Master Program in *Data Science and Business Informatics*

Statistics for Data Science

Lesson 20 - Linear Regression and Least Squares Estimation

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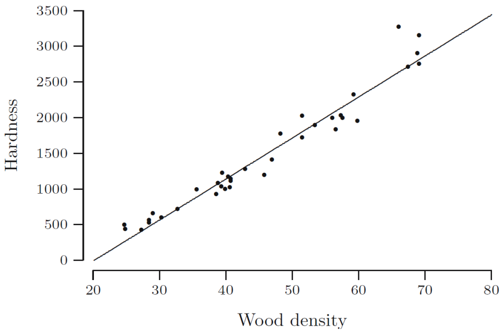
Bivariate dataset

- Consider a bivariate dataset

$$(x_1, y_1), \dots, (x_n, y_n)$$

- It can be visualized in a scatter plot



- This suggests a relation *Hardness* $= \alpha + \beta \cdot$ *Density* $+$ *random fluctuation*

Simple linear regression model

SIMPLE LINEAR REGRESSION MODEL. In a *simple linear regression model* for a bivariate dataset $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, we assume that $x_1, x_2, \ldots, x_n$ are nonrandom and that $y_1, y_2, \ldots, y_n$ are realizations of random variables $Y_1, Y_2, \ldots, Y_n$ satisfying

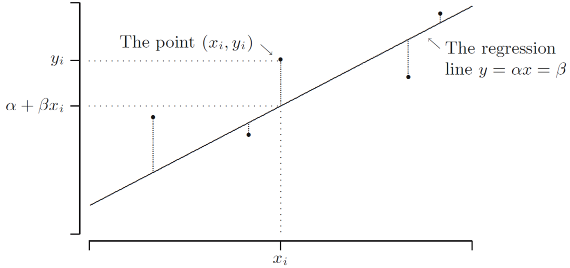
$$Y_i = \alpha + \beta x_i + U_i \quad \text{for } i = 1, 2, \ldots, n,$$

where $U_1, \ldots, U_n$ are *independent* random variables with $\mathrm{E}[U_i] = 0$ and $\mathrm{Var}(U_i) = \sigma^2$.

- *Regression line*: $y = \alpha + \beta x$ with *intercept* α and *slope* β
- x is the *explanatory* (or *independent*) variable, and y the *response* (or *dependent*) variable
- Independence of $U_1, \ldots, U_n$ implies independence of $Y_1, \ldots, Y_n$ *[propagation of ind.]*
  - But Y_i's are not identically distributes, as $E[Y_i] = \alpha + \beta x_i$
- Also, notice the assumption $Var(Y_i) = Var(U_i) = \sigma^2$ *[homoscedasticity]*

Estimation of parameters

- How to estimate α and β? MLE requires to know the distribution of the U_i's



- $y_i - \alpha - \beta x_i$ is called a *residual* (or the *error*), and it is a realization of $U_i = Y_i - \alpha - \beta x_i$
  - recall that $E[U_i] = 0$ and $Var(U_i) = E[U_i^2] = \sigma^2$
- The method of *Least Squares* prescribes to minimize the sum of squares of residuals:

$$\hat{\alpha}, \hat{\beta} = arg \min_{\alpha,\beta} S(\alpha, \beta) \qquad \text{where } S(\alpha, \beta) = \sum_{i=1}^{n} (y_i - \alpha - \beta x_i)^2$$

  - $S(\alpha, \beta)$ also called Sum of Squares of Errors (SSE) or Residual Sum of Squares (RSS)

Least Squares Estimates

$$S(\alpha, \beta) = \sum_{i=1}^{n} (y_i - \alpha - \beta x_i)^2$$

- Partial derivatives:

$$\frac{d}{d\alpha} S(\alpha, \beta) = -\sum_{i=1}^{n} 2(y_i - \alpha - \beta x_i) \qquad \frac{d}{d\beta} S(\alpha, \beta) = -\sum_{i=1}^{n} 2(y_i - \alpha - \beta x_i) x_i$$

- Equal to 0 for:

$$n\alpha + \beta \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i \qquad \alpha \sum_{i=1}^{n} x_i + \beta \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i$$

  and solving, we get:

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

- $\hat{y}_i = \hat{\alpha} + \hat{\beta} x_i$ are called the *fitted values*

Ordinary Least Squares (OLS) Estimates

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

- Equivalent form of $\hat{\beta}$ **[prove it!]**

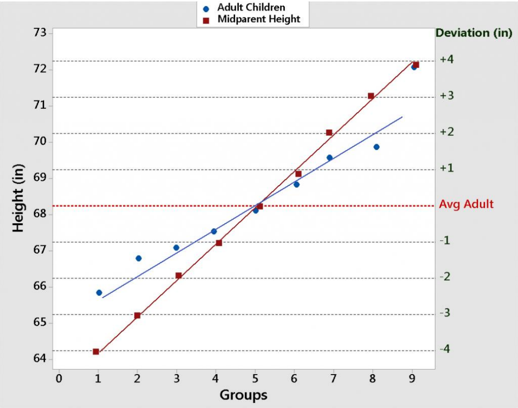
$$\hat{\beta} = \frac{\sum_1^n (x_i - \bar{x}_n)(y_i - \bar{y}_n)}{SXX} = r_{xy}\frac{s_y}{s_x}$$

  where:
  - $SXX = \sum_1^n (x_i - \bar{x}_n)^2$
  - $r_{xy} = \frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)\cdot(y_i - \bar{y}_n)}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x}_n)^2 \cdot \sum_{i=1}^{n}(y_i - \bar{y}_n)^2}}$ is the Pearson's correlation coefficient
  - $s_x = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x}_n)^2}$ is the sample standard deviations of x_i's
  - $s_y = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(y_i - \bar{y}_n)^2}$ is the sample standard deviations of y_i's
- The line $y = \hat{\alpha} + \hat{\beta}x$ always passes through the *center of gravity* $(\bar{x}_n, \bar{y}_n)$
  - Since $\hat{\alpha} = \bar{y}_n - \hat{\beta}\bar{x}_n$, we have $\hat{\alpha} + \hat{\beta}\bar{x}_n = \bar{y}_n - \hat{\beta}\bar{x}_n + \hat{\beta}\bar{x}_n = \bar{y}_n$

See R script

Why 'regression'?

So, why is it called 'regression' anyway?



"**See Francis Galton** concluded that as heights of the parents deviated from the average height, [...] the heights of the children *regressed* to the average height of an adult."

Unbiasedness of estimators: $\hat{\beta}$

- Consider the least square estimators:

$$\hat{\alpha} = \bar{Y}_n - \hat{\beta}\bar{x}_n \qquad \hat{\beta} = \frac{\sum_1^n (x_i - \bar{x}_n)(Y_i - \bar{Y}_n)}{SXX}$$

where $SXX = \sum_1^n (x_i - \bar{x}_n)^2$. Since $\sum_1^n (x_i - \bar{x}_n) = 0$,we can rewrite $\hat{\beta}$ as:

$$\hat{\beta} = \frac{\sum_1^n (x_i - \bar{x}_n) Y_i - \sum_1^n (x_i - \bar{x}_n) \bar{Y}_n}{SXX} = \frac{\sum_1^n (x_i - \bar{x}_n) Y_i}{SXX} \tag{1}$$

- We have:

$$E[\hat{\beta}] = \frac{\sum_1^n (x_i - \bar{x}_n) E[Y_i]}{SXX} = \frac{\sum_1^n (x_i - \bar{x}_n)(\alpha + \beta x_i)}{SXX} = \frac{\beta \sum_1^n (x_i - \bar{x}_n) x_i}{SXX} = \beta$$

where the last step follows since $\sum_1^n (x_i - \bar{x}_n) x_i = \sum_1^n (x_i - \bar{x}_n) x_i - \sum_1^n (x_i - \bar{x}_n) \bar{x}_n = SXX$.

- Moreover:

$$Var(\hat{\beta}) = \frac{\sum_1^n (x_i - \bar{x}_n)^2 Var(Y_i)}{SXX^2} = \sigma^2 \frac{\sum_1^n (x_i - \bar{x}_n)^2}{SXX^2} = \frac{\sigma^2}{SXX}$$

Unbiasedness of estimators: $\hat{\alpha}$

- Consider the least square estimators:

$$\hat{\alpha} = \bar{Y}_n - \hat{\beta}\bar{x}_n \qquad \hat{\beta} = \frac{\sum_1^n (x_i - \bar{x}_n)(Y_i - \bar{Y}_n)}{SXX}$$

- We have:

$$\begin{aligned} E[\hat{\alpha}] &= E[\bar{Y}_n] - \bar{x}_n E[\hat{\beta}] = \frac{1}{n}\sum_{i=1}^{n} E[Y_i] - \bar{x}_n \beta \\ &= \frac{1}{n}\sum_{i=1}^{n}(\alpha + \beta x_i) - \bar{x}_n\beta = \alpha + \bar{x}_n\beta - \bar{x}_n\beta = \alpha \end{aligned}$$

- Moreover:

$$Var(\hat{\alpha}) = Var(\bar{Y}_n - \hat{\beta}\bar{x}_n) = Var(\bar{Y}_n) + \bar{x}_n^2 Var(\hat{\beta}) - 2\bar{x}_n Cov(\bar{Y}_n, \hat{\beta}) = \sigma^2(\frac{1}{n} + \frac{\bar{x}_n^2}{SXX})$$

where $Cov(\bar{Y}_n, \hat{\beta}) = 0$ [**prove it** or see sdsln.pdf Chpt. 2]

An estimator for σ^2, and standard errors

- $Var(\hat{\alpha})$ and $Var(\hat{\beta})$ use σ^2, which is unknown
- We cannot use $\frac{1}{(n-1)}\sum_1^n (Y_i - \bar{Y}_n)^2$ as an estimator of σ^2, because $E[Y_i]$ is not constant
- An unbiased estimate of σ^2 is:

$$\hat{\sigma}^2 = \frac{1}{n-2}\sum_1^n (y_i - \hat{\alpha} - \hat{\beta}x_i)^2$$

$\hat{\sigma}$ is called the *residual standard error*. A close measure is the Root Mean Squared Error:

$$RMSE = \sqrt{\frac{1}{n}\sum_1^n (y_i - \hat{\alpha} - \hat{\beta}x_i)^2}$$

- The *standard errors* of the coefficient estimators are defined as the estimates of the standard deviations:

$$se(\hat{\alpha}) = \hat{\sigma}\sqrt{(\frac{1}{n} + \frac{\bar{x}_n^2}{SXX})} \qquad se(\hat{\beta}) = \frac{\hat{\sigma}}{\sqrt{SXX}}$$

See R script

LSE: Relation with MLE

$$Y_i = \alpha + \beta x_i + U_i$$

- In case $U_i \sim N(0, \sigma^2)$, we have $Y_i \sim N(\alpha + \beta x_i, \sigma^2)$
- Log-likelihood is
  $\ell(\alpha, \beta) = \sum_{i=1}^n \log\left(\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{y_i - \alpha - \beta x_i}{\sigma^2}\right)^2}\right) = -n \log\left(\sigma\sqrt{2\pi}\right) - \frac{1}{2\sigma^2}\sum_{i=1}^n (y_i - \alpha - \beta x_i)^2$
- It turns out that $\textit{arg}\max_{\alpha,\beta} \ell(\alpha, \beta) = \hat{\alpha}, \hat{\beta}$ *[same estimators as LSE]*

Total variability = explained variability + unexplained variability

- Total variability in the data. Sum of Squares Total (SST):

$$SST = \sum_{1}^{n} (y_i - \bar{y}_n)^2$$

- Variability explained by regression. Sum of Squares of Regression (SSR):

$$SSR = \sum_{1}^{n} (\hat{\alpha} + \hat{\beta} x_i - \bar{y}_n)^2 = \sum_{1}^{n} (\hat{y}_i - \bar{\hat{y}}_n)^2$$

  because $\bar{\hat{y}}_n = \frac{1}{n} \sum_1^n (\hat{\alpha} + \hat{\beta} x_i) = \hat{\alpha} + \hat{\beta} \hat{x}_n = \bar{y}_n$

- Unexplained variability. Sum of Squares of Errors (SSE):

$$SSE = \sum_{1}^{n} (y_i - \hat{\alpha} - \hat{\beta} x_i)^2$$

- It turns out: $SST = SSR + SSE$ **[Prove it!]**
- $1 - SSE/SST$ (or SSR/SST) is the fraction of explained variability over total variability

Residuals and R^2 (fraction of explained variability)

- $1 - SSE/SST$ (or SSR/SST) is the fraction of explained variability over total variability
- When taking empirical variances:

$$\sigma_y^2 = \frac{1}{n-1}\sum_1^n (y_i - \bar{y}_n)^2 = \frac{SST}{n-1} \qquad \sigma_{res}^2 = \frac{1}{n-1}\sum_1^n (y_i - \hat{y}_i)^2 = \frac{SSE}{n-1}$$

  we define the *coefficient of determination* $R^2 = 1 - \sigma_{res}^2/\sigma_y^2$

  - **Exercise:** show σ_{res}^2 is the empirical variance of residuals, i.e., $\frac{1}{n}\sum_1^n (y_i - \hat{\alpha} - \hat{\beta}x_i) = 0$

- Using the variance of the fitted:

$$\sigma_{\hat{y}}^2 = \frac{1}{n-1}\sum_1^n (\hat{y}_i - \bar{\hat{y}}_n)^2 = \frac{SSR}{n-1}$$

  alternative definition is $R^2 = \sigma_{\hat{y}}^2/\sigma_y^2$

- For simple (one independent r.v.) linear regression: **[Prove it!]**

$$R^2 = r_{y\hat{y}}^2 = \frac{[\sum_{i=1}^n (y_i - \bar{y}_n)\cdot(\hat{y}_i - \bar{\hat{y}}_n)]^2}{\sum_{i=1}^n (y_i - \bar{y}_n)^2 \cdot \sum_{i=1}^n (\hat{y}_i - \bar{\hat{y}}_n)^2}$$

Adjusted R^2

- $1 - SSE/SST$ (or SSR/SST) is the fraction of explained variability over total variability
- When taking adjusted variances:

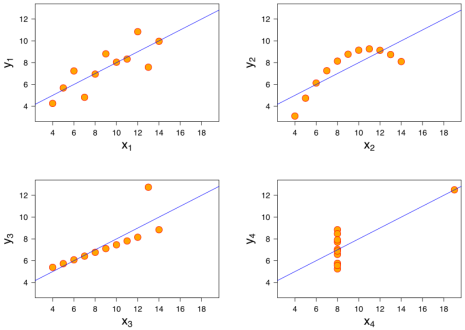
$$\sigma_y^2 = \frac{1}{n-1}\sum_1^n (y_i - \bar{y}_n)^2 = \frac{SST}{n-1} \qquad \hat{\sigma}^2 = \frac{1}{n-2}\sum_1^n (y_i - \hat{y}_i)^2 = \frac{SSE}{n-2}$$

(where $\hat{\sigma}$ is the residual standard error), we define the *adjusted coefficient of determination*:

$$adjR^2 = 1 - \frac{\hat{\sigma}^2}{\hat{\sigma}_y^2} = 1 - \frac{\sigma_{res}^2}{\hat{\sigma}_y^2}\frac{n-1}{n-2}$$

See R script

Anscombe's quartet



- Same regression line $y = 3 + x/2$
  - Top left: linear regression
  - Top right: non-linear regression
  - Bottom left: linear regression with outliers (requires robust regression approaches)
  - Bottom right: single **high-leverage** point produces correlation
- Look at data graphically before starting to analyze them with a specific technique!

See R script

Optional references

Michael H. Kutner, Christopher J. Nachtsheim, John Neter, and William Li (2005)
Applied Linear Statistical Models.
5th edition *McGraw-Hill*