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_1 : At least one suit has a probability that is not 0.25

$$H_1: P \neq (0.25, 0.25, 0.25, 0.25)$$

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
  2 ouros
           50 51
           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)

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

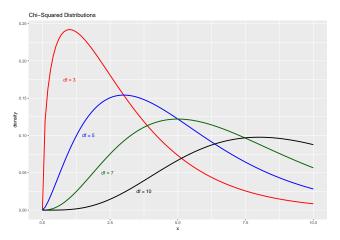
- If X^2 is small, unlikely to reject null hypothesis - Differences will be too small to justify this

```
(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

- χ^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 χ^2 distribution

Mathematical Demonstration

• 3 normally distributed variables

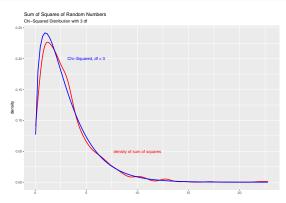
```
norm1 <- rnorm(n = 1000)
norm2 <- rnorm(n = 1000)
norm3 <- rnorm(n = 1000)
```

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")
```



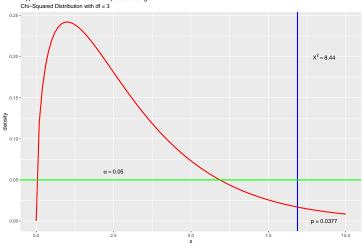
Complete Hypothesis Test

- Compare our X^2 to where the 95th percentile of the χ^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

 χ^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
- H_1 : elderly and others have different chances of dying from COVID-19
 - ▶ H_1 : p(elderly & death = TRUE) \neq 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

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

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

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 χ^2 Tests: Yates Continuity Corretion and Cramér's V

- Yates continuity correction
 - ▶ When you have a 2×2 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

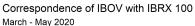
- Solve problems of regression with the Least Squares method
- Invented by Carl Friedrich Gauss (1777 1855)
- Method minimizes the differences between predicted linear values and the values based on the data
- Achieves the best relation between the real dependent variable and the predicted values of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

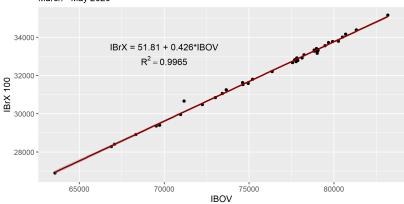
Purpose

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
- β_0 = intercept
- β_1 = slope of the regression line
- X_i = value of the independent variable
- ϵ_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 (ϵ)

- 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
```

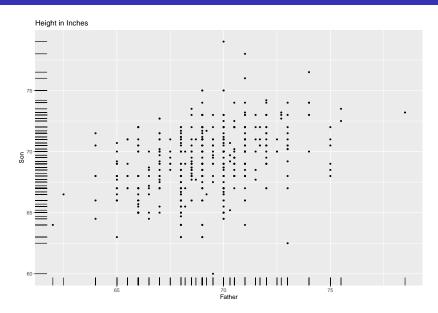
\$ father <dbl> 78.5, 75.5, 75.5, 75.0, 75.0, 75.0, 75.0, 75.0, 75.0, 74.0, ... ## \$ height <dbl> 73.2, 73.5, 72.5, 71.0, 70.5, 68.5, 72.0, 69.0, 68.0, 76.5, ...

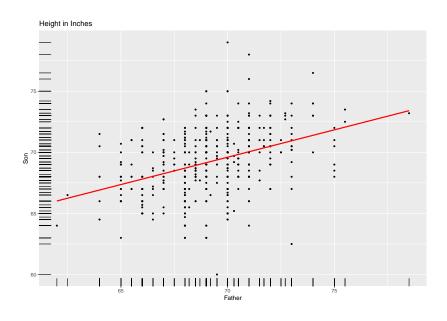
- father is the independent variable
- height is the dependent variable

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?

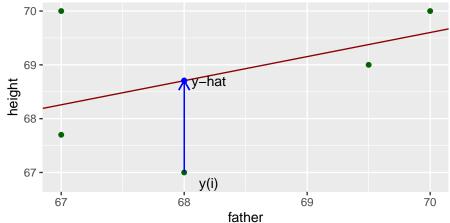
- Seems that taller the fathers, taller the sons
- Descriptive statistics of the 2 variables
 - And, correlation

```
## 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



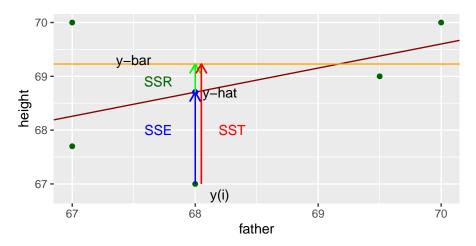
SSE – A Component of Total Sum of Squares (SST)

$$SST = SSE + SSR$$

- 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 β_0 & β_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 β_1 (slope of the line) were 0, what would be the equation?

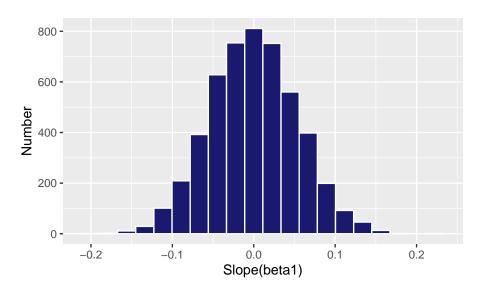
$$Y_i = \beta_0 + \epsilon_i$$

- 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

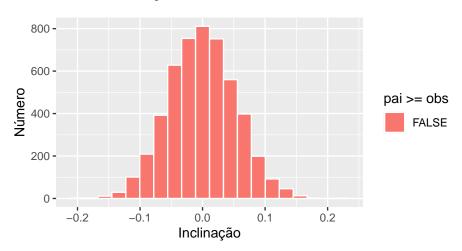
- We will make a simulation of the null hypothesis
- If we do not reject the null, any son's height could have occurred for any father's height
- We can calculate the regression model 5,000 times shuffling around the son's heights
- ullet As a result, we can focus on the values of the slope, eta_1
- 2nd, we will compare our observed value of β_1 (0.4477479) 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 (β_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

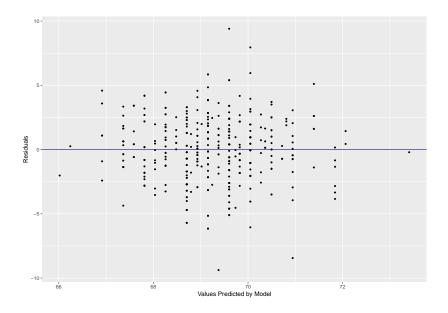
Assumptions of Linear Regression and How to Test
Them

Assumptions of Linear Regression

- All independent variables must have the same variance
 - ▶ Graph of residuals should avoid patterns when looking from left to right
- 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

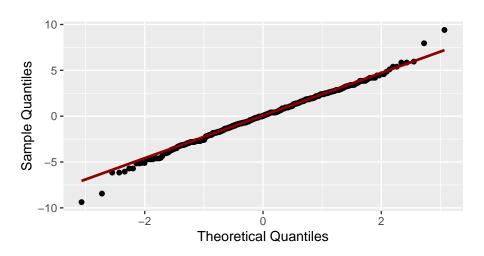


Importance of Residuals

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

Q-Q Graph

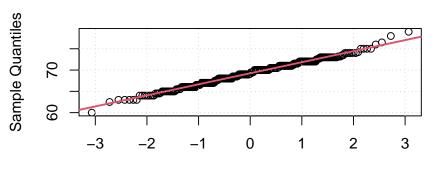
- Verifies the normality of the residuals
 - Closer the curve to a straight line, the better the "fit" with a normal distribution



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 ***

---

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

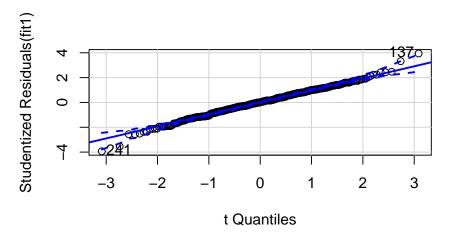
Importance of R^2

- If 100% of the variance in Y can be explained by the regression
- SSR = SST
- $\therefore R^2 = SSR/SST = 1$
- 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

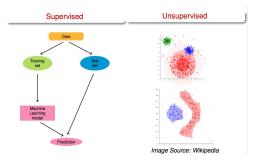
Multiple Linear Regression - MLR

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

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

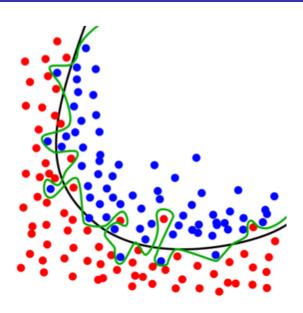
Types of Machine Learning



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

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 parameter set 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 (-)

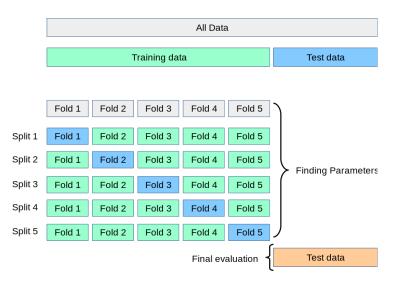
```
train_data <- galton[indice, ]
test_data <- galton[-indice, ]</pre>
```

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

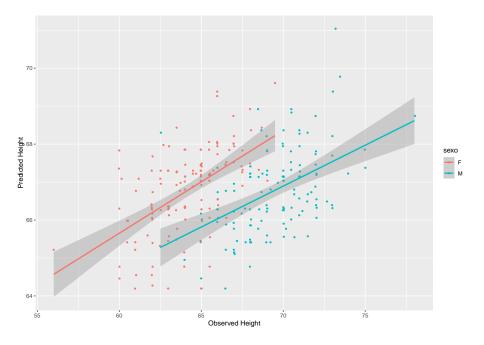
• caret::train() the function that determines the parameters of the regression model

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
##
```

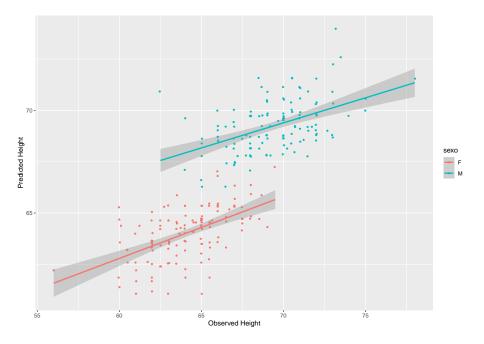
Residual standard error: 1.7 on 6 degrees of freedom
Multiple R-squared: 0.4388, Adjusted R-squared: 0.2518
F-statistic: 2.346 on 2 and 6 DF, p-value: 0.1767

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

- Model predicts 69% of the heights within the standard we set
 - ▶ Double the previous model
- R² 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*₁: Life Expectancy has a relationship with at least one of the three covariates

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

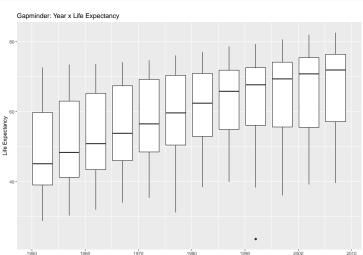
Loading Gapminder

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
##
                                            Min
                        Mean
                             Std.Dev
                                                       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"
```

Boxplot of life_exp against year

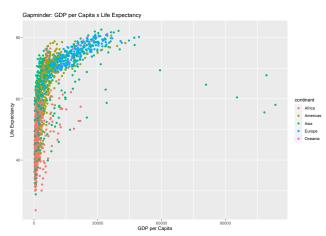
```
ggplot(gm, aes(x = year, y = life_exp, group = year)) +
geom_boxplot() +
labs(title = "Gapminder: Year x Life Expectancy", x = "Year", y = "Life Expectancy")
```



Year

Scatterplot of life_exp against gdp_percap

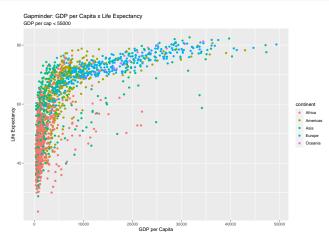
```
ggplot(gm, aes(x = gdp_percap, y = life_exp, color = continent)) +
   geom_point() +
   labs(title = "Gapminder: GDP per Capita x Life Expectancy", x = "GDP per Capita", y = "Life Expectancy")
```



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

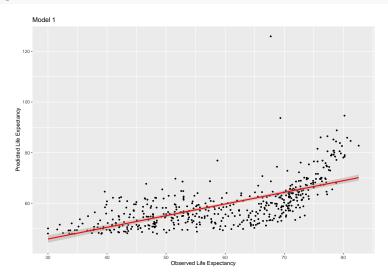
summary(fit_gm_1)

```
##
## 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

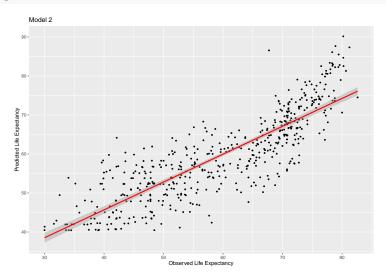
- Only captures 47% of the variance in life expectancy
- Continents seem to play a role
 - ▶ They all have different slopes
- Add continent as a variable to the model
- 58% accuracy not terrific
- Weird outliers with predicted age expectancies above 120 years

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

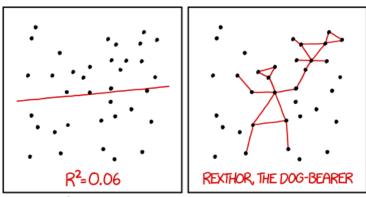
- Set an accuracy standard
 - ▶ Predicted value 2 years ± observed life expectancy

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

Conclusion of This Model

- Better R²
- Graph shows a clearer trend for accuracy (now 63%)
- Continents seem to play important role
 - Mirrors intuitive thought

Danger of Interpretation when R^2 Low



I DON'T TRUST LINEAR REGRESSIONS WHEN IT'S HARDER TO GUESS THE DIRECTION OF THE CORRELATION FROM THE SCATTER PLOT THAN TO FIND NEW CONSTELLATIONS ON IT.

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