Saarland University

The Elements of Stastical Learning

Assignement 4

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Prove that for linear and polynomial least squares regression, the LOOCV estimate for the test MSE can be calculated using the following formula:

$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{y_i - \hat{y}_i}{1 - h_i} \right)^2 \tag{1}$$

Where h_i is the leverage (3.37, ISLR p98)

$$h_i = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_{i'=1}^n (x_i' - \bar{x})^2}$$
 (2)

We first have this equation, that can take long if n is big because it has to fit every model.

$$MSE_i = (y_i - \hat{y_i})^2$$

$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^{n} MSE_i$$

So knowing that $\hat{y} = Hy$ and as it is a Leave One Out cross validation, we fit n times the model with one element out. So we have:

$$H = X(X^T X)^{-1} X^T$$

$$H^{-i} = X_{-i} (X_{-i}^T X_{-i})^{-1} X_{-i}^T$$

The hat matrix with all the data and with one out, respectively

Then we have

$$\hat{y}_i = x_i^T [X(X^T X)^{-1} X^T] y$$

$$\hat{y}_{-i} = x_i^T [X_{-i} (X_{-i}^T X_{-i})^{-1} X_{-i}^T] y_{-i}$$

The fitted values at x_i when using all the data points and when leaving one out. We can then to the following:

$$\hat{y}_{-i} = \sum_{i \neq j} H_{ij} y_j + H_{ii} \hat{y}_{-i}$$

$$\hat{y}_{-i} = \sum_{j}^{m} H_{ij} y_j - H_{ii} y_i + H_{ii} \hat{y}_{-i}$$

$$\hat{y}_{-i} = \hat{y}_i - H_{ii} y_i + H_{ii} \hat{y}_{-i}$$

We substitute the in the prediction error:

$$y_i - \hat{y}_{-i} = y_i - (\hat{y}_i - H_{ii}y_i + H_{ii}\hat{y}_{-i})$$

$$y_{i} - H_{ii}y_{i} - \hat{y}_{-i} - H_{ii}\hat{y}_{-i} = y_{i} - \hat{y}_{i}$$
$$y_{i} - \hat{y}_{-i} = \frac{y_{i} - \hat{y}_{i}}{1 - H_{ii}}$$

Taking the mean square error leads to equation 1.