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Department of Statistics

Statistics 100C

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The fitted values and their variance-covariance matrix

The variance-covariance matrix of the fitted values can be expressed as follows:

$$\text{var}(\hat{\mathbf{Y}}) = \text{var}(\mathbf{X}\hat{\beta}) = \mathbf{X}\text{var}(\hat{\beta})\mathbf{X}' = \sigma^2\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' = \sigma^2\mathbf{H}.$$

Or if we expand this we get:

$$\text{var}(\hat{\mathbf{Y}}) = \begin{pmatrix} \text{var}(\hat{y}_1) & \text{cov}(\hat{y}_1, \hat{y}_2) & \text{cov}(\hat{y}_1, \hat{y}_3) & \cdots & \cdots & \text{cov}(\hat{y}_1, \hat{y}_n) \\ \text{cov}(\hat{y}_2, \hat{y}_1) & \text{var}(\hat{y}_2) & \text{cov}(\hat{y}_2, \hat{y}_3) & \cdots & \cdots & \text{cov}(\hat{y}_2, \hat{y}_n) \\ \cdots & \cdots & \ddots & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \ddots & \cdots & \cdots \\ \text{cov}(\hat{y}_n, \hat{y}_1) & \text{cov}(\hat{y}_n, \hat{y}_2) & \text{cov}(\hat{y}_n, \hat{y}_3) & \cdots & \cdots & \text{var}(\hat{y}_n) \end{pmatrix}$$

$$\text{var}(\hat{\mathbf{Y}}) = \sigma^2 \begin{pmatrix} h_{11} & h_{12} & h_{13} & \cdots & \cdots & h_{1n} \\ h_{21} & h_{22} & h_{23} & \cdots & \cdots & h_{2n} \\ \cdots & \cdots & \ddots & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \ddots & \cdots & \cdots \\ h_{n1} & h_{n2} & h_{n3} & \cdots & \cdots & h_{nn} \end{pmatrix}$$

Where, h_{ij} is the ij_{th} element of the hat matrix \mathbf{H} . Therefore the variance of the i_{th} fitted value is $\text{var}(\hat{y}_i) = \sigma^2 h_{ii}$. Since the variance is always ≥ 0 it means that $h_{ii} \geq 0$. Also from a previous discussion we found that $h_{ii} \leq 1$. Therefore we have $\frac{1}{n} \leq h_{ii} \leq 1$.

The sum of the diagonal elements of the hat matrix is equal to $k + 1$ (in simple regression $k = 1 \Rightarrow \sum_{i=1}^n h_{ii} = 2$).

Proof: The trace of a square matrix is equal to the sum of its diagonal elements. Also a property of the trace is the following: Let \mathbf{A} , \mathbf{B} , \mathbf{C} be matrices. Then $\text{tr}(\mathbf{ABC}) = \text{tr}(\mathbf{BCA}) = \text{tr}(\mathbf{CAB})$. We can apply this result to the hat matrix:

$$\text{tr}(\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}') = \text{tr}(\mathbf{XX}'(\mathbf{X}'\mathbf{X})^{-1}) = \text{tr}(\mathbf{I}_{(k+1) \times (k+1)}) = k + 1.$$

For simple regression it can be shown that

$$h_{ii} = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2}.$$

You can easily verify that $\sum_{i=1}^n h_{ii} = 2$.