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

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

where

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

Proof

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

Since f is deterministic, $\mathrm{E}[f] = f$ and $\mathrm{Var}[f] = 0$.

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

Now

$$\begin{aligned} \mathrm{E}[(\hat{f}-f)^2] &= \mathrm{E}[(\hat{f} - \mathrm{E}[\hat{f}] + \mathrm{E}[\hat{f}] - f)^2] \\ &= \mathrm{E}[(\hat{f} - \mathrm{E}[\hat{f}])^2] + (\mathrm{E}[\hat{f}] - f)^2 + 2\mathrm{E}[(\hat{f} - \mathrm{E}[\hat{f}])(\mathrm{E}[\hat{f}] - f)] \\ &= \mathrm{Var}[\hat{f}] + \mathrm{Bias}^2[\hat{f}] + 2\mathrm{E}[(\hat{f} - \mathrm{E}[\hat{f}])(\mathrm{E}[\hat{f}] - f)] \end{aligned}$$

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

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

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