

SHEET - An Introduction to Statistical Learning
Chapter 3 - Linear Regression

4 December 2023

1 Linear Regression

1.1 Courses' Demonstrations

Let $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ be the prediction for Y based on the i th value of X_i . Then $e_i = y_i - \hat{y}_i$ represents the i th residual - this is the difference between the i th observed response value and the i th response value that is predicted by our linear model. We define the residual sum of squares (RSS) as

$$\begin{aligned} \text{RSS} &= e_1^2 + e_2^2 + \cdots + e_n^2 \\ &= (y_1 - \hat{\beta}_0 - \hat{\beta}_1 x_1)^2 + (y_2 - \hat{\beta}_0 - \hat{\beta}_1 x_2)^2 + \cdots + (y_n - \hat{\beta}_0 - \hat{\beta}_1 x_n)^2 \end{aligned}$$

The least squares approach chooses $\hat{\beta}_0$ and $\hat{\beta}_1$ to minimize the RSS. Using some calculus, one can show that the minimizers are

$$\begin{aligned} \hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \end{aligned} \tag{3.4}$$

where \bar{y} is the sample mean, defined as

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$$

Demonstration : $\hat{\beta}_0$ and $\hat{\beta}_1$

We search RSS as

$$f(\hat{\beta}_0, \hat{\beta}_1) = \min_{\hat{\beta}_0, \hat{\beta}_1} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2$$

We get the minimum where

$$\frac{\partial f}{\partial \hat{\beta}_k} = 0 \text{ with } k \in \{0, 1\}$$

We have

$$\begin{aligned} \bar{y} &= \sum_{i=1}^n y_i \\ \bar{x} &= \sum_{i=1}^n x_i \end{aligned}$$

Then

$$\begin{aligned}
& \begin{cases} \frac{\partial f}{\partial \hat{\beta}_0} = -2 \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) = 0 \\ \frac{\partial f}{\partial \hat{\beta}_1} = -2 \sum_{i=1}^n x_i (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) = 0 \end{cases} \\
& \begin{cases} \sum_{i=1}^n y_i = n\hat{\beta}_0 + \hat{\beta}_1 \sum_{i=1}^n x_i = 0 \\ \sum_{i=1}^n x_i y_i = \hat{\beta}_0 \sum_{i=1}^n x_i + \hat{\beta}_1 \sum_{i=1}^n x_i^2 = 0 \end{cases} \\
& \begin{cases} \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \\ \sum_{i=1}^n x_i y_i - n\hat{\beta}_0 \bar{x} - \hat{\beta}_1 \sum_{i=1}^n x_i^2 = 0 \end{cases} \\
& \begin{cases} \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \\ \sum_{i=1}^n x_i y_i - n(\bar{y} - \hat{\beta}_1 \bar{x}) \bar{x} - \hat{\beta}_1 \sum_{i=1}^n x_i^2 = 0 \end{cases} \\
& \begin{cases} \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \\ (\sum_{i=1}^n x_i y_i - n\bar{y}\bar{x}) - \hat{\beta}_1 (\sum_{i=1}^n x_i^2 - n\bar{x}^2) = 0 \end{cases}
\end{aligned}$$

We have

$$\begin{cases} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) = \sum_{i=1}^n (x_i y_i - \bar{y}\bar{x}) \\ \sum_{i=1}^n (x_i^2 - \bar{x}^2) = \sum_{i=1}^n (x_i^2 - \bar{x}^2) \end{cases}$$

Finally

$$\begin{cases} \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 = \frac{\sum_{i=1}^n (y_i - \bar{y})(x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} \end{cases}$$

By developping we can have

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (y_i - \bar{y})(x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{\sum_{i=1}^n (y_i - \bar{y})(x_i)}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{\sum_{i=1}^n (y_i)(x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

Demonstration : $\hat{\beta}_1$

$$\begin{aligned}\hat{\beta}_1 &= \frac{\sum_{i=1}^n (y_i - \bar{y})(x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sum_{i=1}^n (y_i - \bar{y})(x_i)}{\sum_{i=1}^n (x_i - \bar{x})^2} - \frac{\bar{x} \sum_{i=1}^n (y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sum_{i=1}^n (y_i - \bar{y})(x_i)}{\sum_{i=1}^n (x_i - \bar{x})^2} - \frac{\bar{x} n (\bar{y} - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sum_{i=1}^n (y_i - \bar{y})(x_i)}{\sum_{i=1}^n (x_i - \bar{x})^2}\end{aligned}$$

$$\begin{aligned}\hat{\beta}_1 &= \frac{\sum_{i=1}^n (y_i - \bar{y})(x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i)}{\sum_{i=1}^n (x_i - \bar{x})^2} - \frac{\bar{y} \sum_{i=1}^n (x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i)}{\sum_{i=1}^n (x_i - \bar{x})^2} - \frac{\bar{y} n (\bar{x} - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i)}{\sum_{i=1}^n (x_i - \bar{x})^2}\end{aligned}$$

We assume that the True relationship between X and Y takes the form

$$Y = f(X) + \varepsilon$$

for some unknown function f, where ε is a mean-zero random error term. If f is to be approximated by a linear function then we can write the relationship as

$$Y = \beta_0 + \beta_1 X + \varepsilon \quad (3.5)$$

How accurate is the sample mean $\hat{\mu}$ as an estimate of μ ? In general, we answer this question by computing the standard error of $\hat{\mu}$, written as the standard error $SE(\hat{\mu})$. A reasonable estimate is $\hat{\mu} = \bar{y}$. We have the well-known formula :

$$Var(\hat{\mu}) = SE(\hat{\mu}^2) = \frac{\sigma^2}{n} \quad (3.7)$$

where σ is the standard deviation of each of the realizations y_i of Y.

Demonstration : $Var(\hat{\mu})$

We have

$$\hat{\mu} = \bar{y}$$

$$Var(X + Y) = Var(X) + Var(Y)$$

$$Var(aX) = a^2 Var(X) \text{ with } a = \text{cste}$$

$$Var(y_i) = \sigma^2$$

Then

$$\begin{aligned} Var(\hat{\mu}) &= Var(\bar{y}) = Var\left(\frac{1}{n} \sum_{i=1}^n y_i\right) \\ &= \frac{1}{n^2} Var\left(\sum_{i=1}^n y_i\right) = \frac{1}{n^2} \sum_{i=1}^n Var(y_i) \\ &= \frac{1}{n^2} \sum_{i=1}^n \sigma^2 \\ \text{Var}(\hat{\mu}) &= \frac{\sigma^2}{n} \end{aligned}$$

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In a similar vein, we can wonder how close $\hat{\beta}_0$ and $\hat{\beta}_1$ are to the true values β_0 and β_1 . To compute the standard errors associated with β_0 and β_1 , we use the following formulas :

$$SE(\hat{\beta}_0) = \sigma^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right] \quad (3.8)$$

$$SE(\hat{\beta}_1) = \frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \quad (3.8)$$

where $\sigma^2 = Var(\varepsilon)$

Démonstration : $E[\hat{\beta}_1]$

We have

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})y_i}{\sum_{i=1}^n (x_i - \bar{x})^2} = \sum_{i=1}^n w_i y_i \quad \text{with} \quad w_i = \frac{x_i - \bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

$$\sum_{i=1}^n w_i = \frac{\sum_{i=1}^n (x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{n(\bar{x} - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} = 0$$

$$\begin{aligned} \sum_{i=1}^n w_i x_i &= \frac{\sum_{i=1}^n (x_i - \bar{x})x_i}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{\sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x} + \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} + \frac{\sum_{i=1}^n ((x_i - \bar{x})\bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2} + \frac{\bar{x} \sum_{i=1}^n (x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} = 1 + 0 = 1 \\ \sum_{i=1}^n w_i^2 &= \sum_{i=1}^n \frac{(x_i - \bar{x})^2}{(\sum_{i=1}^n (x_i - \bar{x})^2)^2} = \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{(\sum_{i=1}^n (x_i - \bar{x})^2)^2} = \frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ y_i &= \beta_1 x_i + \beta_0 + \varepsilon_i \end{aligned}$$

We can deduce

$$\begin{aligned} E[\hat{\beta}_1] &= E \left[\sum_{i=1}^n w_i y_i \right] = E \left[\sum_{i=1}^n w_i (\beta_1 x_i + \beta_0 + \varepsilon_i) \right] \\ &= E \left[\beta_1 \sum_{i=1}^n w_i x_i + \beta_0 \sum_{i=1}^n w_i + \varepsilon_i \sum_{i=1}^n w_i \right] = \\ &= E[\beta_1 * 1 + \beta_0 * 0 + \varepsilon_i * 0] = E[\beta_1] = \beta_1 \end{aligned}$$

Démonstration : $E[\hat{\beta}_0]$

$$\begin{aligned}
\mathbf{E}[\hat{\beta}_0] &= E[\bar{y} - \hat{\beta}_1 \bar{x}] = E\left[\frac{1}{n} \sum_{i=1}^n (y_i - \hat{\beta}_1 x_i)\right] = \frac{1}{n} \sum_{i=1}^n E[y_i - \hat{\beta}_1 x_i] \\
&= \frac{1}{n} \sum_{i=1}^n E[(\beta_1 x_i + \beta_0 + \varepsilon_i) - \hat{\beta}_1 x_i] = \frac{1}{n} \sum_{i=1}^n (E[(\beta_1)E[x_i] + E[\beta_0] + E[\varepsilon_i]] - E[\hat{\beta}_1]E[x_i]) \\
&= \frac{1}{n} \sum_{i=1}^n (\beta_1 x_i + \beta_0 + 0 - \beta_1 x_i) = \frac{1}{n} \sum_{i=1}^n \beta_0 = \beta_0
\end{aligned}$$

Démonstration : $Var(\hat{\beta}_1)$

We have

$$Var(X + cste) = Var(X)$$

$$Var(X + Y) = Var(X) + Var(Y)$$

$$\text{if } X \text{ and } Y \text{ independent } Var(XY) = Var(X)Var(Y)$$

$$\begin{aligned}
\hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})y_i}{\sum_{i=1}^n (x_i - \bar{x})^2} \\
&= \frac{\sum_{i=1}^n (x_i - \bar{x})(\beta_0 + \beta_1 x_i + \varepsilon_i)}{\sum_{i=1}^n (x_i - \bar{x})^2} \\
&= \frac{\beta_0 \sum_{i=1}^n (x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} + \frac{\sum_{i=1}^n (x_i - \bar{x})(\beta_1 x_i + \varepsilon_i)}{\sum_{i=1}^n (x_i - \bar{x})^2} \\
&= \frac{\beta_0 n(\bar{x} - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} + \frac{\sum_{i=1}^n (x_i - \bar{x})(\beta_1 x_i + \varepsilon_i)}{\sum_{i=1}^n (x_i - \bar{x})^2} \\
&= 0 + \beta_1 \frac{\sum_{i=1}^n (x_i - \bar{x})x_i}{\sum_{i=1}^n (x_i - \bar{x})^2} + \frac{\sum_{i=1}^n (x_i - \bar{x})\varepsilon_i}{\sum_{i=1}^n (x_i - \bar{x})^2} \\
&= \beta_1 \sum_{i=1}^n w_i x_i + \frac{\sum_{i=1}^n (x_i - \bar{x})\varepsilon_i}{\sum_{i=1}^n (x_i - \bar{x})^2} \\
&= \beta_1 1 + \frac{\sum_{i=1}^n (x_i - \bar{x})\varepsilon_i}{\sum_{i=1}^n (x_i - \bar{x})^2} \\
&= \beta_1 + \frac{\sum_{i=1}^n (x_i - \bar{x})\varepsilon_i}{\sum_{i=1}^n (x_i - \bar{x})^2}
\end{aligned}$$

Then

$$\begin{aligned} \text{Var}(\hat{\beta}_1) &= \text{Var}\left(\beta_1 + \frac{\sum_{i=1}^n (x_i - \bar{x})\varepsilon_i}{\sum_{i=1}^n (x_i - \bar{x})^2}\right) \\ &= \text{Var}\left(\frac{\sum_{i=1}^n (x_i - \bar{x})\varepsilon_i}{\sum_{i=1}^n (x_i - \bar{x})^2}\right) \end{aligned}$$

We know that ε_i is independent of x_i

Then

$$\begin{aligned} \text{Var}(\hat{\beta}_1) &= \text{Var}\left(\frac{\sum_{i=1}^n (x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2}\right) \text{Var}(\varepsilon_i) \\ &= \sum_{i=1}^n \text{Var}\left(\frac{(x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2}\right) \text{Var}(\varepsilon_i) \\ &= \sum_{i=1}^n \text{Var}\left(\frac{(x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2}\right) \text{Var}(\varepsilon_i) \\ &= \sum_{i=1}^n \frac{(x_i - \bar{x})^2}{(\sum_{i=1}^n (x_i - \bar{x})^2)^2} \text{Var}(\varepsilon_i) \\ &= \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{(\sum_{i=1}^n (x_i - \bar{x})^2)^2} \text{Var}(\varepsilon_i) \\ &= \frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2} \text{Var}(\varepsilon_i) \\ \mathbf{Var}(\hat{\beta}_1) &= \frac{\sigma^2}{\sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})^2} \end{aligned}$$

Démonstration : $\text{Var}(\hat{\beta}_0)$

We have

$$\begin{aligned} \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \text{Cov}(X, \text{cste}) &= E[(X - E[X])(\text{cste} - E[\text{cste}])] \\ &= E[(X - E[X])(\text{cste} - \text{cste})] \\ &= E[(X - E[X])0] = E[0] = 0 \text{Var}(\bar{y}) = \text{Var}\left(\frac{1}{n} \sum_{i=1}^n y_i\right) \\ &= \frac{1}{n^2} \sum_{i=1}^n \text{Var}(y_i) \\ &= \frac{1}{n^2} n\sigma^2 = \frac{\sigma^2}{n} \end{aligned}$$

Then

$$\begin{aligned}
Var(\hat{\beta}_0) &= Var(\bar{y}) + \bar{x}^2 Var(\hat{\beta}_1) - 2\bar{x}Cov(\bar{y}, \hat{\beta}_1) \\
&= \frac{\sigma^2}{n} + \bar{x}^2 Var(\hat{\beta}_1) \text{ because } \bar{y} = cste \\
&= \frac{\sigma^2}{n} + \bar{x}^2 \frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \\
\mathbf{Var}(\hat{\beta}_0) &= [\frac{1}{\mathbf{n}} + \frac{\bar{\mathbf{x}}^2}{\sum_{\mathbf{i}=1}^{\mathbf{n}} (\mathbf{x}_{\mathbf{i}} - \bar{\mathbf{x}})^2}] \sigma^2
\end{aligned}$$

The estimate of σ is known as the residual standard error, and is given by the formula residual standard error

$$RSE = \frac{\sqrt{RSS}}{n - 2}$$

We have

$$\begin{aligned}
E[\varepsilon_i] &= 0 \\
\hat{\varepsilon}_i &= y_i - \hat{y}_i = (\beta_1 x_i + \beta_0 + \varepsilon_i) - (\hat{\beta}_1 x_i + \hat{\beta}_0) \\
&= (\beta_1 x_i + (\bar{y} - \beta_1 \bar{x}) + \varepsilon_i) - (\hat{\beta}_1 x_i + (\bar{y} - \hat{\beta}_1 \bar{x})) \\
&= \varepsilon_i + (\beta_1 - \hat{\beta}_1)(x_i - \bar{x}) \\
\hat{\beta}_1 &= \beta_1 + \frac{\sum_{i=1}^n (x_i - \bar{x})\varepsilon_i}{\sum_{i=1}^n (x_i - \bar{x})^2}
\end{aligned}$$

Then

$$\begin{aligned}
\sum_{i=1}^n \hat{\varepsilon}_i^2 &= \sum_{i=1}^n [\varepsilon_i + (\beta_1 - \hat{\beta}_1)(x_i - \bar{x})]^2 \\
&= \sum_{i=1}^n [\varepsilon_i^2 + 2\varepsilon_i(\beta_1 - \hat{\beta}_1)(x_i - \bar{x}) + (\beta_1 - \hat{\beta}_1)^2(x_i - \bar{x})^2] \\
&= \sum_{i=1}^n \varepsilon_i^2 + 2(\beta_1 - \hat{\beta}_1) \sum_{i=1}^n \varepsilon_i(x_i - \bar{x}) + (\beta_1 - \hat{\beta}_1)^2 \sum_{i=1}^n (x_i - \bar{x})^2 \\
&= \sum_{i=1}^n \varepsilon_i^2 - 2 \frac{\sum_{i=1}^n (x_i - \bar{x})\varepsilon_i}{\sum_{i=1}^n (x_i - \bar{x})^2} \sum_{i=1}^n \varepsilon_i(x_i - \bar{x}) + \left(\frac{\sum_{i=1}^n (x_i - \bar{x})\varepsilon_i}{\sum_{i=1}^n (x_i - \bar{x})^2} \right)^2 \sum_{i=1}^n (x_i - \bar{x})^2 \\
&= \sum_{i=1}^n \varepsilon_i^2 - 2 \frac{(\sum_{i=1}^n (x_i - \bar{x})\varepsilon_i)^2}{\sum_{i=1}^n (x_i - \bar{x})^2} + \frac{(\sum_{i=1}^n (x_i - \bar{x})\varepsilon_i)^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \\
&= \sum_{i=1}^n \varepsilon_i^2 - \frac{(\sum_{i=1}^n (x_i - \bar{x})\varepsilon_i)^2}{\sum_{i=1}^n (x_i - \bar{x})^2}
\end{aligned}$$

We have

$$\begin{aligned}
\sum_{i=1}^n (\varepsilon_i)^2 &= \sum_{i=1}^n (\varepsilon_i - \bar{\varepsilon})^2 \\
E\left[\sum_{i=1}^n (\varepsilon_i)^2\right] &= \sum_{i=1}^n E[(\varepsilon_i - \bar{\varepsilon})^2] \\
&= \sum_{i=1}^n \text{Var}(\varepsilon_i) = n\sigma^2 \\
\text{Var}(\hat{\beta}_1) &= \frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}
\end{aligned}$$

$$\begin{aligned}
\sum_{i=1}^n \hat{\varepsilon}_i^2 &= \sum_{i=1}^n \varepsilon_i^2 - (\hat{\beta}_1 - \beta_1)^2 \sum_{i=1}^n (x_i - \bar{x})^2 \\
&= \sum_{i=1}^n \varepsilon_i^2 - (\hat{\beta}_1 - \beta_1)^2 \frac{\sigma^2}{\text{Var}(\hat{\beta}_1)}
\end{aligned}$$

$$RSS = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \sum_{i=1}^n (\beta_1 x_i + \beta_0 + \varepsilon_i - \hat{\beta}_1 x_i - \hat{\beta}_0)^2$$

$$\text{Var}(\hat{\beta}_1) = \frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

$$\text{Cov}(\hat{\beta}_1, \hat{\beta}_0) = \frac{-\bar{x}\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

$$\hat{\beta}_1 = \beta_1 + \frac{\sum_{i=1}^n (x_i - \bar{x})\varepsilon_i}{\sum_{i=1}^n (x_i - \bar{x})^2}$$