## Stat 306: Finding Relationships in Data. Lecture 3 Residuals and 2.2 Statistical linear regression model

## t-test





Dependent variable







#### Sample, n=9



Population parameters  $\mu_0, \mu_1, \sigma^2$ Hypothesis Test  $H_0: \mu_0 = \mu_1$  $H_1: \mu_0 \neq \mu_1$  Sample statistics  $\bar{y}_0 = 56$  $\bar{y}_1 = 27$  $\bar{y}_0 - \bar{y}_1 = 29$  $s_p = 10.81$ t = 2.68, df = 7p-value = 0.03 95% C.I. = [3.4, 54.6]



## linear regression



PREDICTOR variable





**RESPONSE** variable



#### Sample, n=9

Population  $\dot{\eta}$   $\dot{$ 

Population parameters  $\beta_0$  ,  $\beta_1$  ,  $\sigma^2$ 

Hypothesis Test  $H_0: \beta_1 = 0$  $H_1: \beta_1 \neq 0$  Sample statistics  $b_0 = 17.7$   $b_1 = 0.55$  s = 15.5  $R^2 = 0.49$ For parameter  $\beta_1$ :

95% C.I. = [0.05, 1.05] *p*-value = 0.036



## Sample statistics

$$\overline{x} = n^{-1} \sum_{i=1}^{n} x_i, \quad s_x = \sqrt{\sum_{i=1}^{n} (x_i - \overline{x})^2 / (n-1)},$$
  
$$\overline{y} = n^{-1} \sum_{i=1}^{n} y_i, \quad s_y = \sqrt{\sum_{i=1}^{n} (y_i - \overline{y})^2 / (n-1)}.$$

$$s_{xy} = (n-1)^{-1} \sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y}).$$

$$r_{xy} = \frac{s_{xy}}{s_x s_y}$$

#### Sample statistics

Formulas as written in the course notes:

$$\overline{x} = n^{-1} \sum_{i=1}^{n} x_i, \quad s_x = \sqrt{\sum_{i=1}^{n} (x_i - \overline{x})^2 / (n-1)},$$
  
$$\overline{y} = n^{-1} \sum_{i=1}^{n} y_i, \quad s_y = \sqrt{\sum_{i=1}^{n} (y_i - \overline{y})^2 / (n-1)}.$$

$$s_{xy} = (n-1)^{-1} \sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y}).$$

 $r_{xy} = \frac{s_{xy}}{s_x s_y}$ 

```
> y <- c(71, 54, 43, 45, 21, 11, 30, 45, 10)
> n < -9
Formulas written in R code:
 > xbar < -(1/n) * sum(x)
 > xbar
 [1] 34.66667
 >
 > sx<-sqrt( sum((x-xbar)^2)/(n-1) )</pre>
 > SX
 [1] 26.03843
 >
 > ybar<-(1/n)*sum(y)</pre>
 > ybar
 [1] 36.66667
 >
 > sy<-sqrt( sum((y-ybar)^2)/(n-1) )
 > sy
 [1] 20.36541
 >
 > sxy<-(1/(n-1))*sum((x-xbar)*(y-ybar))</pre>
 > SXY
 [1] 371.625
 > rxy<-sxy/(sx*sy)</pre>
 > rxy
  [1] 0.7008045
```

> x <- c(82, 45, 71, 22, 29, 9, 12, 18, 24)

The goal is to minimize  $S(b_0, b_1) = \sum_{i=1}^{n} (y_i - b_0 - b_1 x_i)^2$ .



y = 0 + 1x y = 25 + 0.25x y = 30 + 0.5x y = 20 + 1xy = 17.7 + 0.55x S(b0,b1) = 2933.5 S(b0,b1) = 2251.5 S(b0,b1) = 2725.0 S(b0,b1) = 5712.0 S(b0,b1) = 1688.4 The goal is to minimize  $S(b_0, b_1) = \sum_{i=1}^n (y_i - b_0 - b_1 x_i)^2$ .

**Least Squares Solution:** 

$$\hat{b}_0 = \overline{y} - \hat{b}_1 \overline{x}$$
  
 $\hat{b}_1 = r_{xy} s_y / s_x$ 



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$$\hat{b}_1 = r_{xy} s_y / s_x$$

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> b1\_hat<-rxy\*sy/sx > b0\_hat<-ybar-b1\_hat\*xbar > > b1\_hat [1] 0.5481195 > b0\_hat [1] 17.66519 **Least Squares Solution:** 

$$\hat{b}_1 = r_{xy} s_y / s_x$$

$$\hat{b}_0 = \overline{y} - \hat{b}_1 \overline{x}$$

> b1\_hat<-rxy\*sy/sx > b0\_hat<-ybar-b1\_hat\*xbar > > b1\_hat [1] 0.5481195 > b0\_hat [1] 17.66519

**Predicted** values:

$$\hat{y} = \hat{b}_0 + \hat{b}_1 x$$

#### Age vs. Money

#### Sample statistics

 $b_0 = 17.7$ 

 $b_1 = 0.55$ 

S

= 15.5

- The purpose of this observational study was to demonstrate if, and to what extent, age is
  - $R^2 = 0.49$ For parameter  $\beta_1$ : 95% C.I. = [0.05, 1.05]p-value = 0.036

**Results:** We obtained a random sample of n = 9 subjects. There is a statistically significant association between age and money (*p*-value =0.036). For every additional year in age, an individual's amount of money increases on average by an estimated of \$0.55 (95% C.I. = [\$0.05, \$1.05]).

We collected a random sample of individuals and for each

determined their age (recorded in years) and the amount

of money (in dollars) in their accounts. Analysis of

the data was done using linear regression.

**Conclusions:** We found that, as hypothesized, age is associated with money. In our sample age accounted for about half of the variability observed in money (R<sup>2</sup>=0.49). We predict that a 50 year old will have \$45.1 (95% P.I. = [\$5.6, \$84.5]), whereas a 40 year old will have \$39.6 (95% P.I. = [\$0.8, \$78.4]).

#### **Small Print:** The analysis rests on the following assumptions:

associated with money.

**Objective:** 

**Design and** Methods:

- the observations are independently and identically distributed.
- the response variable, money, is normally distributed.
- Homoscedasticity of residuals or equal variance. -
- the relationship between response and predictor variables is linear.

**Least Squares Solution:** 

$$\hat{b}_0 = \overline{y} - \hat{b}_1 \overline{x}$$
  
 $\hat{b}_1 = r_{xy} s_y / s_x$ 

**Predicted values:** 

$$\hat{y} = \hat{b}_0 + \hat{b}_1 x$$

We predict that a 50 year old will have \$45.1, whereas a 40 year old will have \$39.6.

**Least Squares Solution:** 

$$\hat{b}_0 = \overline{y} - \hat{b}_1 \overline{x}$$
  
 $\hat{b}_1 = r_{xy} s_y / s_x$ 

**Predicted values:** 

$$\hat{y} = \hat{b}_0 + \hat{b}_1 x$$



> plot(y~x, pch=20, cex=3, xlim=c(0,100), ylim=c(0,100))
> abline(17.67, 0.548 , col="gold", lwd=6)

$$\hat{b}_0 = \overline{y} - \hat{b}_1 \overline{x} \qquad \qquad \hat{b}_1 = r_{xy} s_y / s_x$$



**Predicted values:** 

$$\hat{y} = \hat{b}_0 + \hat{b}_1 x$$

> yhat<-b0\_hat+b1\_hat\*x</pre>

> points(x,yhat, pch=20, cex=3, col="blue")



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#### Residuals

$$e_i=y_i-\hat{b}_0-\hat{b}_1x_i,\quad i=1,\ldots,n.$$

#### > residuals

[1] 8.389012 11.669432 -13.581674 15.276180 -12.560656 -11.598267 [7] 5.757375 17.468658 -20.820059 Residuals

$$e_i=y_i-\hat{b}_0-\hat{b}_1x_i,\quad i=1,\ldots,n.$$

The goal is to minimize  $S(b_0, b_1) = \sum_{i=1}^{n} (y_i - b_0 - b_1 x_i)^2$ 

We have: 
$$e_i = y_i - \hat{b}_0 - \hat{b}_1 x_i, \quad i = 1, \dots, n.$$

Therefore: 
$$S(b_0,b_1) = \sum_{i=1}^n (e_i)^2$$
  
 $= \sum_{i=1}^n (y_i - b_0 - b_1 x_i)^2$ 

#### 3.8 Residual plots

In this section, residual plots are introduced to check if the model (3.36) is an adequate approximation to (3.33), and also to check the normality and homoscedasticity assumptions.

#### the *residual*

$$e_i=y_i-\hat{b}_0-\hat{b}_1x_i,\quad i=1,\ldots,n.$$

Residual plots include the following.

- (i) Check for homoscedasticity versus heteroscedasticity and possible structural deviations from model (plot of residuals versus predicted values, plots of residuals versus each explanatory variable).
- (ii) Check for normality (normal quantile plot of residuals) if the plots from (i) look OK.

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Residual plots include the following.

 (i) Check for homoscedasticity versus heteroscedasticity and possible structural deviations from model (plot of residuals versus predicted values, plots of residuals versus each explanatory variable).
 (1) (2)

(ii) Check for normality (normal quantile plot of residuals) if the plots from (i) look OK.

#### Age vs. Money

**Objective:** The purpose of this observational study was to demonstrate if, and to what extent, age is associated with money.

**Design and** 

- Methods:We collected a random sample of individuals and for each<br/>determined their age (recorded in years) and the amount<br/>of money (in dollars) in their accounts. Analysis of<br/>the data was done using linear regression.
- Results:We obtained a random sample of n = 9 subjects. There is a<br/>statistically significant association between age and money (p-value =0.036).<br/>For every additional year in age, an individual's amount of money increases<br/>on average by an estimated of \$0.55 (95% C.I. = [\$0.05, \$1.05]).
- **Conclusions:** We found that, as hypothesized, age is associated with money. In our sample age accounted for about half of the variability observed in money (R<sup>2</sup>=0.49). We <u>predict</u> that a 50 year old will have \$45.1 (95% P.I. = [\$5.6, \$84.5]), whereas a 40 year old will have \$39.6 (95% P.I. = [\$0.8, \$78.4]).
- **Small Print:** The analysis rests on the following assumptions:
  - the observations are independently and identically distributed.
  - Homoscedasticity of residuals or equal variance.
  - the response variable, money, is normally distributed.
  - the relationship between response and predictor variables is linear.

(i) Check for homoscedasticity versus heteroscedasticity and possible structural deviations from model

#### **Homoscedasticity:** EQUAL VARIANCE

Heteroscedasticity: NOT EQUAL VARIANCE

(i) Check for homoscedasticity versus heteroscedasticity and possible structural deviations from model

# Homoscedasticity: EQUAL VARIANCEHeteroscedasticity: NOT EQUAL VARIANCE

(i) Check for homoscedasticity versus heteroscedasticity and possible structural deviations from model (<u>plot of residuals versus predicted values</u>, <u>plots of residuals versus each explanatory variable</u>).

(2)

(ii) Check for normality (normal quantile plot of residuals) if the plots from (i) look OK.

(1)

Homoscedasticity of residuals or "equal variance"

(1) Plot of residuals versus predicted values.

(2) Plot of residuals versus explanatory value

## Homoscedasticity of residuals or "equal variance"

(1) Plot of residuals versus predicted values:

plot(residuals~yhat, pch=20, cex=3, col="violet")



yhat

#### 3.8 Residual Plots Heteroscedasticity of residuals or "not equal variance" (1) Plot of residuals versus predicted values:

plot(residuals~yhat, pch=20, cex=3, col="violet")



yhat

## 3.8 Residual Plots Homoscedasticity of residuals or "equal variance"

(2) Plot of residuals versus explanatory value:

> plot(residuals~x, pch=20, cex=3, col="orange")



#### 3.8 Residual Plots Heteroscedasticity of residuals or "not equal variance"

(2) Plot of residuals versus explanatory value:

> plot(residuals~x, pch=20, cex=3, col="orange")



(1) Plot of residuals versus predicted values.(2) Plot of residuals versus explanatory value



(1) Plot of residuals versus predicted values.(2) Plot of residuals versus explanatory value



Homoscedasticity of residuals or "equal variance"



Heteroscedasticity of residuals or "not equal variance"



## The response variable is normally distributed.

#### (3) Normal quantile plot of residuals.

## The response variable is normally distributed.

#### (3) Normal quantile plot of residuals :

Normal Q-Q Plot



**Theoretical Quantiles** 

 (i) Check for homoscedasticity versus heteroscedasticity and possible structural deviations from model (plot of residuals versus predicted values, plots of residuals versus each explanatory variable).

#### (1) (2)

(ii) Check for normality (normal quantile plot of residuals) if the plots from (i) look OK.

(3)

now back to Chapter 2....

#### 2.1.3 ... Residuals

Because the best fitting line goes through the middle of the scatter of points, some  $e_i$  are  $\geq 0$  and others are  $\leq 0$ . It turns out there is some balance and

(2.29) 
$$\sum_{i=1}^{n} e_i = 0,$$

(2.30) 
$$\overline{e} = n^{-1} \sum_{i=1}^{n} e_i = 0.$$

> sum(residuals)
[1] 1.332268e-14
> (1/n)\*sum(residuals)
[1] 1.480297e-15

## Chapter 2

- Section 2.1 has the mathematics leading to the least squares line.
- Section 2.2 introduces the simple linear regression model (prediction with one explanatory variable) that is formulated for a predictive equation. This is needed to quantify the variability of the coefficients of the best-fitting line, when different samples are taken from the population.
- Section 2.5 has intervals for simple linear regression: the confidence interval for the slope of the least square line, confidence intervals for subpopulation means, and prediction intervals for a future or out-of-sample Y given x\*.
- Section 2.6 has an explanation of Student t quantiles used in the interval estimates.

- 1. For i = 1, ..., n,  $(x_i, y_i)$  is a realization of  $(x_i, Y_i)$ , where  $Y_i$  is a random variable and  $x_i$  is non-random.
- 2. The stochastic relationship is:

(2.32) 
$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i, \quad i = 1, ..., n,$$

where the  $\epsilon_i$ 's are independent normal random variables with mean 0 and variance  $\sigma^2$ . Think of  $\epsilon$  as the sum of unmeasured effects.

3. From properties of normal random variables, this implies that

(2.33) 
$$Y_i \sim N(\beta_0 + \beta_1 x_i, \sigma^2).$$

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#### What is a random variable?

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#### What is a random variable?

A quantity for which it is impossible to know with 100% certainty it's value.

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```
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```

#### What is a random variable?

"A random variable, Y, is a variable whose possible values are numerical outcomes of a random phenomenon."

#### **Three Examples of a Random Variable**

"A random variable, Y, is a variable whose possible values are numerical outcomes of a random phenomenon."

**Example 1: Y is the unknown** result of a rolling a die (1, 2, 3, 4, 5 or 6)

Example 2: Y is the unknown result of a coin flip ("heads" or "tails")

**Example 3: Y is the unknown** amount of money that a random person walking on the street has in their bank account.



"A random variable, Y, is a variable whose possible values are numerical outcomes of a random phenomenon."

Example 1: Y is the unknown result of rolling a die (1, 2, 3, 4, 5 or 6)

Y is a random variable. All we can know about Y is that:

$$Pr(Y=1) = 1/6$$
  
 $Pr(Y=2) = 1/6$   
 $Pr(Y=3) = 1/6$   
 $Pr(Y=4) = 1/6$   
 $Pr(Y=5) = 1/6$   
 $Pr(Y=6) = 1/6$ 



"A random variable, Y, is a variable whose possible values are numerical outcomes of a random phenomenon."

Example 2: Y is the unknown result of a coin flip ("heads" or "tails")

Once we observe the result of the coin flip we have "y". "y" is not random variable it is a "realization of a random variable" also known as "data".

Y is a random variable that follows a Bernoulli( $\theta$ ) distribution:

$$Y \sim Bern(\theta)$$

where  $\theta$  is a population parameter. For a "fair coin",  $\theta = 0.5$ 



"A random variable, Y, is a variable whose possible values are numerical outcomes of a random phenomenon."

**Example 3**: Y is the **unknown** amount of money that a random person has in their bank account.

Y is a random variable that may depend on the age (X) of the random person.



Let us assume that this dependence is linear such that:

$$\ell = \beta_0 + \beta_1 X + \epsilon$$
 and  $\epsilon \sim \text{Normal}(0, \sigma^2)$ 

where  $\beta_0$ ,  $\beta_1$ , and  $\sigma^2$  are population parameters.

Y is a random variable that may depend on X.

We assume that this dependence is linear such that:

Y = 
$$β_0$$
 +  $β_1$ X + ε and ε ~ Normal (0,  $σ^2$ )  
where  $β_0$ ,  $β_1$ , and  $σ^2$  are population parameters.

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 and  $\epsilon \sim Normal (0, \sigma^2)$ 

where  $\beta_0$ ,  $\beta_1$ , and  $\sigma^2$  are population parameters.

 $\epsilon$  is not a parameter.  $\epsilon$  is a "random variable".

We have n random variables. For *i* = 1, ..., n :

$$Y_i \sim \text{Normal} (\beta_0 + \beta_1 X_i, \sigma^2)$$

3. From properties of normal random variables, this implies that

(2.33) 
$$Y_i \sim N(\beta_0 + \beta_1 x_i, \sigma^2).$$

#### Conventional notation for probability/statistics

- Y (upper case letter) is a random variable;
- y (lower case letter) is a realization of a random variable;

• boldfaced 
$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}$$
 is a random vector and  $\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$  is a vector of realized values;

3. From properties of normal random variables, this implies that

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- inside  $E(\cdot)$  and  $Var(\cdot)$ , the arguments are random variables and they should be shown in upper case;
- Greek letters are used for parameters such as  $\beta_1, \sigma, \mu$  (an exception is the use of  $\epsilon$  for the random deviation from the line or curve);
- caret or hat on a symbol is used for estimators, for example  $\hat{\mu}, \hat{\sigma}$  (read as mu hat or sigma hat).

#### What is a random variable?

"A random variable, Y, is a variable whose possible values are numerical outcomes of a random phenomenon."

For a Random Variable, Y, we typically want to talk about the Expectation and Variance:

**Example 1:** E[Y] = 3.5 Var(Y) = 2.92

**Example 2:** E[Y] = 0.5 Var(Y) = 0.25

**Example 3:**  $E[Y] = \beta_0 + \beta_1 X$   $Var(Y) = \sigma^2$ 

Questions?

Example 1: All we can know about Y is that: Pr(Y=1) = 1/6 Pr(Y=2) = 1/6 Pr(Y=3) = 1/6 Pr(Y=4) = 1/6 Pr(Y=5) = 1/6 Pr(Y=6) = 1/6



> Y<-sample(c(1,2,3,4,5,6), size=1,prob=c(1/6,1/6,1/6,1/6,1/6,1/6))</pre>

Using the definitions of Expectation and Variance we can calculate:

E[Y] = 3.5 Var(Y) = 2.92

#### or:

> mean(sample(c(1,2,3,4,5,6), size=10000000,prob=c(1/6,1/6,1/6,1/6,1/6,1/6), replace=TRUE)
[1] 3.500276
> var(sample(c(1,2,3,4,5,6), size=10000000,prob=c(1/6,1/6,1/6,1/6,1/6,1/6), replace=TRUE))
[1] 2.918512

**Example 2:** All we can know about Y is that:  $Pr(Y=0) = 1-\theta$  $Pr(Y=1) = \theta$ 



- > theta<-0.5</pre>
- > Y<-sample(c(0,1), 1, prob=c(1-theta, theta))</pre>

Using the definitions of Expectation and Variance we can calculate:

 $E[Y] = \theta$   $Var[Y] = \theta (1-\theta)$ 

or:

> mean(sample(c(0,1), 100000, prob=c(1-theta, theta),replace=TRUE))
[1] 0.50282

# Section 2.2 - Statistical linear regression model Example 3 for a fixed value of X:

Let X=20.



 $Y = β_0 + β_1 20 + ε \quad and \quad ε ~ Normal (0, σ^2)$ 

Therefore: Y ~ Normal ( $\beta_0 + \beta_1 20$ ,  $\sigma^2$ )

Using properties of the Normal distribution:

 $E[Y] = \beta_0 + \beta_1 20 \qquad Var(Y) = \sigma^2$ 

- > beta0<-20
- > beta1<-0.5</pre>
- > X<-20
- > sigma2<-100</pre>

> Y<-rnorm(n=1, mean=beta0+beta1\*X, sd=sqrt(sigma2))</pre>

#### **Example 3 for a fixed value of X:**

- Y ~ Normal ( $β_0$  +  $β_1$ 20 ,  $σ^2$ )
- > beta0<-20</pre>
- > beta1<-0.5</pre>
- > X<-20
- > sigma2<-100</pre>

> Y<-rnorm(n=1, mean=beta0+beta1\*X, sd=sqrt(sigma2))</pre>

Let's take a large sample of Y and look at the distribution with a histrogram:

Y<-rnorm(n=10000000, mean=beta0+beta1\*X, sd=sqrt(sigma2))
hist(Y)</pre>



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## Section 2.2 - Statistical linear regression model Example 3 for a fixed value of X=40:

X = 40 , Y ~ Normal ( $\beta_0 + \beta_1 40$  ,  $\sigma^2$ )



> X<-40

> Y<-rnorm(n=10000000, mean=beta0+beta1\*X, sd=sqrt(sigma2))</pre> > hist(Y)

Histogram of Y



## **Section 2.2** - Statistical linear regression model Example 3 for a fixed value of X=60:

X = 60 , Y ~ Normal ( $\beta_0 + \beta_1 60$  ,  $\sigma^2$ )



> X<-60

> Y<-rnorm(n=10000000, mean=beta0+beta1\*X, sd=sqrt(sigma2))
> hist(Y)



Histogram of Y

## **Section 2.2** - Statistical linear regression model **Example 3 for a fixed value of X=80**:

X = 80, Y ~ Normal ( $\beta_0 + \beta_1 80, \sigma^2$ )



> X<-80

```
> Y<-rnorm(n=10000000, mean=beta0+beta1*X, sd=sqrt(sigma2))
> hist(Y)
```





## **Section 2.2** - Statistical linear regression model Example 3 for a fixed value of X=80:













Homoscedasticity of residuals or "equal variance"



Homoscedasticity of residuals or "equal variance"



Heteroscedasticity of residuals or "not equal variance"



Х

Heteroscedasticity of residuals or "not equal variance"



Х

**Questions?**