Alberto Andrés Valdés González.

Degree: Mathematical Engineer. Work position: Data Scientist.

Mail: anvaldes@uc.cl/alberto.valdes.gonzalez.96@gmail.com

Location: Santiago, Chile.

Linear Regressions

Statistical and Optimization based approach

Modeling

We can present many ways of modeling Linear Regressions and all these ways are equivalents. However, here we will introduce only two perspectives: The based in Statistics and the based in Optimization.

Statistical based approach

We consider the random variable Y and the data X which satisfy the following relation:

$$Y = \beta \cdot X + \alpha + \epsilon$$

Where ϵ are a **normal random variable** which distributes $\epsilon \sim N(0, \sigma^2)$.

On the other hand β , α and σ are **poblational parameters** we have to estimate.

The estimators for these parameters we will denote as $\hat{\beta}$, $\hat{\alpha}$ and $\hat{\sigma}$ respectively.

As we know in the real world, we don't see **random variables** but we see **observations** of random variables.

Let's consider the independent observations $y_1, ..., y_n, \epsilon_1, ..., \epsilon_n$ and the data $x_1, ..., x_n$. We have the following relations:

$$y_i = \beta x_i + \alpha + \epsilon_i \quad \forall i \in \{1, ..., n\}$$

How $\epsilon_i \stackrel{iid}{\sim} N(0, \sigma^2)$ then $y_i \stackrel{iid}{\sim} N(\beta \cdot x_i + \alpha, \sigma^2)$.

We introduce the Likelihood function:

$$L(\beta, \alpha, \sigma) = \mathbb{P}(y_1, ..., y_n | x_1, ..., x_n, \beta, \alpha, \sigma) = \prod_{i=1}^n \mathbb{P}(y_i | x_i, \beta, \alpha, \sigma)$$
$$= \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \cdot exp\left(-\frac{(y_i - [\beta \cdot x_i + \alpha])^2}{2\sigma^2}\right)$$

The values of $\hat{\beta}$, $\hat{\alpha}$ and $\hat{\sigma}$ are the arguments maximize $L(\beta, \alpha, \sigma)$.

A useful fact to maximize the likelihood function is that maximize a positive function is equivalent to maximize the logaritm of that function. Thus we introduce the log-likelihood function:

$$l(\beta, \alpha, \sigma) = ln(L(\beta, \alpha, \sigma)) = \sum_{i=1}^{n} \left(-\frac{1}{2} \cdot ln(2\pi) - ln(\sigma) - \frac{(y_i - [\beta \cdot x_i + \alpha])^2}{2\sigma^2} \right)$$
$$= -\frac{n \cdot ln(2\pi)}{2} - n \cdot ln(\sigma) - \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - [\beta \cdot x_i + \alpha])^2$$

To obtain the values $\hat{\beta}$, $\hat{\alpha}$ we have to maximize $l(\beta, \alpha, \sigma)$ which es equivalent to maximize:

$$-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - [\beta \cdot x_i + \alpha])^2$$

Which es equivalent to minimize:

$$\sum_{i=1}^{n} (y_i - [\beta \cdot x_i + \alpha])^2$$
 (1)

Optimization based approach

Let's consider the data $x_1, ..., x_n, y_1, ..., y_n$. We will assume that satisfy the relation:

$$y_i = \beta \cdot x_i + \alpha \quad \forall i \in \{1, ..., n\}$$

However, actually this relation have a error considered and the following equations are fulfilled.

$$y_i = \beta \cdot x_i + \alpha + \epsilon_i \qquad \forall \ i \in \{1,...,n\}$$

Where ϵ_i are the error component.

In this approach we want to minimize the mean square error (MSE), and the arguments that minimize the MSE are β^* and α^* .

$$MSE(\beta, \alpha) = \frac{1}{n} \sum_{i=1}^{n} (y_i - [\beta \cdot x_i + \alpha])^2$$

We can see that minimize MSE are equivalent to minimize:

$$\left| \sum_{i=1}^{n} (y_i - [\beta \cdot x_i + \alpha])^2 \right|$$
 (2)

As we can see by (1) and (2) the **both approaches are equivalents**.

Probability Review

Let $(\Omega, \zeta, \mathbb{P})$ a probability space and X a random variable over it.

a) If $X_+ \in L^1(\Omega, \zeta, \mathbb{P})$ or $X_- \in L^1(\Omega, \zeta, \mathbb{P})$ the expected value of X its defined as follow:

$$\mathbb{E}(X) = \int X d\mathbb{P} = \int X dF_X$$

Note: $X = X_+ - X_-$ where $X_+ = \max\{X, 0\} = \frac{|X| + X}{2}$ and $X_- = \max\{-X, 0\} = \frac{|X| - X}{2}$.

- b) For all $k \in \mathbb{N}$: $k \geq 1$ the k-th moment is given by $\mathbb{E}(X^k)$. We say X has k-th moment if $X \in L^k(\Omega, \zeta, \mathbb{P})$.
- c) If $X,Y\in L^2(\Omega,\zeta,\mathbb{P})$ we define its covariance as follows:

$$Cov(X, Y) = \mathbb{E}(X \cdot Y) - \mathbb{E}(X) \cdot \mathbb{E}(Y)$$

Note:
$$\mathbb{V}(X) = Cov(X, X), \ \sigma_X = \sqrt{\mathbb{V}(X)} \ \text{and} \ \rho_{X,Y} = \frac{Cov(X, Y)}{\sigma_X(X) \cdot \sigma(Y)}.$$

Estimators

Some **unbiased** estimators to considers are:

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

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

$$S_{X,Y} = \frac{1}{(n-1)} \cdot \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})$$

Linear relation between random variables

If X and Y are random variables which satisfy the next relation:

$$Y = m \cdot X + n$$

then:

$$\rho_{X,Y} = \frac{Cov(X, m \cdot X + n)}{\sqrt{\mathbb{V}(X)} \cdot \sqrt{\mathbb{V}(m \cdot X + n)}} = \frac{m \cdot Cov(X, X)}{\sqrt{\mathbb{V}(X)} \cdot \sqrt{m^2 \cdot \mathbb{V}(X)}} = \frac{m \cdot \mathbb{V}(X)}{|m| \cdot \mathbb{V}(X)} = \frac{m}{|m|} = sign(m)$$

Thus, to see how strong the linearity is between two random variables, the important thing is to see the magnitude of the absolute value of correlation.

Some facts about $\hat{\beta}$ and $\hat{\alpha}$

We can deduce from (1) and (2) that the values of $\hat{\beta}$ and $\hat{\alpha}$ satisfy the next:

$$\hat{\beta} = \frac{\sum_{i=1}^{n} (x_i - \bar{x}) \cdot (y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2}$$
 (3)
$$\hat{\alpha} = \bar{y} - \hat{\beta} \cdot \bar{x}$$
 (4)

First Fact: If instead of x_i and y_i we consider its normalizations, i.e.

$$u_i = \frac{x_i - \bar{x}}{\sqrt{S_X}}, \quad v_i = \frac{y_i - \bar{y}}{\sqrt{S_Y}}$$

then, we have:

$$\bar{u} = 0, \quad \bar{v} = 0$$

Therefore:

$$\hat{\beta} = \frac{\sum_{i=1}^{n} (u_i - \bar{u}) \cdot (v_i - \bar{v})}{\sum_{i=1}^{n} (u_i - \bar{u})^2} = \frac{\sum_{i=1}^{n} u_i \cdot v_i}{\sum_{i=1}^{n} u_i^2} = \frac{\sum_{i=1}^{n} \left(\frac{x_i - \bar{x}}{\sqrt{S_X}}\right) \cdot \left(\frac{y_i - \bar{y}}{\sqrt{S_Y}}\right)}{\sum_{i=1}^{n} \left(\frac{x_i - \bar{x}}{\sqrt{S_X}}\right)^2}$$

$$= \frac{\sqrt{S_X}^2}{\sqrt{S_X} \cdot \sqrt{S_Y}} \cdot \frac{\sum_{i=1}^{n} (x_i - \bar{x}) \cdot (y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2} = \frac{\sqrt{S_X}^2}{\sqrt{S_X} \cdot \sqrt{S_Y}} \cdot \frac{\frac{1}{n-1} \cdot \sum_{i=1}^{n} (x_i - \bar{x}) \cdot (y_i - \bar{y})}{\frac{1}{n-1} \cdot \sum_{i=1}^{n} (x_i - \bar{x})^2}$$

$$= \frac{\sqrt{S_X}^2}{\sqrt{S_X} \cdot \sqrt{S_Y}} \cdot \frac{S_{X,Y}}{S_X} = \frac{S_{X,Y}}{\sqrt{S_X} \cdot \sqrt{S_Y}} = \hat{\rho}_{X,Y}$$

 \Rightarrow

$$\hat{\beta} = \hat{\rho_{X,Y}}$$

On the other hand:

$$\hat{\alpha} = \bar{v} - \hat{\beta} \cdot \bar{u} = 0 - \hat{\rho}_{XY} \cdot 0 = 0$$

 \Rightarrow

$$\hat{\alpha} = 0$$

Second Fact: If instead of x_i and y_i we consider its scaling by its desviations, i.e.

$$u_i = \frac{x_i}{\sqrt{S_X}}, \quad v_i = \frac{y_i}{\sqrt{S_Y}}$$

then, we have:

$$\bar{u} = \frac{\bar{x}}{\sqrt{S_X}}, \quad \bar{v} = \frac{\bar{y}}{\sqrt{S_Y}} \quad \Rightarrow \quad u_i - \bar{u} = \frac{(x_i - \bar{x})}{\sqrt{S_X}}, \quad v_i - \bar{v} = \frac{(y_i - \bar{y})}{\sqrt{S_Y}}$$

Therefore:

$$\hat{\beta} = \frac{\sum_{i=1}^{n} (u_i - \bar{u}) \cdot (v_i - \bar{v})}{\sum_{i=1}^{n} (u_i - \bar{u})^2} = \frac{\sum_{i=1}^{n} \left(\frac{x_i - \bar{x}}{\sqrt{S_X}}\right) \cdot \left(\frac{y_i - \bar{y}}{\sqrt{S_Y}}\right)}{\sum_{i=1}^{n} \left(\frac{x_i - \bar{x}}{\sqrt{S_X}}\right)^2}$$

$$= \frac{\sqrt{S_X}^2}{\sqrt{S_X} \cdot \sqrt{S_Y}} \cdot \frac{\sum_{i=1}^n (x_i - \bar{x}) \cdot (y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{\sqrt{S_X}^2}{\sqrt{S_X} \cdot \sqrt{S_Y}} \cdot \frac{\frac{1}{n-1} \cdot \sum_{i=1}^n (x_i - \bar{x}) \cdot (y_i - \bar{y})}{\frac{1}{n-1} \cdot \sum_{i=1}^n (x_i - \bar{x})^2}$$
$$= \frac{\sqrt{S_X}^2}{\sqrt{S_X} \cdot \sqrt{S_Y}} \cdot \frac{S_{X,Y}}{S_X} = \frac{S_{X,Y}}{\sqrt{S_X} \cdot \sqrt{S_Y}} = \hat{\rho}_{X,Y}$$

 \Rightarrow

$$\hat{\beta} = \hat{\rho_{X,Y}}$$

On the other hand:

$$\hat{\alpha} = \bar{v} - \hat{\beta} \cdot \bar{u} = \frac{\bar{y}}{\sqrt{S_Y}} - \hat{\beta} \cdot \frac{\bar{x}}{\sqrt{S_X}} = 0 - \hat{\rho}_{X,Y} \cdot 0 = 0$$

 \Rightarrow

$$\hat{\alpha} = 0$$

Third Fact: Using the (3) formula, we have that:

$$\hat{\beta} = \frac{\sum_{i=1}^{n} (x_i - \bar{x}) \cdot (y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2} = \frac{\frac{1}{(n-1)} \sum_{i=1}^{n} (x_i - \bar{x}) \cdot (y_i - \bar{y})}{\frac{1}{(n-1)} \sum_{i=1}^{n} (x_i - \bar{x})^2} = \frac{S_{X,Y}}{S_X} = \frac{\sqrt{S_Y}}{\sqrt{S_Y}} \cdot \frac{S_{X,Y}}{\sqrt{S_X}} \cdot \sqrt{S_X}$$

$$= \frac{\sqrt{S_Y}}{\sqrt{S_X}} \cdot \frac{S_{X,Y}}{\sqrt{S_Y}} \cdot \sqrt{S_X} = \frac{\sqrt{S_Y}}{\sqrt{S_X}} \cdot \hat{\rho}_{X,Y}$$

 \Rightarrow

$$\hat{\beta} = \frac{\sqrt{S_Y}}{\sqrt{S_X}} \cdot \hat{\rho}_{X,Y}$$

For this if two variables are strongly lineal relationated $\Rightarrow |\hat{\rho}_{X,Y}| \approx 1 \Rightarrow |\hat{\beta}| \approx \frac{\sqrt{S_Y}}{\sqrt{S_X}}$.

Fourth Fact: If we have the next linear regression:

$$\hat{y}_i = \hat{\beta} \cdot x_i + \hat{\alpha} \quad \forall i \in \{1, ..., n\} \quad (*)$$

And now we want to make other linear regression, but instead of consider y_i, x_i , we want to consider v_i, u_i , where:

$$v_i = c_1 \cdot y_i + c_2$$
 $u_i = d_1 \cdot x_i + d_2$ $\forall i \in \{1, ..., n\}$
$$\hat{v}_i = \hat{\beta}_2 \cdot u_i + \hat{\alpha}_2 \quad \forall i \in \{1, ..., n\}$$

Then the relation of $\hat{\beta}$ and $\hat{\alpha}$ with $\hat{\beta}_2$ and $\hat{\alpha}_2$ are the same if we only had replaced in (*) with x_i and y_i in function of u_i and v_i respectively.

Inference over $\hat{\beta}$

We know that $y_i \stackrel{iid}{\sim} N(\beta \cdot x_i + \alpha, \sigma^2)$ and x_i are data. Also we know that:

$$\hat{\beta} = \frac{\sum_{i=1}^{n} (x_i - \bar{x}) \cdot (y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2}$$
(3)

We going to rewrite this formula using the next:

$$\sum_{i=1}^{n} (x_{i} - \bar{x}) \cdot (y_{i} - \bar{y}) = \sum_{i=1}^{n} (x_{i} \cdot y_{i} - \bar{x} \cdot y_{i} - x_{i} \cdot \bar{y} + \bar{x} \cdot \bar{y})$$

$$= \sum_{i=1}^{n} x_{i} \cdot y_{i} - \bar{x} \cdot \sum_{i=1}^{n} y_{i} - \bar{y} \cdot \sum_{i=1}^{n} x_{i} + \sum_{i=1}^{n} \bar{x} \cdot \bar{y}$$

$$= \sum_{i=1}^{n} x_{i} \cdot y_{i} - \bar{x} \cdot n \cdot \bar{y} - \bar{y} \cdot n \cdot \bar{x} + n \cdot \bar{x} \cdot \bar{y} = \sum_{i=1}^{n} x_{i} \cdot y_{i} - \bar{x} \cdot n \cdot \bar{y}$$

$$= \sum_{i=1}^{n} x_{i} \cdot y_{i} - \bar{x} \cdot \sum_{i=1}^{n} y_{i} = \sum_{i=1}^{n} x_{i} \cdot y_{i} - \sum_{i=1}^{n} \bar{x} \cdot y_{i}$$

$$= \sum_{i=1}^{n} (x_{i} \cdot y_{i} - \bar{x} \cdot y_{i}) = \sum_{i=1}^{n} (x_{i} - \bar{x}) \cdot y_{i}$$

 \Rightarrow

$$\hat{\beta} = \frac{\sum_{i=1}^{n} (x_i - \bar{x}) \cdot y_i}{\sum_{i=1}^{n} (x_i - \bar{x})^2}$$
 (5)

Expected value of $\hat{\beta}$

$$\mathbb{E}[\hat{\beta}] \stackrel{(3)}{=} \mathbb{E}\left[\frac{\sum_{i=1}^{n} (x_{i} - \bar{x}) \cdot (y_{i} - \bar{y})}{\sum_{i=1}^{n} (x_{i} - \bar{x})^{2}}\right] = \frac{1}{\sum_{i=1}^{n} (x_{i} - \bar{x})^{2}} \cdot \mathbb{E}\left[\sum_{i=1}^{n} (x_{i} - \bar{x}) \cdot (y_{i} - \bar{y})\right]$$

$$= \frac{1}{\sum_{i=1}^{n} (x_{i} - \bar{x})^{2}} \cdot \sum_{i=1}^{n} \mathbb{E}\left[(x_{i} - \bar{x}) \cdot (y_{i} - \bar{y})\right] = \frac{1}{\sum_{i=1}^{n} (x_{i} - \bar{x})^{2}} \cdot \sum_{i=1}^{n} (x_{i} - \bar{x}) \cdot \mathbb{E}\left[y_{i} - \bar{y}\right]$$

$$= \frac{1}{\sum_{i=1}^{n} (x_{i} - \bar{x})^{2}} \cdot \sum_{i=1}^{n} (x_{i} - \bar{x}) \cdot (\mathbb{E}\left[y_{i}\right] - \mathbb{E}\left[\bar{y}\right])$$

 \Rightarrow

$$\mathbb{E}[\hat{\beta}] = \frac{1}{\sum_{i=1}^{n} (x_i - \bar{x})^2} \cdot \sum_{i=1}^{n} (x_i - \bar{x}) \cdot (\mathbb{E}[y_i] - \mathbb{E}[\bar{y}])$$
 (6)

We know $\mathbb{E}[y_i] = \beta \cdot x_i + \alpha$, thus:

$$\mathbb{E}\left[\bar{y}\right] = \mathbb{E}\left[\frac{\sum_{j=1}^{n} y_j}{n}\right] = \frac{1}{n} \cdot \mathbb{E}\left[\sum_{j=1}^{n} y_j\right] = \frac{1}{n} \cdot \sum_{j=1}^{n} \mathbb{E}\left[y_j\right] = \frac{1}{n} \cdot \sum_{j=1}^{n} (\beta \cdot x_j + \alpha) = \beta \cdot \bar{x} + \alpha$$

 \Rightarrow

$$\mathbb{E}[y_i] - \mathbb{E}[\bar{y}] = (\beta \cdot x_i + \alpha) - (\beta \cdot \bar{x} + \alpha) = \beta \cdot (x_i - \bar{x})$$

Substituting this in (6) we obtain:

$$\mathbb{E}[\hat{\beta}] = \frac{1}{\sum_{i=1}^{n} (x_i - \bar{x})^2} \cdot \sum_{i=1}^{n} (x_i - \bar{x}) \cdot (\mathbb{E}[y_i] - \mathbb{E}[\bar{y}])$$

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

 \Rightarrow

$$\boxed{\mathbb{E}[\hat{\beta}] = \beta} \tag{7}$$

Variance of $\hat{\beta}$

$$\mathbb{V}[\hat{\beta}] \stackrel{(5)}{=} \mathbb{V}\left[\frac{\sum_{i=1}^{n}(x_{i}-\bar{x})\cdot y_{i}}{\sum_{i=1}^{n}(x_{i}-\bar{x})^{2}}\right] = \frac{1}{\left[\sum_{i=1}^{n}(x_{i}-\bar{x})^{2}\right]^{2}} \cdot \mathbb{V}\left[\sum_{i=1}^{n}(x_{i}-\bar{x})\cdot y_{i}\right] \\
\stackrel{(iid)}{=} \frac{1}{\left[\sum_{i=1}^{n}(x_{i}-\bar{x})^{2}\right]^{2}} \cdot \sum_{i=1}^{n} \mathbb{V}\left[(x_{i}-\bar{x})\cdot y_{i}\right] = \frac{1}{\left[\sum_{i=1}^{n}(x_{i}-\bar{x})^{2}\right]^{2}} \cdot \sum_{i=1}^{n}(x_{i}-\bar{x})^{2} \cdot \mathbb{V}\left[y_{i}\right] \\
= \frac{1}{\left[\sum_{i=1}^{n}(x_{i}-\bar{x})^{2}\right]^{2}} \cdot \sum_{i=1}^{n}(x_{i}-\bar{x})^{2} \cdot \sigma^{2} = \frac{\sigma^{2}}{\left[\sum_{i=1}^{n}(x_{i}-\bar{x})^{2}\right]^{2}} \cdot \sum_{i=1}^{n}(x_{i}-\bar{x})^{2} \\
= \frac{\sigma^{2}}{\sum_{i=1}^{n}(x_{i}-\bar{x})^{2}}$$

 \Rightarrow

$$\mathbb{V}[\hat{\beta}] = \frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}$$
 (8)

Statistical for Hypothesis Test

If we have to test the next hypotesis:

$$H_0: \beta = \beta_0$$

We use the statistical:

$$T = \frac{\hat{\beta} - \beta_0}{\sqrt{\mathbb{V}(\hat{\beta})}} = \frac{\hat{\beta} - \beta_0}{\sqrt{\frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}}} = \sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \cdot \left(\frac{\hat{\beta} - \beta_0}{\sigma}\right)$$

Often we don't know the value of σ , for this reason we use $\hat{\sigma}$ and the statistical finally is:

$$T = \sqrt{\sum_{i=1}^{n} (x_i - \bar{x})^2} \cdot \left(\frac{\hat{\beta} - \beta_0}{\hat{\sigma}}\right) \sim N(0, 1)$$