Bias Variance Outline

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Average Prediction Error at x_0

$$E_{\text{train}}\left[\left(y_0 - f_{\hat{\beta}}(x_0)\right)^2\right] = \sigma^2 + \left[\text{Bias}\left(f_{\hat{\beta}}(x_0)\right)\right]^2 + \text{Var}\left(f_{\hat{\beta}}(x_0)\right)$$

The notation $E_{\text{train}}\left[\left(y_0 - f_{\hat{\beta}}(x_0)\right)^2\right]$ defines the *expected test MSE*, and refers to the average test MSE that we would obtain if we repeatedly estimated f using a large number of training sets, and tested each at x_0. The overall expected test MSE can be computed by averaging $E_{\text{train}}\left[\left(y_0 - f_{\hat{\beta}}(x_0)\right)^2\right]$ over all possible values of x_0 in the test set.

Derivation

$$E_{\text{train}}\left[\left(y_0 - f_{\hat{\beta}}(x_0)\right)^2\right] = E_{\text{train}}\left[\left((y_0 - f_{\beta}(x_0)) + (f_{\beta}(x_0) - f_{\hat{\beta}}(x_0))\right)^2\right]$$

Note that

$$E\left[(a+b)^2\right] = E\left[a^2 + 2ab + b^2\right]$$

Derivation Continued

$$\begin{aligned} E_{\textsf{train}}\left[\left(y_0 - f_\beta(x_0)\right)^2\right] + 2E_{\textsf{train}}\left[\left(y_0 - f_\beta(x_0)\right)\left(f_\beta(x_0) - f_{\hat{\beta}}(x_0)\right)\right] \\ + E_{\textsf{train}}\left[\left(f_\beta(x_0) - f_{\hat{\beta}}(x_0)\right)^2\right] \end{aligned}$$

Bullet

Consider shortening the notation for the middle term:

$$2E_{\textsf{train}}\left[\big(y_0 - f_\beta(x_0)\big)\big(f_\beta(x_0) - f_{\hat{\beta}}(x_0)\big)\right] = 2E\left[\big(y - f\big)\big(f - \hat{f}\big)\right]$$

Note that $y - f = \epsilon$ and that $E(\epsilon) = 0$ so the middle term is 0 and we are left with the first and third terms.

First and Third Terms

$$E\left[(y-f)^2\right] + E\left[(f-\hat{f})^2\right]$$

Note that:

- $E\left[(y-f)^2\right] = E\left[(\epsilon - E(\epsilon))^2\right] = \sigma^2$
- $E\left[(f-\hat{f})^2\right] = MSE(\hat{f})$.
- $MSE(\hat{f}) = E\left[(f-\hat{f})^2\right] = E\left[\left((f-\bar{f}) + (\bar{f}-\hat{f})\right)^2\right]$

MSE

Using the same trick as before. . . the middle term drops out!

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

That is $2E\left[(f-\bar{f})(\bar{f}-\hat{f})\right]=0$ since $E\left[\bar{f}-\hat{f}\right]=\bar{f}-\bar{f}=0$.

More

- $MSE(\hat{f}) = E\left[(f - \bar{f})^2\right] + E\left[(\bar{f} - \hat{f})^2\right]$
- $MSE(\hat{f}) = \left[\text{Bias}(\hat{f})\right]^2 + \text{Var}\left[\hat{f}\right]$

So,

$$E_{\text{train}}\left[\left(y_0 - f_{\hat{\beta}}(x_0)\right)^2\right] = \sigma^2 + \left[\text{Bias}\left(f_{\hat{\beta}}(x_0)\right)\right]^2 + \text{Var}\left(f_{\hat{\beta}}(x_0)\right)$$

Or

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