

# 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 ( $O_1 \dots O_{200}$ )

```
naipes <- readRDS(here("naipes.rds"))  
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))
```

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

```
n <- 200
expected <- n * probs
diff <- observed - expected
df <- tibble(suit = names(observed),
             expected,
             observed,
             diff)

df
```

## # A tibble: 4 x 4

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

# Goodness of Fit Statistic - $\chi^2$

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

$$\chi^2 = \sum_{i=1}^k \frac{(O_i - E_i)^2}{E_i}$$

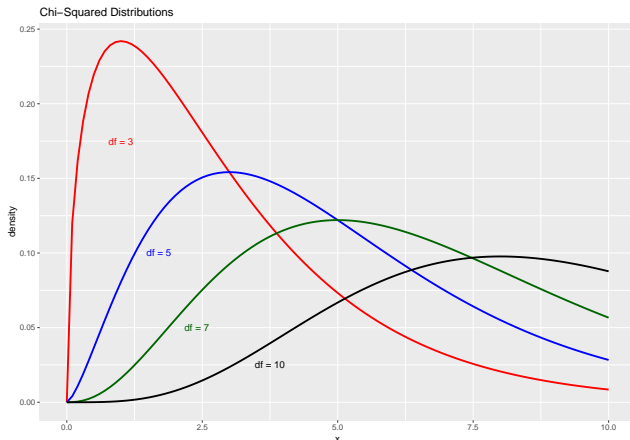
- If  $\chi^2$  is small, unlikely to reject null hypothesis - Differences will be too small to justify this

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

```
## [1] 8.44
```

# Sampling Distribution of $\chi^2$

- This statistic ( $\chi^2$ ) follows a **chi-squared distribution**
  - ▶ *Qui-quadrado*
  - ▶  $\chi^2$
  - ▶ 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

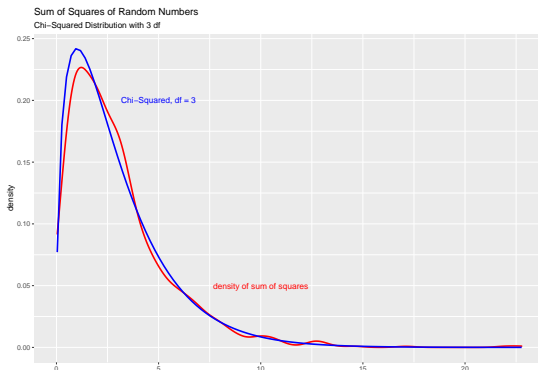
```
norm1 <- rnorm(n = 1000)
norm2 <- rnorm(n = 1000)
norm3 <- rnorm(n = 1000)
```

- 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
- $X^2 = 8.44$ ;  $\chi^2 = 7.8147279$
- $\therefore$  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

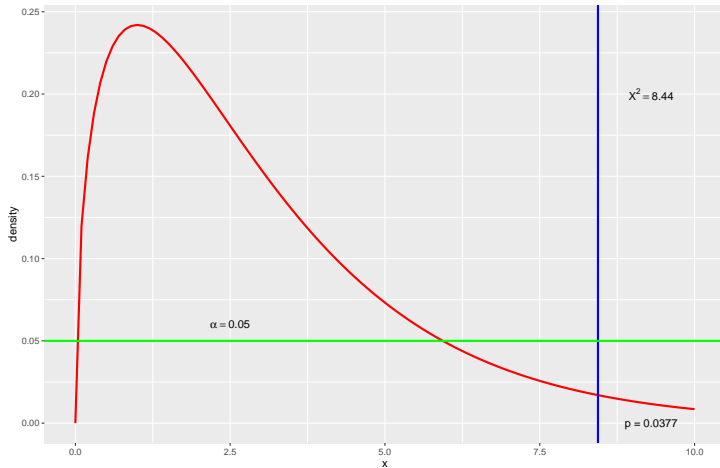
```
pchisq(q = X_sq, df = 3, lower.tail = FALSE) ## only calculate
```

```
## [1] 0.03774185
```

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

```
## [1] 0.03774185
```

Hypothesis Test of Student Naïpe Guessing  
Chi-Squared Distribution with  $df = 3$



# 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  $2 \times 2$  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"))  
summarytools::ctable(comorbid$death, comorbid$age_group, prop = "c")
```

```
## 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%)  
## -----
```

# Hypotheses

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

# Calculate Expected Values

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

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

```
## 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%)
## -----
```



# Estimated Values

```
estim <- data.frame(death = integer(length = 2),
                    age_group = integer(length = 2))
ct <- tab_comorb$cross_table
n <- nrow(comorbid)
for(i in 1:2){
  for(j in 1:2){
    estim[i,j] <- sum(ct[i,1:2]) * sum(ct[1:2,j]) / n
  }
}
rownames(estim) <- c("FALSE", "TRUE")
colnames(estim) <- c("elderly", "other")
estim
```

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

# $\chi^2$ 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
  - ▶  $(r - 1)(c - 1)$

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

# 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

```
gmodels::CrossTable(comorbid$death, comorbid$age_group, expected = TRUE, chisq = TRUE,  
                    format = "SPSS")
```

Cell Contents			
	Count	Expected Values	
	Chi-square contribution		
	Total	Percent	
Total Observations in Table: 300			
comorbid\$death	comorbid\$age_group		Row Total
	elderly	other	
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			
Pearson's Chi-squared test			
Chi^2 = 8.618043	d.f. = 1	p = 0.003328492	
Pearson's Chi-squared test with Yates' continuity correction			
Chi^2 = 7.903174	d.f. = 1	p = 0.004934813	

# Results with `lsr::associationTest()`

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

```
comorbid <- comorbid %>%  
  mutate(age_group = factor(age_group),  
         death = factor(death))  
lsr::associationTest(~ age_group + death, data = comorbid)
```

```
##
##      Chi-square test of categorical association
##
## Variables:   age_group, death
##
## Hypotheses:
##   null:      variables are independent of one another
##   alternative: some contingency exists between variables
##
## Observed contingency table:
##           death
## age_group FALSE TRUE
##   elderly   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 Correction and Cramér's V

- Yates continuity correction

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

$$\chi^2 = \sum_{i=1} \frac{(|O_i - E_i| - 0.5)^2}{E_i}$$

- 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



- 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

- 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

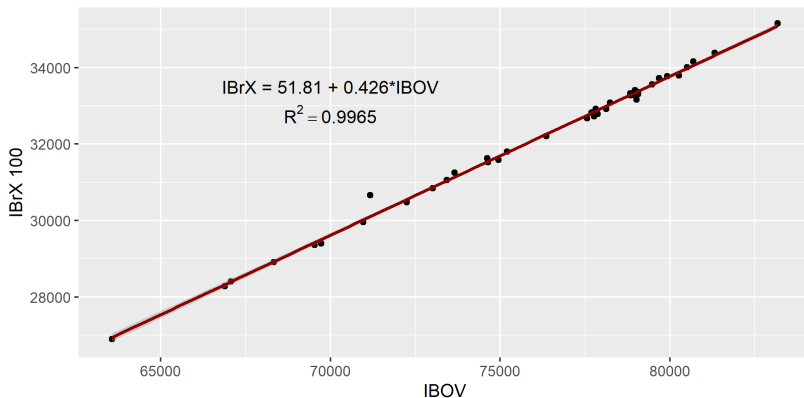
*Predict a result on a dependent variable based on one or more independent variables*

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

# Visualização de Regressão

## Correspondence of IBOV with IBrX 100

March - May 2020



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

- $\beta_1 = \mathbf{Slope}$  of the line
- $\beta_0 = \mathbf{Intercept}$  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”?

- 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

```
galton <- readRDS(here::here("galton.rds"))  
str(galton)
```

```
## 'data.frame':    898 obs. of  6 variables:  
## $ family: Factor w/ 197 levels "1","10","100",...: 1 1 1 1 108 108 108 108 123 1  
## $ father: num  78.5 78.5 78.5 78.5 75.5 75.5 75.5 75.5 75 75 ...  
## $ mother: num  67 67 67 67 66.5 66.5 66.5 66.5 64 64 ...  
## $ sex    : Factor w/ 2 levels "F","M": 2 1 1 1 2 2 1 1 2 1 ...  
## $ height: num  73.2 69.2 69 69 73.5 72.5 65.5 65.5 71 68 ...  
## $ nkids  : int   4 4 4 4 4 4 4 4 2 2 ...
```

- 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
```

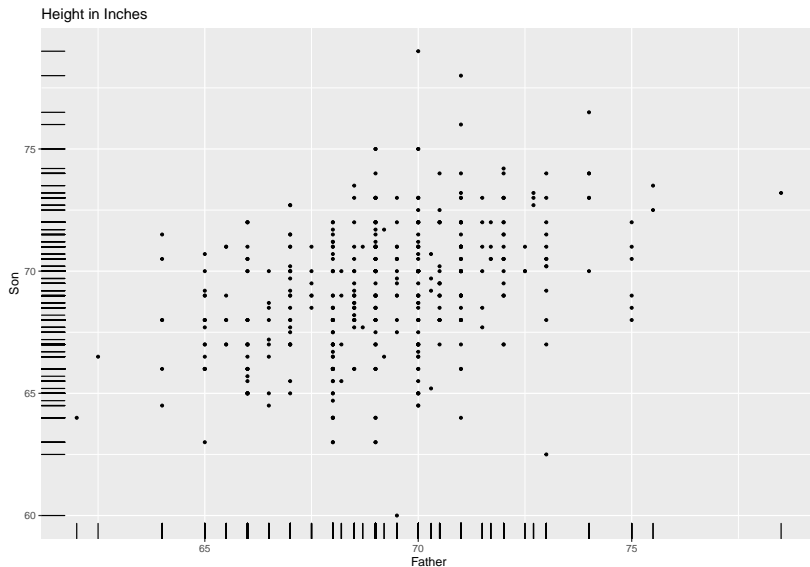
```
## Columns: 2
```

```
## $ father <dbl> 78.5, 75.5, 75.5, 75.0, 75.0, 75.0, 75.0, 75.0, 75.0, 74.0, ...
```

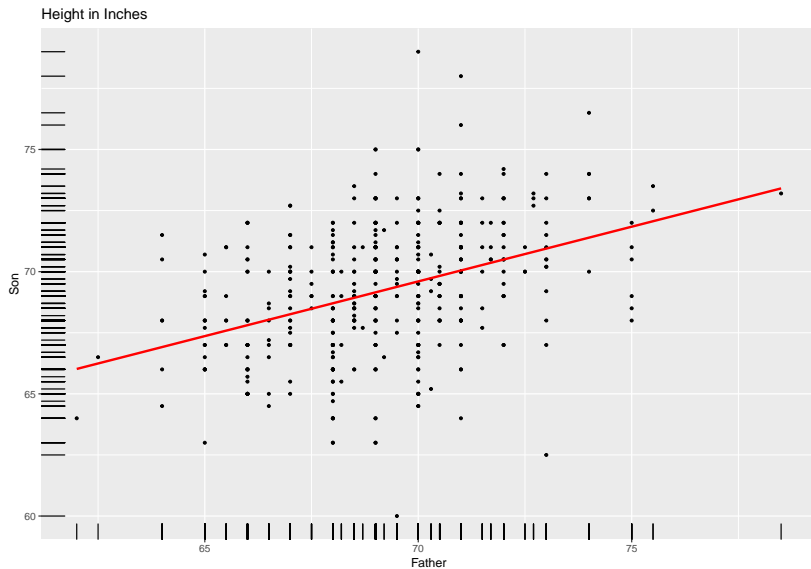
```
## $ height <dbl> 73.2, 73.5, 72.5, 71.0, 70.5, 68.5, 72.0, 69.0, 68.0, 76.5, ...
```

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

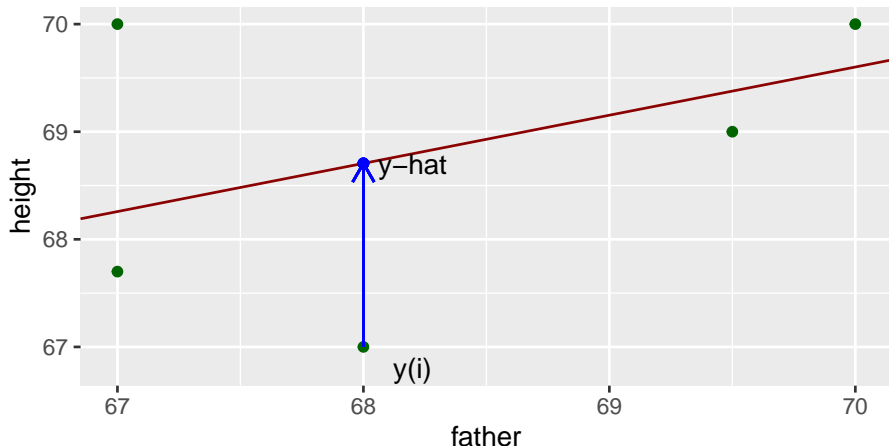
- **Seems** that taller the fathers, taller the sons
- Descriptive statistics of the 2 variables
  - ▶ And, correlation

```
## Descriptive Statistics
## boys
## N: 465
##
##           Mean   Std.Dev   Min      Q1   Median      Q3      Max      IQR      CV
## -----
##   father  69.17     2.30   62.00   68.00   69.00   70.50   78.50   2.50   0.03
##   height  69.23     2.63   60.00   67.50   69.20   71.00   79.00   3.50   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



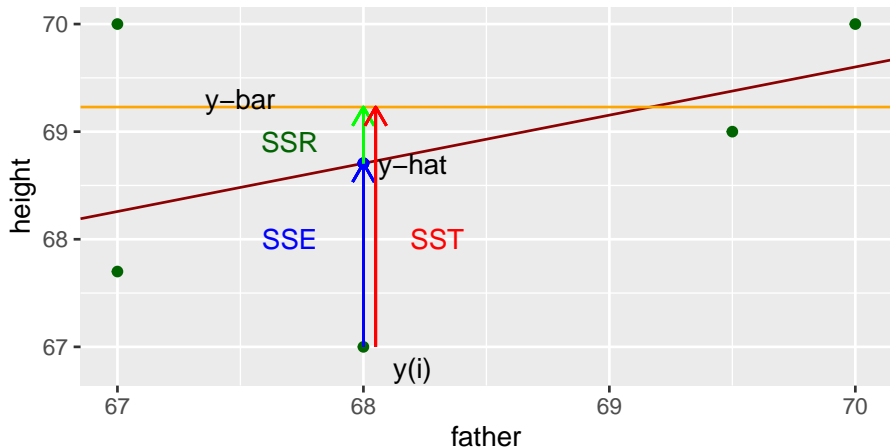
# SSE – A Component of Total Sum of Squares (SST)

$$SST = SSE + SSR$$

- 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
- Set the partial derivatives of the SSE with respect to  $\beta_0$  and  $\beta_1$

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

- 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 `lm` 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       1Q   Median       3Q      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 '**' 0.01 '*' 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
```

# 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
##   <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?

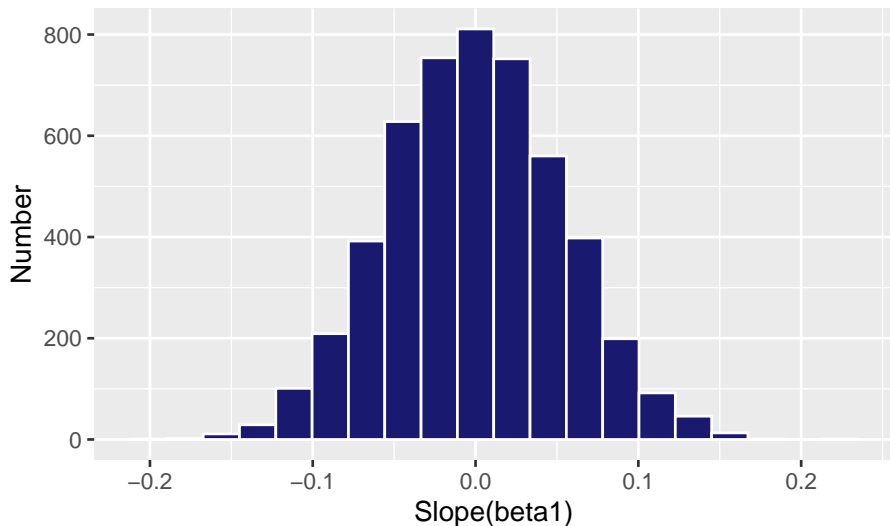
$$Y_i = \beta_0 + \epsilon_i$$

- X disappears
- 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
- As a result, we can focus on the values of the slope,  $\beta_1$
- 2nd, we will compare our observed value of  $\beta_1$  (`'r coef(fit1)[2]`) to see where it falls in the simulated values

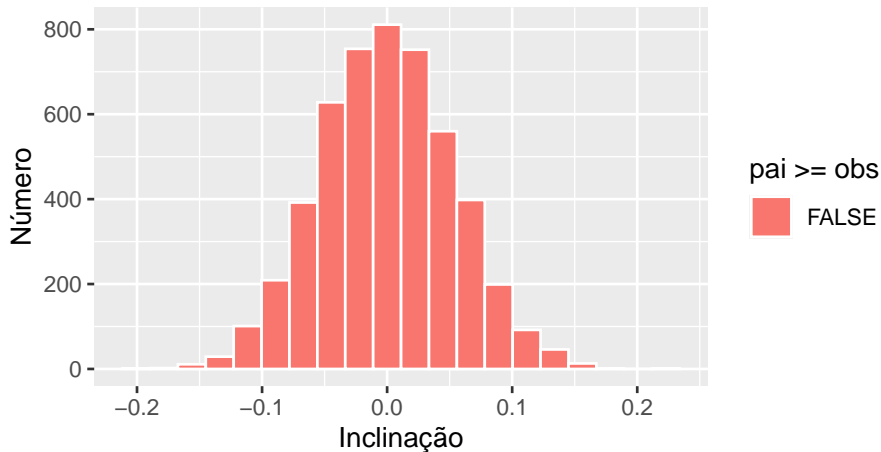
# Histogram of the Slopes of the Simulated Models





# Histogram with Values Above and Below Observed Slope

## Número de simulações com  $\text{beta1} \geq \text{obs}$ : 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

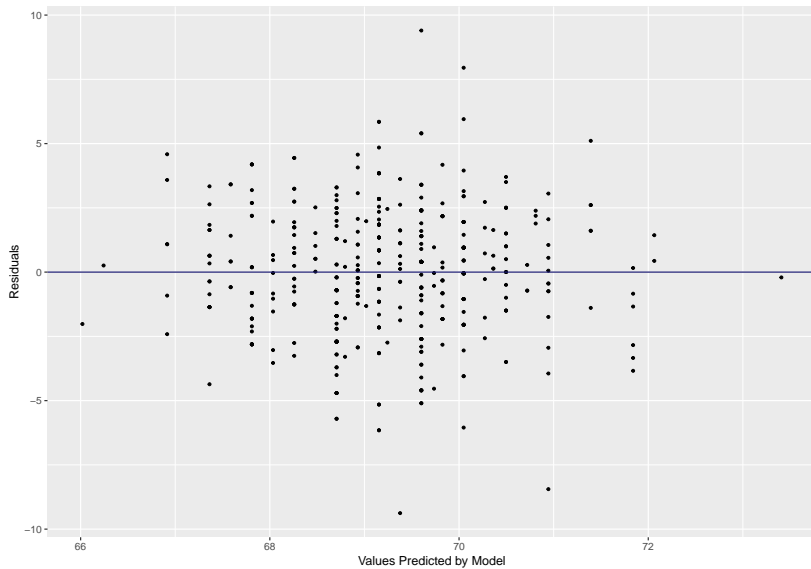
# Assumptions of Linear Regression

- ① 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
- ③ 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 multivariate normal distribution
- ④ 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

```
mods <- broom::augment(fit1)
residgr <- ggplot(data = mods, mapping = aes(x = .fitted, y = .resid))
residgr <- residgr + geom_point(shape = 20)
residgr <- residgr + geom_hline(yintercept = 0, color = "midnightblue")
residgr <- residgr + labs(x = "Values Predicted by Model",
                        y = "Residuals")
```



# Importance of Residuals

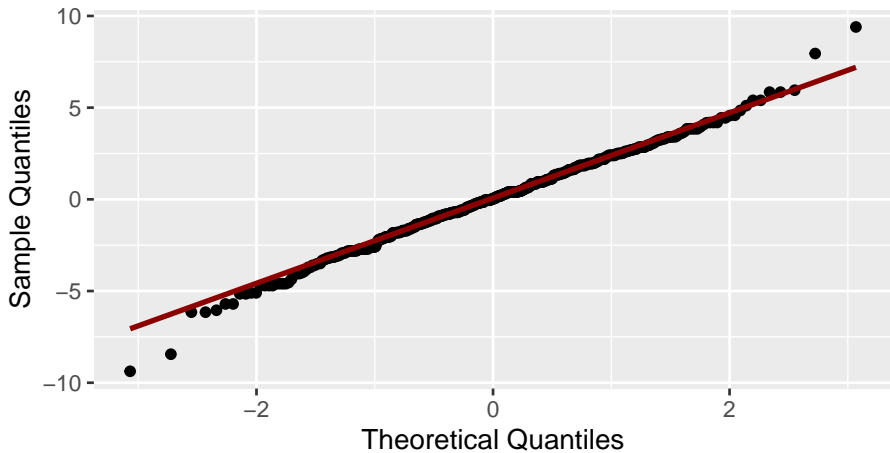
- Can use the residuals to verify if the model respects the assumptions of regression
- Should not show any linear trend

# Q-Q Graph

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

```
grqq <- ggplot(data = mods, aes(sample = .resid))  
grqq <- grqq + stat_qq()  
grqq <- grqq + stat_qq_line(color = "darkred", size = 1)  
grqq <- grqq + labs(x = "Theoretical Quantiles",  
                    y = "Sample Quantiles")
```

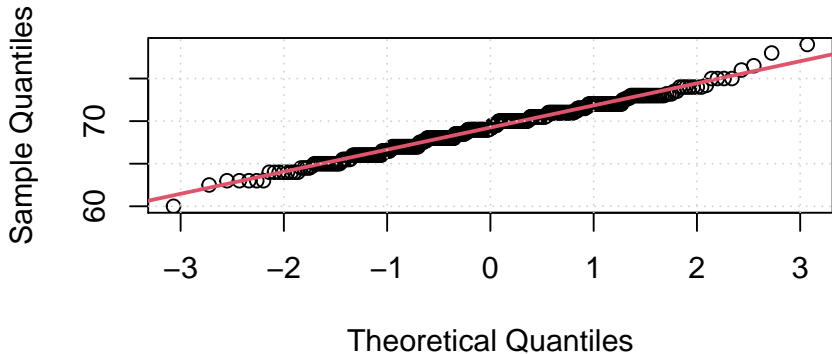




## Q-Q Graphs Also Directly Available in Base R

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

## Normal Q-Q Plot



# 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



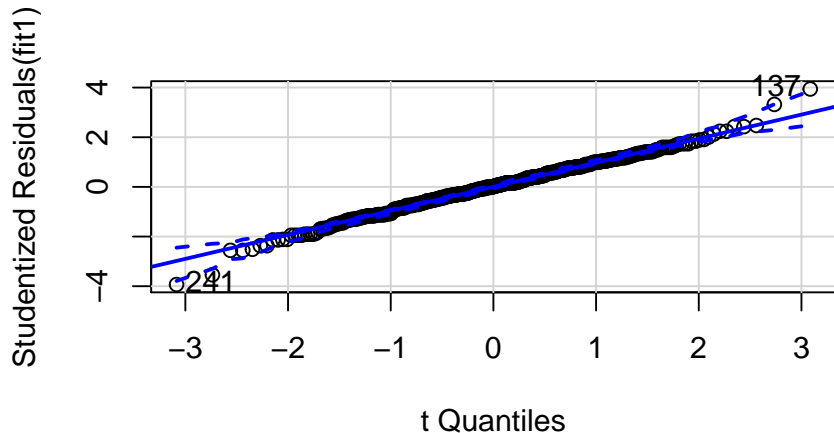
# Importance of $R^2$

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

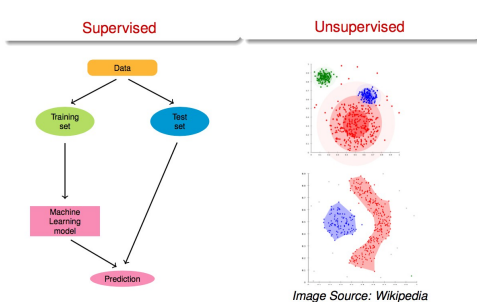
# Multiple Linear Regression - MLR

# 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

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \dots + \beta_k X_{ik} + \epsilon_i$$

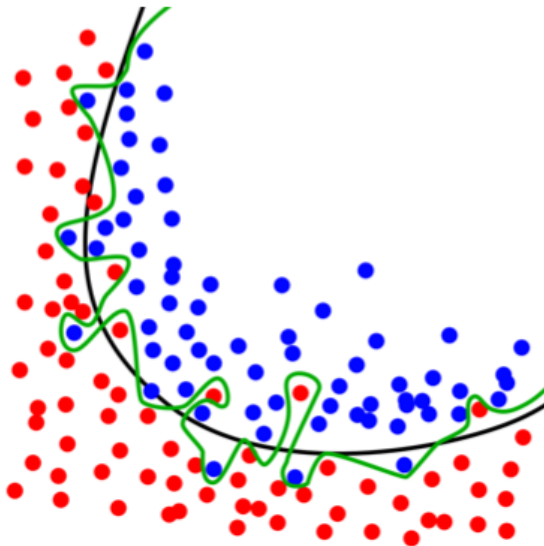
# Types of *Machine Learning*



# 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





- 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

- 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

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

```
glimpse(galton)
```

```
## Rows: 898
## Columns: 6
## $ family <fct> 1, 1, 1, 1, 2, 2, 2, 2, 3, 3, 4, 4, 4, 4, 4, 5, 5, 5, 5, 5, ...
## $ father <dbl> 78.5, 78.5, 78.5, 78.5, 75.5, 75.5, 75.5, 75.5, 75.0, 75.0, ...
## $ mother <dbl> 67.0, 67.0, 67.0, 67.0, 66.5, 66.5, 66.5, 66.5, 64.0, 64.0, ...
## $ sex    <fct> M, F, F, F, M, M, F, F, M, F, M, M, F, F, F, M, M, M, F, F, ...
## $ height <dbl> 73.2, 69.2, 69.0, 69.0, 73.5, 72.5, 65.5, 65.5, 71.0, 68.0, ...
## $ nkids  <int> 4, 4, 4, 4, 4, 4, 4, 4, 2, 2, 5, 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
```

- 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)
```

```
## [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 (-)

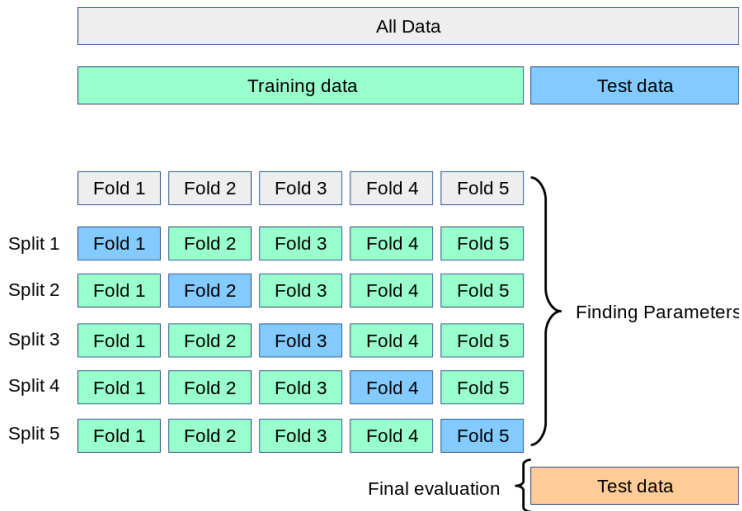
```
train_data <- galton[indice, ]  
test_data <- galton[-indice, ]
```

- 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](https://scikit-learn.org)

- 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

```
fit_pai_mae <- caret::train(height ~ father + mother,  
                             method = "lm",  
                             data = train_data,  
                             trControl = trainControl(method = "repeatedcv",  
                                                       number = 5,  
                                                       repeats = 10,  
                                                       savePredictions = "none",  
                                                       verboseIter = FALSE))
```

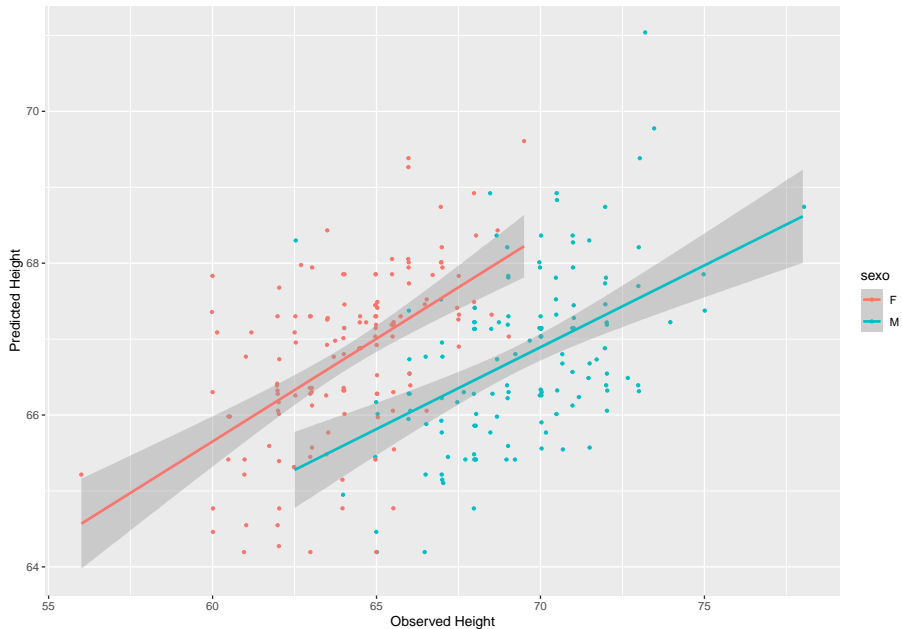
```
summary(fit_pai_mae)
```

```
##
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##      Min       1Q   Median       3Q      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 '**' 0.01 '*' 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

```
# previsões
prv <- predict(fit_pai_mae, test_data)
# comparar
gg_pai_mae_1 <- data.frame(obs = test_data$height,
                           previs = prv,
                           sexo = test_data$sex) %>%
  ggplot(aes(x = obs, y = previs, color = sexo)) +
  geom_jitter(shape = 20) +
  geom_smooth(method = "lm") +
  labs(x = "Observed Height", y = "Predicted Height")
```



# 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)

```
pred <- predict(fit_pai_mae, test_data)
res <- tibble(pred = pred,
              obs = test_data$height,
              dif = obs - pred)

padrao_in <- 2
# teste de bom, ruim
res <- res %>%
  mutate(bomruim = ifelse(abs(dif) <= padrao_in, "bom", "ruim"))
tabyl(res$bomruim) %>% adorn_pct_formatting()
```

```
## 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)
  - ▶ 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),
                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       1Q   Median       3Q      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 '**' 0.01 '*' 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

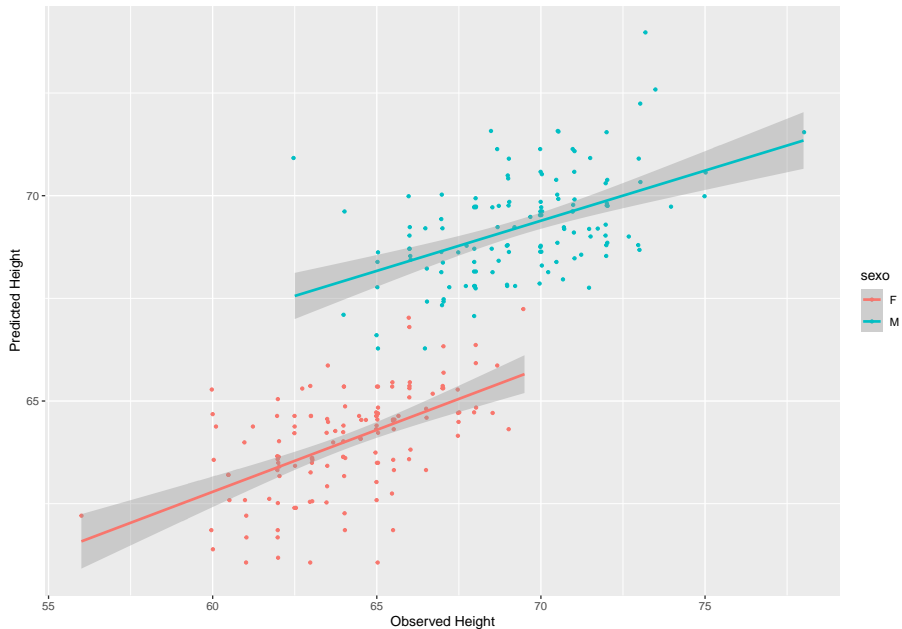
```
fit_pms <- caret::train(height ~ father + mother + sex,  
  method = "lm",  
  data = train_data,  
  trControl = trainControl(method = "repeatedcv",  
    number = 5,  
    repeats = 10,  
    savePredictions = "none",  
    verboseIter = FALSE))
```

```
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|)
## (Intercept) 15.05115     3.29308   4.571 0.00000586 ***
## 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 '**' 0.01 '*' 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

```
# previsões
prv <- predict(fit_pms, test_data)
# comparar
gg_pms_1 <- data.frame(obs = test_data$height,
                        previs = prv,
                        sexo = test_data$sex) %>%
  ggplot(aes(x = obs, y = previs, color = sexo)) +
  geom_jitter(shape = 20) +
  geom_smooth(method = "lm") +
  labs(x = "Observed Height", y = "Predicted Height")
```





# How Accurate Was the Model?

```
pred <- predict(fit_pms, test_data)
res_pms <- tibble(pred = pred,
                  obs = test_data$height,
                  dif = obs - pred)

padrao_in <- 2
# teste de bom, ruim
res_pms <- res_pms %>%
  mutate(bomruim = ifelse(abs(dif) <= padrao_in, "bom", "ruim"))
tabyl(res_pms$bomruim) %>% adorn_pct_formatting()
```

```
## res_pms$bomruim    n percent
##                bom 183    68.5%
##                ruim  84    31.5%
```

- Model predicts 69% of the heights within the standard we set
  - ▶ Double the previous model
- $R^2$  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

```
varImp(fit_pms)
```

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

## 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.*

- 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

```
gm <- gapminder::gapminder %>%  
  janitor::clean_names()  
glimpse(gm)
```

```
## Rows: 1,704  
## Columns: 6  
## $ country    <fct> Afghanistan, Afghanistan, Afghanistan, Afghanistan, Afgh...  
## $ continent  <fct> Asia, Asia, Asia, Asia, Asia, Asia, Asia, Asia, Asia, Asia, As...  
## $ year       <int> 1952, 1957, 1962, 1967, 1972, 1977, 1982, 1987, 1992, 19...  
## $ life_exp   <dbl> 28.801, 30.332, 31.997, 34.020, 36.088, 38.438, 39.854, ...  
## $ pop        <int> 8425333, 9240934, 10267083, 11537966, 13079460, 14880372...  
## $ gdp_percap <dbl> 779.4453, 820.8530, 853.1007, 836.1971, 739.9811, 786.11...
```

# Descriptive Statistics

```
gm %>%  
  select(year, pop, gdp_percap) %>%  
  mutate(pop = log10(pop)) %>%  
  descr(stats = c("mean", "sd", "min", "q1", "med", "q3", "max", "iqr", "cv"),  
         transpose = TRUE)
```

```
## Descriptive Statistics
```

```
## gm
```

```
## N: 1704
```

```
##
```

	Mean	Std.Dev	Min	Q1	Median	Q3	Max	IQR	CV
gdp_percap	7215.33	9857.45	241.17	1201.92	3531.85	9325.86	113523.13	8123.40	1.37
pop	6.85	0.70	4.78	6.45	6.85	7.29	9.12	0.85	0.10
year	1979.50	17.27	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)))
```

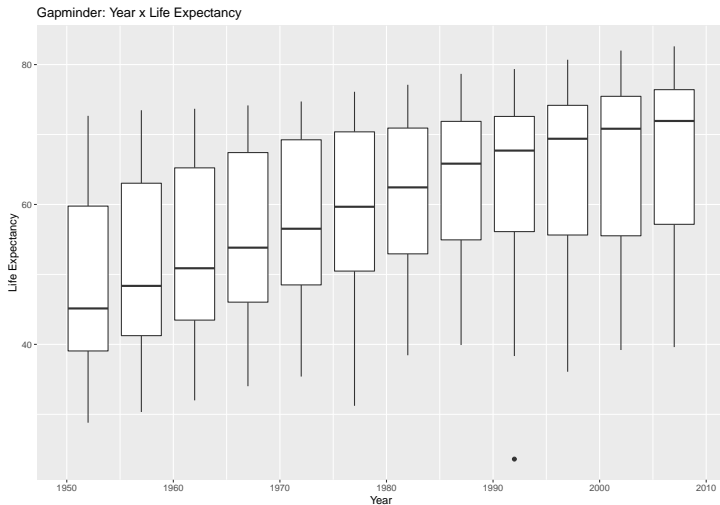
```
## [1] "Correlation Coefficient (life x gdp): 0.584"
```

```
paste("Correlation Coefficient (gdp x life):", with(gm, round(cor(gdp_percap, year), 3)))
```

```
## [1] "Correlation Coefficient (gdp x life): 0.227"
```

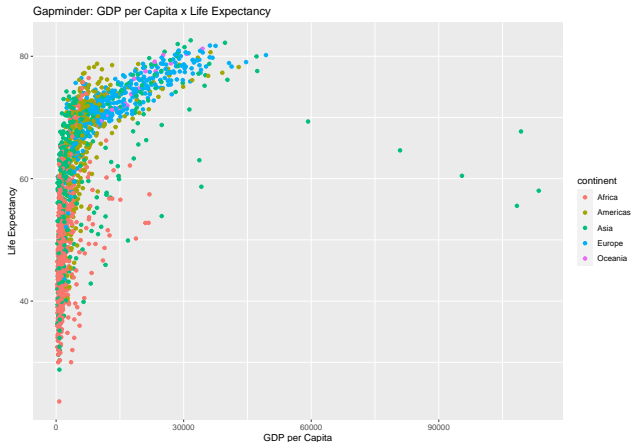
# Boxplot of life\_exp against year

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



# Scatterplot of life\_exp against gdp\_percap

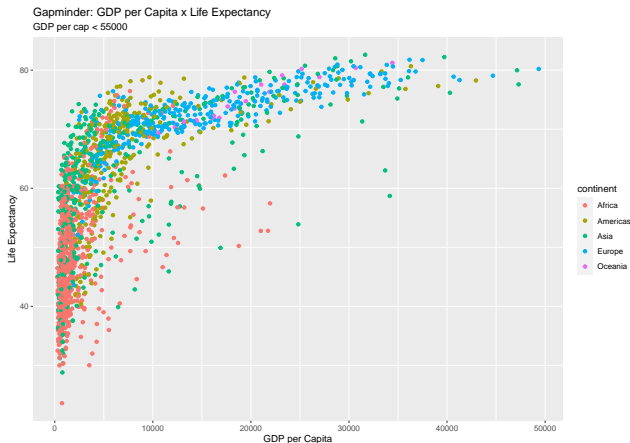
```
ggplot(gm, aes(x = gdp_percap, y = life_exp, color = continent)) +  
  geom_point() +  
  labs(title = "Gapminder: GDP per Capita x Life Expectancy", x = "GDP per Capita", y = "Life Expectancy")
```



# 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

```
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, ]
gm_test <- gm[-index, ]
```

# 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

```
fit_gm_1 <- caret::train(life_exp ~ year + gdp_percap,  
  method = "lm",  
  data = gm_train,  
  trControl = trainControl(method = "repeatedcv",  
    number = 10,  
    repeats = 10,  
    savePredictions = "none",  
    verboseIter = FALSE))
```

```
summary(fit_gm_1)
```

```
##
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##      Min       1Q   Median       3Q      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         0.25233666     0.01663001    15.17  <2e-16 ***
## gdp_percap   0.00066984     0.00002919    22.94  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 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
```

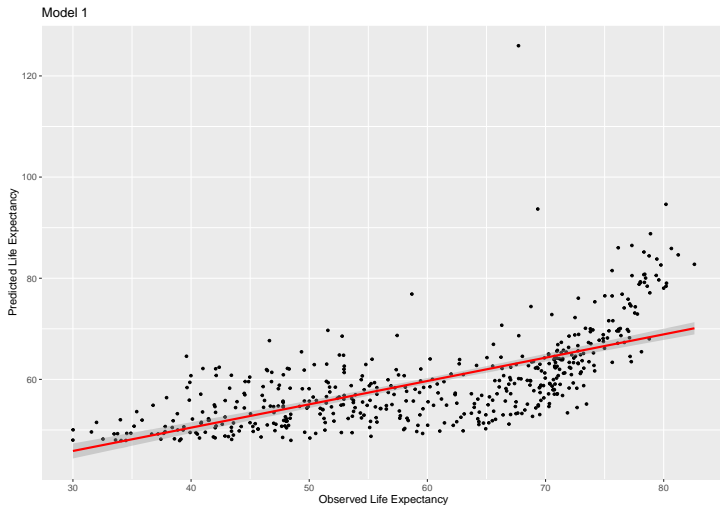
# How Did the Model Do?

- Applying model to test data

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

```
## predictions
pred_1 <- predict(fit_gm_1, gm_test)
## compare
gm_pred_1 <- data.frame(obs = gm_test$life_exp,
                        preds = pred_1)
gm_1_plot <- ggplot(gm_pred_1, aes(x = obs, y = preds)) +
  geom_jitter(shape = 20) +
  geom_smooth(method = "lm", color = "red") +
  labs(title = "Model 1", x = "Observed Life Expectancy", y = "Predicted Life Expectancy")
```

## gm\_1\_plot



# Accuracy of Model 1

- Set an accuracy standard
  - ▶ Predicted value 2 years  $\pm$  observed life expectancy

```
# calculate difference between predicted and observed
gm_pred_1 <- gm_pred_1 %>%
  mutate(dif = obs - preds,
         goodbad = ifelse(abs(dif) <= 2), "good", "bad"))
tabyl(gm_pred_1$goodbad) %>% adorn_pct_formatting()
```

```
## 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

```
fit_gm_2 <- caret::train(life_exp ~ year + gdp_percap + continent,  
  method = "lm",  
  data = gm_train,  
  trControl = trainControl(method = "repeatedcv",  
    number = 10,  
    repeats = 10,  
    savePredictions = "none",  
    verboseIter = FALSE))
```

```
summary(fit_gm_2)
```

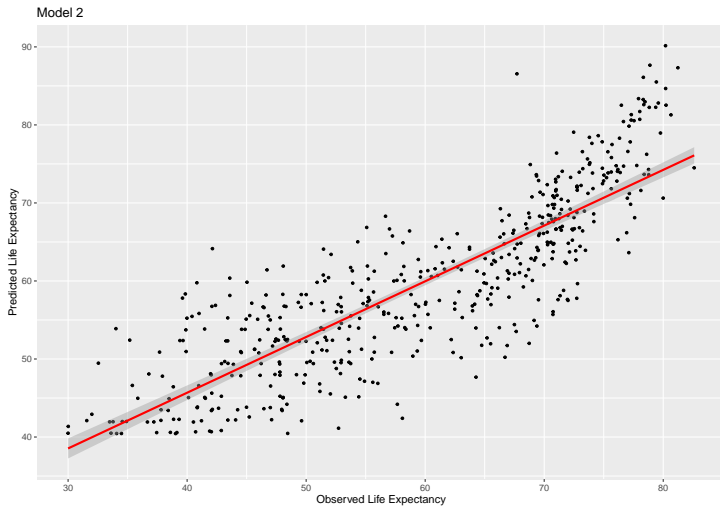
```
##
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -28.7132  -4.1337   0.0507   4.4951  19.7608
##
## Coefficients:
##              Estimate      Std. Error t value Pr(>|t|)
## (Intercept)   -533.19986541    23.47738883  -22.71  <2e-16 ***
## year           0.29382541     0.01186453   24.77  <2e-16 ***
## gdp_percap     0.00028746     0.00002394   12.01  <2e-16 ***
## 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 '**' 0.01 '*' 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)?

```
## predictions
pred_2 <- predict(fit_gm_2, gm_test)
## compare
gm_pred_2 <- data.frame(obs = gm_test$life_exp,
                        preds = pred_2)
gm_2_plot <- ggplot(gm_pred_2, aes(x = obs, y = preds)) +
  geom_jitter(shape = 20) +
  geom_smooth(method = "lm", color = "red")+
  labs(title = "Model 2", x = "Observed Life Expectancy", y = "Predicted Life Expectancy")
```

## gm\_2\_plot



# Accuracy of Model 2

- Set an accuracy standard
  - ▶ Predicted value 2 years  $\pm$  observed life expectancy

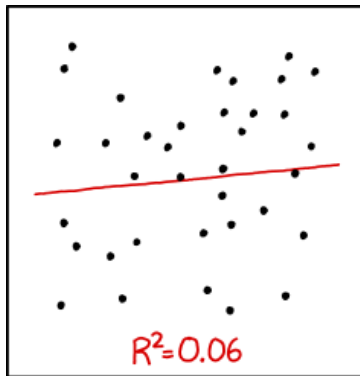
```
# calculate difference between predicted and observed
gm_pred_2 <- gm_pred_2 %>%
  mutate(dif = obs - preds,
         goodbad = ifelse(abs(dif) <= 2), "good", "bad"))
tabyl(gm_pred_2$goodbad) %>% adorn_pct_formatting()
```

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

# Conclusion of This Model

- Better  $R^2$
- 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.

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



Today    Weekly edition     Menu

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## Forecasting the US elections

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## 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