# MAD – Data Analysis & Biostatistics in R Inference & Regression

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#### Section 1

Inference with Categorical Variables

## Focus on Categorical Variables Only

- Case of categorical x numeric variables
  - Covered last week
  - Case of penguin body mass x species
  - Use of t-test
- First, single categorical variable
  - Example from Psychology
  - D. Navarro, LSR, v0.6
- Second, two-way table of categorical variables
  - From SEADE comorbidity tables

## Single Variable – Goodness of Fit Test

- Experiment to see if people can choose randomly
- 200 students asked to pick a card from a virtual deck (baralho) at random
- Then asked to pick a 2nd card from the virtual deck
- We are only interested in the suits (naipes) they chose
- Initial focus on 1st card they chose (choice\_1)
- If they had chosen purely randomly, all the probabilities should be equal

#### Look at the data

• Get a table of the observed values  $(O_1...O_{200})$ 

```
naipes <- readRDS(here("naipes.rds"))</pre>
head(naipes) # View initial cases
        id choice 1 choice 2
##
## 1 subj1
           espadas
                        paus
## 2 subj2
              ouros
                    paus
## 3 subj3 copas
                    paus
## 4 subj4 espadas
                        paus
## 5 subj5
           copas
                    espadas
## 6 subj6
            paus
                       copas
(observed <- table(naipes$choice_1))</pre>
##
##
      paus
                     copas espadas
             ouros
##
        35
                51
                        64
                                 50
```

## Hypothesis Test

Null hypothesis

 $H_0$ : All four suits chosen with equal probability

Another, more mathematical, format

$$H_0: P = (0.25, 0.25, 0.25, 0.25)$$

Alternative hypothesis

 $H_0$ : At least one suit has a probability that is not 0.25

$$H_0: P \neq (0.25, 0.25, 0.25, 0.25)$$

## Probabilities and Expected Values

- We have a set of probabilities we want to test P = (0.25, 0.25, 0.25, 0.25)
  - Store them in a vector

```
(probs <- c(copas = 0.25, ouros = 0.25, paus = 0.25, espadas = 0.25))
```

```
## copas ouros paus espadas
## 0.25 0.25 0.25 0.25
```

## Calculating Goodness of Fit

- Goodness of fit means how close are the observed data to the null hypothesis
- Need to translate the probabilities of null hypothesis to an expected frequency (E) for each suit (N = 200)

$$E_i = N \times P_i$$

• Then calculate how far the observed value  $(O_i)$  for each case differs from the expected value  $(E_i)$ :  $(O_i - E_i)$ 

#### Do This in R

## 1 paus

## 2 ouros

## 3 copas

50 35

50 51

50 64

## 4 espadas 50 50

-15

14

0

## Not Quite There

- Remember when we measured difference from mean in variance
  - ▶ Difference always equals 0
  - ▶ Differences: -15, 1, 14, 0
  - Sum of Differences: 0
- Avoid that consequence by squaring the difference

```
df$diff_sq <- df$diff^2
df
## # A tibble: 4 x 5</pre>
```

```
suit
         expected observed diff
                           diff_sq
   <chr>
           <dbl>   
             50 35 -15
                            225
 1 paus
           50 51
  2 ouros
           50 64
                    14
## 3 copas
                            196
## 4 espadas 50 50
                             0
```

## Goodness of Fit Statistic - $X^2$

- Next step: divide differences squared by expected
- Finally: sum the adjusted squared differences
- k = number of categories (naipes)

$$X^{2} = \sum_{i=1}^{k} \frac{(O_{i} - E_{i})^{2}}{E_{i}}$$

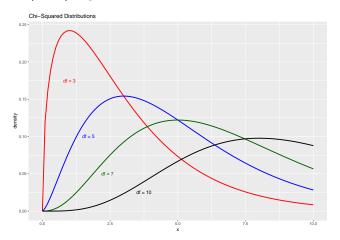
- If  $X^2$  is small, unlikely to reject null hypothesis - Differences will be too small to justify this

```
(X_sq <- sum((observed - expected)^2/expected))</pre>
```

## [1] 8.44

## Sampling Distribution of $X^2$

- This statistic  $(X^2)$  follows a chi-squared distribution
  - ► Qui-quadrado
  - $\sim \chi^2$
  - with (k-1) degrees of freedom



## What is Going On – Statistical Sidebar

- $\chi^2$  Distribution is quite common
- If you have multiple variables that are normally distributed
  - Square their values
  - Sum the squares
- The result will have a  $\chi^2$  distribution

#### Mathematical Demonstration

• 3 normally distributed variables

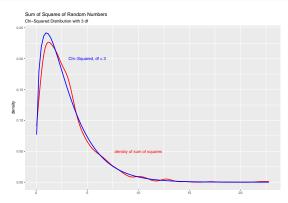
```
norm1 <- rnorm(n = 1000)
norm2 <- rnorm(n = 1000)
norm3 <- rnorm(n = 1000)
```

Sum the squares of the values

```
final_dist <- norm1^2 + norm2^2 + norm3^2
```

## Graph of Results

```
tibble(final_dist) %>%
ggplot(aes(x = final_dist)) +
geom_density(color = "red", size = 1) +
stat_function(fun = dchisq, args = list(df = 3), color = "blue", size = 1) +
labs(title= "Sum of Squares of Random Numbers",
    subtitle = "Chi-Squared Distribution with 3 df",
    x = "") +
annotate("text", x = 10, y = .05, label = "density of sum of squares", color = "red") +
annotate("text", x = 5, y = .2, label = "Chi-Squared, df = 3", color = "blue")
```



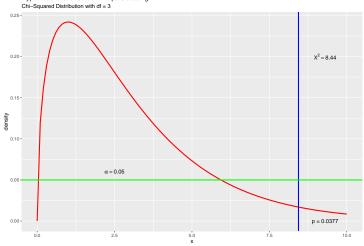
## Complete Hypothesis Test

- Compare our  $X^2$  to where the 95th percentile of the  $\chi^2$  distribution with 3 degrees of freedom (4 naipes 1)
- qchisq(p = .95, df = 3) = 7.8147279
  - Quantile function for the chi-squared distribution
- If our  $X^2$  is larger than 7.8147279, we should reject the null hypothesis
- $X^2 = 8.44$ ;  $\chi^2 = 7.8147279$
- ... we should reject null hypothesis
  - ► People cannot guess randomly
- Exact probability can be shown with pchisq()
  - ▶ Takes the quantile  $(X^2)$  as its p argument

```
pchisq(q = X_sq, df = 3, lower.tail = FALSE) ## only calculate
## [1] 0.03774185

1-pchisq(q = X_sq, df = 3) ## calculate 1 - lower tail
## [1] 0.03774185
```

#### Hypothesis Test of Student Naipe Guessing



## Running the Test in R

Doesn't get easier

chisq.test(x = observed)

```
##
## Chi-squared test for given probabilities
##
## data: observed
## X-squared = 8.44, df = 3, p-value = 0.03774
```

### Section 2

 $\chi^2$  Test of Independence

## Return to SEADE Comorbidity Data

- Question: Are people with more than 60 years more likely to die from COVID-19?
- Exists a numeric age variable
- Create a categorical variable for ages: age\_group
  - ▶ elderly: 60 years old or older
  - others: less than 60 years
    - ★ Note: only 1 child in sample (newborn)
- This is a 2 x 2 test, but could have any dimensions
  - ▶ All cells in test *should* have at least **5** cases

#### **Table**

```
comorbid <- readRDS(here("seade_comorbid_sample.rds")) %>%
 mutate(age_group = ifelse(age < 60, "other", "elderly"))</pre>
summarytools::ctable(comorbid$death, comorbid$age group, prop = "c")
## Cross-Tabulation, Column Proportions
## death * age_group
## Data Frame: comorbid
##
##
                           elderly other
                                                           Total
            age_group
##
    death
##
    FALSE
                     107 (59.4%) 91 (75.8%) 198 (66.0%)
                       73 (40.6%) 29 (24.2%) 102 (34.0%)
##
     TRUE
    Total
                       180 (100.0%) 120 (100.0%) 300 (100.0%)
##
```

## Hypotheses

- $\bullet$   $H_0$ : elderly and others have equal chance of dying from COVID-19
  - ▶  $H_0$ : p(elderly & death = TRUE) = p(others & death = TRUE) =  $P_1$
- $\bullet$   $H_1$ : elderly and others have different chances of dying from COVID-19
  - ▶  $H_1$ : p(elderly & death = TRUE) = p(others & death = TRUE)  $\neq P_1$

## Calculate Expected Values

- Here a little more tricky
  - Must estimate the probability from the data
- Multiply the column total x the probability of the row
  - Probability of row is the proportion for that row of the total
  - $ightharpoonup \hat{P}_i = \frac{R_i}{N}$
- Estimated values = product of margins \* N

$$E_{ij} = \frac{R_i \times C_j}{N}$$

### **Estimated Values**

```
## elderly other
## FALSE 118.8 79.2
## TRUE 61.2 40.8
```

## $X^2$ Statistic for Independence

- Same as for Goodness of Fit
- Need double summation over rows and columns both
- Need to adjust degrees of freedom for both dimensions

$$(r-1)(c-1)$$

$$X_{df}^2 = \sum_{i=1}^r \sum_{j=1}^c \frac{\left(E_{ij} - Oij\right)}{Eij}$$

## Executing Test in R

- Three ways with different amounts of information
- 1st: summarytools::ctable()

```
summarytools::ctable(comorbid$death, comorbid$age_group, prop = "c", chisq = TRUE)
## Cross-Tabulation, Column Proportions
## death * age_group
## Data Frame: comorbid
##
##
##
          age_group elderly other
                                                      Total
##
    death
    FALSE
                   107 (59.4%) 91 (75.8%) 198 (66.0%)
##
   TRUE
                    73 (40.6%) 29 (24.2%) 102 (34.0%)
##
    Total
              180 (100.0%) 120 (100.0%) 300 (100.0%)
##
##
   Chi.squared df p.value
##
      7.903 1 0.0049
```

## Results with gmodels::CrossTable()

#### Shows results in format similar to SPSS and SAS

Cell Contents

Count
Expected Values
Chi-square contribution
Total Percent

Total Observations in Table: 300

comorbid\$death	comorbid\$a elderly	ge_group other	Row Total
FALSE	107 118.800 1.172 35.667%	91 79.200 1.758 30.333%	198
TRUE	73 61.200 2.275 24.333%	29 40.800 3.413 9.667%	102
Column Total	180	120	300

Statistics for All Table Factors

### Results with lsr::associationTest()

- Adjunct to Learning Statistics with R book
- Uses formula interface

```
##
       Chi-square test of categorical association
## Variables:
              age_group, death
## Hypotheses:
##
     nu11:
                  variables are independent of one another
     alternative: some contingency exists between variables
##
## Observed contingency table:
##
           death
## age_group FALSE TRUE
    elderlv
              107
                    73
   other
               91
                     29
## Expected contingency table under the null hypothesis:
##
           death
## age_group FALSE TRUE
    elderly 118.8 61.2
##
    other
             79 2 40 8
##
## Test results:
##
     X-squared statistic: 7.903
##
     degrees of freedom: 1
     p-value: 0.005
##
## Other information:
     estimated effect size (Cramer's v): 0.162
##
     Yates' continuity correction has been applied
```

# Notes on $\chi^2$ Tests: Yates Continuity Corretion and Cramér's V

- Yates continuity correction
  - ▶ When you have a 2 x 2 table, the  $X^2$  statistic tends to be too big
  - ➤ Yates proposed a *hack* that subtracts 0.5 from all the deviations (before squaring)

$$X^{2} = \sum_{i=1}^{\infty} \frac{(|O_{i} - E_{i}| - 0.5)^{2}}{E_{i}}$$

- Cramér's V
  - ▶ Measures correlation between two categorical variables
  - Also can be called "effect size"
  - Varies between 0 and 1
  - Our 0.162 suggests overall association between variables not very strong
    - ★ Although clearly not 0
    - ★ Because they are not independent

### Section 3

## Machine Learning Models

## Flavors Machine Learning

- If there is a dependent variable
  - Supervised
    - Supervised because the model's results can be evaluated in terms of the dependent variable
  - 2 subtypes
    - Classification Put each case in a group based on values of the independent variables
    - Regression Determine a dependent value based on a combination of the independent variables
- If there is *not* a dependent variable
  - Unsupervised
    - Explore the structure among the cases and try to group them in a cluster of cases
    - ★ Cluster Analysis

#### Section 4

## Simple Linear Regression

## Regression – History

- Term comes from eugenics (eugenismo) proposed by Sir Francis Galton.
- Studied heights on individuals within families
- Observed that children of
  - ► Children of tall parents tended to be shorter than the parents
  - ▶ Children of shorter parents tended to be taller than the parents
- Called this trend regression to the mean

## Method of Least Squares

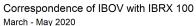
- Solve problems of regression with the Least Squares method
- Invented by Carl Friedrich Gauss (1777 1855)
- Method minimizes the differences between predicted linear values and the values based on the data
- Achieves the best relation between the real dependent variable and the predicted values of the variable
- In this course, focus on linear model forms
  - Many other types of regression exist

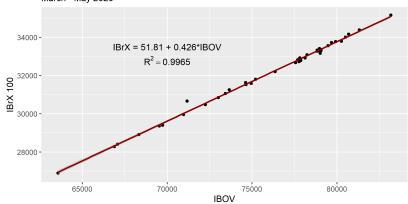
## Purpose

Predict a result on a dependent variable based on one or more indepedent variables

- One *simple* linear regression
- More *multiple* linear regression

# Visualização de Regressão





# Straight Line

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

- $\beta_1 =$ Slope of the line
- $\beta_0 =$ **Intercept** of the line (where it crosses the *y* axis)
- Two parameters of regression
- Optimizing these parameters, Least Squares finds the straight line
- Best predicts the value of the dependent variable (y) based on the value of the independent variable (x)

#### Does "Best" Mean "Good"?

- ullet Despite being the best way to predict y,
  - ▶ Possible that it does **not** describe *y* well
- Good depends on the data
- Best depends on the algorithm

# Regression Equation

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$$

- $Y_i$  = value of the dependent variable
- $\beta_0$  = intercept
- $\beta_1$  = slope of the regression line
- $X_i$  = value of the independent variable
- $\epsilon_i$  = error term for each case

# Regression Equation - Estimation

$$\hat{Y}_i = b_0 + b_1 X_i + e_i$$

- $\hat{Y}_i$  = value of the dependent variable (estimated)
- $b_0$  = intercept (estimated)
- $b_1$  = slope of the regression line (estimated)
- $X_i$  = value of the independent variable
- $e_i$  = error term for each case

# "Error" Term $(\epsilon)$

- Also called residual
- Responsible for variability in y the the line cannot explain
- Does not mean "wrong"
- Only means "difference from a mean"
- Similar to what we saw with hypothesis tests

## Least Squares

- Makes the calculation that minimizes the error sum of squares
- Errors = residuals = differences between the observed value and the expected value

$$min\sum(y_i-\hat{y}_i)^2$$

- $y_i$  = observed value of the dependent variable
- $\hat{y}_i$  = estimated value of the dependent variable

## Example

- Data set of Galton about height in families
- Question is if children are taller or shorter than their parents
- He measured 898 sons/daughters in 197 families
- Original data records are in University College, London (UCL)

#### **Variables**

• height, father, mother - all are height in inches

#### Focus on Fathers and Sons

```
boys <- galton %>%
  filter(sex == "M") %>%
  select(-family, -mother, -sex, -nkids)
glimpse(boys)
## Rows: 465
```

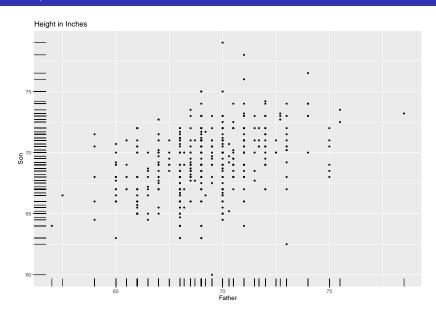
## \$ father <dbl> 78.5, 75.5, 75.5, 75.0, 75.0, 75.0, 75.0, 75.0, 75.0, 74.0, ... ## \$ height <dbl> 73.2, 73.5, 72.5, 71.0, 70.5, 68.5, 72.0, 69.0, 68.0, 76.5, ...

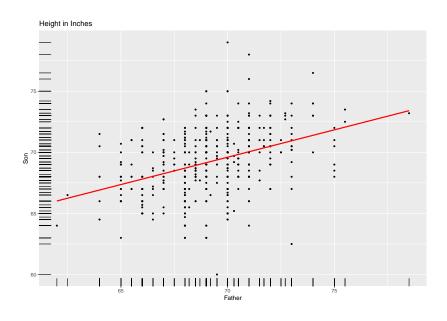
- father is the independent variable
- height is the dependent variable

## Columns: 2

• We want to see if the height of the father predicts the height of the son

# Father/Son – Scatterplot





# What Have We Learned from the Scatterplot?

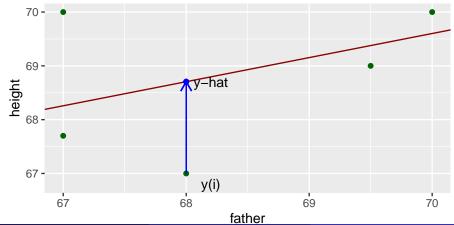
- Seems that taller the fathers, taller the sons
- Descriptive statistics of the 2 variables
  - And, correlation

```
## Descriptive Statistics
## boys
## N · 465
                          Std.Dev
                   Mean
                                      Min
                                                     Median
                                                                        Max
                                                                                IQR
                             2.30
                                                              70.50
                                                                      78.50
                                                                               2.50
         father
                  69.17
                                    62.00
                                             68.00
                                                      69.00
                                                                                      0.03
                  69.23
                             2.63
                                            67.50
                                                      69.20
                                                              71.00
                                                                               3.50
        height
                                    60.00
                                                                      79.00
                                                                                      0.04
```

## [1] "Correlation Coefficient: 0.391"

# How Do We Calculate the Regression Line?

- A line that minimizes the difference between  $y_i$  and  $\hat{y}$
- Need to work with squared differences
  - ▶ To not end up with a sum of 0
- SSE Error Sum of Squares



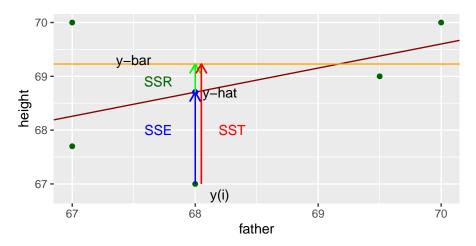
# SSE – A Component of Total Sum of Squares (SST)

$$SST = SSE + SSR$$

- SST - Total - SSE - Related to errors/residuals - SSR - Related to/Explained by regression

# SST – What Does It Represent?

• The total variance is the difference between the model value for each value of X and the mean of the values of the dependent variable  $(\hat{y})$ 



# Sum of Squares

- Refer to the sum of squares we want to minimize as the SSE
   Error sum of squares
- SSE is a component of the total sum of squares (SST)como componente da soma dos quadrados total
- SSE -- the of the squares related to the residuals
- SSR -- sum of squares related to the regression
- Expression for the SSE

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

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

# To Determine the Formula for $\beta_0$ & $\beta_1$

- To minimize the SSE (determine the most efficient line), we need to use calculus cálculo
- ullet Set the partial derivatives of the SSE with respect to  $eta_0$  and  $eta_1$

$$\frac{\partial}{\partial \beta_0} SSE = \frac{\partial}{\partial \beta_1} SSE = 0$$

- Called the normal equations
- We let the software calculate the parameters of the equation

#### Function in R

- Function lm() ("linear model")
- lm(formula, data, subset, weights, na.action, method =
  "qr", model = TRUE, x = FALSE, y = FALSE, qr = TRUE,
  singular.ok = TRUE, contrasts = NULL, offset, ...)
- Important arguments are formula, data, subset, weights, na.action
  - formula: where you show which variables you are modelling
    - ★ Dependent variable comes first
    - ★ Separated from the independent by " ~ "
  - ▶ For the boys: height ~ father
  - data: data frame or tibble that contains the variables
  - subset, weights: parameters that permit customization of the variables
  - ▶ na.action: how you will deal with missing data in the model variables

# Function Applied to Fathers and Sons

Function 1m produces a list of 12 items in a special format

```
fit1 <- lm(height ~ father, data = boys)
summary(fit1)
##
## Call:
## lm(formula = height ~ father, data = boys)
##
## Residuals:
      Min 10 Median 30
##
                                    Max
## -9.3774 -1.4968 0.0181 1.6375 9.3987
##
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) 38.25891 3.38663 11.30 <2e-16 ***
## father
          0.44775 0.04894 9.15 <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.424 on 463 degrees of freedom
## Multiple R-squared: 0.1531, Adjusted R-squared: 0.1513
## F-statistic: 83.72 on 1 and 463 DF, p-value: < 2.2e-16
```

# What Does This Model Say?

$$\hat{y} = 38.259 + 0.448x$$

- If a father had 0 height, the son would be 38.259 inches tall
  - Doesn't make practical sense
  - Establishes a base for the height calculation
  - For each incremental inch on the father's height, the son would be 0.448 inches taller

#### Extract the Coefficient Values

- Option 1: use broom::tidy
  - Automatically extracts the key information and puts in a tibble

```
broom::tidy(fit1) %>% knitr::kable()
```

term	estimate	std.error	statistic	p.value
(Intercept)	38.2589122	3.3866340	11.297032	0
father	0.4477479	0.0489353	9.149788	0

Option 2: use coef

coef(fit1)

```
## (Intercept) father
## 38.2589122 0.4477479
```

#### Predictions of New Values

- You can use the model parameters to predict new values of the heights of sons
- Use broom::augment
- How tall would the son of a 72 inch father be?

```
fit1 %>% broom::augment(newdata = data_frame(father = 72))

## # A tibble: 1 x 2
## father fitted
```

```
## father .fitted
## <dbl> <dbl>
## 1 72 70.5
```

#### Section 5

What Does the Model Mean? How to Interpret It?

# Does There Exist a Relationship between the Independent and Dependent Variables?

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$$

• If  $\beta_1$  (slope of the line) were 0, what would be the equation?

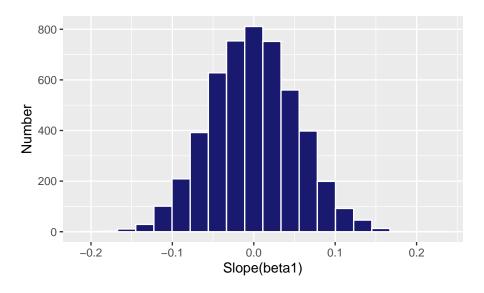
$$Y_i = \beta_0 + \epsilon_i$$

- X disappears
- $\bullet$  There would be no relationship between X and Y
  - Only an intercept and an error term
- Makes possible an efficient test of the existence of a relationship between X & Y (or not)
- Create a null hypothesis  $H_0: \beta_1 = 0$

# Test of the Null Hypothesis

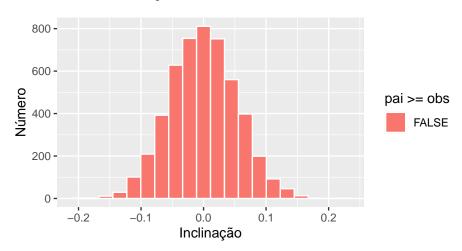
- We will make a simulation of the null hypothesis
- If we do not reject the null, any son's height could have occurred for any father's height
- We can calculate the regression model 5,000 times shuffling around the son's heights
- ullet As a result, we can focus on the values of the slope,  $eta_1$
- 2nd, we will compare our observed value of  $\beta_1$  ('r coef(fit1)[2]) to see where it falls in the simulated values

# Histogram of the Slopes of the Simulated Models



# Histogram with Values Above and Below Observed Slope

## Número de simulações com beta1 >= obs: 0



# The p-value of the Slope $(\beta_1)$

- Because **none** of the simulations produced a value higher than our observed value (0.448)
- We can conclude that the p-value of this test is 0
- There is **no** chance that the slope = 0
- Thus, we reject the null hypothesis and conclude that a linear relationship does exist between the heights of fathers and sons

#### Section 6

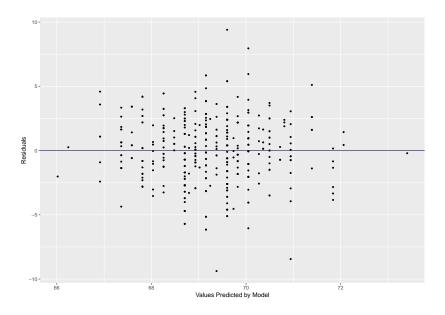
Assumptions of Linear Regression and How to Test
Them

# Assumptions of Linear Regression

- All independent variables must have the same variance
  - ▶ Graph of residuals should avoid patterns when looking from left to right
- ② All the observations, residuals and independent variables must be independent of each other
  - Graph of residuals should not show a sinuous pattern
- Residuals should have a near-normal distribution
  - Q-Q graph of the standardized residuals should be a straight line
  - ▶ Shows that the variables have a multivarite normal distribution
- Independent variables should avoid multicollinearity
  - ▶ They should not have high correlations between them

## Residuals Graph

- Graph that shows the value predicted by the model ("fitted value") vs. the residual
- Use the function broom::augment()
  - Extracts efficiently the values used in the model tests

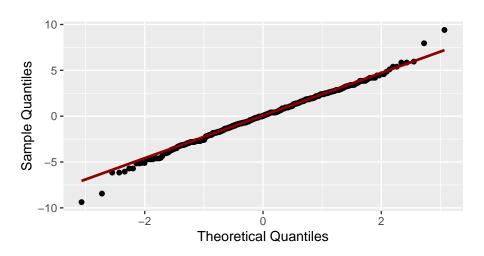


# Importance of Residuals

- Can use the residuals to verify if the model respects the assumptions of regression
- Should not show any linear trend

## Q-Q Graph

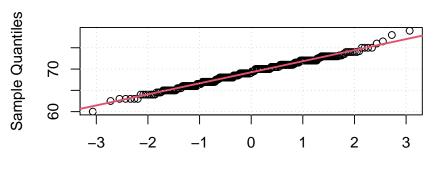
- Verifies the normality of the residuals
  - Closer the curve to a straight line, the better the "fit" with a normal distribution



## Q-Q Graphs Also Directly Available in Base R

```
qqnorm(boys$height)
qqline(boys$height, col = 2, lwd = 2)
grid()
```

### Normal Q-Q Plot



**Theoretical Quantiles** 

### F-Test of Model Variance

- F-Test is a test that verifies that the variances of variables are close to equal
- Uses the F Distribution
  - ▶ With 2 degrees of freedom as parameters
- Serves as a test of significance for the model as a whole
- Shown in the summary() function output for the lm() function

## F-Test for the Son-Father Heights Model

```
Coefficients:

Estimate Std. Error t value Pr(>|t|)

(Intercept) 38.25891  3.38663  11.30  <2e-16 ***

father  0.44775  0.04894  9.15  <2e-16 ***

---

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.424 on 463 degrees of freedom

Multiple R-squared: 0.1531, Adjusted R-squared: 0.1513

F-statistic: 83.72 on 1 and 463 DF, p-value: < 2.2e-16
```

# Summary of the Sum of Squares

Total Sum of Squares

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

Error Sum of Squares

$$SSE = \sum (y_i - \hat{y})^2$$

Regression Sum of Squares

$$SSR = \sum (\hat{y}_i - \bar{y})^2 = SST - SSE$$

### $R^2$ – Coefficient of Determination

- Measure of how much the regression line explains the variance in Y
- Ratio of SSR to SST

$$R^2 = \frac{SSR}{SST}$$

- Calculated by lm()
- Appears in summary(lm)
- Varies between 0 and 1
- $\sqrt{R^2} = r$  (correlation coefficient)

```
Coefficients:

Estimate Std. Error t value Pr(>|t|)

(Intercept) 38.25891 3.38663 11.30 <2e-16 ***

father 0.44775 0.04894 9.15 <2e-16 ***

---

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.424 on 463 degrees of freedom

Multiple R-squared: 0.1531, Adjusted R-squared: 0.1513

F-statistic: 83.72 on 1 and 463 DF, p-value: < 2.2e-16
```

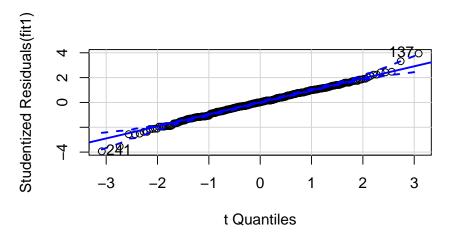
# Importance of $R^2$

- If 100% of the variance in Y can be explained by the regression
- SSR = SST
- $\therefore R^2 = SST/SST = 1$
- Variance completely explained by the regression
  - Means there is no error
- In general, the degree to which the regression explains the model variance

### Section 7

## More Advanced Graph

# qqPlot() Function from the car Package



## [1] 137 241

### Section 8

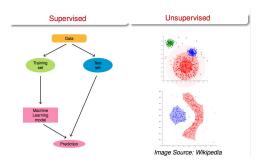
## Multiple Linear Regression - MLR

## Multiple Linear Regression - MLR

- Regression with more than 1 independent variable
- Now we can also call the independent variables "covariates"
- 1st real machine learning model
- Change in the Equation of the Regression Model

$$Y_i = \beta_0 + \beta_1 X_i + \beta_2 X_i + \dots + \beta_k X_i + \epsilon_i$$

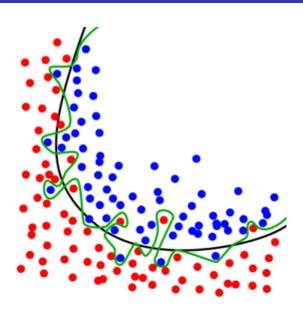
## Types of Machine Learning



## Training x Testing of Models

- Divide data frames into different parts
- To avoid overfitting
- NEVER, EVER, USE THE SAME CASES FOR TESTING THAT YOU USED FOR TRAINING A MODEL

# Overfitting



### Model Characteristics

- Covariates
- How many are sufficient for construction of a model?
  - ▶ Too few model does not describe the condition being modelled
  - ▶ Too many overfitting

## Strengthening a Model

- Bootstrapping
- k-fold Cross Validation
  - ▶ Pull out a group (fold) from the training group
  - Train the model
  - Test the model with the training cases
  - ▶ Do the same with all the other groups
- Use as the final model that which shows the best performance

## Machine Learning in Biological/Medical Modelling

- Typically, projects with "big data"
- Model can provide information quickly and correctly
  - ▶ Clinicians can use the information to design treatments or diagnostics
- Applications in personalized or precision medicine
- Example:
  - Diagnosis of breast cancer with help from a computer model

### Can We Have Confidence in Machine Learning Models?

- ML algorithms model interactions among variables
- Interpretation of results of ML models can be difficult
- ML algorithms' "black box" hide how they make choices
  - For some algorithms (e.g. neural networks)
- Thus, we need models that mean something to the
  - Builders
  - Users
- "Meaningful Models"

## What Makes a Model a "Meaningful Model"

- Being able to generalize based on the model
- Offer an answer to the original motivating question
  - with sufficient precision to be trusted
- The level of precision depends on the nature of the problem

#### Covariates – Features

- The independent variables
- Variables we use to train the model
- Select the **right** variables
- More features not necessarily good
  - Danger of "overfitting"

### Section 9

### Mãos na Massa

#### Data

- Continue with the galton data
- Bring the mother's height into the analysis

## \$ nkids <int> 4, 4, 4, 4, 4, 4, 4, 2, 2, 5, 5, 5, 5, 5, 6, 6, 6, 6, 6, ...

#### Section 10

The caret Method of Machine Learning

## Organized Workflow

- Methodology comes from caret package
- Step 1
  - Divide the cases in 2 groups: training, test
  - Random division
- Train the model with the training data
- After, test the predictions of the model with the values from the test data
- Objective: Make accurate predictions
  - More important than the elegance of the model

## Method Requires a Number of Packages

- caret: Classification And REgression Training
- ggplot: graphs
- broom: functions for showing and comparing models
- nortest: statistical normality tests
- janitor: help with tables

```
pacman::p_load(caret, ggplot2, broom, nortest, janitor)
```

#### The caret Process

- An efficient workflow for regression and classification problems
- Models built with the function caret::train

```
1 Define sets of model parameter values to evaluate
2 for each parameter set do
3 | for each resampling iteration do
4 | Hold-out specific samples
5 | [Optional] Pre-process the data
6 | Fit the model on the remainder
7 | Predict the hold-out samples
8 | end
9 | Calculate the average performance across hold-out predictions
10 | end
11 | Determine the optimal parameter set
12 | Fit the final model to all the training data using the optimal parameter set
```

#### caret Division of Data

- Function caret::createDataPartition()
- Give the function the dependent variable galton\$height
- Proportion (p) that you want in the training sample (70%)
  - Can be between 50% and 70%
  - ▶ Higher percentage can cause overfitting
- Function returns the indices of cases for the training set
- Give it the argument list = FALSE

```
set.seed(42)
indice <- createDataPartition(galton$height, p = 0.70, list = FALSE)
head(indice[, 1], 25)</pre>
```

## [1] 2 3 4 6 7 8 9 13 14 15 17 18 20 21 23 24 25 26 27 28 29 30 31 33 34

## Create train\_data and test\_data

- VSS Remember the comma after the indice
  - ► Why?
- For the test\_data, you want the data that are NOT in the train\_data
  - ► Thus, you need to use the minus sign (-)

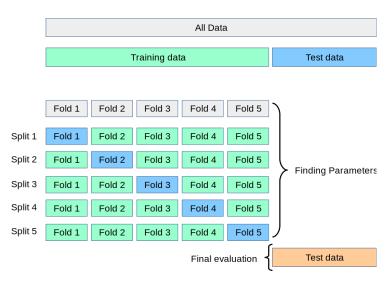
```
train_data <- galton[indice, ]
test_data <- galton[-indice, ]</pre>
```

### Cross-Validation

- Validation of the calculation of the model parameters
  - Using bits of each case repeatedly
- Mathematical equivalent of amplifying biological samples
- Related to the process of resampling called bootstrap
- caret selects the model that has the best performance

### k-fold Cross-Validation – Process

- Divide the training sample into k equal subgroups
- Train the model with k-1 of the folds
- Software tests this model with the cases of the fold left out
  - ► Test is of the predictive performance (precision)
- Repeat until you have left out all the folds
- Can repeat the entire process a number of times



Source: scikit.learn.org

### **Pre-Processing**

- If there are signs that some variables are non-normal
- You can reduce the non-normality of the curves with
  - Centralization (subtract the mean from the value)  $(x_i \bar{x})$
  - Normalization (divide the centralized value by the std. deviation)  $\frac{(x_i \bar{x})}{s}$
- caret will perform these for you

### train() Heights Model

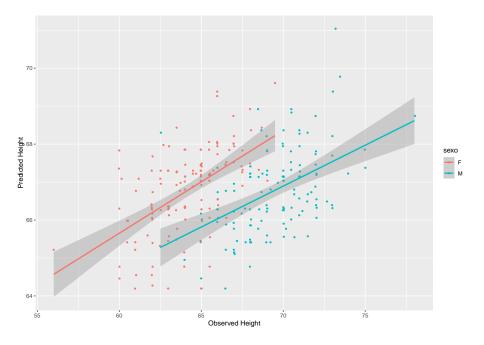
• caret::train() the function that determines the parameters of the regression model

#### summary(fit\_pai\_mae)

```
##
## Call:
## lm(formula = .outcome ~ .. data = dat)
##
## Residuals:
##
     Min
            10 Median 30
                                Max
## -8.480 -2.740 -0.179 2.807 11.699
##
## Coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 23.59851 5.08952 4.637 4.31e-06 ***
## father
          0.37731 0.05589 6.751 3.34e-11 ***
## mother 0.26601 0.05870 4.532 7.00e-06 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3.404 on 628 degrees of freedom
## Multiple R-squared: 0.1052, Adjusted R-squared: 0.1023
## F-statistic: 36.9 on 2 and 628 DF, p-value: 7.022e-16
```

### How Did the Model Do?

- Apply the model to the data from test\_data
- Until now, the model has not seen these data
- Shows what you can do with any data that measures the same phenomenon
- predict calculates the predicted values using the model parameters



### How Accurate Was the Model?

- Look at the difference between the real (observed) values and the predicted values
- How many of these differences were less than a reasonable standard (?
   2 inches)

```
## res$bomruim n percent
## bom 95 35.6%
## ruim 172 64.4%
```

### Model Is Not Good

- Very low accuracy
  - ▶ 36% within our standard of 2 inches
- $R^2$  very low (0.1023)
  - $\blacktriangleright$  Only 10% of the variance in the model was explained by the covariates

### Can We Do Better?

- Gender could be having an effect on height
- Gender is a categorical variable
- Regression compares distributions of numbers
- But, it can include categorical variables

# Categorical Variables in Regression

- Divide the variable into a series of "dummy" variables
  - ▶ 1 *dummy* variable for each level of the categorical variable (less the 1st level)
  - ▶ k 1 dummy variables
- If there are 3 levels (high, medium, low), the system will create 2 new variables
  - medium and low
  - high will be a reference value that represents the case when none of the other variables is present

```
notas <- tibble(x = rep(c("alto", "media", "baixo"), 3),</pre>
              y = c(3, 2, 1, 3, 2, 1, 7, 5, 2))
summary(lm(y ~ x, data = notas))
##
## Call:
## lm(formula = y ~ x, data = notas)
##
## Residuals:
##
      Min 10 Median 30
                                   Max
## -1.3333 -1.0000 -0.3333 0.6667 2.6667
##
## Coefficients:
##
             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 4.3333 0.9813 4.416 0.00449 **
## xbaixo -3.0000 1.3878 -2.162 0.07390 .
## xmedia -1.3333 1.3878 -0.961 0.37377
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
```

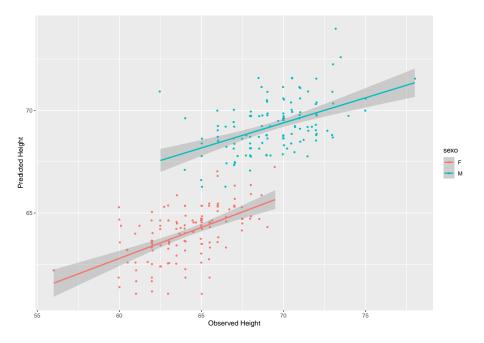
## Residual standard error: 1.7 on 6 degrees of freedom
## Multiple R-squared: 0.4388, Adjusted R-squared: 0.2518
## F-statistic: 2.346 on 2 and 6 DF, p-value: 0.1767

# Include sex in the Heights Regression

#### summary(fit\_pms)

```
##
## Call:
## lm(formula = .outcome ~ .. data = dat)
##
## Residuals:
##
     Min 1Q Median 3Q
                                Max
## -9.4833 -1.5274 0.0932 1.5369 9.1510
##
## Coefficients:
##
            Estimate Std. Error t value Pr(>|t|)
## father 0.40976 0.03604 11.369 < 2e-16 ***
## mother 0.32157 0.03788 8.489 < 2e-16 ***
## sexM 5.21288 0.17527 29.742 < 2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.194 on 627 degrees of freedom
## Multiple R-squared: 0.6288, Adjusted R-squared: 0.627
## F-statistic: 354.1 on 3 and 627 DF, p-value: < 2.2e-16
```

### Model Performance



### How Accurate Was the Model?

##

##

bom 183 68.5% ruim 84 31.5%

### Result

- ullet Model predicts 69% of the heights within the standard we set
  - Double the previous model
- R<sup>2</sup> increased to 0.627 (a lot)
- Gender has an important role in determining the heights of the offspring
  - ► The model captures this characteristic

# varImp() Function in caret

- Function evaluates the relative importance of variables in the model
  - ► Most important 100%
  - ► Least important 0%
- Our Second Model

```
## lm variable importance
##
## Overall
## sexM 100.00
## father 13.55
## mother 0.00
```

varImp(fit\_pms)

### Section 11

# Final Example - gapminder

# What Is Gapminder?

- R package derived from the site https://www.gapminder.org/
- Monitors socio-economic conditions around the world
- Result of research by Hans Rosling and his family
- They find that poverty in the world can be eliminated by 2030
- Have a look at the video: https://www.gapminder.org/videos/dont-panic-end-poverty/
- Inspiring!

### What Can We Learn from This?

- Life Expectancy (lifeExp) dependent variable
  - Measured by country
- Our hypothesis is that life expectancy depends on
  - ► The year surveyed (1952 2007 every five years)
    - ★ As time passes (year increases), life expectancy naturally increases
  - ▶ Gross domestic product per capita

Life expectancy as a measure of the health of countries increases based on the economic well being of the population. It has become better over time since the 1950's.

## Philosophical Issue

- Objective of Machine Learning models: accurate prediction
  - ► Niceties of obeying all the assumptions and statistical hypothesis tests not as important
- Objective of Statistical models: relate the data of the sample to a larger truth about a population
  - Assumptions, hypothesis tests, confidence intervals, etc. all very important

# Null and Alternative Hypotheses

- If we were building a strictly statistical model, we would first establish a null hypothesis
- $H_0$ : Life expectancy does not vary due to these three variables

$$H_0: Y_i = b_0 + \epsilon_i$$

• *H*<sub>1</sub>: Life Expectancy has a relationship with at least one of the three covariates

$$H_1: Y_i = \left(\sum_{k=1}^K b_k X_{ik}\right) + b_0 + \epsilon_i$$

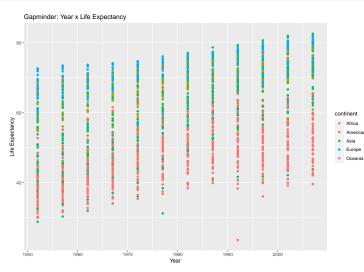
# Loading Gapminder

# **Descriptive Statistics**

```
gm %>%
  select(year, pop, gdp_percap) %>%
  mutate(pop = log10(pop)) %>%
  descr(stats = c("mean", "sd", "min", "q1", "med", "q3", "max", "igr", "cv"),
     transpose = TRUE)
## Descriptive Statistics
## N: 1704
##
                        Mean
                             Std.Dev
                                            Min
                                                       Q1
                                                             Median
                                                                                              TOR
        gdp_percap
                    7215.33 9857.45
                                         241.17 1201.92
                                                           3531.85
                                                                                           8123.40
##
                                                                      9325.86
                                                                               113523.13
                                                                                                   1 37
                        6.85
                                 0.70 4.78
                                                     6.45
                                                              6.85
                                                                        7.29
                                                                                    9.12
                                                                                                    0.10
##
               pop
                                                                                              0.85
                     1979.50 17.27
##
              year
                                        1952.00 1964.50 1979.50
                                                                     1994.50
                                                                                 2007.00
                                                                                             27.50
                                                                                                    0.01
paste("Correlation Coefficient (year x life):", with(gm, round(cor(life exp, year), 3)))
## [1] "Correlation Coefficient (year x life): 0.436"
paste("Correlation Coefficient (life x gdp):", with(gm, round(cor(life_exp, gdp_percap), 3)))
## [1] "Correlation Coefficient (life x gdp): 0.584"
paste("Correlation Coefficient (gdp x life):", with(gm, round(cor(gdp_percap, year), 3)))
## [1] "Correlation Coefficient (gdp x life): 0.227"
```

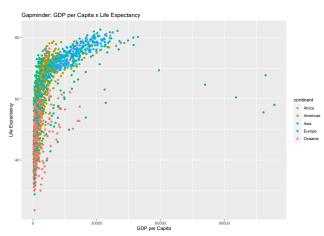
# Scatterplot of life\_exp against year

```
ggplot(gm, aes(x = year, y = life_exp, color = continent)) +
geom_point() +
labs(title = "Gapminder: Year x Life Expectancy", x = "Year", y = "Life Expectancy")
```



# Scatterplot of life\_exp against gdp\_percap

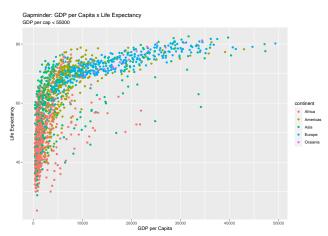
```
ggplot(gm, aes(x = gdp_percap, y = life_exp, color = continent)) +
   geom_point() +
   labs(title = "Gapminder: GDP per Capita x Life Expectancy", x = "GDP per Capita", y = "Life Expectancy")
```



# Scatterplot of life\_exp against gdp\_percap - 2

• Get rid of very high GDP's per capita to see mass more clearly

```
gm %>%
filter(gdp_percap < 55000) %>%
ggplot( aes(x = gdp_percap, y = life_exp, color = continent)) +
geom_point() +
labs(title = "Gapminder: GDP per Capita x Life Expectancy", x = "GDP per Capita", y = "Life Expectancy", su
```



# Initializing caret and Related Packages

```
pacman::p_load(caret, tidyverse, broom, nortest, janitor)
```

# Setup Training and Test Sets

gm\_test <- gm[-index, ]</pre>

```
set.seed = 1946
index <- createDataPartition(gm$life_exp, p = 0.7, list = FALSE)
head(index[, 1], 25)
## [1] 1 2 3 5 6 9 10 12 14 15 16 17 18 19 20 21 24 25 26 27 28 30 31 32 33
gm_train <- gm[index, ]</pre>
```

### Plan for Cross-Validation

- Given 142 countries, divide data into 10 folds
  - ▶ 14.2 countries per fold
- Repeats of cross-validation
  - Stick with the 10 repeats of heights analysis

### train Command to Build Model

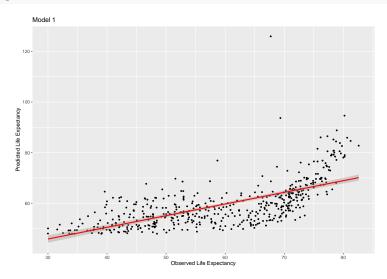
#### summary(fit\_gm\_1)

```
##
## Call:
## lm(formula = .outcome ~ .. data = dat)
##
## Residuals:
##
      Min
             10 Median
                           30
                                 Max
## -66.947 -7.035 1.302 7.644 19.946
##
## Coefficients:
##
                 Estimate Std. Error t value Pr(>|t|)
## (Intercept) -444.88582782 32.88263874 -13.53 <2e-16 ***
## year
              ## gdp_percap 0.00066984 0.00002919 22.94 <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 9.691 on 1193 degrees of freedom
## Multiple R-squared: 0.4386, Adjusted R-squared: 0.4377
## F-statistic: 466 on 2 and 1193 DF. p-value: < 2.2e-16
```

### How Did the Model Do?

- Applying model to test data
  - ▶ Up to now, model has not seen test data

### gm\_1\_plot



# Accuracy of Model 1

- Set an accuracy standard
  - ▶ Predicted value 2 years ± observed life expectancy

```
## gm_pred_1$goodbad n percent
## bad 231 45.5%
## good 277 54.5%
```

### Conclusion of This Model

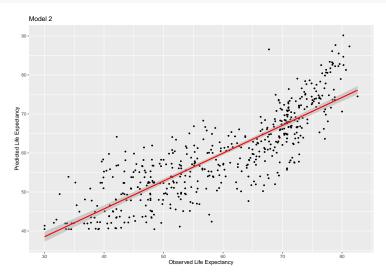
- Only captures 47% of the variance in life expectancy
- Continents seem to play a role
  - ▶ They all have different slopes
- Add continent as a variable to the model
- 58% accuracy not terrific
- Weird outliers with predicted age expectancies above 120 years

## Model # 2 – Three Covariates

```
##
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##
      Min
               1Q
                   Median
                               30
                                      Max
## -28.7132 -4.1337 0.0507 4.4951 19.7608
##
## Coefficients:
##
                      Estimate
                                 Std. Error t value Pr(>|t|)
## (Intercept)
                  -533.19986541
                                23.47738883 -22.71 <2e-16 ***
## year
                    0.00028746 0.00002394 12.01
                                                   <2e-16 ***
## gdp_percap
## continentAmericas 14.34155249 0.58768275 24.40 <2e-16 ***
## continentAsia
                8.89348649 0.54472749 16.33 <2e-16 ***
## continentEurope 19.45248558 0.61794077 31.48 <2e-16 ***
## continentOceania 20.91883484 1.90370803 10.99
                                                   <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 6.868 on 1189 degrees of freedom
## Multiple R-squared: 0.7189, Adjusted R-squared: 0.7175
## F-statistic: 506.9 on 6 and 1189 DF, p-value: < 2.2e-16
```

# How Did We Do (This Time)?

### $gm_2_plot$



# Accuracy of Model 2

- Set an accuracy standard
  - ▶ Predicted value 2 years ± observed life expectancy

```
## gm_pred_2$goodbad n percent
## bad 202 39.8%
## good 306 60.2%
```

### Conclusion of This Model

- Better R<sup>2</sup>
- Graph shows a clearer trend for accuracy (now 63%)
- Continents seem to play important role
  - Mirrors intuitive thought

# Interesting New Machine Learning Site

https://projects.economist.com/us-2020-forecast/president



### Section 12

Next Week's Theme

- Continue with regression
- Focus on Logistic Regression
  - Applying regression to problem of classification
- Remember project topics to Prof. this week
- Problem Set 2 Available
  - ▶ Due 16/10