An Observation About Subsection 6.6: On Average Training MSE Underestimates Validation MSE

The validating mean squared error is often used to evaluate the performance of a predictor. The expected value of the validating mean squared error, taken over the distribution of training data y and validating data y_v is shown in equation (6.65) on page 285:

$$\mathrm{E}_{y,y_v}(\mathrm{MSE}_v) = \sigma^2 + \frac{1}{N}\sum_i \mathrm{Var}(\hat{y}_{v,i}) + \mathrm{bias}^2. \tag{6.65}$$

On the other hand, the expected value of the training mean squared error, taken over the distribution of training data y is shown in equation (6.66):

$$\mathrm{E}_y(\mathrm{MSE}_t) = \sigma^2 + \frac{1}{N}\sum_i \mathrm{Var}(\hat{y}_i) + \mathrm{bias}^2 - \frac{2}{N}\sum_i \mathrm{Cov}(y_i, \hat{y}_i), \tag{6.66}$$

indicating that the training mean squared error

$$\mathrm{MSE}_t = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

is a poor estimate of (6.65).

The predicted values in training and validating data are $\hat{y}_i = \hat{f}(x_i)$ and $\hat{y}_{v,i} = \hat{f}(x_{v,i})$, a function of known covariates x_i and $x_{v,i}$, respectively. These covariates are not necessarily the same. However with common covariates such as genetic markers, for a given number of these covariates, as the number of records increases the second terms after the equal sign of equations (6.65) and (6.66) become smaller and more alike. Regardless of the number of records, if predictions are evaluated at the same values of the covariates in the training and validating data, $E(y_i) = E(y_{v,i})$, $\hat{y}_{v,i} = \hat{y}_i$ and $\frac{1}{N}\sum_i \mathrm{Var}(\hat{y}_{v,i}) = \frac{1}{N}\sum_i \mathrm{Var}(\hat{y}_i)$. This is not made explicit in the book. Then it follows that

$$\mathrm{E}_y(\mathrm{MSE}_t) = \mathrm{E}_{y,y_v}(\mathrm{MSE}_v) - \frac{2}{N}\sum_i \mathrm{Cov}(y_i, \hat{y}_i). \tag{6.67}$$

Evaluation of training and validating MSE at the same value of the covariates is not as unrealistic as it may seem at first glance. When the objective is to obtain a measure of the validating MSE committing all the records as training data, it is reasonable to perform the calculations at the value of the covariates available in the training data.

References