Bias variance decomposition

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Let $y = f(x) + \varepsilon$ where ε is iid noise with zero mean and variance σ^2 .

We estimate f using \hat{f} . Then the expected MSE for a new y at x_0 will be equal to

$$E[(y - \hat{f}(x_0))^2] = [Bias(\hat{f}(x_0))]^2 + Var(\hat{f}(x_0)) + \sigma^2$$

where

$$\begin{aligned} \operatorname{Bias}(\hat{f}(x_0)) &= \operatorname{E}[\hat{f}(x_0)] - f(x_0) \\ \operatorname{and} & \operatorname{Var}(\hat{f}(x_0)) &= \operatorname{E}\left[\left(\hat{f}(x_0) - \operatorname{E}[\hat{f}(x_0)]\right)^2\right]. \end{aligned}$$

Proof

We will abbreviate $f = f(x_0)$ and $\hat{f} = \hat{f}(x_0)$.

Since f is deterministic, E[f] = f and Var[f] = 0.

$$\begin{split} \mathbf{E}[(y-\hat{f})^2] &= \mathbf{E}[(y-f+f-\hat{f})^2] \\ &= \mathbf{E}[(y-f)^2 + (f-\hat{f})^2 + 2(y-f)(f-\hat{f})] \\ &= \sigma^2 + \mathbf{E}[(\hat{f}-f)^2] + 2\mathbf{E}[(y-f)(f-\hat{f})] \end{split}$$

Now

$$E[(\hat{f} - f)^{2}] = E[(\hat{f} - E[\hat{f}] + E[\hat{f}] - f)^{2}]$$

$$= E[(\hat{f} - E[\hat{f}])^{2}] + (E[\hat{f}] - f)^{2} + 2E[(\hat{f} - E[\hat{f}])(E[\hat{f}] - f)]$$

$$= Var[\hat{f}] + Bias^{2}[\hat{f}] + 2E[(\hat{f} - E[\hat{f}])(E[\hat{f}] - f)]$$

Both cross-product terms are equal to zero as can be shown by expansion:

$$\begin{split} \mathbf{E}[(y-f)(f-\hat{f})] &= \mathbf{E}[yf-f^2-y\hat{f}+f\hat{f}] \\ &= f^2-f^2-\mathbf{E}[y\hat{f}]+f\mathbf{E}[\hat{f}] \\ &= -\mathbf{E}[(f+\varepsilon)\hat{f}]+f\mathbf{E}[\hat{f}] \\ &= -\mathbf{E}[f\hat{f}]-\mathbf{E}[\varepsilon\hat{f}]+f\mathbf{E}[\hat{f}] \\ &= 0 \end{split}$$

$$\begin{split} \mathbf{E}[(\hat{f} - \mathbf{E}[\hat{f}])(\mathbf{E}[\hat{f}] - f)] &= \mathbf{E}\left[\hat{f}\mathbf{E}[\hat{f}] - \mathbf{E}[\hat{f}]\mathbf{E}[\hat{f}] - \hat{f}f + \mathbf{E}[\hat{f}]f\right] \\ &= \mathbf{E}[\hat{f}]\mathbf{E}[\hat{f}] - \mathbf{E}[\hat{f}]\mathbf{E}[\hat{f}] - \mathbf{E}[\hat{f}]f + \mathbf{E}[\hat{f}]f \\ &= 0 \end{split}$$