Bias Variance Tradeoff

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Definitions

Definition (*Average Hypothesis at x*)**.** For each point $x \in X$ define the average hypothesis at x as the expectation of $g^{(D)}(x)$ with respect to $\mathcal{D}$ as

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

Definition (*Prediction Error at x*)**.** For each point $x \in X$ define the prediction error at x as the expected squared error between the ground truth $f(x)$ at x and the learned hypothesis $g^{(D)}(x)$ at x as

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

where the expectation is with respect to the set of data sets $\mathcal{D}$.

Derivation

To derive the bias variance decomposition at x, we "insert" the average hypothesis $\bar{g}(x)$ in the prediction error at x.

$$\begin{aligned}
\mathbb{E}_{\mathcal{D}}\left[\left(f(x) - g^{(D)}(x)\right)^2\right] &= \mathbb{E}_{\mathcal{D}}\left[\left(f(x) - \bar{g}(x) + \bar{g}(x) - g^{(D)}(x)\right)^2\right] \\
&= \mathbb{E}_{\mathcal{D}}\left[(f(x) - \bar{g}(x))^2 + (\bar{g}(x) - g^{(D)}(x))^2\right] && \text{(I)} \\
&= \mathbb{E}_{\mathcal{D}}\left[(f(x) - \bar{g}(x))^2\right] + \mathbb{E}_{\mathcal{D}}\left[(\bar{g}(x) - g^{(D)}(x))^2\right] \\
&= (f(x) - \bar{g}(x))^2 + \mathbb{E}_{\mathcal{D}}\left[(\bar{g}(x) - g^{(D)}(x))^2\right] && \text{(II)} \\
&= \quad \text{bias(x)} \quad + \quad \text{variance(x)},
\end{aligned}$$

where in (I) we used that $2\,\mathbb{E}_{\mathcal{D}}\left[g(x) - \bar{g}(x)\right] = 0$ and in (II) we used that neither f nor $\bar{g}$ depends on $D \in \mathcal{D}$. Taking the expectation with respect to the domain X yields:

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$$\begin{aligned}
\mathbb{E}_{\mathcal{D},X}\left[\left(f(x) - g^{(D)}(x)\right)^2\right] &= \mathbb{E}_X\left[(f(x) - \bar{g}(x))^2\right] + \mathbb{E}_{\mathcal{D},X}\left[(\bar{g}(x) - g^{(D)}(x))^2\right] \\
&= \quad \text{bias} \quad + \quad \text{variance}
\end{aligned}$$