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

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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 ith value of X_i. Then $e_i = y_i - \hat{y}_i$ represents the ith residual - this is the difference between the ith observed response value and the ith response value that is predicted by our linear model. We define the residual sum of squares (RSS) as

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

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

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

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

$$\frac{\partial f}{\partial \hat{\beta}_k} = 0$$

Then

$$\begin{cases} \dfrac{\partial f}{\partial \hat{\beta}_0} = 0 \\ \dfrac{\partial f}{\partial \hat{\beta}_1} = 0 \end{cases}$$

$$\begin{cases} \dfrac{\partial(\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2)}{\partial \hat{\beta}_0} = 0 \\ \dfrac{\partial(\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2)}{\partial \hat{\beta}_1} = 0 \end{cases}$$

$$\begin{cases} -2\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) = 0 \\ -2\sum_{i=1}^{n}x_i(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) = 0 \end{cases}$$

$$\begin{cases} \sum_{i=1}^{n} y_i - n\hat{\beta}_0 - \hat{\beta}_1 \sum_{i=1}^{n} x_i = 0 \\ \sum_{i=1}^{n} x_i y_i - \hat{\beta}_0 \sum_{i=1}^{n} x_i - \hat{\beta}_1 \sum_{i=1}^{n} x_i^2 = 0 \end{cases}$$

We know that

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

$$\bar{x} = \sum_{i=1}^{n} x_i$$

Then

$$\begin{cases} n\bar{y} - n\hat{\beta}_0 - n\hat{\beta}_1 \bar{x} = 0 \\ \sum_{i=1}^{n} x_i y_i - n\hat{\beta}_0 \bar{x} - \hat{\beta}_1 \sum_{i=1}^{n} x_i^2 = 0 \end{cases}$$

$$\begin{cases} \bar{y} - \hat{\beta}_0 - \hat{\beta}_1 \bar{x} = 0 \\ \sum_{i=1}^{n} x_i y_i - n\hat{\beta}_0 \bar{x} - \hat{\beta}_1 \sum_{i=1}^{n} x_i^2 = 0 \end{cases}$$

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

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

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

We have

$$\begin{aligned} E[(X - E[X])(Y - E[Y])] &= E[XY - XE[Y] - E[X]Y + E[X]E[Y]] \\ &= E[XY] - E[XE[Y]] - E[E[x]Y] + E[E[X]E[Y]] \\ &= E[XY] - E[X]E[Y] - E[X]E[Y] + E[X]E[Y] \\ &= E[XY] - E[X]E[Y] \end{aligned}$$

Then

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

We have

$$\begin{aligned} E[(X - E[X])^2] &= E[X^2 - 2XE[X] + E[X]^2] \\ &= E[X^2] - E[2XE[X]] + E[E[X]^2] \\ &= E[X^2] - 2E[X]E[X] + E[X]^2 \\ &= E[X^2] - E[X]^2 \end{aligned}$$

Then

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

Then

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

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

Finally

$$\begin{cases} \hat{\beta}_{\mathbf{0}} = \bar{\mathbf{y}} - \hat{\beta}_{\mathbf{1}}\bar{\mathbf{x}} \\ \hat{\beta}_{\mathbf{1}} = \dfrac{\sum_{\mathbf{i=1}}^{\mathbf{n}}(\mathbf{y_i} - \bar{\mathbf{y}})(\mathbf{x_i} - \bar{\mathbf{x}})}{\sum_{\mathbf{i=1}}^{\mathbf{n}}(\mathbf{x_i} - \bar{\mathbf{x}})^{\mathbf{2}}} \end{cases}$$

By developping we can have

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

Demonstration: $\hat{\beta}_1$

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

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

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

$$Y = \beta_0 + \beta_1 X + \varepsilon \tag{3.5}$$

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:

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

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

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

We have

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

$$\bar{\mu} = \frac{1}{n}\sum_{i=1}^{n} \mu_i$$

$$E[\bar{\mu}] = E\left[\frac{1}{n}\sum_{i=1}^{n} \mu_i\right] = \frac{1}{n}\sum_{i=1}^{n} E[\mu_i] = \mu$$

Then

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

We set

$$a_i = y_i - E[y_i]$$

So

$$Var(\hat{\mu}) = \frac{1}{n^2} E\left[\left(\sum_{i=1}^{n} a_i\right)^2\right] = \frac{1}{n^2} E\left[\left(\sum_{i=1}^{n} a_i\right)\left(\sum_{j=1}^{n} a_j\right)\right]$$
$$= \frac{1}{n^2} E\left[\sum_{i=1}^{n} a_i^2 + 2 \sum_{1\leq i<j\leq n} a_i a_j\right]$$
$$= \frac{1}{n^2}\left(\sum_{i=1}^{n} E[a_i^2] + 2 \sum_{1\leq i<j\leq n} E[a_i a_j]\right)$$

We have

$$E[a_i] = E[y_i - E[y_i]] = E[y_i] - E[y_i] = 0$$
$$E[a_i a_j] = E[a_i]E[a_j] \textbf{ since } a_i \textbf{ and } a_j \textbf{ are independent}$$

$$\textbf{So } Var(\hat{\mu}) = \frac{1}{n^2} \sum_{i=1}^{n} E[(y_i - E[y_i])^2]$$

Because σ is the standard deviation of each of the realizations y_i of Y
We have finally

$$\mathbf{Var}(\hat{\mu}) = \frac{\boldsymbol{\sigma^2}}{\mathbf{n}}$$

In a similar vein, we can wonder how close $\hat{\beta}_0$ and $\hat{\beta}_0$ 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:

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

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

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

Démonstration : $E[\hat{\beta}_1]$

We have

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

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

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

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

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

$$y_i = \beta_1 x_i + \beta_0 + \varepsilon_i$$

We can deduce

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

Démonstration : $E[\hat{\beta}_0]$

$$\mathbf{E}[\hat{\beta}_\mathbf{0}] = E[\bar{y} - \hat{\beta}_1\bar{x}] = E[\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{\beta}_1 x_i)] = \frac{1}{n}\sum_{i=1}^{n}E[y_i - \hat{\beta}_1 x_i]$$
$$= \frac{1}{n}\sum_{i=1}^{n}E[(\beta_1 x_i + \beta_0 + \varepsilon_i) - \hat{\beta}_1 x_i] = \frac{1}{n}\sum_{i=1}^{n}(E[(\beta_1]E[x_i] + E[\beta_0] + E[\varepsilon_i]) - E[\hat{\beta}_1]E[x_i])$$
$$= \frac{1}{n}\sum_{i=1}^{n}(\beta_1 x_i + \beta_0 + 0 - \beta_1 x_i) = \frac{1}{n}\sum_{i=1}^{n}\beta_0 = \beta_\mathbf{0}$$

Démonstration : $Var(\hat{\beta}_1)$

We have

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

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

Then

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

We know that ε_i is independent of x_i

Then

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

Démonstration : $Var(\hat{\beta}_0)$

We have

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

Then

$$\begin{aligned}
Var(\hat{\beta}_0) &= Var(\bar{y}) + \bar{x}^2 Var(\hat{\beta}_1) - 2\bar{x}Cov(\bar{y}, \hat{\beta}_1) \\
&= \frac{\sigma^2}{n} + \bar{x}^2 Var(\hat{\beta}_1) \text{ because } \bar{y} = cste \\
&= \frac{\sigma^2}{n} + \bar{x}^2 \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \\
\mathbf{Var}(\hat{\beta}_{\mathbf{0}}) &= [\frac{\mathbf{1}}{\mathbf{n}} + \frac{\bar{\mathbf{x}}^{\mathbf{2}}}{\sum_{\mathbf{i=1}}^{\mathbf{n}}(\mathbf{x_i} - \bar{\mathbf{x}})^{\mathbf{2}}}]\sigma^{\mathbf{2}}
\end{aligned}$$