

Ex. 6.7

$$CV(\hat{f}) = \frac{1}{N} \sum_{i=1}^N (y_i - \hat{f}^{(-i)}(x_i))^2$$

for $\hat{f}(x_0) = b(x_0)^T (B^T W(x_0) B)^{-1} B^T W(x_0) Y$,

We will show that:

$$CV(\hat{f}) = \frac{1}{N} \sum_{i=1}^N \frac{(y_i - \hat{f}(x_i))^2}{(1 - h_i)^2}, \quad \text{where } h_i \text{ is a function of } x_i.$$

Notation: For a matrix or vector A , $A^{(-i)}$ is the corresponding matrix or vector with the i^{th} row/element removed. Additionally, $A^{(i)}$ refers to that i^{th} row/element.

The proof is split into 2 parts:

Part 1/

Wish to show that:

$$(*) \quad \hat{f}^{(-i)}(x_i) = \frac{\hat{f}(x_i) - h_i y_i}{1 - h_i}$$

First some results we will use later:

The Sherman-Morrison Formula states that for V an invertible $P \times P$ matrix; a P -vector q ; and λ constant:

$$(1) \quad (V + \lambda q q^T)^{-1} = V^{-1} - \frac{\lambda V^{-1} q q^T V^{-1}}{1 + \lambda q^T V^{-1} q}$$

for B an $N \times P$ matrix and W a diagonal $N \times N$ matrix with i^{th} diagonal element w_i :

$$(2) \quad \sum_{i=1}^N w_i B^{(i)T} B^{(i)} = B^T W B$$

Since $B^{(i)}$ is simply the basis expansion of x_i we can follow the book's notation in referring to it as $b(x_i)$ from here on.

We will need to Prove one more identity:

Now, using ② We can see that:

$$\begin{aligned} (B^{(-i)T} W^{(-i)} B^{(-i)})^{-1} &= (B^T W B - b(x_i) W(x_i) b(x_i)^T)^{-1} \\ &= (B^T W B)^{-1} + \frac{W(x_i) (B^T W B)^{-1} b(x_i) b(x_i)^T (B^T W B)^{-1}}{1 - W(x_i) b(x_i)^T (B^T W B)^{-1} b(x_i)} \quad (\text{using ②}) \end{aligned}$$

$$\begin{aligned} \Rightarrow (B^{(-i)T} W^{(-i)} B^{(-i)})^{-1} b(x_i) W(x_i) &= (B^T W B)^{-1} b(x_i) W(x_i) \\ &+ (B^T W B)^{-1} b(x_i) W(x_i) \left(\frac{b(x_i)^T (B^T W B)^{-1} b(x_i) W(x_i)}{1 - b(x_i)^T (B^T W B)^{-1} b(x_i) W(x_i)} \right) \end{aligned}$$

Giving:

$$\textcircled{3} (B^{(-i)T} W^{(-i)} B^{(-i)})^{-1} b(x_i) W(x_i) = (B^T W B)^{-1} b(x_i) W(x_i) \left(\frac{1}{1 - h_i} \right)$$

$$\text{Where } h_i = b(x_i)^T (B^T W B)^{-1} b(x_i) W(x_i)$$

finally, We can make some progress on the original Problem. From the definition of $\hat{\beta}$ in 6.8 we have:

$$\hat{\beta} = (B^T W B)^{-1} B^T W y$$

$$\Rightarrow (B^T W B) \hat{\beta} = B^T W y$$

$$\begin{aligned} \Rightarrow (B^{(-i)T} W^{(-i)} B^{(-i)} + b(x_i) W(x_i) b(x_i)^T) \hat{\beta} &= B^{(-i)T} W^{(-i)} y^{(-i)} + b(x_i) W(x_i) y_i \quad \left(\begin{array}{l} \text{similar logic} \\ \text{to ②} \end{array} \right) \end{aligned}$$

$$\Rightarrow (I + (B^{(-i)T} W^{(-i)} B^{(-i)})^{-1} b(x_i) W(x_i) b(x_i)^T) \hat{\beta}$$

$$= \hat{\beta}^{(-i)} + (B^{(-i)T} W^{(-i)} B^{(-i)})^{-1} b(x_i) W(x_i) y_i$$

Now the residual of observation i is defined as:

$$r_i = y_i - b(x_i)^T \hat{\beta} \quad \text{implying} \quad y_i = b(x_i)^T \hat{\beta} + r_i \quad (4)$$

Now when we expand y_i in the previous equation some convenient cancellation occurs and we are left with:

$$\hat{\beta} = \hat{\beta}^{(-i)} + (B^{(-i)T} W^{(-i)} B^{(-i)})^{-1} b(x_i) W(x_i) r_i$$

$$\Rightarrow b(x_i)^T \hat{\beta} = b(x_i)^T \hat{\beta}^{(-i)} + b(x_i)^T (B^{(-i)T} W^{(-i)} B^{(-i)})^{-1} b(x_i) W(x_i) r_i \quad (\text{using } (3))$$

$$\Rightarrow \hat{f}(x_i) = \hat{f}^{(-i)}(x_i) + b(x_i)^T (B^T W B)^{-1} b(x_i) W(x_i) \left(\frac{1}{1 - h_i} \right) r_i$$

$$\Rightarrow \hat{f}(x_i) = \hat{f}^{(-i)}(x_i) + \left(\frac{h_i}{1 - h_i} \right) r_i \quad (\text{From definition of } h_i)$$

$$\Rightarrow \hat{f}^{(-i)}(x_i) = \hat{f}(x_i) - \left(\frac{h_i}{1 - h_i} \right) (y_i - \hat{f}(x_i)) \quad (\text{using } (4) \text{ again})$$

$$= \hat{f}(x_i) \left(1 - \frac{h_i}{1 - h_i} \right) - \frac{h_i y_i}{1 - h_i}$$

$$\hat{f}^{(-i)}(x_i) = \frac{\hat{f}(x_i) - h_i y_i}{1 - h_i} \quad \text{Proving } (*) \text{ as required}$$

Part 2//

The next step is to Sub (*) into the original Cross Validation expression. In Particular:

$$y_i - \hat{f}^{(-i)}(x_i) = y_i - \frac{\hat{f}(x_i) - h_i y_i}{1 - h_i}$$

$$= \frac{y_i - h_i y_i - \hat{f}(x_i) + h_i y_i}{1 - h_i}$$

$$= \frac{y_i - \hat{f}(x_i)}{1 - h_i}$$

Proving that the leave-one-out cross-validated residual sum-of-squares for local Polynomial regression is given by

$$CV(\hat{f}) = \frac{1}{N} \sum_{i=1}^N (y_i - \hat{f}^{(-i)}(x_i))^2 = \frac{1}{N} \sum_{i=1}^N \left(\frac{y_i - \hat{f}(x_i)}{1 - h_i} \right)^2$$

$$\text{where } h_i = b(x_i)^T (B^T W B)^{-1} b(x_i) W(x_i)$$