

Identities for the Leave-one-out LS estimates

To calculate these jackknife (or leave-one-out) LS estimates, such as $\hat{\boldsymbol{\beta}}_{(i)}$ and $\hat{\sigma}_{(i)}$, we don't need to run the model n times. Using the Sherman-Morrison formula (a.k.a. Woodbury matrix identity), we have

$$[\mathbf{X}_{(i)}^t \mathbf{X}_{(i)}]^{-1} = (\mathbf{X}^t \mathbf{X})^{-1} + \frac{(\mathbf{X}^t \mathbf{X})^{-1} \mathbf{x}_i \mathbf{x}_i^t (\mathbf{X}^t \mathbf{X})^{-1}}{1 - h_i}.$$

Consequently,

$$\begin{aligned} \mathbf{x}_i^t (\mathbf{X}_{(i)}^t \mathbf{X}_{(i)})^{-1} \mathbf{x}_i &= \frac{h_i}{1 - h_i} & \hat{\boldsymbol{\beta}}_{(i)} &= \hat{\boldsymbol{\beta}} - \frac{(\mathbf{X}^t \mathbf{X})^{-1} \mathbf{x}_i r_i}{1 - h_i} \\ y_i - \hat{y}_{(i)} &= \frac{1}{1 - h_i} (y_i - \hat{y}_i), & \hat{\sigma}_{(i)}^2 &= \hat{\sigma}^2 \frac{(n - p) - (r_i^*)^2}{n - p - 1} \end{aligned}$$

$$\begin{aligned} \text{Jackknife Residual } t_i &= \frac{y_i - \hat{y}_{(i)}}{\hat{\sigma}_{(i)} [1 + \mathbf{x}_i^t (\mathbf{X}_{(i)}^t \mathbf{X}_{(i)})^{-1} \mathbf{x}_i]^{1/2}} \\ &= \frac{r_i}{\hat{\sigma}_{(i)} \sqrt{1 - h_i}} = r_i^* \left[\frac{n - p - 1}{n - p - (r_i^*)^2} \right]^{1/2} \\ \text{Cook's distance } D_i &= \frac{\|\mathbf{X} \hat{\boldsymbol{\beta}} - \mathbf{X} \hat{\boldsymbol{\beta}}_{(i)}\|^2}{p \hat{\sigma}^2} = \frac{(\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{(i)})^t (\mathbf{X}^t \mathbf{X}) (\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{(i)})}{p \hat{\sigma}^2} \\ &= \frac{r_i^2}{p \hat{\sigma}^2} \frac{h_i}{(1 - h_i)^2} = \frac{(r_i^*)^2}{p} \left(\frac{h_i}{1 - h_i} \right) \end{aligned}$$

where $r_i^* = r_i / (\hat{\sigma} \sqrt{1 - h_i})$ is the standardized residual for the i th sample.

The Leave-one-out Prediction Error

We provide an alternative proof for the leave-one-out prediction error

$$y_i - \hat{y}_{(i)} = \frac{1}{1 - h_i} (y_i - \hat{y}_i). \quad (1)$$

Consider **two** regression models:

- *Model I*: the regression model on the n data points $\mathbf{y}_{n \times 1}$, where

$$\hat{y}_i = h_i y_i + \sum_{j \neq i} H_{ij} y_j. \quad (2)$$

- *Model II*: the regression model on a set of new data points $\mathbf{y}_{n \times 1}^*$, which are almost the same as the original data \mathbf{y} except the i th element,

$$y_i^* = \hat{y}_{(i)} = \mathbf{x}_i^t \hat{\boldsymbol{\beta}}_{(i)},$$

where $\hat{\beta}_{(i)}$ denotes the leave-one-out (leave the i th sample out) LS coefficient. Note that the two regression models have the same projection matrix since their design matrices are the same. We have

$$\hat{y}_i^* = h_i y_i^* + \sum_{j \neq i} H_{ij} y_j^* = h_i y_i^* + \sum_{j \neq i} H_{ij} y_j, \quad (3)$$

where H_{ij} 's and h_i are the same as the ones in (2).

We can show that the LS line for *Model II* passes the i -th sample, that is

$$\hat{y}_i^* = y_i^* = \hat{y}_{(i)}. \quad (4)$$

Then (3) becomes

$$\hat{y}_{(i)} = h_i \hat{y}_{(i)} + \sum_{j \neq i} H_{ij} y_j = h_i \hat{y}_{(i)} - h_i y_i + \sum_j H_{ij} y_j = h_i \hat{y}_{(i)} - h_i y_i + \hat{y}_i.$$

Then you can get the conclusion (1) by re-arranging the terms above.

Proof for eq (4): Let $\hat{\alpha}$ denote the corresponding LS coefficient for *Model II*, that is,

$$\begin{aligned} \hat{\alpha} &= \arg \min_{\alpha} \sum_{j=1}^n (y_j^* - \mathbf{x}_j^t \alpha)^2 \\ &= \arg \min_{\alpha} \left[(\hat{y}_{(i)} - \mathbf{x}_i^t \alpha)^2 + \sum_{j \neq i} (y_j - \mathbf{x}_j^t \alpha)^2 \right]. \end{aligned}$$

It is not difficult to show that $\hat{\beta}_{(i)}$ the minimizer of the optimization above since it'll make the first term equal to zero and meanwhile minimize the 2nd term. So we have

$$\hat{\beta}_{(i)} = \hat{\alpha}.$$

So the LS fit for the i th sample (in *Model II*) is

$$\hat{y}_i^* = \mathbf{x}_i^t \hat{\alpha} = \mathbf{x}_i^t \hat{\beta}_{(i)} = \hat{y}_{(i)}.$$