Biomedical Engineering Degree

6. Linear Regression

Felipe Alonso Atienza

✉felipe.alonso@urjc.es

@FelipeURJC

Escuela Técnica Superior de Ingeniería de Telecomunicación
Universidad Rey Juan Carlos

References

1. R. Bernard. *Fundamentals of Biostatistics*. Ed.: Thompson. Chapter 11
2. D. Díez, M Cetinkaya-Rundel and CD Barr. *OpenIntro Statistics*. Chapter 8, 9.
3. J. James, D. Witten, T Hastie and R. Tibshirani. *An Introduction to Statistical Learning*. Chapter 3.

Introduction

- A **regression model** is a model that allows us to describe an effect of a variable X on a variable Y

$$Y = f(X)$$

  - X: **independent** or **explanatory** or **exogenous** or **predictor** variable
  - Y: **dependent** or **response** or **endogenous** or **target** variable

- Examples:
  - Estimate the price of an apartment depending on its size
  - Estimate the weight of individuals depending on their height
  - Estimate the voltage depending on the current through a real resistor

- The objective is to obtain reasonable estimates of Y for X based on a sample of n **observations** $(x_1, y_1), \ldots, (x_n, y_n)$

Outline

Deterministic

- Given a value of X, the value of Y can be perfectly identified

$$Y = f(X)$$

  - Example: Ohm's law relationship for Voltage and Current through a Resistor:

$$V = I \cdot R$$

  notice that in the real practice, this relationship expressed in the Ohm's law **physical model** will not be a perfect due to the resistor tolerance

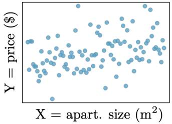
Nondeterministic (random/stochastic)

- Given a value of X, the value of Y **cannot** be perfectly identified

$$Y = f(X) + U$$

where U is an unknown (random) perturbation (random variable).

  - Example: Estimate the price of an apartment depending on its size



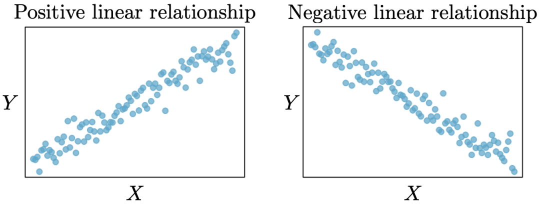
notice that there is a linear pattern, but not perfect. This means that the *apartment size* is not enough to linearly model the price. We might want to add more exogenous/predictor variables to reduce the uncertainty.

Linear

- When the function $f(X)$ is linear, then

$$f(X) = \beta_0 + \beta_1 X$$

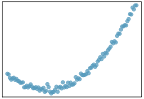
  - if $\beta_1 > 0$ there is a positive linear relationship
  - if $\beta_1 < 0$ there is a negative linear relationship



Nonlinear

- When the function $f(X)$ is nonlinear. For example:

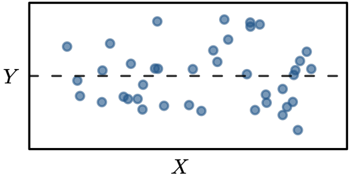
$$
\begin{aligned}
f(X) &= \beta_0 + \beta_1 X + \beta_2 X^2 \\
f(X) &= \log\left(X^2\right) \\
&\dots
\end{aligned}
$$



  - Notice that in the first case, $f(x)$ is nonlinear with respect to the exogenous variable, but it is linear with respect to the β's!

Lack of relationship

- When $f(X) = 0$

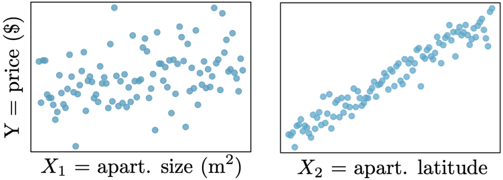


Multiple linear

- When the function $f(\cdot)$ depends on **two or more variables**: $X_1, X_2, \ldots$

$$f(X_1, X_2) = \beta_0 + \beta_1 X_1 + \beta_2 X_2$$

  - Example: Estimate the price of an apartment depending on its size (X_1) and location (X_2).



Outline

Covariance

- It is used to quantify the relationship between two random variables

$$\text{Cov}(X, Y) = \mathsf{E}\left[(X - \mu_X)(Y - \mu_Y)\right] = \mathsf{E}\left[XY\right] - \mu_X \mu_Y$$

which can be calculated using the observations $(x_1, y_1), \ldots, (x_n, y_n)$ as

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

  - If there is a **positive linear** relationship, Cov > 0
  - If there is a **negative linear** relationship, Cov < 0
  - If there is no relationship or the relationship is nonlinear, Cov ≈ 0: uncorrelated variables

- Covariance depends on the units of X and Y

Correlation coefficient

- Normalize the covariance by the standard deviation

$$\rho = r(X, Y) = \mathsf{Cor}(X, Y) = \frac{\mathsf{Cov}(X, Y)}{\sigma_X \sigma_Y}$$

which can be calculated using the observations $(x_1, y_1), \ldots, (x_n, y_n)$ as

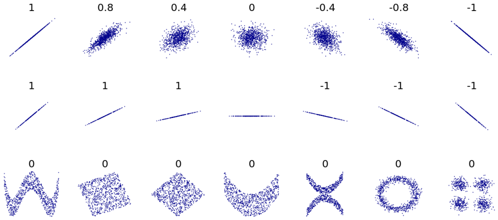
$$\mathsf{cor}(x, y) = \frac{\mathsf{cov}(x, y)}{s_x s_y}$$

where

$$s_x^2 = \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n-1} \quad \text{and} \quad s_y^2 = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n-1}$$

Correlation coefficient

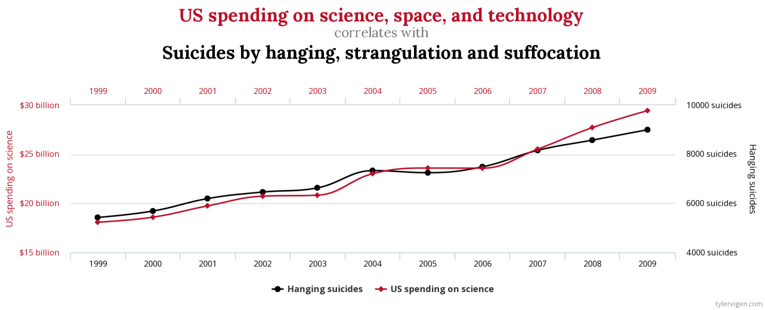
- Also known as Pearson correlation coefficient
- The correlation coefficient is unitless
- Symmetric: $\text{cor}(x, y) = \text{cor}(y, x)$
- $-1 \leq \text{cor}(x, y) \leq 1$
  - $\text{cor}(x, y) = 1$, perfect (positive) linear relationship
  - $\text{cor}(x, y) = -1$, perfect (negative) linear relationship
  - $\text{cor}(x, y) = 0$, no linear relationship



Correlation coefficient

- If X and Y are statistically independent then they are uncorrelated
  - Independent variables: $\mathsf{E}[XY] = \mathsf{E}[X]\mathsf{E}[Y]$
  - Uncorrelated variables $\mathsf{Cov}(X, Y) = \mathsf{E}[XY] - \mathsf{E}[X]\mathsf{E}[Y] = 0$

- **Correlation does not imply causation**[1]!



[1] Figure extracted from *Spurious correlations*

Other correlation measures

- *Spearman's* rank correlation: assesses monotonic relationships (whether linear or not)
- *Kendall's tau* (rank) coefficient: measures the similarity of the orderings of the data when ranked by each of the quantities

Outline

Simple linear regression model

- The simple linear regression model assumes that

$$\boxed{y_i = \beta_0 + \beta_1 x_i + u_i}$$

  where

  - y_i is the $i-$th observation of the dependent variable Y when the random variable X takes the observation value x_i
  - x_i is the $i-$th observation of the exogenous variable X
  - u_i is the error term, which is a **random variable** that accounts for the uncertainty on the observations, an it is assumed to be normal with a mean 0 and an unknown variance σ^2, that is

$$U \sim \mathcal{N}(0, \sigma^2)$$

  - β_0 and β_1 are the regression (population) coefficients:
    - β_0 is the intercept
    - β_1 is the slope
- The (population) parameters need to be estimated: β_0, β_1 and σ^2

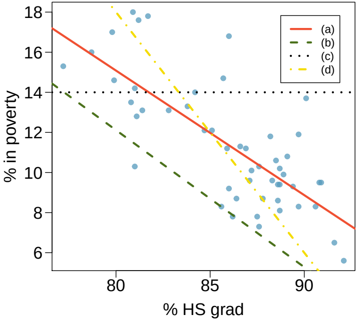
Simple linear regression model

- Based on the observed data $(x_1, y_1), \ldots, (x_n, y_n)$, we want to find the estimates $\hat{\beta}_0$, $\hat{\beta}_1$, in order to obtain the regression line

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$$

which is the best fit to the data with a linear pattern

- Example: High School (HS) graduate rate vs % of residents who live below the poverty line

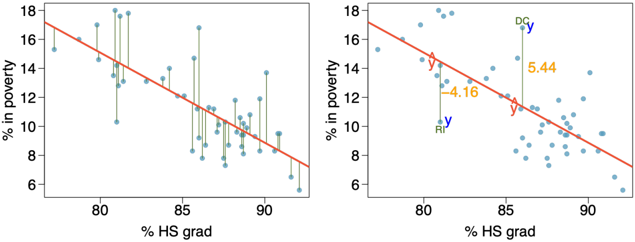


Simple linear regression model

- **Residual** is the difference between the observed y_i and predicted $\hat{y}_i$

$$e_i = y_i - \hat{y}_i$$

- Example: High School (HS) graduate rate vs % of residents who live below the poverty line



  - %living in poverty in DC is 5.44 % more than predicted.
  - % living in poverty in RI is 4.16 % less than predicted.

Simple linear regression model: model assumptions

1. **Linearity**: the relationship between the explanatory and the response variable should be linear.
2. **Homogeneity**: the errors have zero mean

$$\mathsf{E}[u_i] = 0$$

3. **Homoscedasticity**: the variance of the errors is constant

$$\mathsf{Var}(u_i) = \sigma^2$$

4. **Independence**: the errors are independent

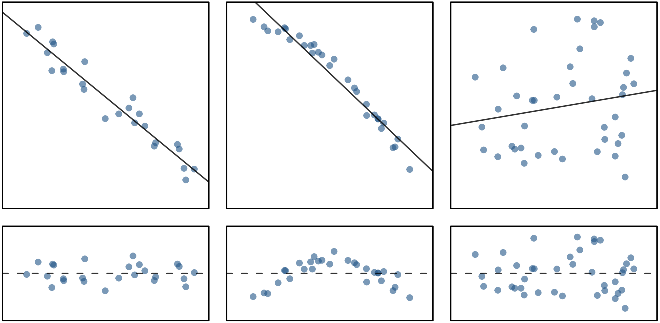
$$\mathsf{E}[u_i u_j] = 0$$

5. **Normality**: the errors should be nearly normal

$$u_i \sim \mathcal{N}(0, \sigma^2)$$

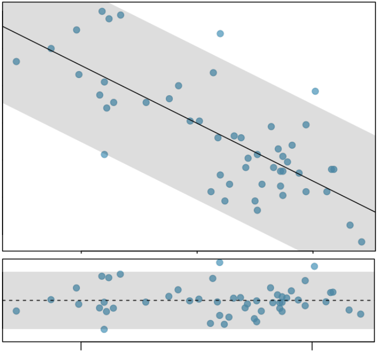
Model assumptions: linearity

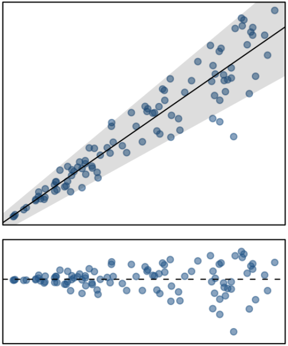
- The relationship between the explanatory and the response variable should be linear.
- Check using a scatterplot of the data, or a **residuals plot**.



Model assumptions: homoscedasticity

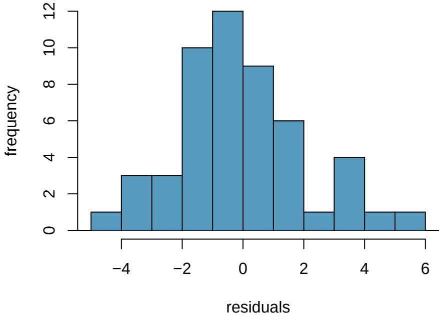
- The variability of points around the (prediction) line should be roughly constant.
- This implies that the variability of residuals around the 0 line should be roughly constant as well.
- If that's not the case, **heteroscedasticity** is present





Model assumptions: normality

- The residuals should be nearly normal
- This condition may not be satisfied when there are unusual observations that don't follow the trend of the rest of the data.
- Check using a histogram



Model assumptions: independence

- The observations should be independent
- One observation doesn't imply any information about another.
- In general, time series fail this assumption.

Outline

Fitting the regression line

- Our aim is to obtain the estimator $\hat{\beta}_0$ and $\hat{\beta}_1$ that provide **the best fit**

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 \hat{x}_i$$

- There are several criteria to obtain the best fit:
  1. Minimize the sum of magnitudes (absolute values) of residuals

$$|e_1| + |e_2| + \ldots + |e_n| = \sum_{i=1}^{n} |e_i|$$

  2. Minimize the **residual sum of squares** (RSS), also known as least squares

$$\text{RSS} = e_1^2 + e_2^2 + \ldots + e_n^2 = \sum_{i=1}^{n} e_i^2$$

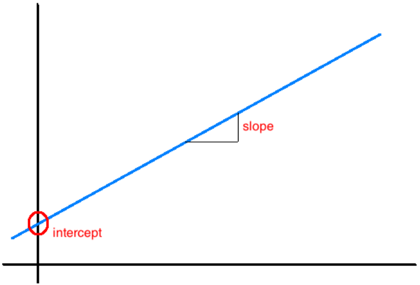
- The least squares method was proposed by Gauss in 1809

$$\text{RSS} = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} \left(y_i - \left(\hat{\beta}_0 + \hat{\beta}_1 \hat{x}_i \right) \right)^2$$

Least squares estimators

- The resulting estimators are

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

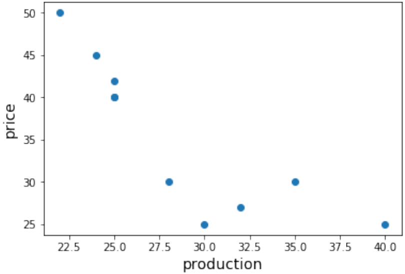


Example

For the Spanish wheat production data from the 80's with production (X) and price per kilo in pesetas (Y) we have the following table

production	30	28	32	25	25	25	22	24	35	40
price	25	30	27	40	42	40	50	45	30	25

- Fit a least squares regression line to the data



Example solution

- We have $n = 10$, $\bar{x} = 28.6$, $\bar{y} = 35.4$, so

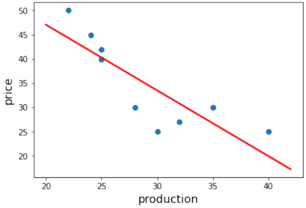
$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} = \frac{-390.4}{288.4} = -1.357$$

- On the other hand

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} = 74.115$$

- Thus

$$\boxed{\hat{y} = 74.115 - 1.3537x}$$



Prediction

production	30	28	32	25	25	25	22	24	35	40
price	25	30	27	40	42	40	50	45	30	25

What is the estimated price value for a production value of 26?

Prediction

production	30	28	32	25	25	25	22	24	35	40
price	25	30	27	40	42	40	50	45	30	25

What is the estimated price value for a production value of 26?

$$\hat{y} = 74.115 - 1.3537 \times 26 = 38.92$$

Goodness-of-fit of the model

- The quality of a linear regression fit is typically assessed using two related quantities:

  1. The residual standard error (RSE): an (unbiased) estimate of σ, the standard deviation of u_i

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

     notice that RSE it is measured in the units of Y, thus it is not always clear what constitutes a good RSE

  2. The R^2 statistic, which is calculated as

     $$\text{R}^2 = 1 - \frac{\text{RSS}}{\text{TSS}}$$

     where $\text{TSS} = \sum_{i=1}^{n}(y_i - \bar{y})^2$ is the **total sum of squares**

R^2 coefficient

- R^2 measures the proportion of variability in Y that can be explained using X
  - RSS measures the amount of **variability that is left unexplained** after performing the regression
  - TSS measures the total variance in the response Y, and can be thought of as the **amount of variability inherent in the response before the regression is performed**
- $R^2 \in [0, 1]$
  - An $R^2 \approx 1$ indicates that a large proportion of the variability in the response has been explained by the regression (good fit).
  - An $R^2 \approx 0$ indicates that the regression did not explain much of the variability in the response (bad fit)
  - In the real practice, less than 0.6, not so good

Outline

Inference in simple linear regression

- Up to this point we only talked about **point estimation**
- With **confidence intervals** for model parameters, we can obtain information about the estimation error.
- And **hypothesis tests** will help us to decide if a given parameter is statistically significant.
- We will use a $t-$test in inference for regression, and remember

$$\text{test statistic} = \frac{\text{point estimate} - \text{null value}}{\text{SE}}$$

Inference for the slope β_1

- It can be demonstrated that

$$\hat{\beta}_1 \sim \mathcal{N}\left(\beta_1, \frac{\sigma^2}{(n-1)s_x^2}\right)$$

- In general, σ^2 is not known, but can be estimated from the RSE ($\sigma^2 = \mathsf{RSE}^2$). So, we can approximate the SE of $\hat{\beta}_1$ by

$$\mathsf{SE}_{\hat{\beta}_1} = \sqrt{\frac{\mathsf{RSE}^2}{(n-1)s_x^2}}$$

- Since we use the *sample* SE, thus

$$t = \frac{\hat{\beta}_1 - \beta_1}{\mathsf{SE}_{\hat{\beta}_1}} \sim t_{n-2}$$

- Notice that we lose 1 df for each parameter we estimate, and in simple linear regression we estimate 2 parameters, β_0 and β_1.

Confidence interval for the slope β_1

- $1-\alpha$ confidence interval

$$\hat{\beta}_1 \pm t_{n-2,1-\alpha/2} \times \underbrace{\sqrt{\frac{\mathsf{RSE}^2}{(n-1)s_x^2}}}_{\mathsf{SE}_{\hat{\beta}_1}}$$

- The length of the interval decreases if
  - The sample size increases
  - The variance of X increases
  - The RSE decreases

Hypothesis test on β_1

H_0 : There is no relationship between X and Y

H_1 : There is some relationship between X and Y

- Mathematically, this corresponds to testing

$$H_0 : \beta_1 = 0 \quad \text{vs} \quad H_1 : \beta_1 \neq 0$$

- Thus, we calculate our statistic

$$t = \frac{\hat{\beta}_1 - 0}{\mathsf{SE}_{\hat{\beta}_1}} \sim t_{n-2}$$

- Then, for a α significance level
  - We reject the null hypothesis if $|t| > t_{n-2,1-\alpha/2}$

Inference for the intercept β_0

- In this case

$$\hat{\beta}_0 \sim \mathcal{N}\left(\beta_0, \sigma^2\left(\frac{1}{n} + \frac{\bar{x}^2}{(n-1)s_x^2}\right)\right)$$

- In general, σ^2 is not known, but can be estimated from the RSE ($\sigma^2 = \mathsf{RSE}^2$). So, we can approximate the SE of $\hat{\beta}_0$ by

$$\mathsf{SE}_{\hat{\beta}_0} = \sqrt{\mathsf{RSE}^2\left(\frac{1}{n} + \frac{\bar{x}^2}{(n-1)s_x^2}\right)}$$

- Since we use the *sample* SE, thus

$$t = \frac{\hat{\beta}_0 - \beta_0}{\mathsf{SE}_{\hat{\beta}_0}} \sim t_{n-2}$$

Inference for the intercept β_0

- $1-\alpha$ confidence interval

$$\hat{\beta}_0 \pm t_{n-2,1-\alpha/2} \times \underbrace{\sqrt{\mathsf{RSE}^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{(n-1)s_x^2} \right)}}_{\mathsf{SE}_{\hat{\beta}_0}}$$

- Hypothesis testing: if the true value of β_0 is 0, it means that the population regression line goes through the origin.

$$H_0 : \beta_0 = 0 \quad \text{vs} \quad H_1 : \beta_0 \neq 0$$

using the statistic

$$t = \frac{\hat{\beta}_0 - 0}{\mathsf{SE}_{\hat{\beta}_0}} \sim t_{n-2}$$

Example

For the Spanish wheat production data from the 80's with production (X) and price per kilo in pesetas (Y) we have the following table

production	30	28	32	25	25	25	22	24	35	40
price	25	30	27	40	42	40	50	45	30	25

- Find a 95 % CI for the slope of the (population) regression model
- Test the hypothesis that the price of wheat depends linearly on the production at a 0.05 significance level

Example solution

- Find a 95 % CI for the slope of the (population) regression model

$$\hat{\beta}_1 \pm t_{n-2,1-\alpha/2} \times \underbrace{\sqrt{\frac{\mathsf{RSE}^2}{(n-1)s_x^2}}}_{\mathsf{SE}_{\hat{\beta}_1}}$$

where $n = 10$, $\alpha = 0.05$ and therefore

$$t_{n-2,1-\alpha/2} = t_{8,0.975} = \texttt{t(df=8).ppf(0.975)} = 2.306$$

- On the other hand

$$\begin{aligned} \mathsf{RSE}^2 &= \frac{RSS}{n-2} = 25.99 \\ s_x^2 &= 32.04 \end{aligned}$$

- Thus $\boxed{-2.046 \leq \beta_1 \leq -0.661}$

Example solution

- Test the hypothesis that the price of wheat depends linearly on the production at a 0.05 significance level

$$t = \frac{\hat{\beta}_1 - 0}{\mathsf{SE}_{\hat{\beta}_1}} = \frac{-1.3537}{\sqrt{\frac{25.99}{(10-1)\times 32.04}}} = 4.509$$

- We can calculate the $p-$value (two-sided)

$$p = \texttt{2*t(df=8).cdf(-4.509)} = 0.001978$$

- Thus, **we reject the null hypothesis**. X and Y are not independent.

Example solution

Using Python

```
import statsmodels.api as sm

X = [30, 28, 32, 25, 25, 25, 22, 24, 35, 40]
Y = [25, 30, 27, 40, 42, 40, 50, 45, 30, 25]

X = sm.add_constant(X)
model = sm.OLS(Y,X)

results = model.fit()
results.summary()
```

	coef	std err	t	P>|t|	[0.025	0.975]
const	74.1151	8.736	8.484	0.000	53.970	94.260
x1	-1.3537	0.300	-4.509	0.002	-2.046	-0.661