Approximation-generalization tradeoff

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

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

Less complex $\mathcal{H} \Longrightarrow$ 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

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

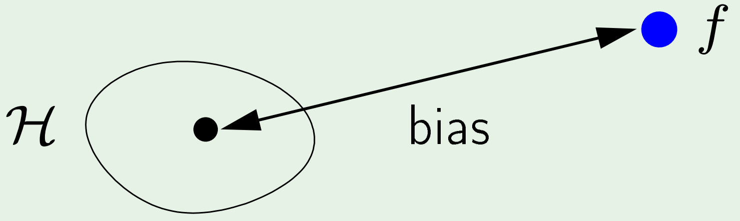
Therefore, $\mathbb{E}_{\mathcal{D}}\left[E_{\text{out}}(g^{(\mathcal{D})})\right] = \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]\right]$

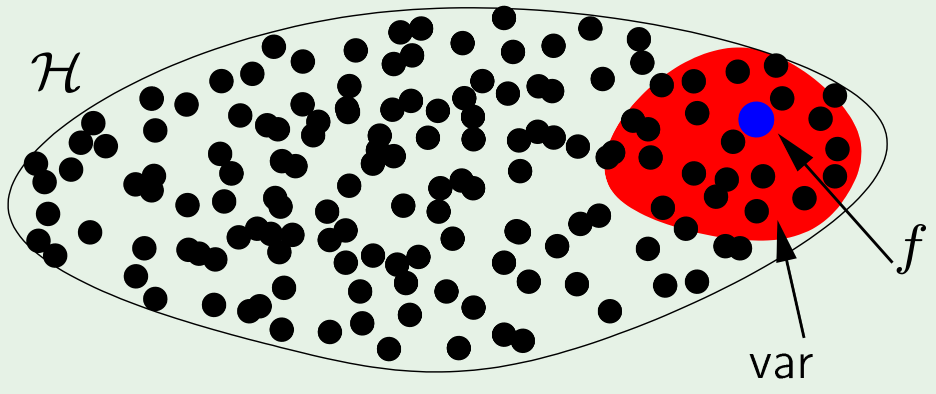
$$= \mathbb{E}_{\mathbf{x}}[\textsf{bias}(\mathbf{x}) + \textsf{var}(\mathbf{x})]$$

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

The tradeoff

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





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