

# Statistical Modeling

CH.1 - Simple Linear Regression

SS 2021 || Prof. Dr. Buchwitz

Wir geben Impulse

**1** Organizational Information

**2** Introduction

**3** Simple Linear Regression

### Lecturer

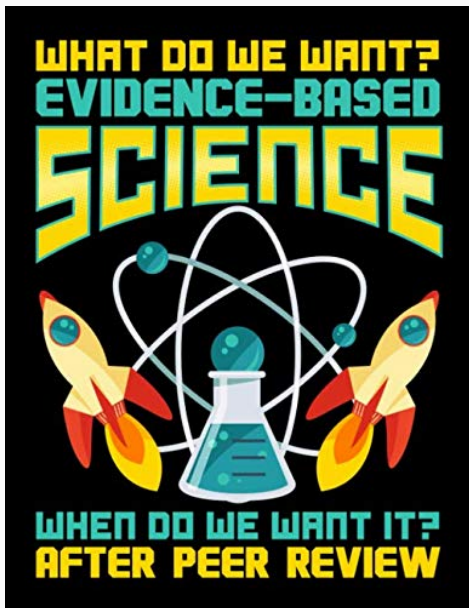
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## Unit objectives

- 1 To obtain an understanding of common statistical methods used in statistical modeling.
- 2 To develop the computer skills required to model relationships found in business, economic and social sciences contexts;
- 3 To gain insights into the problems of implementing and conducting analyses for professional use.

Session	Topic
1	Simple Linear Regression
2	Multiple Linear Regression
3	Regression Diagnostics
4	Qualitative Variables as Predictors
5	Transformation of Variables
6	Weighted Least Squares
7	Correlated Errors
8	Analysis of Collinear Data
9	Working with Collinear Data
10	Variable Selection Procedures
11	Logistic Regression
12	Further Topics



## Install R

<https://cloud.r-project.org/>

## Install RStudio

<https://www.rstudio.com/products/rstudio/download/#download>

Grading is based on a portfolio examination with three parts:

- 1 One Lecture Recap Presentation (20%)
- 2 Hand-in Exercises (40%)
- 3 Final Case Study (40%)



**1** Organizational Information

**2** Introduction

**3** Simple Linear Regression

# What is Regression Analysis?

- Regression analysis is a conceptually simple method for investigating functional relationships among variables.
- The relationship is expressed in the form of an equation or a model connecting the **response** or **dependent variable** with one or more **explanatory** or **predictor** variables.
- We denote the response variable by  $Y$  and the set of predictor variables by  $X_1, X_2, \dots, X_p$ , where  $p$  denotes the number of predictor variables.
- The **true** relationship between the response and its predictors can be approximated by the regression model, where  $\epsilon$  represents the random discrepancy in the relation.

$$Y = f(X_1, X_2, \dots, X_p) + \epsilon$$

- The function  $f(X_1, X_2, \dots, X_p)$  describes the relationship between  $Y$  and  $X_1, X_2, \dots, X_p$  and can take any functional form.
- One example of a function is the linear regression model:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots \beta_p X_p + \epsilon$$

- Here  $\beta_0, \beta_1, \dots, \beta_p$  are called the regression parameters or coefficients, which are unknown constants and need to be estimated from data.

## Data Example: River Data

- Nitrogen: Mean nitrogen concentration (*mg/l*) based on samples taken at regular intervals during the spring, summer and fall months
- Agr: Percentage of land area currently in agricultural use
- Forest: Percentage of forest land
- Rsdntial: Percentage of land area in residential use
- ConIndl: Percentage of land area in either commercial or industrial use

```
head(P010)
```

##	Agr	Forest	Rsdntial	ComIndl	Nitrogen
## Olean	26	63	1.2	0.29	1.10
## Cassadaga	29	57	0.7	0.09	1.01
## Oatka	54	26	1.8	0.58	1.90
## Neversink	2	84	1.9	1.98	1.00
## Hackensack	3	27	29.4	3.11	1.99
## Wappinger	19	61	3.4	0.56	1.42

# Data Example: Motor Trend US Car Magazine

```
# see help(mtcars) for variable description
```

```
mtcars
```

##	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
## Mazda RX4	21.0	6	160.0	110	3.90	2.620	16.46	0	1	4	4
## Mazda RX4 Wag	21.0	6	160.0	110	3.90	2.875	17.02	0	1	4	4
## Datsun 710	22.8	4	108.0	93	3.85	2.320	18.61	1	1	4	1
## Hornet 4 Drive	21.4	6	258.0	110	3.08	3.215	19.44	1	0	3	1
## Hornet Sportabout	18.7	8	360.0	175	3.15	3.440	17.02	0	0	3	2
## Valiant	18.1	6	225.0	105	2.76	3.460	20.22	1	0	3	1
## Duster 360	14.3	8	360.0	245	3.21	3.570	15.84	0	0	3	4
## Merc 240D	24.4	4	146.7	62	3.69	3.190	20.00	1	0	4	2
## Merc 230	22.8	4	140.8	95	3.92	3.150	22.90	1	0	4	2
## Merc 280	19.2	6	167.6	123	3.92	3.440	18.30	1	0	4	4
## Merc 280C	17.8	6	167.6	123	3.92	3.440	18.90	1	0	4	4
## Merc 450SE	16.4	8	275.8	180	3.07	4.070	17.40	0	0	3	3
## Merc 450SL	17.3	8	275.8	180	3.07	3.730	17.60	0	0	3	3
## Merc 450SLC	15.2	8	275.8	180	3.07	3.780	18.00	0	0	3	3
## Cadillac Fleetwood	10.4	8	472.0	205	2.93	5.250	17.98	0	0	3	4
## Lincoln Continental	10.4	8	460.0	215	3.00	5.424	17.82	0	0	3	4
## Chrysler Imperial	14.7	8	440.0	230	3.23	5.345	17.42	0	0	3	4
## Fiat 128	22.4	4	78.7	66	4.08	2.200	19.47	1	1	4	1

## Steps in Regression Analysis

- 1 Statement of the problem
- 2 Selection of potentially relevant variables
- 3 Data collection
- 4 Model specification
- 5 Choice of fitting method
- 6 Model fitting
- 7 Model validation and criticism
- 8 Using the chosen model(s) for the solution of the proposed problem

- Every analysis starts with the definition of the problem, which includes formulation of questions addressed by the analysis.
- Ill-defined problems or misformulated questions can lead to wasted effort or the selection of a wrong model.
- Finding and formulating suitable questions is probably the hardest part in an analysis.

## Example: Problem Statement Definition

- Assume we want to research whether or not an employer is discriminating against a group of employees, e.g. women and data on salary, gender and qualification is available.
- There are multiple definitions of discriminations available in the literature (a) women are paid less than equally qualified men, or (b) women are more qualified than equally paid men.



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### Your turn

What is the modeling implication of the definition?

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### Your turn

What is the modeling implication of the definition?

a)  $salary = f(qualification, gender) + \epsilon$

b)  $qualification = f(salary, gender) + \epsilon$



**1** Organizational Information

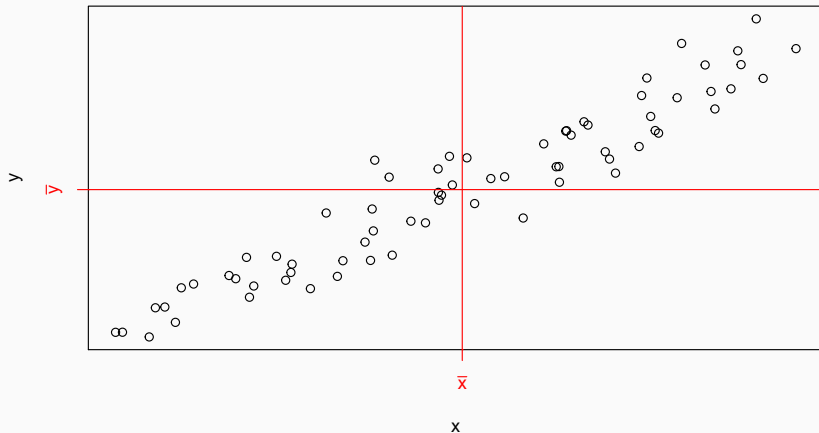
**2** Introduction

**3** Simple Linear Regression

$$Y = f(X) + \epsilon$$

- We start with the simple case to study the relationship between the response  $Y$  and a single predictor  $X$ .
- As we only have one regressor variable we drop the subscript to simplify the notation ( $X_1 = X$ ).
- We derive and formulate the regression model and focus on the key results but favor numerical examples over mathematical derivations.

# Covariance



## Determine the sign:

- $y_i - \bar{y}$  the deviation of each observation  $y_i$  from the mean of the response variable,
- $x_i - \bar{x}$  the deviation of each observation  $x_i$  from the mean of the predictor variable, and
- the product of the above quantities,  $(y_i - \bar{y})(x_i - \bar{x})$

Quadrant	$y_i - \bar{y}$	$x_i - \bar{x}$	$(y_i - \bar{y})(x_i - \bar{x})$
1 (top right)			
2 (top left)			
3 (bottom left)			
4 (bottom right)			

## Positive Relationship

- If the linear relationship between  $Y$  and  $X$  is **positive** (when  $X$  increases,  $Y$  also increases), then there are more points in the first and third quadrants than in the second and fourth.
- The sum over the elements in the last column is likely to be positive, that is  $\text{Cov}(Y, X) > 0$ .



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## Negative Relationship

- If the linear relationship between  $Y$  and  $X$  is **negative** (as  $X$  increases  $Y$  decreases), then there are more points in the second and fourth quadrants than in the first and third.
- The sum over the elements in the last column is likely to be negative, that is  $\text{Cov}(Y, X) < 0$ .

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

- The quantity calculated using the above formula is called the covariance.
- The sign of the covariance indicates the relationship between  $Y$  and  $X$ .
- The covariance can **only indicate the direction** of a relationship, and does not tell much about the strength of the relationship.
- the covariance is unit sensitive, changing the unit of a measurement (e.g. from Euro to kEuro) changes the value of the covariance.

### Your turn

What happens if we calculate  $\text{Cov}(X, Y)$  instead of  $\text{Cov}(Y, X)$ ?

- To avoid the obvious disadvantages of the covariance we can standardize (z-transform) each variable before computing the covariance.
- Standardizing  $Y$  means subtracting the mean  $\bar{y}$  and dividing by the associated sample standard deviation  $s_y$ .
- The resulting variable  $z_i$  has mean zero and unit standard deviation.

$$z_i = \frac{y_i - \bar{y}}{s_y} \quad \text{with} \quad s_y = \sqrt{\frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n - 1}}$$

$$\text{Cor}(Y, X) = \frac{1}{n-1} \sum_{i=1}^n \left( \frac{y_i - \bar{y}}{s_y} \right) \left( \frac{x_i - \bar{x}}{s_x} \right) = \frac{\text{Cov}(Y, X)}{s_y s_x}$$

- Calculating the covariance of the standardized values yields the correlation coefficient.
- $\text{Cov}(Y, X)$  can be interpreted in two ways, either as
  - the covariance between two standardized variables or as
  - ratio between of the covariance to the standard deviations of the two variables
- Opposed to the covariance,  $\text{Cor}(Y, X)$  is scale invariant so that it is not affected by unit changes. It also satisfies  $-1 \geq \text{Cor}(Y, X) \geq 1$  and therefore indicates **direction** and **strength**.

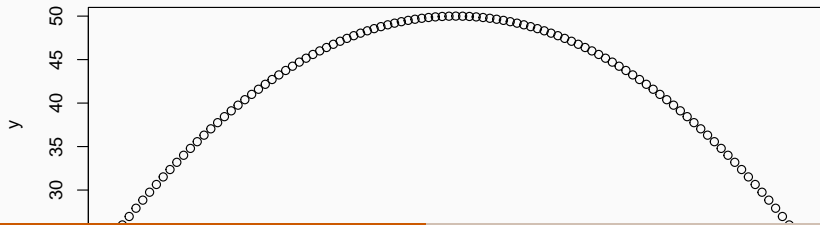
# Correlation Coefficient

$\text{Cor}(Y, X) = 0$  does not necessarily mean that the variables are not related!

```
x <- seq(from=-5, to=5,by=.1)
y <- 50 - x^2
cor_yx = cor(y,x)
round(cor_yx, digits=4)
```

```
## [1] 0
```

```
plot(x,y)
```



## Example: Anscombe Quartet

```
knitr::kable(anscombe[,c("y1", "x1", "y2", "x2", "y3", "x3", "y4", "x4")], booktabs=T)
```

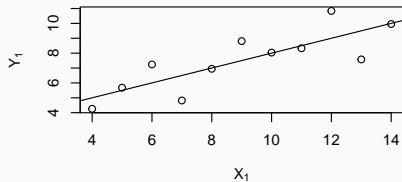
y1	x1	y2	x2	y3	x3	y4	x4
8.04	10	9.14	10	7.46	10	6.58	8
6.95	8	8.14	8	6.77	8	5.76	8
7.58	13	8.74	13	12.74	13	7.71	8
8.81	9	8.77	9	7.11	9	8.84	8
8.33	11	9.26	11	7.81	11	8.47	8
9.96	14	8.10	14	8.84	14	7.04	8
7.24	6	6.13	6	6.08	6	5.25	8
4.26	4	3.10	4	5.39	4	12.50	19
10.84	12	9.13	12	8.15	12	5.56	8
4.82	7	7.26	7	6.42	7	7.91	8
5.68	5	4.74	5	5.73	5	6.89	8

### Your turn

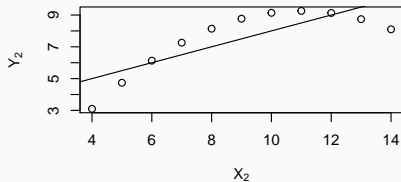
Choose one of the datasets (e.g.  $i = 3$ ) and calculate  $\bar{y}_i$ ,  $\bar{x}_i$ ,  $\text{Cov}(y_i, x_i)$  and  $\text{Cor}(y_i, x_i)$  using R (**Hint:** mean, cov, cor).

# Results: Anscombe Quartet

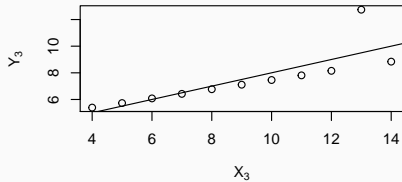
(a)



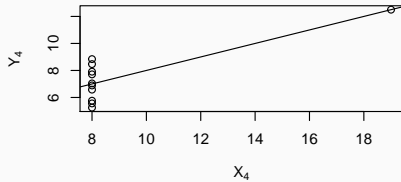
(b)



(c)



(b)



- Like many other summary statistics the correlation coefficient can be substantially influenced by one or a few outlier in the data.
- All four datasets in the Anscombe quartet have almost the **same summary** statistics, despite being inherently different.
- A purely descriptive analysis can not reveal the different patterns **we need to plot the data before starting an analysis.**
- Findings:
  - a) can be adequately described by a linear model
  - b) is nonlinear and would be better fitted by a quadratic function
  - c) one outlier distorts the slope and intercept of the lines
  - d) is unsuitable for linear fitting as the line is determined by a single extreme observation



## Example: Computer Repair Data

```
# Minutes = Duration of the service operation  
# Units = Number of computers repaired during service operation  
head(P031)
```

##	Minutes	Units
## 1	23	1
## 2	29	2
## 3	49	3
## 4	64	4
## 5	74	4
## 6	87	5

### Your turn

Calculate  $\text{Cov}(Y, X)$  and  $\text{Cor}(Y, X)$  manually (step-by-step) using R by avoiding the internal functions `cov` and `cor`.

# The Simple Linear Regression Model

- The correlation coefficient is useful to measure the strength of a pairwise relationship, it **cannot be used for prediction purposes**.
- That means that we cannot use  $\text{Cor}(Y, X)$  to predict one variable, when the other one is given.
- Regression is an extension to correlation analysis and can not only measure direction, but allows for **numerically describing** that relationship.

# The Simple Linear Regression Model

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

- $\beta_0$  and  $\beta_1$  are constants called the regression coefficients, and  $\epsilon$  is the error term.
  - $\beta_0$  is called the intercept. It is the prediction value, when  $X = 0$ .
  - $\beta_1$  is called the slope. It can be interpreted as the change in  $Y$ , when  $X$  changes by one unit.
- Each observation in the data can therefore be written as:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i \quad \text{with} \quad i = 1, 2, \dots, n$$

# The Simple Linear Regression Model

- We assume that (in the range of our observations studied), the linear equation provides an **acceptable approximation** to the real relationship:  $Y$  is approximately a linear function of  $X$ .
- The error term  $\epsilon$  measures the discrepancy of the approximation.
- That simple linear regression model is linear in two ways:
  - the relationship between  $X$  and  $Y$  is linear
  - more generally the word linear describes that the regression parameters  $\beta_0$  and  $\beta_1$  enter the equation in a linear fashion
  - $Y = \beta_0 + \beta_1 X^2 + \epsilon$  is still a linear model but with a quadratic term!
- In correlation  $X$  and  $Y$  are of equal “importance” which is reflected in the symmetry  $\text{Cor}(Y, X) = \text{Cor}(X, Y)$ .
- In regression we want to explain  $Y$ , hence the importance of the predictor  $X$  lies on its ability to account for the variability of the response.

## Example: Computer Repair Data

Reconsidering the computer repair data and assuming we want to predict the numbers of support engineers that will be required for a task, we can now formulate an equation in form of a linear model that is assumed to represent the relationship between the length of service calls and the number of electronic components in the computer that must be repaired.

$$\text{Minutes} = \beta_0 + \beta_1 \text{ Units} + \epsilon$$

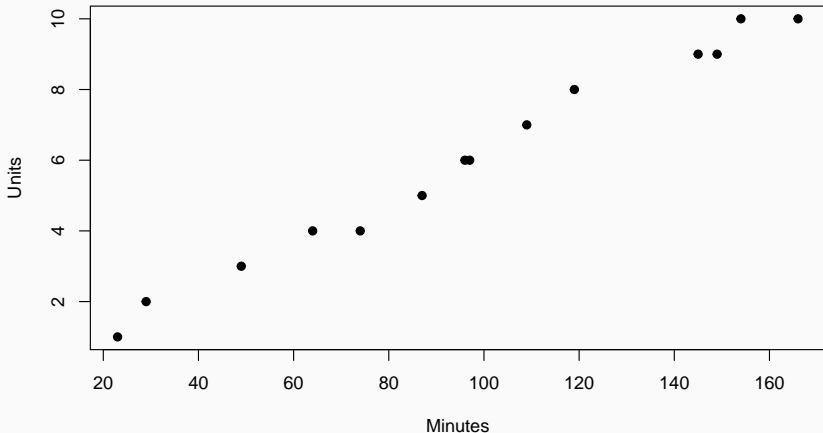
### Your turn

Consult the scatter plot (plot) of the data (P031) and check whether the straight linear relationship is a reasonable assumption.

How do we  
determine  $\beta_0$  and  $\beta_1$ ?

# Parameter Estimation

```
plot(P031$Minutes,P031$Units,xlab="Minutes",ylab="Units", pch=19)
```



- We want values for  $\beta_0$  and  $\beta_1$  that give the *best fit* or the *best representation* for the points in the graph.
- This can be achieved using the **least squares method** that minimizes the sum of squares of **vertical distances**.
- Those vertical distances from each point to the line represent the errors  $\epsilon_i$  and can be obtained by:

$$\epsilon_i = y_i - \beta_0 - \beta_1 x_i \quad \text{for } i = 1, 2, \dots, n$$



- As  $\beta_0$  and  $\beta_1$  are unknown, but required to calculate the errors and therefore the sum of squared errors, we can devise a function for that:

$$S(\beta_0, \beta_1) = \sum_{i=1}^n \epsilon_i^2 = \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$$

- This is a quadratic function that can be minimized. The analytical solution for the values  $\hat{\beta}_0$  and  $\hat{\beta}_1$  that minimize the function  $S(\ )$  are

$$\hat{\beta}_1 = \frac{\sum (y_i - \bar{y})(x_i - \bar{x})}{\sum (x_i - \bar{x})^2} \quad \text{and} \quad \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

- Both,  $\hat{\beta}_0$  and  $\hat{\beta}_1$  are called the **least squares estimates** and give the line with the smallest possible sum of squares of vertical distances.

- The **least squares regression line** can always be found (does always exist) and is given by

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$$

- For each observation we can compute a **fitted value**, which is given by

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i \quad \text{for } i = 1, 2, \dots, n$$

- Each point  $(x_i, \hat{y}_i)$  is a point **on the regression line**
- The corresponding vertical distances are called **ordinary least squares residuals** and can be computed like

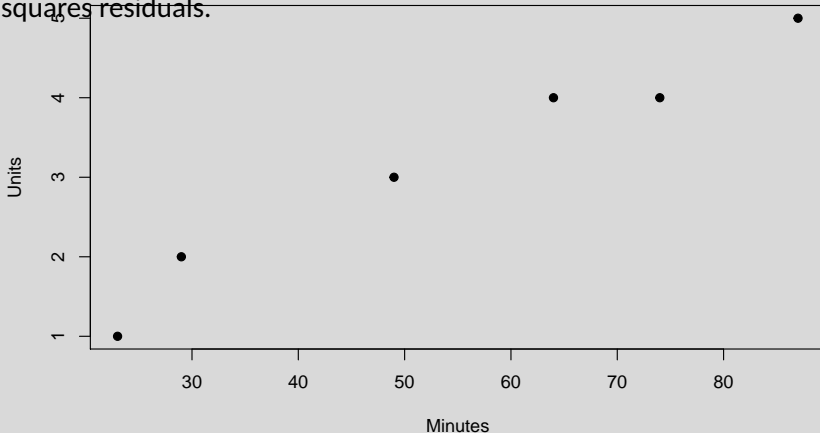
$$\hat{\epsilon}_i = y_i - \hat{y}_i \quad \text{for } i = 1, 2, \dots, n$$

# Parameter Estimation

```
plot(head(P031$Minutes), head(P031$Units), xlab="Minutes", ylab="Units", pch=19)
```

## Your turn

Add a sketch of the least squares regression line to the plot above and include, mark and annotate the the fitted values and the ordinary least squares residuals.



## Your turn

- Calculate  $\hat{\beta}_0$  and  $\hat{\beta}_1$  twice using R.
  - 1) Manually (abstain from `cor` and `cov`) using R
  - 2) Using the functions mentioned above
- Plot the data and add your calculated regression line to that plot  
(**Hint:** `abline`)

- So far we only made one assumption or hypothesis about the relationship between the response and predictor variables, which is called the **linearity assumption**.
- An early step in an analysis should always be the validation of this assumption: *We wish to determine if the data at hand supports the assumption that  $Y$  and  $X$  are linearly related.*
- An **informal** way to check this assumption is to check the scatter plot.
- A more **formal** way to check the assumption and to measure the usefulness of  $X$  as a predictor for  $Y$  is to conduct a hypothesis test about the regression parameter  $\beta_1$ .

- Testing for the postulated relationship can be done by checking the hypothesis that  $\beta_1 = 0$ , which means that there is **no linear relationship** between  $X$  and  $Y$ .
- Finding that  $\beta_1 > 0$  or  $\beta_1 < 0$  is equivalent to  $\beta_1 \neq 0$  and would provide **evidence (not proof!) for an existing linear relationship**.
- Testing of this hypothesis requires the assumption that the errors  $\epsilon_i$  are independent random quantities originating from a normal distribution with mean zero and common variance  $\sigma^2$ .
  - $\epsilon \sim N(0, \sigma^2)$
  - $\epsilon_i$  are independent

- Given that the assumptions for the error term  $\epsilon$  hold,  $\hat{\beta}_0$  and  $\hat{\beta}_1$  are unbiased estimates of  $\beta_0$  and  $\beta_1$ .
- This means that  $\hat{\beta}_0$  and  $\hat{\beta}_1$  allow to draw conclusions about the unobserved and unknown parameters  $\beta_0$  and  $\beta_1$  in the population, hence  $E(\hat{\beta}) = \beta$ .
- Under the mentioned circumstances the variances of the regression coefficients are

$$\text{Var}(\hat{\beta}_0) = \sigma^2 \left[ \frac{1}{n} + \frac{\bar{x}^2}{\sum (x_i - \bar{x})^2} \right] \quad \text{and} \quad \text{Var}(\hat{\beta}_1) = \frac{\sigma^2}{\sum (x_i - \bar{x})^2}$$

- The variances of  $\hat{\beta}_0$  and  $\hat{\beta}_1$  depend on the unknown and unobservable parameter  $\sigma^2$ , which needs to be estimated from the data before we can proceed.

- An unbiased estimate of  $\sigma^2$  is given by

$$\hat{\sigma}^2 = \frac{\sum \epsilon_i^2}{n - 2} = \frac{\sum (y_i - \hat{y}_i)^2}{n - 2} = \frac{SSE}{n - 2}$$

- Here *SSE* is an abbreviation for Sum of Squares Error (Residuals).
- The number  $n - 2$  is called *degrees of freedom (df)* and is equal to the number of observations  $n$  minus the number of estimated regression coefficients.



- Plugging  $\hat{\sigma}^2$  into  $\text{Var}(\hat{\beta}_0)$  and  $\text{Var}(\hat{\beta}_1)$  yields unbiased estimates of the respective variances.
- The estimate of the standard deviation is called the **standard error (s.e.)**

$$\text{s.e.}(\hat{\beta}_0) = \hat{\sigma}^2 \sqrt{\frac{1}{n} + \frac{\bar{x}^2}{\sum (x_i - \bar{x})^2}} \quad \text{and} \quad \text{s.e.}(\hat{\beta}_1) = \frac{\hat{\sigma}^2}{\sqrt{\sum (x_i - \bar{x})^2}}$$

- The standard error of  $\hat{\beta}_1$  is a measure of how precisely the slope has been estimated. The smaller  $\text{s.e.}(\hat{\beta}_1)$ , the more precise is the estimator.

We are now in the position to perform statistical analysis concerning the usefulness of  $X$  as a predictor of  $Y$ . Under the assumption of normality, an appropriate test for testing the hypothesis is the t-test.

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

The test statistic follows a Student t distribution with  $n - 2$  degrees of freedom and we need a specified significance value (e.g.  $\alpha = 0.05$ ) to perform the test.

$$t_1 = \frac{\hat{\beta}_1}{s.e.(\hat{\beta}_1)}$$

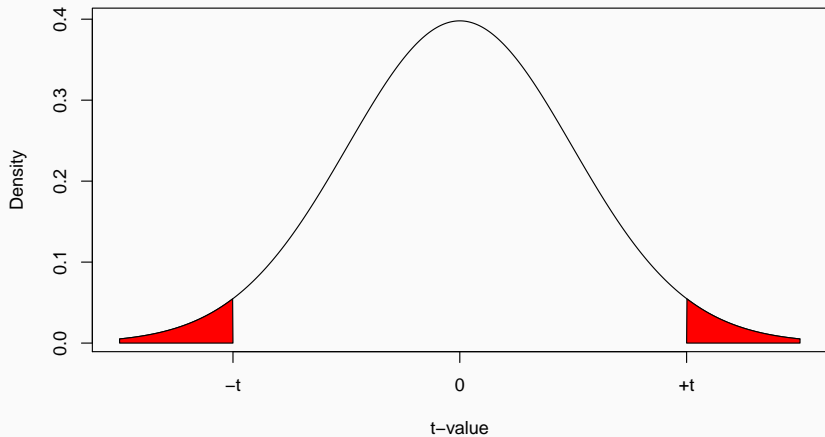
Carrying out the test is done by comparing the value  $t_1$  against the appropriate critical value obtained from the t-table, which is  $t_{(n-2, \alpha/2)}$  (Note that we divide  $\alpha$  by 2 as we have a two-sided test).

**Reject  $H_0$  at the given significance level if:**

$$t_1 \geq t_{(n-2, \alpha/2)} \quad \text{or} \quad t_1 \leq -t_{(n-2, \alpha/2)}$$

One condition is fulfilled if  $|t_1| \leq t_{(n-2, \alpha/2)}$ . A criterion equivalent to that is to compare the pvalue (implicit probability value) for the t-test with  $\alpha$  and reject  $H_0$  if  $p(|t_1|) \leq \alpha$ , where  $p(|t_1|)$ , called the p-value, is the sum of the two shaded areas under the following curve. This value is also provided by R.

# Tests of Hypotheses



The t-test can be generalized to test the more general hypothesis  $H_0 : \beta_1 = \beta_1^0$ , where  $\beta_1^0$  is a constant chosen by the data analyst.

$$t_1 = \frac{\hat{\beta}_1 - \beta_1^0}{s.e.(\hat{\beta}_1)}$$

The t-test can also be used for the testing the intercept  $\beta_0$  in the same fashion.

# Tests of Hypotheses

```
summary(lm(P031$Minutes ~ 1 + P031$Units))
```

```
##
## Call:
## lm(formula = P031$Minutes ~ 1 + P031$Units)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -9.2318 -3.3415 -0.7143  4.7769  7.8033
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)      4.162       3.355   1.24    0.239
## P031$Units      15.509       0.505  30.71 8.92e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5.392 on 12 degrees of freedom
## Multiple R-squared:  0.9874, Adjusted R-squared:  0.9864
## F-statistic: 943.2 on 1 and 12 DF,  p-value: 8.916e-13
```

- Confidence Intervals
- Predictions
- Quality of Fit
- Regression Line through the Origin
- Trivial Models