Bi-variate analysis and linear regression

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Bivariate Data and Linear Regression

Ref: D. Diez, M. Cetinkaya-Rundel, C. Barr, *OpenIntro Statistics* (4th Edition), OpenIntro, 2019 [available for download at www.openintro.org/book/os/, accessed 27/01/2020]

Content

- Bivariate Data
- Measuring Associations between variables
- Linear Regression
  - Finding the 'best straight line'
- Visualisation
- Residuals
- Generalisations

Bivariate Data

- Bivariate – involving 2 variables
  - Data consists of pairs of values (x,y)
  - Where x is a value of some variable X and y is a corresponding value of some variable Y
- Examples
  - People’s size: height and weight
  - Pressure and temperature measured at a number of locations
  - GPS location: latitude and longitude
  - Game result: goals for team 1 and goals for team 2.

Goals

- Individual variables X and Y can be analysed independently using univariate methods
  - But independent analysis of each variable does not make use of the information about pairs
- The relationship between the 2 variables can be discovered, visualised and quantified

Measures of Association

- Covariance

$$\sigma(x, y) = \frac{\sum_{i=1}^{N}(x_i - \bar{x}) * (y_i - \bar{y})}{N}$$

- Measure of how much two variables vary together.

Covariance interpretation

- **Positive:** there is a positive association between variables x and y.
  - x tends to be higher than average when y is higher than average
- **Negative:** there is a negative association.
  - x tends to be lower than average when y is higher than average
- **0:** no association between x and y

Notes on Covariance

- The covariance is here averaged over N data points
- Can also define covariance as the expected value for a theoretical distribution
  - Data can be treated as sample (cf. St. Dev.)
- Related to variance by $\boldsymbol{\sigma(x, x) = \sigma^2(x)}$
  - Variance is square of standard deviation

Correlation

- Not obvious what size of covariance means
  - When is it close to zero?
- Can normalise by dividing by standard deviation of the variables
  - This is the correlation (coefficient)
  - $R(x, y) = \frac{\sigma(x,y)}{\sigma(x) * \sigma(y)}$
  - $-1 \leq R \leq 1$

Interpretation of Correlation

- **1:** perfect linear relationship with positive gradient
- **-1:** perfect linear relationship with negative gradient
- **0:** no (linear) relationship
- R is sometimes called the **product-moment correlation coefficient**

Linear Regression

- It is often useful to fit some function $\mathrm{y}(\mathrm{x})$ to the data
- In regression, we assume some general functional form and fit parameters to the data
- For example, **linear regression**
  - Assume form is $\boldsymbol{y} = \boldsymbol{\beta_0} + \boldsymbol{\beta_1}\,\boldsymbol{x}$
  - Use the data to determine best values of coefficients $\boldsymbol{\beta_0}$ and $\boldsymbol{\beta_1}$

Terminology

- X is the predictor (variable) and Y is the response (variable)
- We are regressing Y on X
  - NOT X on Y
- If we swap the roles of Y and X, we get a different line with
  - Y as predictor and X as response
  - Regression of X on Y

Assumptions

- y obeys the model

$$y = \beta_0 + \beta_1 x + \varepsilon$$

Where ε is a random variable and individual ε_i are

- Independently
- Identically
- Distributed according to a Normal distribution
  - with zero mean

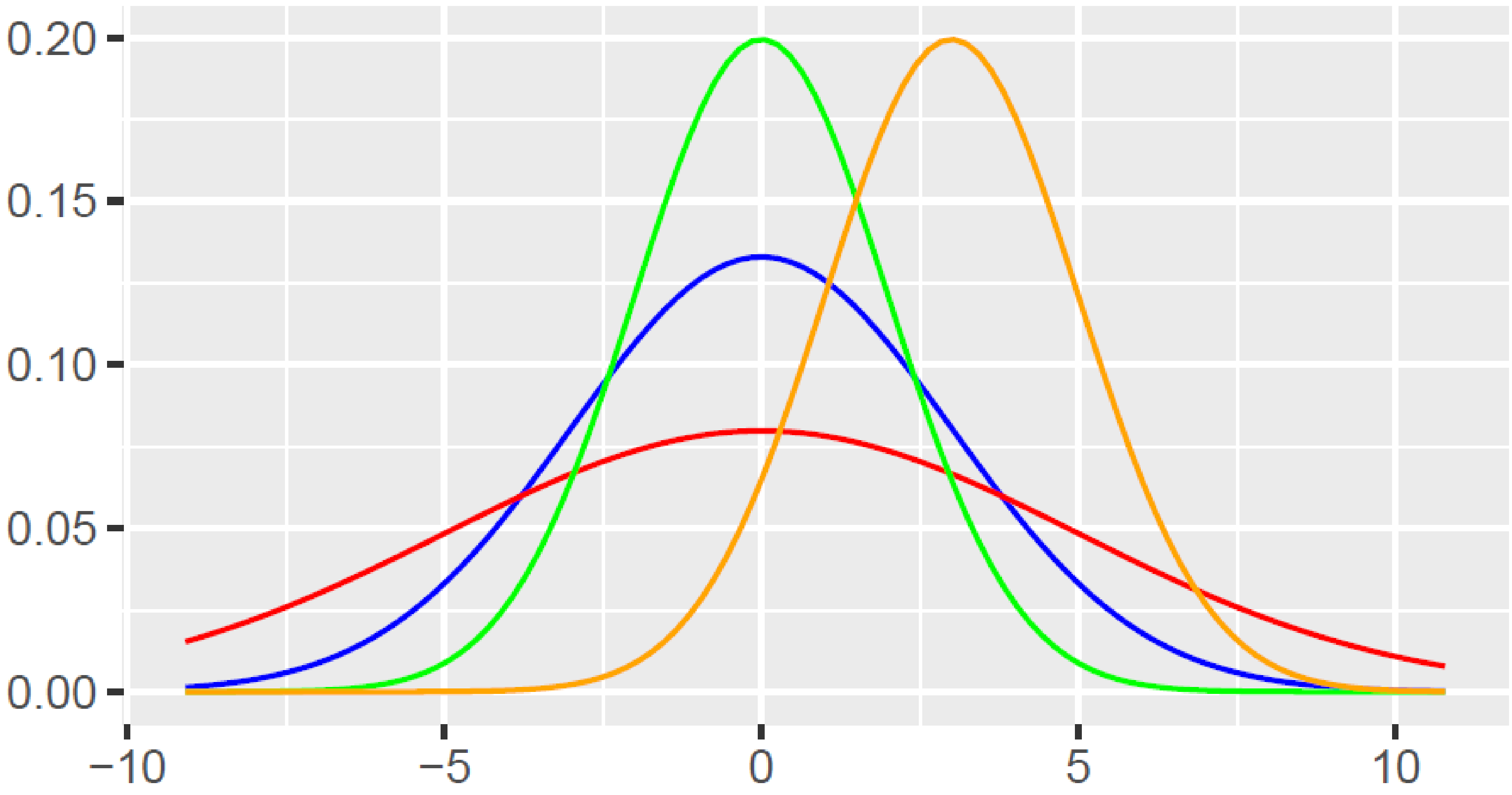
… assumptions

- **Identically distributed** - randomly drawn from the same distribution
- **Independently** - the result of one draw does not affect the others
- The distribution is assumed to be a **normal** (Gaussian) distribution of zero mean
    - Note: precisely the same distribution for every point

Normal Distribution

- Continuous bell-shaped, symmetrical distribution
- It frequently appears in nature and in industrial applications
- It is also of great theoretical importance
- It is uniquely defined by its mean and standard deviation

Example Normal Distributions

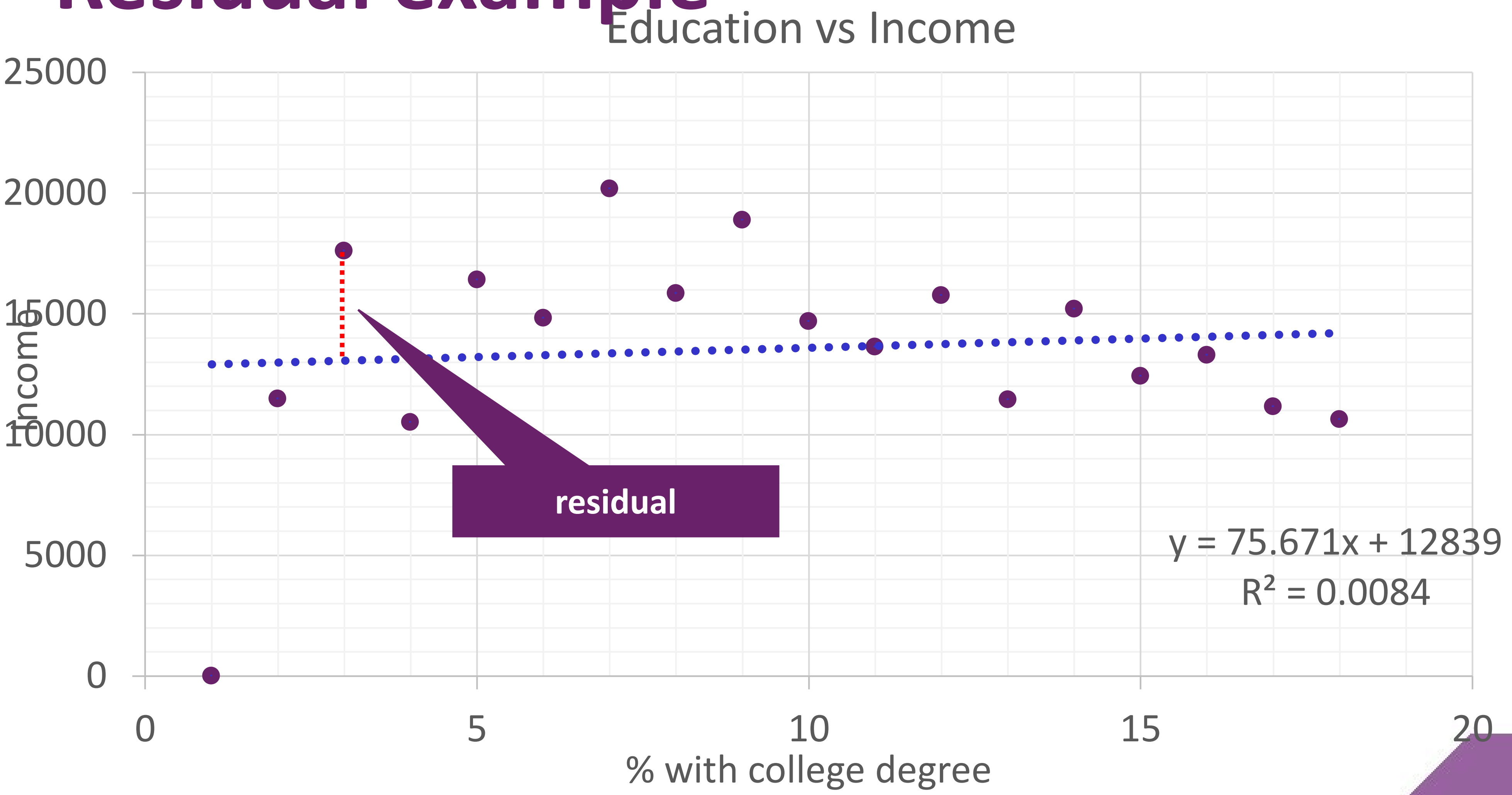


Green: $\bar{x} = 0, \sigma = 2$
Blue: $\bar{x} = 0, \sigma = 3$
Red: $\bar{x} = 0, \sigma = 5$
Orange: $\bar{x} = 3, \sigma = 2$

Residuals and Least Squares

- The *residuals* are the differences between the data values and the predictions of the linear model, i.e.
  - For a linear regression $y = \beta_0 + \beta_1 x$
  - For a data point (x_i, y_i)
    - $residual_i = y_i - (\beta_0 + \beta_1 xi)$
- The best fitting straight line is the one that minimises the sum of the squares of the residuals
  - The 'least squares' line

Residual example



How Good is Our Model?

- Coefficient of Determination R^2
  - Proportion of spread (variance) in Y explained by linear model
  - Square of Correlation Coefficient
  - Values close to 1 indicate strong linear relationship
  - Values close to 0 indicate no linear relationship

Statistical Inference

- Linear regression model follows
  - $y = \beta_0 + \beta_1 x + \varepsilon$
- Consider our data as a sample of a much larger population
- Can we reject (with x% confidence) the null hypothesis that $\beta_1 = 0$?
  - F Test (see lab)
- Find an interval estimate for the model coefficients
  - With x% confidence, each coefficient lies in a certain interval (formulae for this known).

Linear Regression Formulae

$$\boldsymbol{y = \beta_0 + \beta_1 x + \varepsilon}$$

$$\beta_1 = \frac{n\sum xy - (\sum x)(\sum y)}{n\sum x^2 - (\sum x)^2}$$

$$\beta_0 = \bar{y} - \beta_1 \bar{x}$$

$$R^2 = \frac{\left(n\sum xy - (\sum x)(\sum y)\right)^2}{\left(n\sum x^2 - (\sum x)^2\right)\left(n\sum y^2 - (\sum y)^2\right)}$$

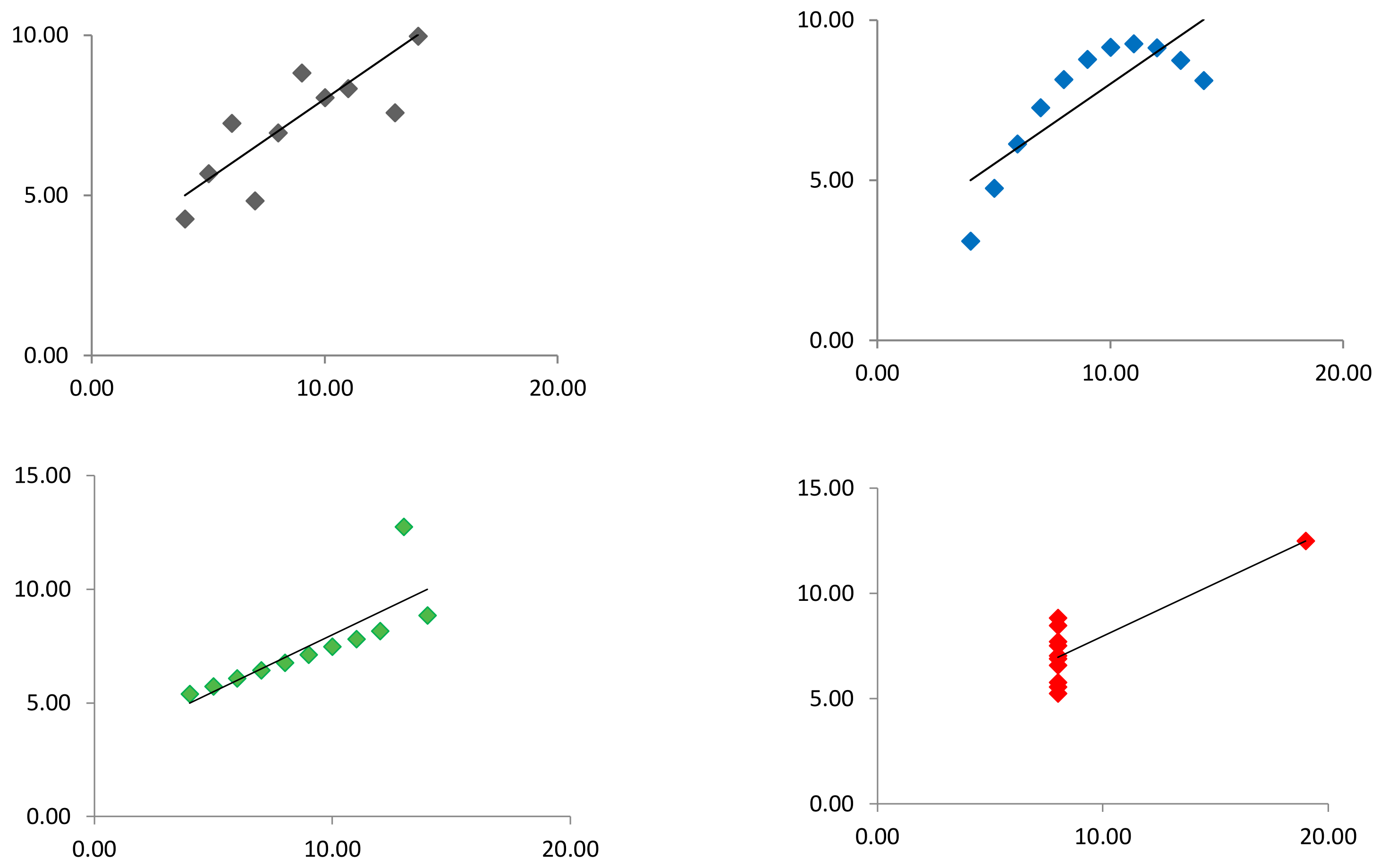
Example Calculation

- Note formulae depend on number of (pairs of) observations n and the sums
  - $\sum x, \sum y, \sum x^2, \sum y^2, \sum xy$
- Consider data for which:
  - $n = 11, \sum x = 99, \sum y = 82.5$,
  - $\sum x^2 = 1001, \ \sum y^2 = 660, \sum xy = 796.6$
  - Then $\beta_0 = 3, \ \beta_1 = 0.5, \ R^2 = 0.67$

Value is positive, but not really close to 1 so model is not ideal

- Best linear fit with moderate linear correlation
  - $\boldsymbol{y = \beta_0 + \beta_1 x + \varepsilon = 3 + 0.5\,x + \varepsilon}$
  - But, must visualise to check

Why Visualise? Visualisation shows differences!



Anscombe quartet

Anscombe’s Quartet

- Black points are what we expected
- Blue points show clear non-linear relationship
  - Should fit higher order polynomial
- Green points: outlier in Y spoils perfect fit and drags line upwards
  - Should seek to explain outlier
- Red points: outlier in X has undue influence
  - Should we be fitting this at all?

Graphing Residuals

- Since the residuals correspond to the random variable $\boldsymbol{\varepsilon}$, they should look like iind samples
- We can check this by graphing
  - Residuals vs X
    - should look random
  - Residuals vs Y
    - should look random
  - Residuals vs theoretical normal distribution.
    - should be close to straight line

Reality Checks

- Consider plausibility of linear model at outset
  - If appropriate, before collecting data
- Visualise your data
- Examine Residuals

Prediction using Linear Regression

- To predict the y-value corresponding to a particular x, we just use the straight line
- Should be interpolation – x value in range of X data used to find line
- **Extrapolation (x value outside range) is inadvisable**
- **Do not use y on x line to predict x from y!**

Generalisations

- Can fit other functions, e.g.
  - Polynomial (quadratic, cubic etc.)
  - Exponential
  - Logistic (used for probabilities)
- Multivariate Linear Regression
  - Consider multiple predictor variables

Summary

- When each data point involves 2 variables the analysis can be extended
  - Covariance $\sigma(x, y)$
  - Correlation coefficient $R(x, y)$
  - Linear regression $y = \beta_0 + \beta_1 x$
  - Coefficient of determination , R^2
- What if one of our variables is time?
  - Special case requiring separate treatment
  - Data of this type is called a **time series**
  - A series of values of the same variable at different times