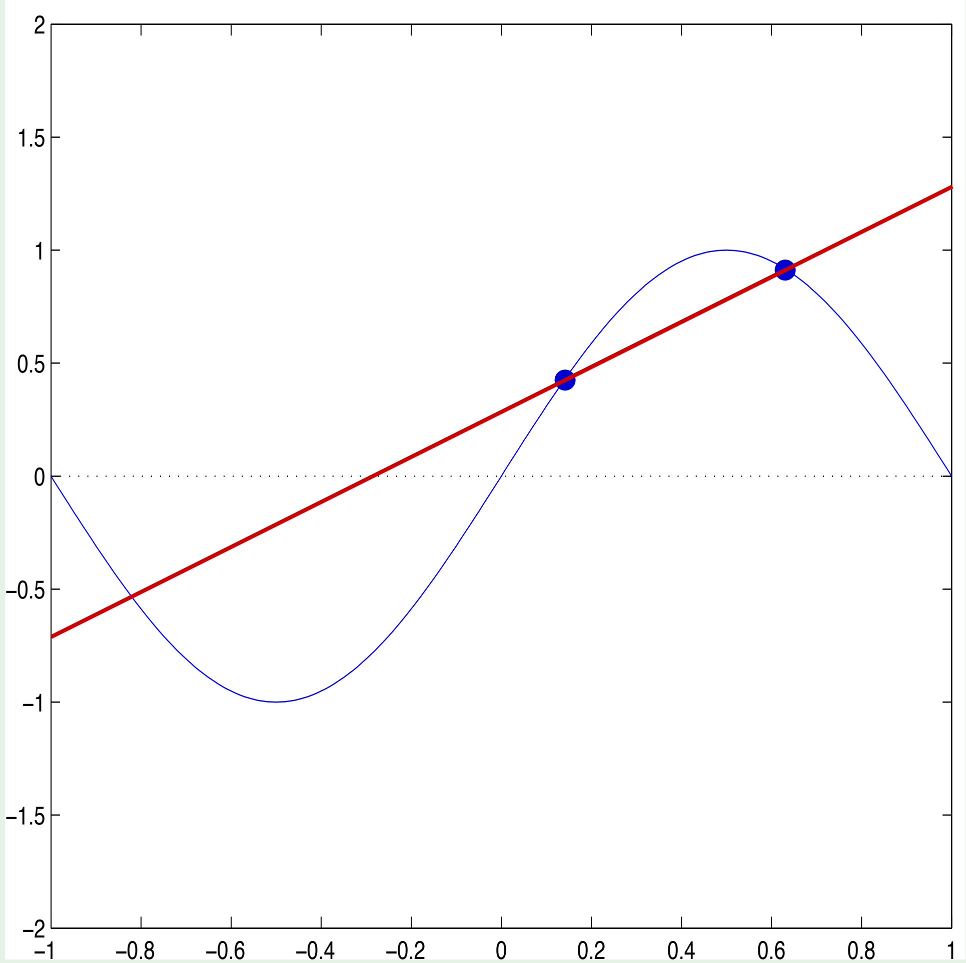


Learning - $\mathcal{H}_0$ versus $\mathcal{H}_1$

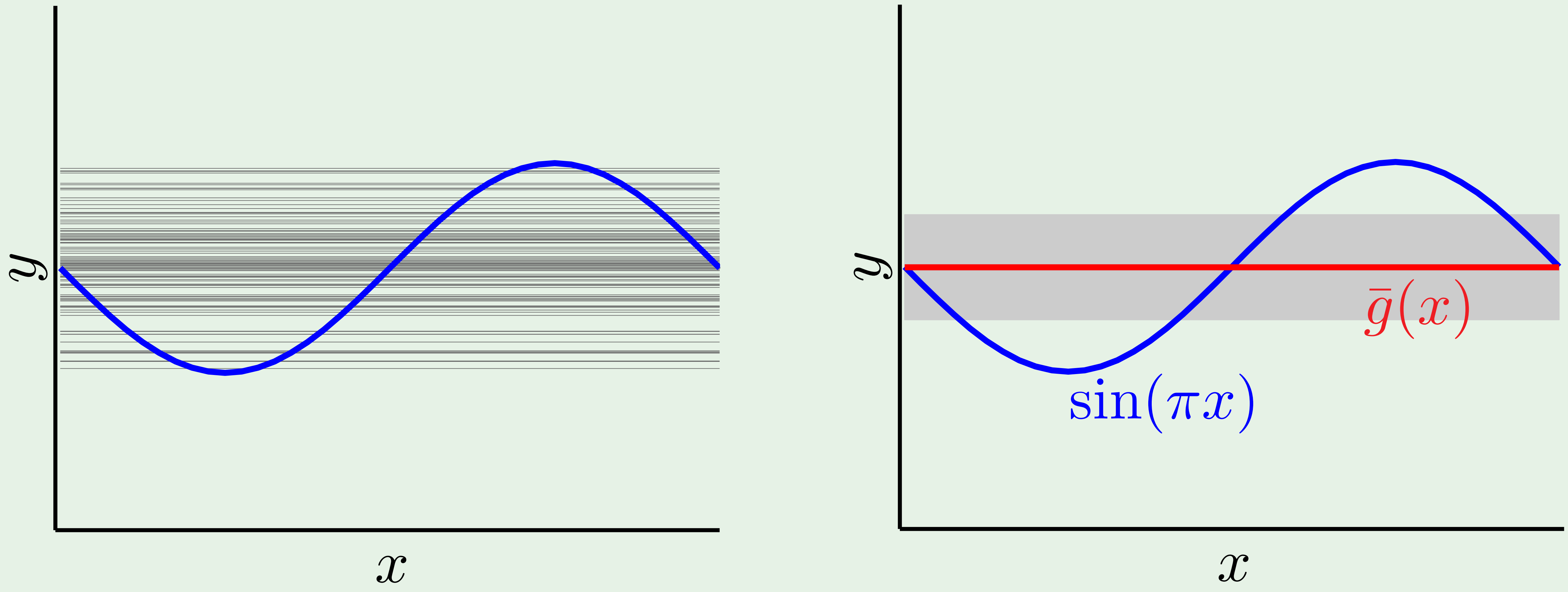
$\mathcal{H}_0$



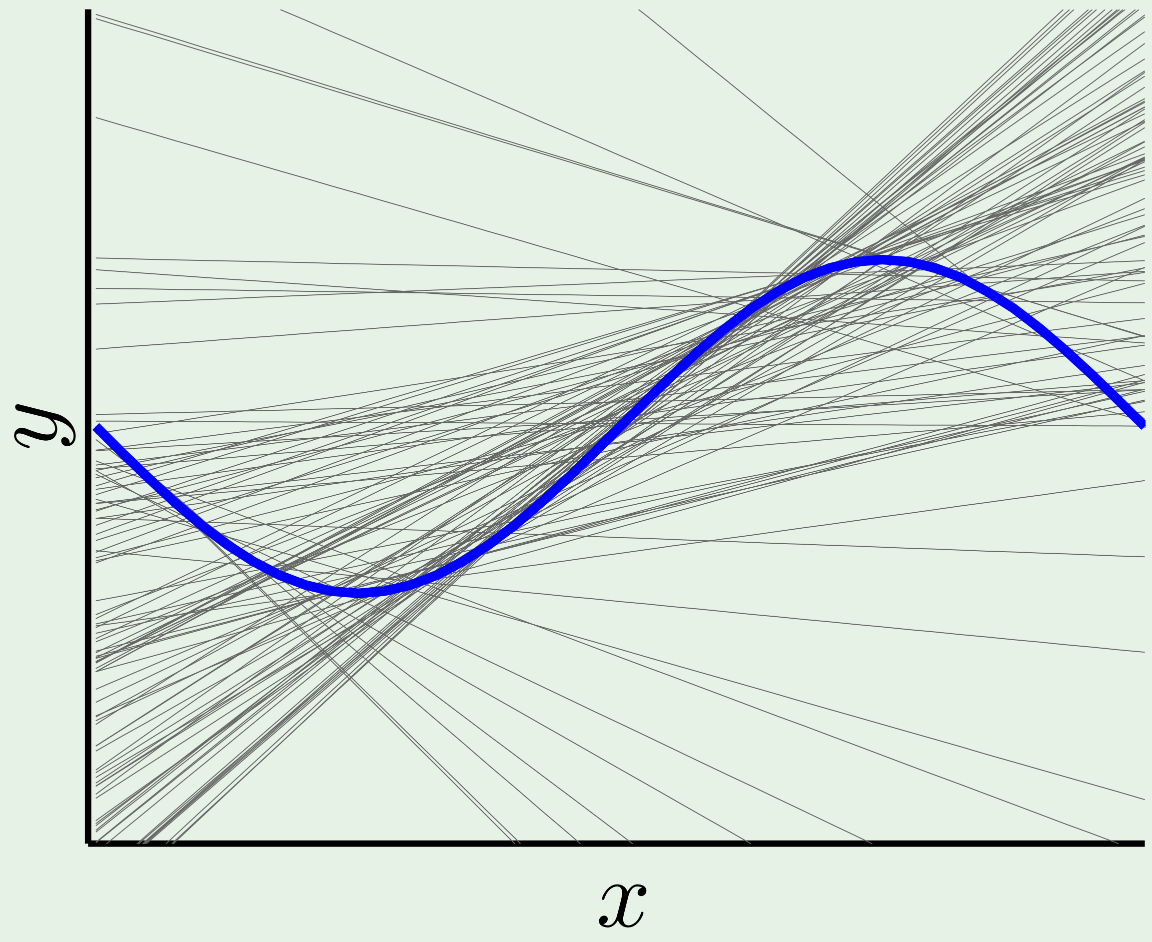
$\mathcal{H}_1$

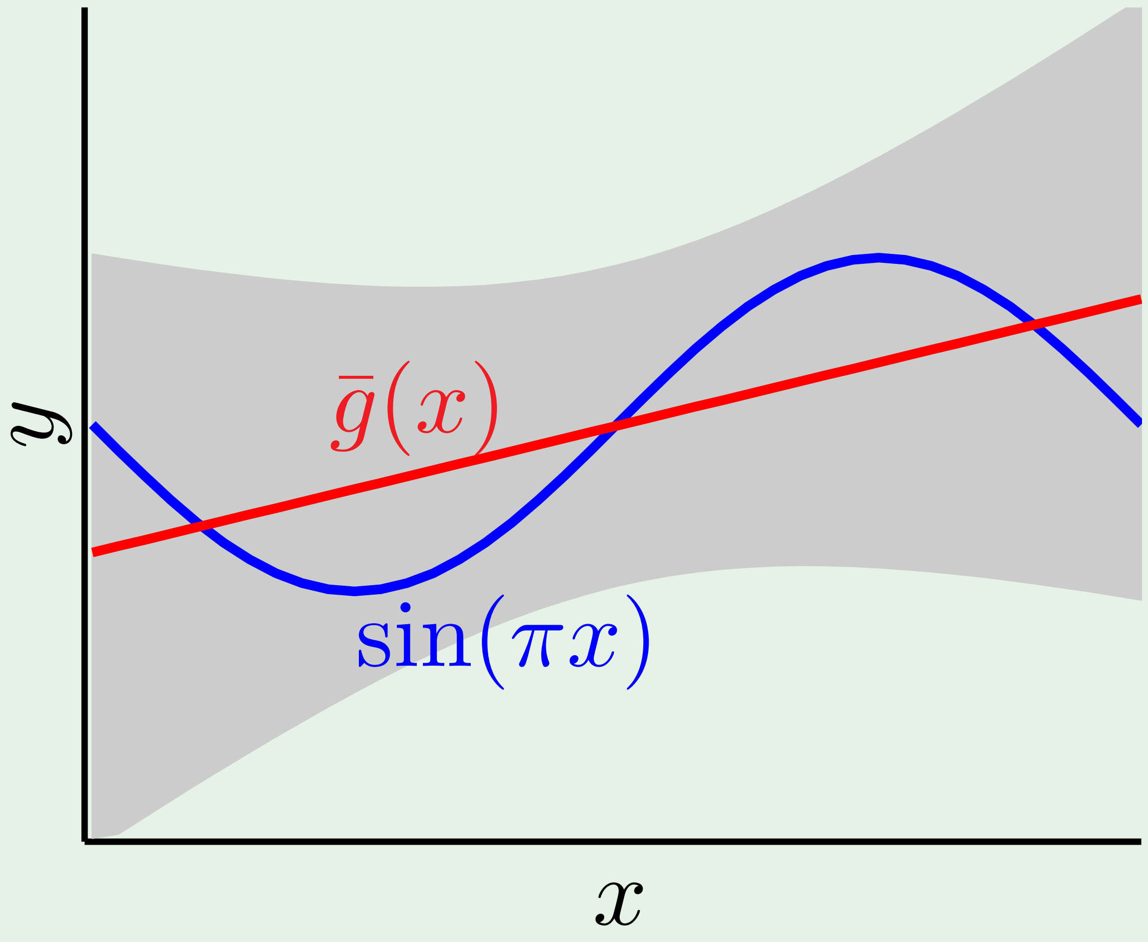


Bias and variance - $\mathcal{H}_0$

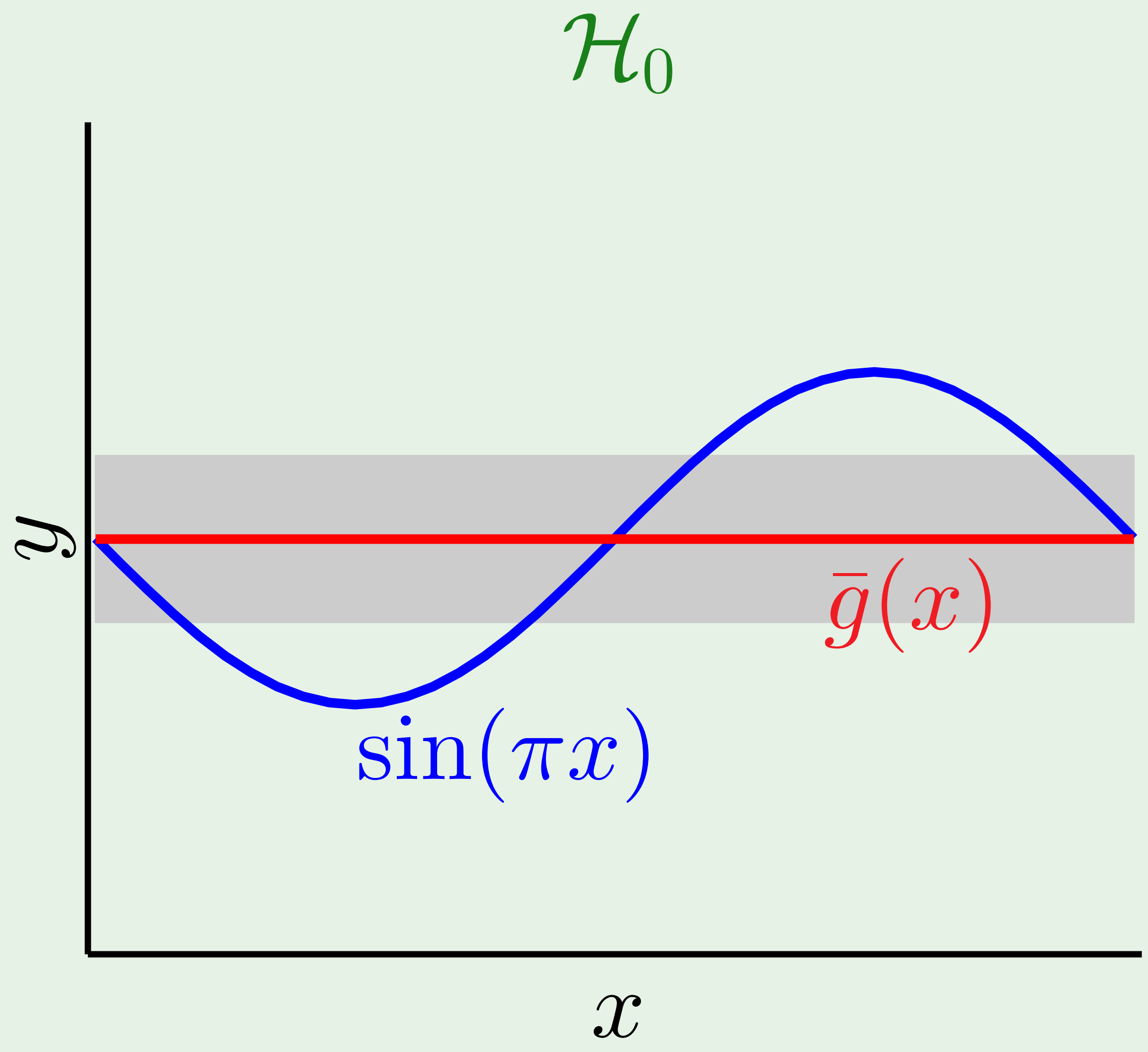


Bias and variance - $\mathcal{H}_1$

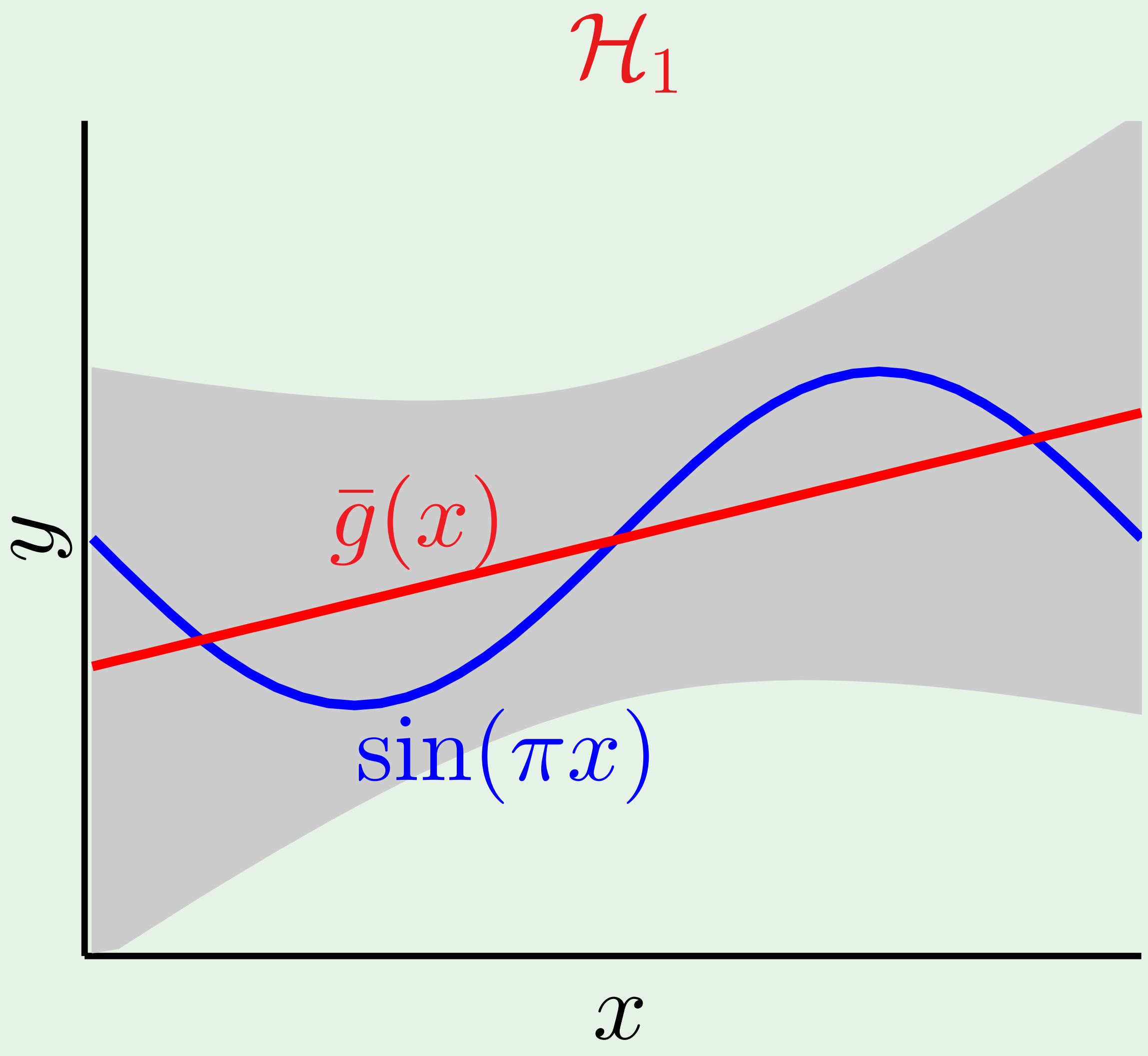




and the winner is ...



bias $=$ **0.50** var $=$ **0.25**



bias $=$ **0.21** var $=$ **1.69**

Lesson learned

Match the '**model complexity**'

to the **data resources**, not to the **target complexity**

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- Learning Curves

Expected E_{out} and E_{in}

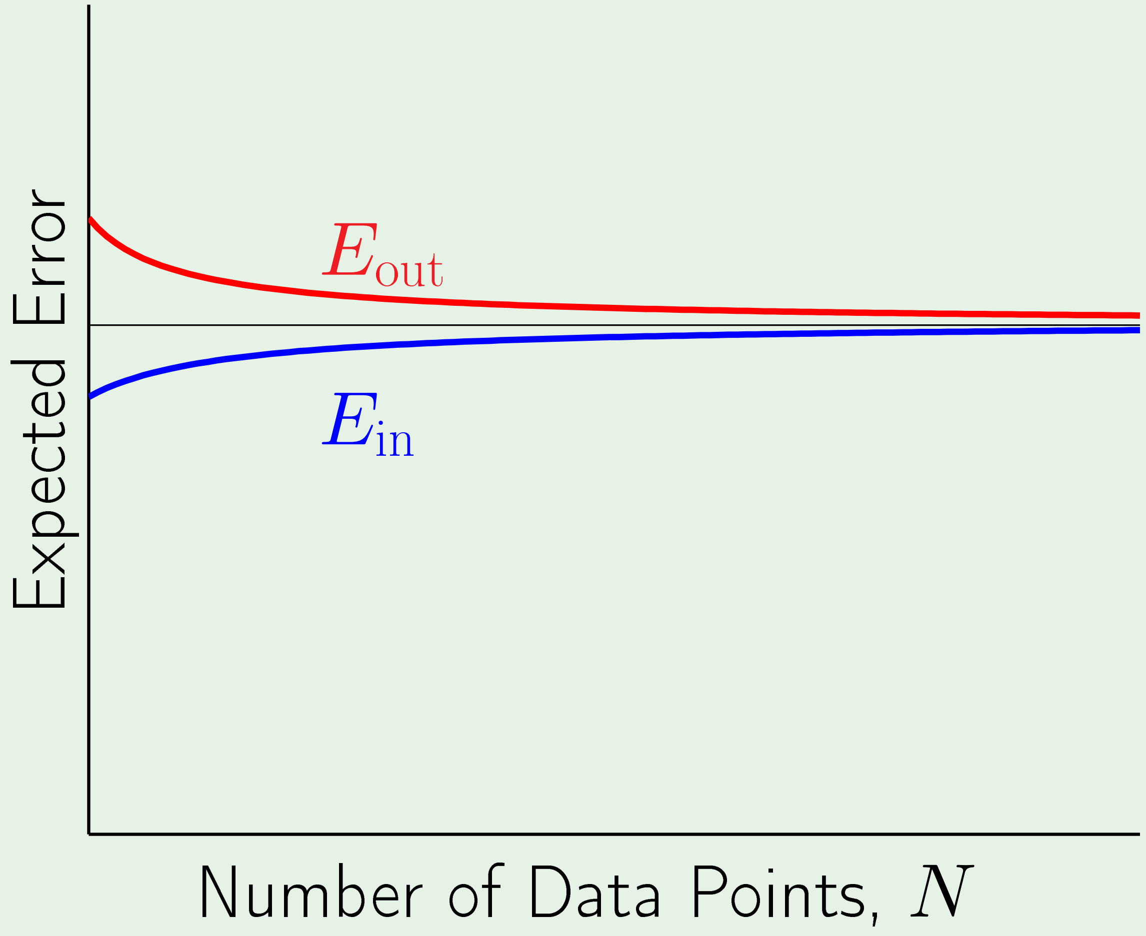
Data set $\mathcal{D}$ of size N

Expected out-of-sample error $\mathbb{E}_{\mathcal{D}}[E_{\text{out}}(g^{(\mathcal{D})})]$

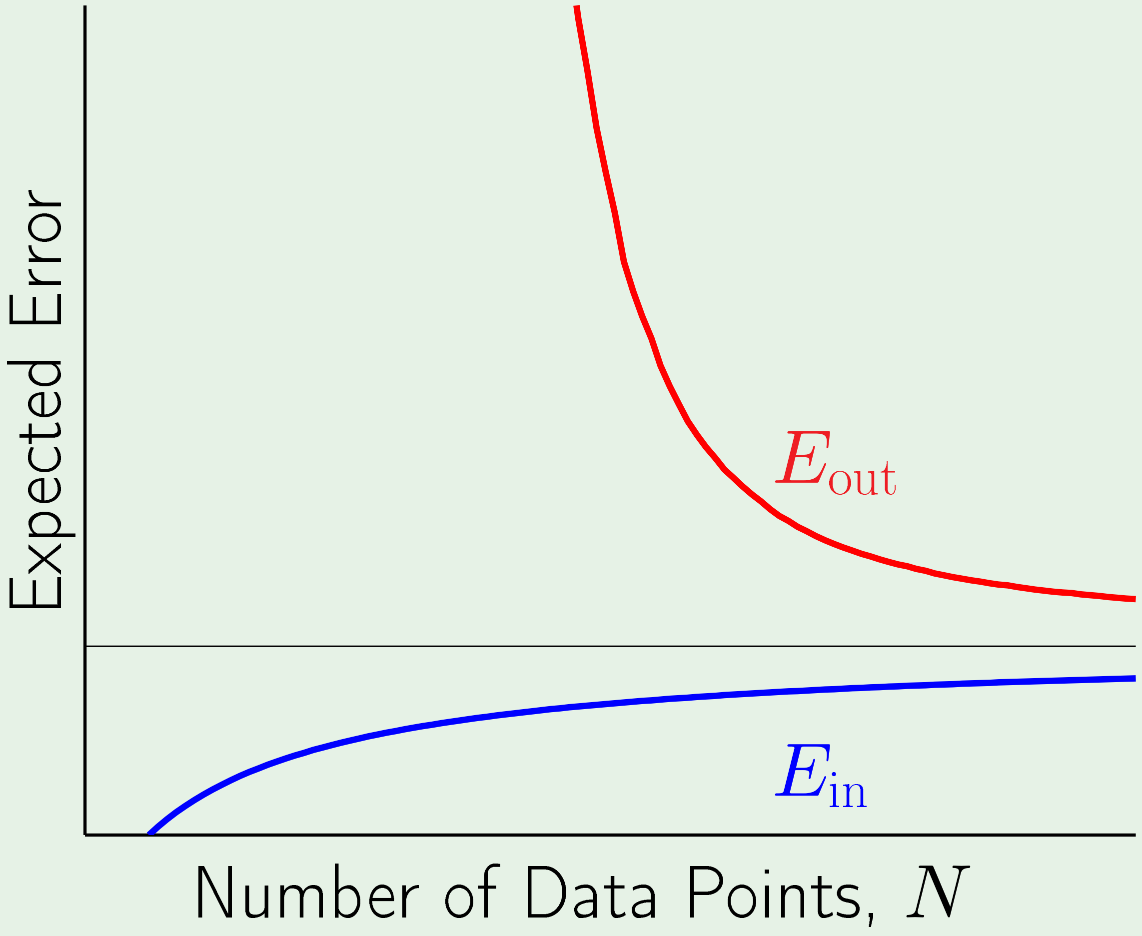
Expected in-sample error $\mathbb{E}_{\mathcal{D}}[E_{\text{in}}(g^{(\mathcal{D})})]$

How do they vary with N?

The curves

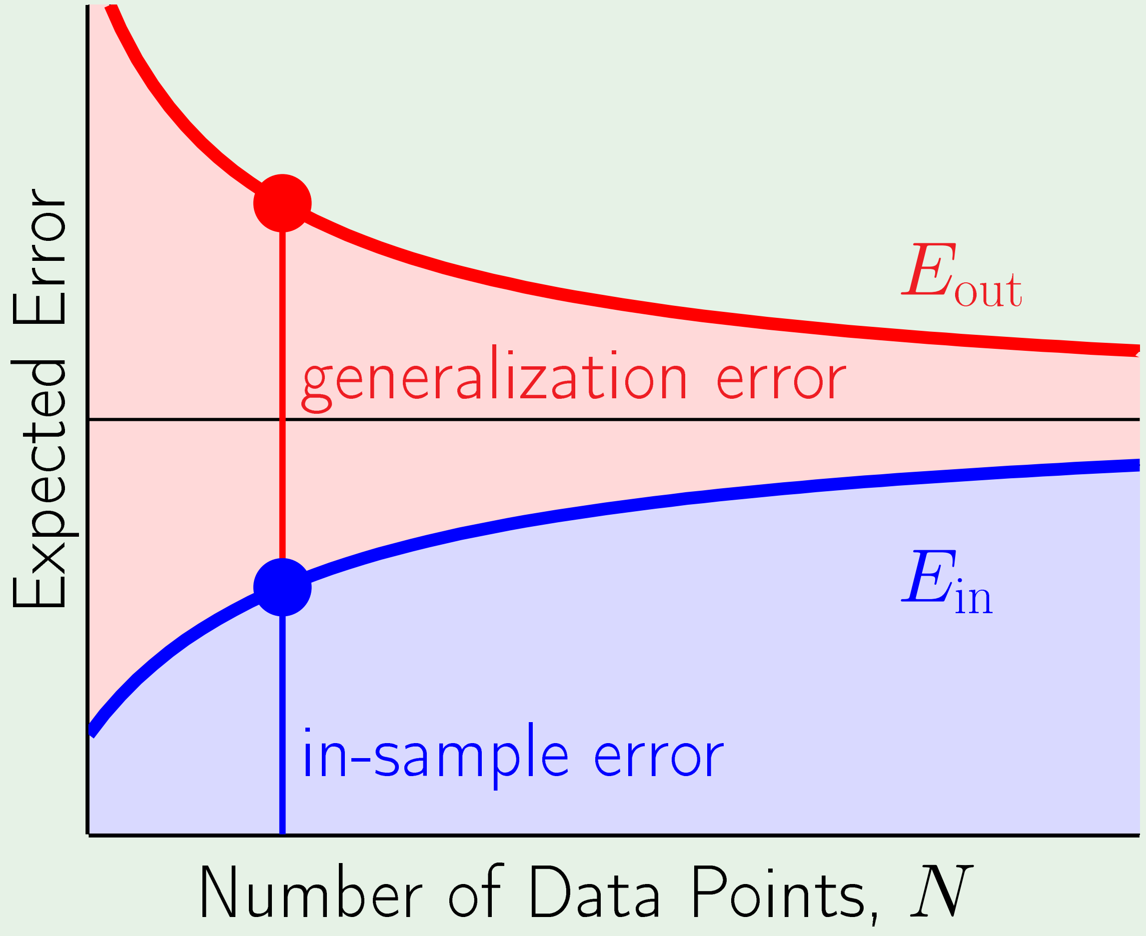


Simple Model

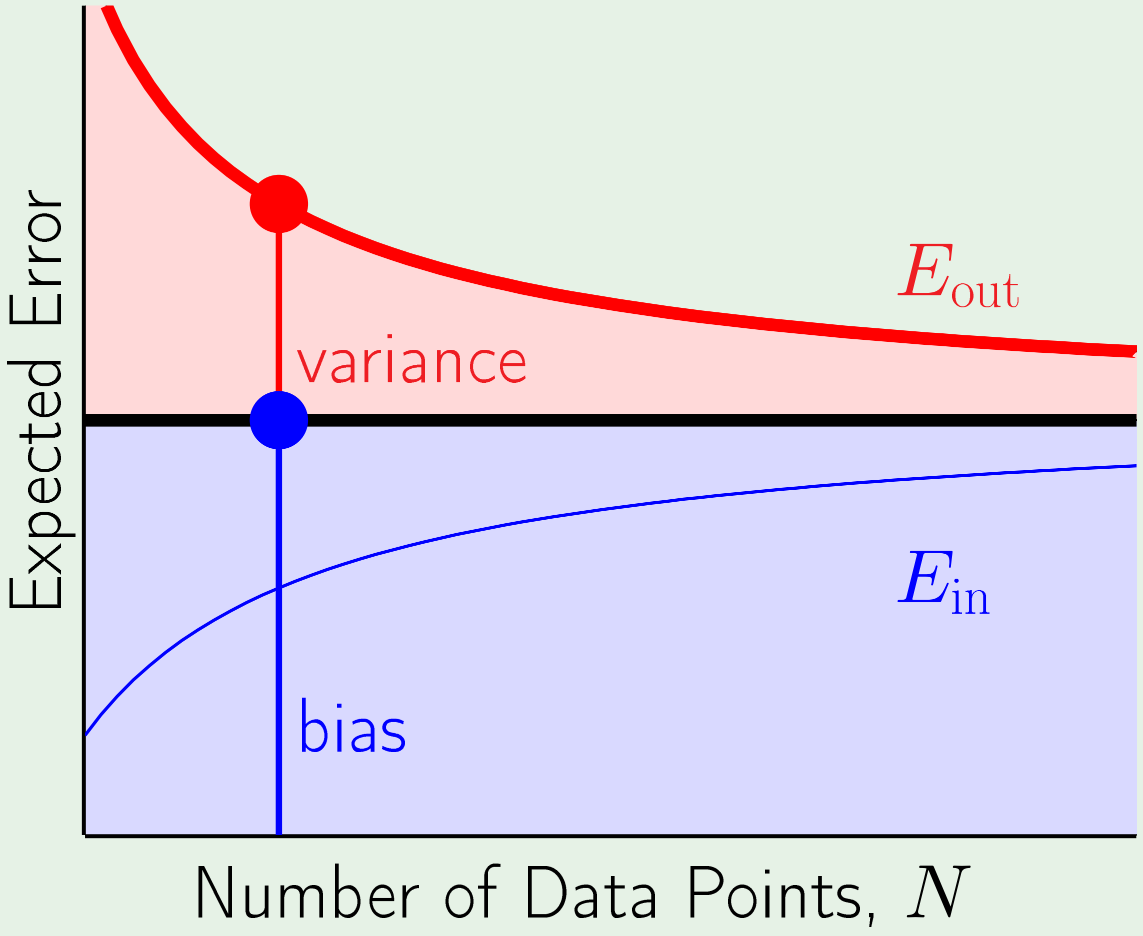


Complex Model

VC versus bias-variance



VC analysis



bias-variance

Linear regression case

Noisy target $y = \mathbf{w}^{*\intercal}\mathbf{x} + \text{noise}$

Data set $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$

Linear regression solution: $\mathbf{w} = (\mathrm{X}^\intercal\mathrm{X})^{-1}\mathrm{X}^\intercal\mathbf{y}$

In-sample error vector $= \mathrm{X}\mathbf{w} - \mathbf{y}$

'Out-of-sample' error vector $= \mathrm{X}\mathbf{w} - \mathbf{y}'$

Learning curves for linear regression

Best approximation error $= \sigma^2$

Expected in-sample error $= \sigma^2 \left(1 - \frac{d+1}{N}\right)$

Expected out-of-sample error $= \sigma^2 \left(1 + \frac{d+1}{N}\right)$

Expected generalization error $= 2\sigma^2 \left(\frac{d+1}{N}\right)$