3 OCT - LEC 2

SIMPLE LINEAR MODEL VIA ORDINARY LEAST SQUARES (OLS)

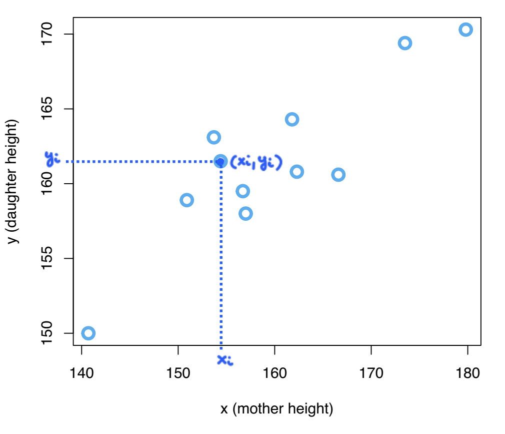
Assume that on n statistical units (individuals) we observe (x_i, y_i), $i=1,\dots,n$.
Hence the data are $\underline{y}=(y_1,\dots,y_n)$ and $\underline{x}=(x_1,\dots,x_n)$
We consider that each y_i is realization of a r.v. Y_i, $i=1,\dots,n$ $\rightarrow$ sample space $S=\mathcal{Y}^n=\mathbb{R}^n$

We do not specify a distribution for $(Y_1,\dots,Y_n)$: we only make assumptions about the first two moments $\mathbb{E}[Y_i]$ and $var(Y_i)$.

We specify a <u>simple</u> linear model (only 1 covariate)
We estimate the model parameters only through "intuitive" considerations and a simple optimization ("ordinary least squares" method)

We start with a simple example
relationship between the height of 11 mothers (x_i) and the height of their daughters (y_i).

	x	y
1	153.7	163.1
2	156.7	159.5
3	173.5	169.4
4	157.0	158.0
5	161.8	164.3
6	140.7	150.0
7	179.8	170.3
8	150.9	158.9
9	154.4	161.5
10	162.3	160.8
11	166.6	160.6



Intuition:
the simplest way to describe the relationship between two quantities is a straight line:
$$Y_i = \beta_1 + \beta_2 x_i \qquad i=1,\dots,n$$
However, such a relationship does not hold exactly: the points are not PERFECTLY ALIGNED.
hence we add an error term to take into account this discrepancy:
$$Y_i = \beta_1 + \beta_2 x_i + \varepsilon_i \qquad i=1,\dots,n$$

1st step: MODEL SPECIFICATION

Consider the model:
$$\underbrace{Y_i}_{\text{height of the i-th daughter}} = \underbrace{\beta_1 + \beta_2 x_i}_{\text{systematic component}} + \underbrace{\varepsilon_i}_{\text{ERROR TERM}} \qquad i=1,\dots,n$$
ERROR TERM: the linear relationship is not exact

(β_1, β_2) are the REGRESSION COEFFICIENTS
We specified a straight line with the intercept (β_1)
We only observe 1 covariate, but we also introduce one additional "variable" taking value 1 for each individual.
The model matrix then is:
$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

$\Rightarrow$ β_1 is the INTERCEPT (coefficient of $\underline{1}$)
β_2 is the COEFFICIENT of x (slope)

ASSUMPTIONS on the independent variables
1. $x_1,\dots,x_n$ fixed and non-stochastic
2. the x_i can not be all equal (sample variance of $(x_1,\dots,x_n)$ must be $\neq 0$)

The systematic component is now fully specified, we need to define the stochastic component (ε).

ASSUMPTIONS on the STOCHASTIC COMPONENT
1. $\mathbb{E}[\varepsilon_i]=0$ for $i=1,\dots,n$
2. $Var(\varepsilon_i)=\sigma^2>0$ $i=1,\dots,n$ (common variance across subjects)
3. $Cov(\varepsilon_i,\varepsilon_k)=0$ if $i\neq k$, $i=1,\dots,n$ $k=1,\dots,n$

1. $\mathbb{E}[\varepsilon_i]=0$ $i=1,\dots,n$ ABSENCE OF SYSTEMATIC ERROR

Implications for Y_i
$$\mathbb{E}[Y_i]=\mathbb{E}[\beta_1+\beta_2 x_i+\varepsilon_i] \overset{\text{linearity of } \mathbb{E}}{=} \mathbb{E}[\underbrace{\beta_1+\beta_2 x_i}_{\text{non-stochastic}}]+\underbrace{\mathbb{E}[\varepsilon_i]}_{0} = \beta_1+\beta_2 x_i$$

What happens if there is a systematic error? i.e. $\mathbb{E}[\varepsilon_i]=c\neq 0$
$\mathbb{E}[Y_i]=\beta_1+\beta_2 x_i + c = (\beta_1+c)+\beta_2 x_i$
the systematic error c is inglobated into the intercept (not a problem)
it is equivalent to a model
$Y_i = \beta_1^* + \beta_2 x_i + \varepsilon_i^*$ where $\beta_1^* = \beta_1 + c$
$\varepsilon_i^* = \varepsilon_i - c \Rightarrow \mathbb{E}[\varepsilon_i^*]=0$

2. $Var(\varepsilon_i)=\sigma^2>0$ for all $i=1,\dots,n$ HOMOSCEDASTICITY OF THE ERRORS

Implications for Y_i:
$$var(Y_i)=var(\underbrace{\beta_1+\beta_2 x_i}_{\text{non-stoch.}}+\varepsilon_i)=var(\varepsilon_i)=\sigma^2 \quad \forall i=1,\dots,n$$
$\Rightarrow$ homoscedasticity of the response

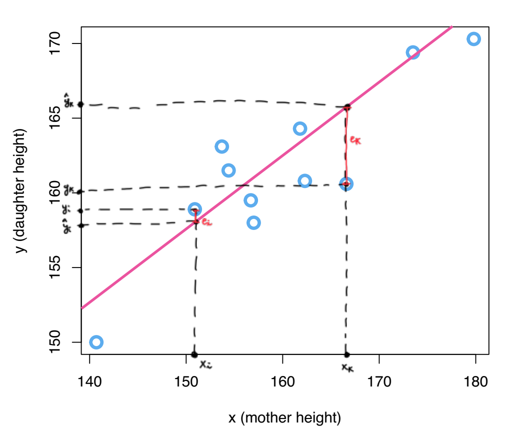
3. $cov(\varepsilon_i,\varepsilon_k)=0$ for $i\neq k$ THE ERRORS ARE UNCORRELATED

Implication for Y_i
$$cov(Y_i,Y_k)=cov(\underbrace{\beta_1+\beta_2 x_i}_{\text{non-stochastic}}+\varepsilon_i \,;\, \underbrace{\beta_1+\beta_2 x_k}+\varepsilon_k) = cov(\varepsilon_i,\varepsilon_k)=0$$

2nd step: ESTIMATE

what do we need to estimate? Unknown quantities are $(\beta_1,\beta_2,\sigma^2)$
Hence the PARAMETER SPACE is $\Theta = \mathbb{R}^2\times(0,+\infty)$

Every combination of (β_1,β_2) determines a specific line: how do we select the "best" line?
We need a criterion of what is a "good" line.
We want a line which is the <u>closest</u> to the observed points.



Consider this line: at each value of x_i corresponds one value of y_i that lies on the line
$\Rightarrow$ given x_i and fixed (β_1,β_2) we can compute the corresponding value of y_i (according to the line)
$$\hat{y}_i = \beta_1 + \beta_2 x_i \qquad \text{"predicted value"}$$

The discrepancy between the observed and the predicted value (at the observed locations x_i)
RESIDUAL: $e_i = y_i - \hat{y}_i$

A good line will have small residuals OVERALL.
- we could consider the sum of the residuals $\sum_{i=1}^n e_i$ and select the (β_1,β_2) that minimize it
  $\rightarrow$ not a good idea: positive and negative values cancel out.
- we could consider the sum of the absolute values $\sum_{i=1}^n |e_i|$ $\rightarrow$ mathematically not very practical
- we consider instead the sum of the SQUARED residuals
$$\sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i-\hat{y}_i)^2 = \sum_{i=1}^n (y_i-\beta_1-\beta_2 x_i)^2 = S(\beta_1,\beta_2)$$
  and take as an estimate of (β_1,β_2) the combination that minimizes it.

<u>DEF</u>: the LEAST SQUARES estimate of (β_1,β_2) is the combination of values $(\hat\beta_1,\hat\beta_2)$ that minimizes $S(\beta_1,\beta_2)$
$$(\hat\beta_1,\hat\beta_2) = \underset{(\beta_1,\beta_2)\in\mathbb{R}^2}{\arg\min}\ S(\beta_1,\beta_2) = \underset{(\beta_1,\beta_2)\in\mathbb{R}^2}{\arg\min}\ \sum_{i=1}^n (y_i-\beta_1-\beta_2 x_i)^2$$
We have hence turned a problem of estimation into an optimization.

<u>THM</u>: The least squares estimate of (β_1,β_2) is
$$\hat\beta_1 = \bar{y} - \hat\beta_2\bar{x}$$
$$\hat\beta_2 = \frac{\sum_{i=1}^n (x_i-\bar{x})(y_i-\bar{y})}{\sum_{i=1}^n (x_i-\bar{x})^2}$$
where $\bar{x}=\frac{1}{n}\sum_{i=1}^n x_i$
$\bar{y}=\frac{1}{n}\sum_{i=1}^n y_i$ (sample mean).

Remark:
recall that the sample variance of $(x_1,\dots,x_n)$ is $s_x^2=\frac{1}{n-1}\sum_{i=1}^n (x_i-\bar{x})^2$
(and similarly for s_y^2)
the sample covariance is $s_{xy}=\frac{1}{n-1}\sum_{i=1}^n (x_i-\bar{x})(y_i-\bar{y})$
Hence $\hat\beta_2=\frac{s_{xy}}{s_x^2}$

<u>Proof</u>: we want to show that $\hat\beta_1,\hat\beta_2$ minimize $S(\beta_1,\beta_2)=\sum_{i=1}^n (y_i-\beta_1-\beta_2 x_i)^2$.
We need to find the critical points (1st derivative $=0$)
and then check that $(\hat\beta_1,\hat\beta_2)$ is a minimum (2nd derivative >0)
$$\begin{cases} \frac{\partial S(\beta_1,\beta_2)}{\partial\beta_1}=0 \\ \frac{\partial S(\beta_1,\beta_2)}{\partial\beta_2}=0 \end{cases} \qquad \begin{cases} \sum_{i=1}^n 2(y_i-\beta_1-\beta_2 x_i)(-1)=0 \\ \sum_{i=1}^n 2(y_i-\beta_1-\beta_2 x_i)(-x_i)=0 \end{cases}$$
$$\begin{cases} \sum_{i=1}^n (y_i-\beta_1-\beta_2 x_i)=0 & (A) \\ \sum_{i=1}^n x_i(y_i-\beta_1-\beta_2 x_i)=0 & (B) \end{cases}$$

(A) $\cancel{n}\bar{y}-\cancel{n}\beta_1-\cancel{n}\beta_2\bar{x}=0$ (since $\sum_{i=1}^n y_i = n\bar{y}$)
$\beta_1=\bar{y}-\beta_2\bar{x}$

(B) $\sum_{i=1}^n x_i y_i - n\bar{x}\beta_1 - \beta_2\sum_{i=1}^n x_i^2 = 0$ substituting $\beta_1=\bar{y}-\beta_2\bar{x}$
$\sum_{i=1}^n x_i y_i - n\bar{x}\bar{y} + n\beta_2\bar{x}^2 - \beta_2\sum_{i=1}^n x_i^2 = 0$
$$\hat\beta_2 = \frac{\sum_{i=1}^n x_i y_i - n\bar{x}\bar{y}}{\sum_{i=1}^n x_i^2 - n\bar{x}^2}$$
but since
$(n-1)s_x^2 = \sum_{i=1}^n (x_i-\bar{x})^2 = \sum_{i=1}^n x_i^2 - n\bar{x}^2$ and
$\sum(x_i^2+\bar{x}^2-2x_i\bar{x}) = \sum x_i^2 + n\bar{x}^2 - 2\bar{x}\sum x_i = \sum x_i^2 + n\bar{x} - 2n\bar{x}$
$(n-1)s_{xy} = \sum_{i=1}^n (x_i-\bar{x})(y_i-\bar{y}) = \sum_{i=1}^n x_i y_i - n\bar{x}\bar{y}$
$\sum(x_i y_i - x_i\bar{y} - y_i\bar{x} + \bar{x}\bar{y}) = \sum x_i y_i - n\bar{x}\bar{y} - \cancel{n\bar{x}\bar{y}} + \cancel{n\bar{x}\bar{y}}$

we obtain $\hat\beta_2 = \frac{s_{xy}}{s_x^2}$
and $\hat\beta_1 = \bar{y} - \hat\beta_2\bar{x}$

Is $(\hat\beta_1,\hat\beta_2)$ a minimum? We compute the Hessian
$$H = \begin{bmatrix} \frac{\partial^2 S(\beta_1,\beta_2)}{\partial\beta_1^2} & \frac{\partial^2 S(\beta_1,\beta_2)}{\partial\beta_1\partial\beta_2} \\ \frac{\partial^2 S(\beta_1,\beta_2)}{\partial\beta_2\partial\beta_1} & \frac{\partial^2 S(\beta_1,\beta_2)}{\partial\beta_2^2} \end{bmatrix} = \begin{bmatrix} 2n & 2n\bar{x} \\ 2n\bar{x} & 2\sum_{i=1}^n x_i^2 \end{bmatrix}$$
$$\det(H) = 4n\sum_{i=1}^n x_i^2 - 4n^2\bar{x}^2 = 4n\left(\sum_{i=1}^n x_i^2 - n\bar{x}^2\right) = 4n\sum_{i=1}^n (x_i-\bar{x})^2 > 0$$
since $\det(H)>0$ and $H_{1,1}=2n>0$, $(\hat\beta_1,\hat\beta_2)$ is a minimum of $S(\beta_1,\beta_2)$
Moreover, it is the global minimum. □

Remarks:
- we did not use the assumptions on ε_i
- we used the assumption on the x_i: what happens if $x_i=x_0$ for all $i=1,\dots,n$?
  $(x_i-\bar{x})=0$ $\forall i \Rightarrow s_x^2=0$ and $s_{xy}=0 \Rightarrow \hat\beta_2=\frac{0}{0}$ not defined
- once we estimate $(\hat\beta_1,\hat\beta_2)$, we automatically obtain $\hat{y}=\hat\beta_1+\hat\beta_2 x$, i.e. the estimated regression line.
- $\hat{y}$ allows us to make predictions: given a generic value x, we predict the corresponding value of the response.
  As usual, careful with extrapolation, i.e., estimating the response for a value of x outside of the observed range of $(x_1,\dots,x_n)$.

- INTERPRETATION of $(\hat\beta_1,\hat\beta_2)$

we have estimated a line $\hat{y}=\hat\beta_1+\hat\beta_2 x$

$\hat\beta_1$ is the intercept, i.e., the predicted value of y when $x=0$.
Not always interpretable! E.g. with the heights example: height $=0$ is meaningless

Now consider two individuals observed at $x_1=x_0$ and $x_2=x_0+1$
The predicted values are
$$\hat{y}_1=\hat\beta_1+\hat\beta_2 x_0$$
$$\hat{y}_2=\hat\beta_1+\hat\beta_2(x_0+1)$$
let's study the difference in their predicted values
$$\hat{y}_2-\hat{y}_1 = \cancel{\hat\beta_1}+\hat\beta_2(x_0+1)-\cancel{\hat\beta_1}-\hat\beta_2 x_0 = \cancel{\hat\beta_2 x_0}+\hat\beta_2-\cancel{\hat\beta_2 x_0} = \hat\beta_2$$
Hence $\hat\beta_2$ is the expected change in y when I increase x of 1 unit