

Bias variance decomposition

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Let $y_i = f(x_i) + \varepsilon_i$ 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

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

where

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

Proof

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

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

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

Now

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

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

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

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