# STAT 420: Methods of Applied Statistics

### Simple Linear Regression II

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Course website: https://sites.google.com/site/teazrq/teaching/STAT420

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### **Simple Linear Regression**

 From last lecture, we learned how to perform linear regression on one predictor and an intercept:

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

· The regression coefficients can be obtained through

$$\widehat{\beta}_{0} = \bar{y} - \widehat{\beta}_{1}\bar{x}$$

$$\widehat{\beta}_{1} = \frac{\sum_{i=1}^{n} (y_{i} - \bar{y})(x_{i} - \bar{x})}{\sum_{i=1}^{n} (x_{i} - \bar{x})^{2}} = r_{xy}\frac{s_{y}}{s_{x}}$$

 We can calculate these estimations without knowing the complete data, but only some key statistics.

### What's next?

- · Properties of the least squares estimator
- Evaluating the goodness-of-fit of the model
- Estimating the error variance

### Simple Linear Regression

- Load the skin cancer dataset and perform a simple linear regression and answer the following questions:
  - 1). Predict the mortality rates, i.e.,  $\hat{y}$ , for states with latitude at 30 and 45.
  - 2). Calculate the sum of squared errors produced by this regression line
  - Suppose another researcher claims that the regression line should be

$$y = 389 - 6x$$

which line fits the data better?

- Learn how to plot using R
- Source code provided in SIR II.r

### Coefficient of determination: $R^2$

```
| | cancer = read.table("skincancer.txt", header = TRUE)
|x| > x = cancer Lat
| > y = cancer Mort
|x| > ybar = mean(y)
| > xbar = mean(x)
|s| > beta1 = sum((x - xbar)*(y - ybar))/sum((x - xbar)^2)
7 |> beta0 = ybar - beta1 * xbar
8
9 # predicted values at 30 and 45
| > beta0 + beta1 * c(30, 45) 
11 [1] 209.8603 120.1957
12
13 # sum of squared errors
|x| > sum((y - beta0 - beta1 * x)^2)
15 [1] 17173.07
16
17 # another fit
|x| > sum((y - 389 + 6*x)^2)
19 [1] 17230.04
```

# Properties of the least squares estimator

The sum of errors (not squared) is 0. Why?

$$\sum_{i=1}^{n} e_i = \sum_{i=1}^{n} (y_i - \hat{y}_i) = 0$$

 $\bullet$  The predictor vector  ${\bf x}$  is orthogonal to the error vector  ${\bf e}.$  Why?

$$\mathbf{x}^{\mathsf{T}}\mathbf{e} = \sum_{i=1}^{n} x_i e_i = 0$$

• The regression line passes through the centroid  $(\bar{x}, \bar{y})$ . Why?

- We partition observed variation by expressing  $y_i = \hat{y}_i + e_i$ .
- The total variance (corrected for mean) SST is defined as

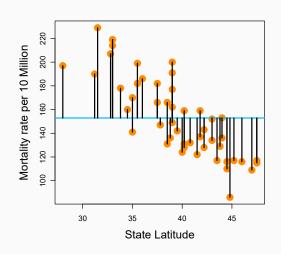
$$SST = \sum_{i} (y_i - \bar{y})^2$$

which can be partitioned into

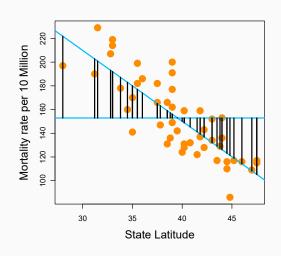
$$\begin{split} \sum_{i=1}^{n} (y_i - \bar{y})^2 &= \sum_{i=1}^{n} (y_i - \hat{y}_i + \hat{y}_i - \bar{y})^2 \\ &= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 + \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^{n} 2(y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) \\ &= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 + \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2 + 0 \\ &= \text{SS of Error} + \text{SS of Regression,} \end{split}$$

i.e., the sum of squares explained by the regression (SSR) and the sum of squared errors (SSE). This is the essential idea of the analysis of variance (ANOVA).

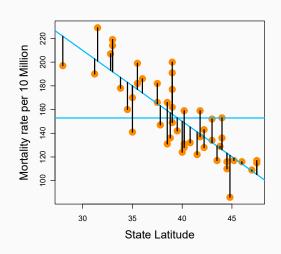












### Coefficient of determination $R^2$

- SST is a fixed value for a given dataset. SSR and SSE changes depending on the regression coefficient.
- · We can create a descriptive measure of linear association,

$$R^2 = \frac{\text{SSR}}{\text{SST}} = 1 - \frac{\text{SSE}}{\text{SST}}$$

- $0 \le R^2 \le 1$
- Interpretation: R<sup>2</sup> tells us the percentage of variance explained by the regression line when the relationship is indeed linear. It represents the goodness-of-fit.
- Remark 1:  $\mathbb{R}^2$  does not necessarily tell us that we can make accurate predictions even when  $\mathbb{R}^2$  is large.
- Remark 2: Reasons for R<sup>2</sup> being close to 0?

### **Simple Linear Regression**

Load the "cheddar" data using library(faraway) and data(cheddar). Perform the regression model:

Taste = 
$$\beta_0 + \beta_1$$
Lactic acid concentration

#### Calculate:

- The parameter estimates of  $\beta_0$  and  $\beta_1$  using the least square method we introduced
- · Calculate the residual sum of squares SSE
- Calculate the coefficient of determination  $\mathbb{R}^2$ .  $\mathbb{R}^2$  is:

A: 
$$\leq 0.3$$
; B:  $\in (0.3, 0.5]$ ; C:  $\in (0.5, 0.7]$ ; D:  $> 0.7$ ;

#### Coefficient of determination: $R^2$

• Fit a linear model to the skin cancer data and calculate the SST, SSE and  $\mathbb{R}^2$ .

```
# Calculate the coefficient of determination
> n = nrow(cancer)
> SSR = var(beta0 + beta1*x)*(n-1)
> SST = var(y)*(n-1)
> SSR/SST
[1] 0.6798296
```

• Fit the model using the variable "longitude" instead, what is the  $\mathbb{R}^2$ ?

A: 
$$\leq 0.3$$
; B:  $\in (0.3, 0.5]$ ; C:  $\in (0.5, 0.7]$ ; D:  $> 0.7$ ;

### Estimating the error variance

- There is an other part of the model that we haven't analyzed:  $\epsilon$
- We approximate these error terms using  $e_i = y_i \hat{y}_i$
- Hence, to estimate the variance  $\sigma^2$  of the error term  $\epsilon$ .

$$\widehat{\sigma}^2 = \frac{\text{SSE}}{\text{degrees of freedom}} = \frac{\text{SSE}}{\frac{n}{n-2}} = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)}{\frac{n-2}{n-2}}$$

We call this the mean square error (MSE).

• Why the degrees of freedom is n-2?

| Source of Variation | DF  | Sum of Squares  |
|---------------------|-----|---|
| Regression          | 1   | $SSR = \sum_{i=1}^{n} (\widehat{y}_i - \overline{y})^2$ |
| Residual error      | n-2 | $SSE = \sum_{i=1}^{n} (y_i - \widehat{y}_i)^2$          |
| Total               |     | $SST = \sum_{i=1}^{n} (y_i - \bar{y})^2$                |

• We have n observations, where is that last degree of freedom?

#### The "cats" data

Load the "cats" data using library(MASS) and data(cats). "MASS" is a pre-installed package in R. Calculate the following statistics:  $\bar{x}$ ,  $\bar{y}$ ,  $s_x$ ,  $s_y$ ,  $r_{xy}$ ,  $\sum_i^n x_i y_i$ . Consider the regression model:

$$\mathsf{Height} = \beta_0 + \beta_1 \mathsf{Weight}$$

- Use 4 of these statistics to calculate both  $\widehat{\beta}_0$  and  $\widehat{\beta}_1$
- Use only 3 of these statistics to calculate  $\widehat{\beta}_1$

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- Use only 3 of these statistics to calculate  $\widehat{\beta}_1$
- Calculate the coefficient of determination R<sup>2</sup>.

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- Use 4 of these statistics to calculate both  $\widehat{\beta}_0$  and  $\widehat{\beta}_1$
- Use only 3 of these statistics to calculate  $\widehat{\beta}_1$
- Calculate the coefficient of determination  $\mathbb{R}^2$ .
- Calculate the MSE  $\hat{\sigma}^2$ , and it is

$$A: > 2;$$
  $B: \leq 2;$   $C: \Omega$ 

#### The "cheddar" data

Load the "cheddar" data using library(faraway) and data(cheddar). Use "taste" as the outcome variable and compare two models

model 1: 
$$taste = \beta_0 + \beta_1 Acetic$$
  
model 2:  $taste = \beta_0 + \beta_1 Lactic$ 

 If we use the coefficient of determination as the criterion, which variable seems to fit the data better?

A: Acetic; B: Lactic; C: Equally well

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 If we use the coefficient of determination as the criterion, which variable seems to fit the data better?

• Which model gives smaller estimation  $\hat{\sigma}^2$ 

A: Acetic model; B: Lactic model; C: Equally well

### Inference about the coefficients

 If we model the mortality rate using longitude instead of latitude, it gives a regression line

$$y = 182.7696 - 0.3287x$$
.

But, does this mean the regression line, especially the slope  $\beta_1 = -0.3287$ , is truly meaningful?

- How to test whether  $\beta_1$  is zero or not?
- We will develop some new techniques of linear regression using matrix representation and derive the property of the parameter estimations.
- · Let's first use a simulation study to analyze it.

· We want to test the hypothesis:

$$H_0: \beta_1 = 0$$
 vs.  $H_0: \beta_1 \neq 0$ 

- Similar to the hypothesis testing of means (such as t-test), we want to obtain a p-value (meaning?).
  - In the current data we obtained  $\hat{\beta}_1 = -0.3287$ .
  - The idea of p-value is: if we repeatedly generate new datasets under the Null hypothesis, and calculate  $\widehat{\beta}_1$ , how many of them (proportion) have an estimation "more extreme" than -0.3287, i.e., <-0.3287 or >0.3287
  - How to setup the simulation study?

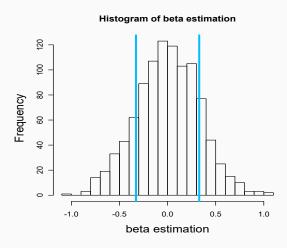
- There could be many different ways to setup the simulation. Here I give one choice:
- · We want to generate new dataset from the model:

$$Y = \beta_0 + 0X + \epsilon$$

- Take the longitude values in the skin cancer dataset as x values
- Use the mean of mortality rates as the true  $\beta_0$ , 152.8776
- Take  $\epsilon$  i.i.d. from  $\mathcal{N}(0,\sigma^2)$ , where we use the MSE in our current data: 1116.829
- Generate 1000 independent datasets, with 49 observations in each dataset, and perform the regression. Record all estimations of  $\beta_1$

```
# Setup the underlying data generater
  > x = cancer$Long
  > beta0 = mean(cancer$Mort)
| > n = nrow(cancer)
_{5} | > sigma2 = sum(Im(Mort ~ Long, data= cancer)\$residuals^2)/(n-2)
6
7 # Generate 10000 independent datasets and perform the regression
8 # Record the estimation \widehat{\beta}_1 from each dataset
| > \text{ hatb } = \text{rep}(NA, 10000)
| > for (i in 1:10000)
11 + {
|y| = beta0 + rnorm(n, mean = 0, sd = sqrt(sigma2))
|x| + hatb[i] = lm(y \sim x) \cdot coef[2]
14 + }
15
16 # Check how many of them have more extreme value than -0.3287
| > mean(abs(hatb) > 0.3287)
18 [1] 0.314
```

## A simulation study



```
_{1} | # Compare it to the theoretical p-value obtained in the lm()
      function
 > summary(Im(Mort ~ Long, data= cancer))
3
 Call:
5 Im(formula = Mort ~ Long, data = cancer)
6
  Residuals:
      Min
              1Q Median
                               3Q
                                      Max
8
  -63.898 -25.995 -5.952 21.856 78.444
10
  Coefficients:
              Estimate Std. Error t value Pr(>|t|)
12
13 (Intercept) 182.7696 29.8893 6.115 1.8e-07 ***
         -0.3287 0.3245 -1.013
                                              0.316
14 Long
15
  Signif. codes: 0 ?**?0.001 ?*?0.01 ??0.05 ??0.1 ??1
  Residual standard error: 33.42 on 47 degrees of freedom
19 Multiple R-squared: 0.02137, Adjusted R-squared: 0.0005491
 F-statistic: 1.026 on 1 and 47 DF, p-value: 0.3162
```