

Chapter 11: Linear regression

(Section 2.1.1 and 3.1 of ISLR¹)

<https://dzwang91.github.io/stat324/>



¹An Introduction to Statistical Learning with Applications in R

Outline



- 1 What is statistical learning
- 2 Pearson correlation coefficient
- 3 Simple linear regression
- 4 Estimating the coefficients
- 5 Assessing the accuracy of the coefficient estimates
- 6 Assessing the accuracy of the model
- 7 Simple linear regression in R

A motivating example: advertising data



- Suppose we are statistical consultants hired by a client to provide advice on how to improve sales of a particular product.
- The Advertising data set ² consists of the sales of that product in 200 different markets, along with advertising budgets for the product in each of those markets for three different media: TV, radio, and newspaper.

²download the data set at <http://www-bcf.usc.edu/~gareth/ISL/data.html>

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```
> setwd("/Users/peterwang/Desktop/LinearReg")
> advertising=read.csv("Advertising.csv")
> head(advertising)
  X    TV radio newspaper sales
1 1 230.1 37.8    69.2  22.1
2 2  44.5 39.3    45.1  10.4
3 3  17.2 45.9    69.3   9.3
4 4 151.5 41.3    58.5  18.5
5 5 180.8 10.8    58.4  12.9
6 6   8.7 48.9    75.0   7.2
```

Figure: Advertising data

²download the data set at <http://www-bcf.usc.edu/~gareth/ISL/data.html>

A motivating example: advertising data



- It is impossible for our client to directly increase sales of the product. But they can control the advertising expenditure in each of the three media.
- Therefore, if we determine that there is an association between advertising and sales, then we can instruct our client to adjust advertising budgets, thereby indirectly increasing sales.
- In other words, our goal is to develop an accurate model that can be used to predict sales on the basis of the three media budgets.

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We want to find a good function f such that

$$\text{Sales} \approx f(\text{TV}, \text{Radio}, \text{Newspaper})$$

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Input variable and output variable



- The advertising budgets: input variables/predictors/independent variables/features
- Typically we use X to denote the input variables. For example, X_1 =TV budget, X_2 =radio budget, X_3 =newspaper budget

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- The sales: output variable/response/dependent variable
- Typically we use Y to denote the output variable. For example, Y = sale

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- The sales: **output variable/response/dependent variable**
- Typically we use Y to denote the output variable. For example, Y = sale
- In general, suppose we have a **quantitative** response Y and p different predictors, X_1, \dots, X_p . Then

$$Y = f(X_1, \dots, X_p) + \epsilon$$

- f is some **fixed but unknown** function of X_1, \dots, X_p , and it's called **regression function**
- f represents the **systematic** information that X provides about Y
- ϵ is a random error term, independent of X and has mean 0

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Example: income data

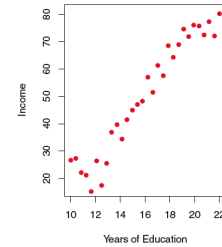


Figure: The red dots are the observed values of income (in tens of thousands of dollars) and years of education for 30 individuals.

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Example: income data

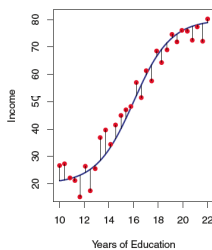


Figure: The blue curve represents the underlying relationship between income and years of education.

$$\text{Income} = f(\text{Years of education}) + \epsilon$$

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Why estimate f : prediction



- In many situations, a set of input X are readily available, but the output Y cannot be easily obtained.

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Why estimate f : prediction



- In many situations, a set of input X are readily available, but the output Y cannot be easily obtained.
- We can predict Y using

$$\hat{Y} = \hat{f}(X)$$

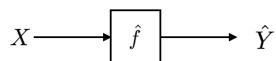


Figure: \hat{f} is treated as a black box

- \hat{f} represents our estimate for f
- \hat{Y} represents the prediction of Y

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The accuracy of prediction



- We use mean squared error (MSE) to measure the accuracy of the prediction:

$$\text{MSE} = \mathbb{E}(Y - \hat{Y})^2$$

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The accuracy of prediction



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$$\text{MSE} = \mathbb{E}(Y - \hat{Y})^2$$

- MSE decomposition:

$$\begin{aligned}
 \text{MSE} &= \mathbb{E}(f(X) + \epsilon - \hat{f}(X))^2 \\
 &= \mathbb{E}[(f(X) - \hat{f}(X))^2 + 2(f(X) - \hat{f}(X))\epsilon + \epsilon^2] \\
 &= (f(X) - \hat{f}(X))^2 + 2(f(X) - \hat{f}(X))\mathbb{E}(\epsilon) + \mathbb{E}(\epsilon^2) \\
 &= \underbrace{(f(X) - \hat{f}(X))^2}_{\text{Reducible}} + \underbrace{\text{Var}(\epsilon)}_{\text{Irreducible}}
 \end{aligned}$$

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 \end{aligned}$$

- Our goal for estimating f is to minimize the reducible error

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- We are interested in
 - which predictors are associated with the response? Only a small fraction of the available predictors are substantially associated with Y , want to identify the important predictors
 - what is the relationship between the response and each predictor?
 - Can the relationship between Y and each predictor be adequately summarized using a linear equation, or is the relationship more complicated?
- Example: for the advertising data, we are interested in
 - which media contribute to sales?
 - how much increase in sales is associated with a given increase in TV advertising?



How can we estimate f ?



How can we estimate f ?

The most popular method: linear regression

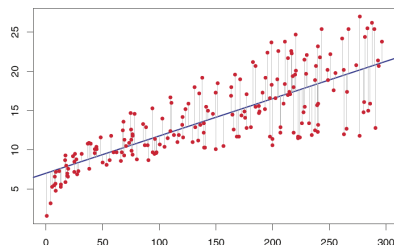


What is the relationship between TV/Radio/newspaper advertising budgets and sales?

Back to advertising data



What is the relationship between TV/Radio/newspaper advertising budgets and sales?



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"All models are wrong, but some are useful"

George Box



- True regression functions are never linear!

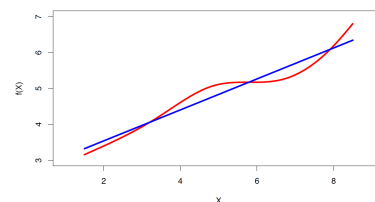


Figure: the red curve is the true regression function

- But linear regression is easy to implement and interpret!

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Motivation



A natural question: for two random variables X and Y , how can we measure their association?

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Pearson correlation coefficient



- For two random variables X and Y , Pearson correlation coefficient is defined as

$$\rho_{X,Y} = \frac{\text{cov}(X, Y)}{\sigma_X \sigma_Y},$$

where

- $\text{cov}(X, Y) = \mathbb{E}(X - \mu_X)(Y - \mu_Y)$, and μ_X and μ_Y are expectations of X and Y .
- $\sigma_X = \sqrt{\text{Var}(X)}$: standard deviation of X
- $\sigma_Y = \sqrt{\text{Var}(Y)}$: standard deviation of Y

- Range of $\rho_{X,Y}$:

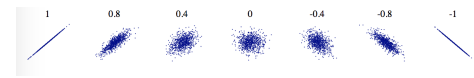
$$-1 \leq \rho_{X,Y} \leq 1$$

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Pearson correlation coefficient continued



- Visualization of $\rho_{X,Y}$:

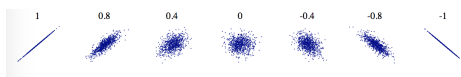


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Pearson correlation coefficient continued



- Visualization of $\rho_{X,Y}$:



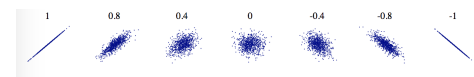
- When $\rho_{X,Y} = 1$, scatter is perfect straight line sloping up
- When $\rho_{X,Y} = -1$, scatter is perfect straight line sloping down
- When $\rho_{X,Y} = 0$, there is no linear association, then we call X and Y are uncorrelated.

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Pearson correlation coefficient continued



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- Conclusion: Pearson correlation coefficient measures the **linear** association

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Pearson correlation coefficient continued



- Visualization of $\rho_{X,Y}$:



- When $\rho_{X,Y} = 1$, scatter is perfect straight line sloping up
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- When $\rho_{X,Y} = 0$, there is no linear association, then we call X and Y are uncorrelated.
- Conclusion: Pearson correlation coefficient measures the **linear** association
- When $\rho_{X,Y} > 0$, we say X and Y have a positive linear association
- When $\rho_{X,Y} < 0$, we say X and Y have a negative linear association

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Sample Pearson correlation coefficient



- Given n pairs of data $(x_1, y_1), \dots, (x_n, y_n)$, sample Pearson correlation coefficient is defined as

$$r_{xy} = \frac{S_{xy}}{S_x S_y} = \frac{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2}} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}}$$

where $\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$ and $\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$.

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Correlation is not causation³

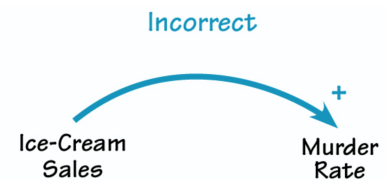


- A famous example: Ice cream sales is correlated with homicides in New York,

Correlation is not causation³



- A famous example: Ice cream sales is correlated with homicides in New York, **but ice cream is not causing the death of people.**



³Reading: Why correlation does not imply causation?

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³Reading: Why correlation does not imply causation?

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Correlation is not causation continued



- Why are ice cream sales and homicides correlated?

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Correlation is not causation continued



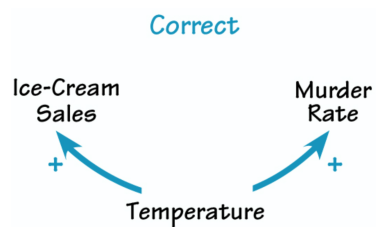
- Why are ice cream sales and homicides correlated?
- There are some hidden factors which cause both of ice cream sales and homicides.

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Correlation is not causation continued



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Example



- Sir Francis Galton (1822-1911) was interested in how children resemble their parents. One simple measure of this is height.
- Galton measured the heights of father son pairs (in inches) at maturity.
- In the actual study, 1078 pairs were measured. For convenience, we will use a small subsample of $n = 14$ pairs:

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Example continued



Family	Father's Height	Son's Height
1	71.3	68.9
2	65.5	67.5
3	65.9	65.4
4	68.6	68.2
5	71.4	71.5
6	68.4	67.6
7	65.0	65.0
8	66.3	67.0
9	68.0	65.3
10	67.3	65.5
11	67.0	69.8
12	69.3	70.9
13	70.1	68.9
14	66.9	70.2

- Goal: predict sons' height from father's height.

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Example continued



- Which variable is input variable?

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Example continued



- Which variable is input variable? Father's height

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Example continued



- Which variable is input variable? Father's height
- Which variable is output variable?

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Example continued



- Which variable is input variable? Father's height
- Which variable is output variable? Son's height

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Example continued



- Which variable is input variable? Father's height
- Which variable is output variable? Son's height
- A simple linear regression:
Son's height = $\beta_0 + \beta_1 \cdot \text{Father's height} + \text{Random error}$
 $Y = \beta_0 + \beta_1 X + \epsilon$

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Example continued



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Son's height = $\beta_0 + \beta_1 \cdot \text{Father's height} + \text{Random error}$
 $Y = \beta_0 + \beta_1 X + \epsilon$
- Denote the height of son i by y_i , the height of father i by x_i , and the random error by ϵ_i , so that the model becomes:
 $y_i = \beta_0 + \beta_1 x_i + \epsilon_i$.

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Example continued



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- Why do we add a random error term?

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Example continued



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- Denote the height of son i by y_i , the height of father i by x_i , and the random error by ϵ_i , so that the model becomes:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i.$$

- Why do we add a random error term? The random error term picks up sources of variation in an individual son's height that are not due to his father's height (mother's genetics, environmental factors, etc.) and which cause the points to be "off line."

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Intercept and slope



- β_0 is the **intercept**. It is the expected value of Y when $X = 0$.
- β_1 is the **slope**. It is the average increase of Y associated with a one-unit increase in X .
- Our goal: estimate the values of β_0 and β_1 from data. (**what is the available (training) data?**)

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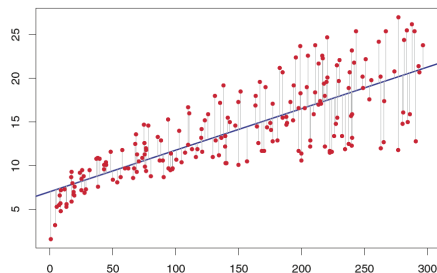
Simple linear regression



- We assume a model

$$Y = \beta_0 + \beta_1 X + \epsilon$$

- Let $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ be n observation pairs, each of which consists of a measurement of X and a measurement of Y .



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Residual sum of squares



- Suppose $\hat{\beta}_0$ and $\hat{\beta}_1$ are estimates, then the **estimated (fitted) value** for given x_i is:

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

- The i -th **residual**: the difference between \hat{y}_i and the observed y_i .

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

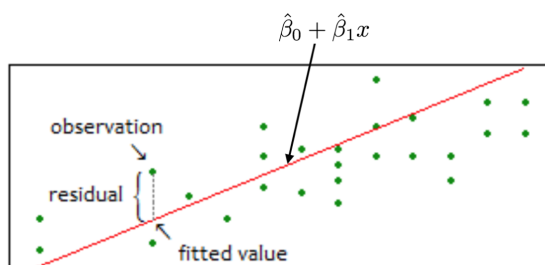
- Residual sum of squares (RSS)**:

$$\text{RSS} = e_1^2 + e_2^2 + \dots + e_n^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2.$$

- RSS measures how well the line fits the data.

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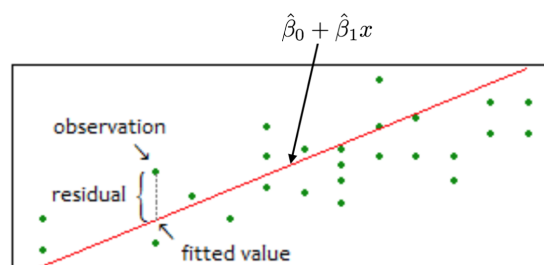
Ordinary least squares



- How can we decide the line?

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Ordinary least squares



- How can we decide the line?
- Ordinary least squares (OLS):

$$\text{minimize } \text{RSS}(\hat{\beta}_0, \hat{\beta}_1) = \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2$$

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- OLS estimator:

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

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

where $\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$ and $\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$.

- We call $\hat{\beta}_0 + \hat{\beta}_1 x$ the **least squares/best fit/regression line**.
- The residual sum of squares for the least squares line is also called **the sum of squared errors (SSE)**. SSE is the smallest possible residual sum of squares in the universe of all possible lines.



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- Exercise: calculate $\hat{\beta}_0$ and $\hat{\beta}_1$ for the father and son data. ($\hat{\beta}_1 = 0.65$ and $\hat{\beta}_0 = 23.64$)



- OLS estimator of slope:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{S_{xy}}{S_x^2} = \frac{S_{xy}}{S_x S_y} \frac{S_x S_y}{S_x^2} = r_{xy} \frac{S_y}{S_x}$$



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- We have

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i = (\bar{y} - \hat{\beta}_1 \bar{x}) + \hat{\beta}_1 x_i,$$

Back to Pearson correlation



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Back to Pearson correlation



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Back to Pearson correlation



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- Conclusion: r_{xy} is the slope of the regression line for **standardized** data points.

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Unbiasedness



- The OLS estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ are unbiased:

$$\mathbb{E}(\hat{\beta}_0) = \beta_0, \mathbb{E}(\hat{\beta}_1) = \beta_1$$

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Unbiasedness



- The OLS estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ are unbiased:

$$\mathbb{E}(\hat{\beta}_0) = \beta_0, \mathbb{E}(\hat{\beta}_1) = \beta_1$$

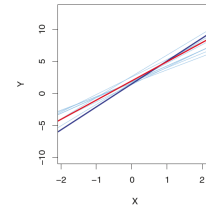


Figure: The simple linear regression is $Y = 2 + 3X + \epsilon$. The red line is the true regression function $2 + 3X$. The light blue lines are least squares lines for different sample. On average, the least squares lines are close to the true regression function.

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Standard error of OLS estimator ⁴



- Standard error of $\hat{\beta}_0$:

$$SE(\hat{\beta}_0) = \sqrt{\text{Var}(\hat{\beta}_0)} = \sqrt{\sigma^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right]}$$

where $\sigma^2 = \text{Var}(\epsilon)$.

- Standard error of $\hat{\beta}_1$:

$$SE(\hat{\beta}_1) = \sqrt{\text{Var}(\hat{\beta}_1)} = \sqrt{\frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}}$$

⁴Proofs are not required. See the extra slides in our course website.

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- When σ is unknown, we need to estimate the standard error. Replace σ^2 by its estimator $\frac{SSE}{n-2}$ where $SSE = \sum_{i=1}^n e_i^2$

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Confidence interval



- If
 - The linear model is correct.
 - The observations are independent.
 - The variance around the true regression line is constant for all values of x .
 - The random error around the true line is normal.
 Assumptions 2-4 are equivalent to $\epsilon_i \sim N(0, \sigma^2)$ with an **unknown** σ and ϵ_i are i.i.d.

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Then

$$\frac{\hat{\beta}_1 - \beta_1}{\widehat{SE}(\hat{\beta}_1)} \sim t_{n-2}$$

where $\widehat{SE}(\hat{\beta}_1)$ is the estimated standard error of $\hat{\beta}_1$.

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- Therefore,

$$\mathbb{P}(-t_{n-2, \alpha/2} \leq \frac{\hat{\beta}_1 - \beta_1}{\widehat{SE}(\hat{\beta}_1)} \leq t_{n-2, \alpha/2}) = 1 - \alpha$$

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Confidence interval continued ⁵



- 100(1 - α)% confidence interval of β_1 is

$$[\hat{\beta}_1 - t_{n-2, \alpha/2} \widehat{SE}(\hat{\beta}_1), \hat{\beta}_1 + t_{n-2, \alpha/2} \widehat{SE}(\hat{\beta}_1)]$$

⁵The CI formulas here are slightly different with those in Section 3.1 of ISLR.

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Confidence interval continued ⁵



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- Similarly, the 100(1 - α)% confidence interval of β_0 is

$$[\hat{\beta}_0 - t_{n-2, \alpha/2} \widehat{SE}(\hat{\beta}_0), \hat{\beta}_0 + t_{n-2, \alpha/2} \widehat{SE}(\hat{\beta}_0)]$$

⁵The CI formulas here are slightly different with those in Section 3.1 of ISLR.

Hypothesis testing



- The most common hypothesis test in the simple linear regression is
 H_0 : There is no relationship between X and Y

vs.

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$$H_0 : \beta_1 = 0 \text{ vs. } H_A : \beta_1 \neq 0,$$

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$$t = \frac{\hat{\beta}_1}{SE(\hat{\beta}_1)}$$
- Under same assumptions with confidence interval, if H_0 is true, then t has a t distribution with $n - 2$ degrees of freedom.
- Exercise: For the father and son data, $\hat{\sigma} = 1.78$, so $SE(\hat{\beta}_1) = 0.24$, and $t_{obs} = 2.70$. Comparing this to a t_{12} , the p-value is 0.0193. So we would reject at the 5% level, and conclude that father's height is related to son's height.

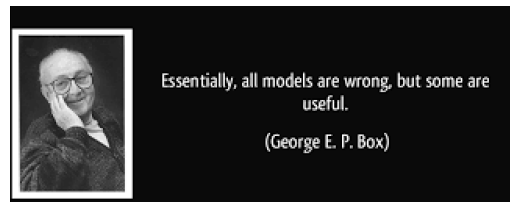
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Outline



- 1 What is statistical learning
- 2 Pearson correlation coefficient
- 3 Simple linear regression
- 4 Estimating the coefficients
- 5 Assessing the accuracy of the coefficient estimates
- 6 Assessing the accuracy of the model
- 7 Simple linear regression in R

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Essentially, all models are wrong, but some are useful.

(George E. P. Box)

How good does the linear model fit the data?

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R squared



- Total sum of squares:

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

- Regression sum of squares:

$$SSReg = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2$$

- Residual sum of squares/ sum of squares error:

$$SSE = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

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- Sum of squares law:

$$SSTot = SSReg + SSE$$

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R squared continued



- R squared is defined as

$$R^2 = \frac{SSTot - SSE}{SSTot} = \frac{SSReg}{SSTot}$$

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R squared continued



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- It's interpreted as the fraction of total sum of squares (variability) that is explained by the regression line.

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$$R^2 = \frac{SSTot - SSE}{SSTot} = \frac{SSReg}{SSTot}.$$

- It's interpreted as the fraction of total sum of squares (variability) that is explained by the regression line.
- Exercise: for the father and son data, $R^2 = 0.38$. So we can say that about 38% of the variability in sons' heights can be explained by fathers' heights.

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Lab: simple linear regression



See R code at our course website.

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