### Class 5: Classification

BUS 696

Prof. Jonathan Hersh

### Class 5: Announcements

Will post Problem Set 2 tomorrow,
 Due Oct 9

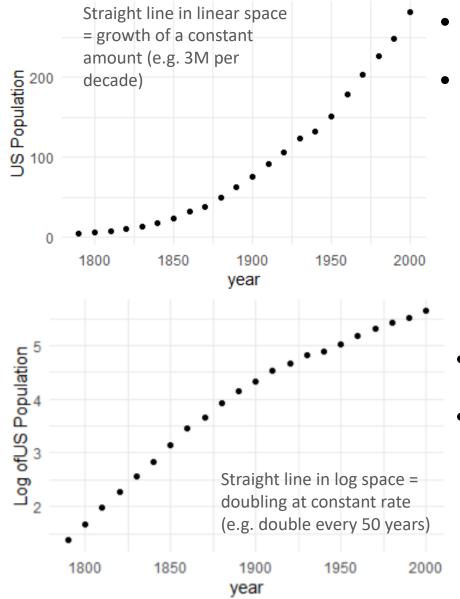
- 2. Office Hours
  - 1. TA: Wed: 12-1, Th 5-6
  - 2. Instructor: M: 4-5, W 5-6
- 3. Post October 5<sup>th</sup> In Person

### Class 5: Outline

- Log Transformations and Interpreting log-log Regressions
- 2. Model Evaluation
  - Testing and Training Sets, RMSE, and R-Squared
- 3. Why not regression for classification?
- 4. Logistic Function
- 5. Log Odds Ratio
- 6. Estimating Logistic Regressions in R
- 7. Classification Lab 1

- 8. False/True Positives False/True Negatives
- 9. Confusion Matrices
- 10. ROC Curves and AUC
- 11. Classification Lab 2

### Log Transformations



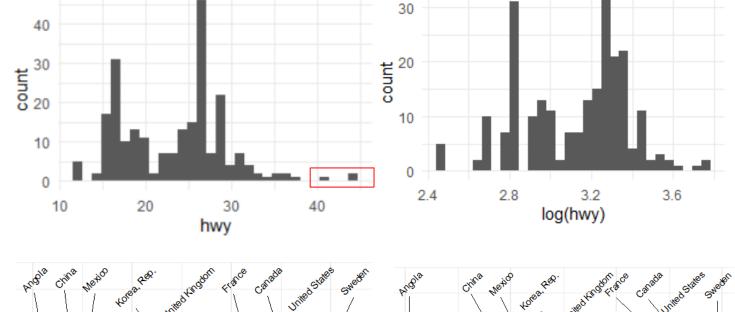
- Recall that log is the inverse of exponentiation
- Logging a number answers the question "what is the exponent I must raise the base of the log to produce this number"

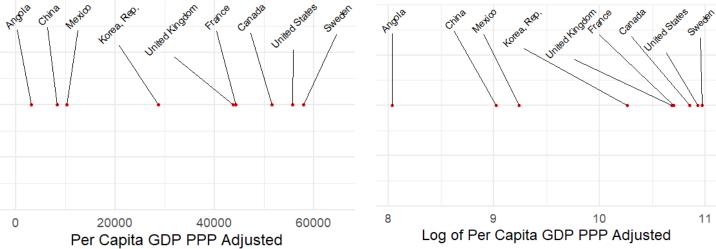
• 
$$\log_{10} 100 = 2 \rightarrow 10^2 = 100$$

• 
$$\log_{10} 1000 = 3 \rightarrow 10^3 = 1000$$

- The natural log is  $\log_e x = \ln(x)$  where e=2.718...
- Each unit increase of ln(x) = a doubling of x
  - This is a useful data transformation because we often want to incorporate data that increases rapidly in our regression analysis

### Why Log Transformations For Regression Data





- Log transforming our data is often very useful if our data is particularly "spread out"
- In particular if there are outlier values this will improve model performance
- Some data like income should usually be logged

Model accuracy often improves when logging dependent variable but interpretation can suffer

### Log-Log Regression Model Coefficients = Elasticities!

```
\log(hwy_i) = \beta_0 + \beta_1 \log(displ_i) + \beta_2 year_i + \epsilon_i
```

```
mod1 <- lm(log(hwy) ~ log(displ) + year,
           data = mpq)
  summary(mod1)
Call:
lm(formula = log(hwy) ~ log(displ) + year, data = mpg)
Residuals:
    Min
              1Q Median
-0.46033 -0.09856 -0.00202 0.08837 0.48681
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -10.874596 4.551216
log(displ) -0.560514 0.027052 -20.720 < 2e-16
             0.007314 0.002274
                                 3.217 0.00148 **
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' '1
Residual standard error: 0.1547 on 231 degrees of freedom
Multiple R-squared: 0.6502, Adjusted R-squared: 0.6471
F-statistic: 214.7 on 2 and 231 DF, p-value: < 2.2e-16.
```

- Suppose we log our hwy regression model
- How do we now interpret the coefficient  $eta_{\log(displ)}$ 
  - $y = \exp(\beta_0 + \beta_1 \log(x) + \epsilon)$
  - $\frac{dy}{dx} = \frac{\beta_1}{x} \exp(\beta_0 + \beta_1 \log(x) + \epsilon)$
  - $\bullet \quad \Rightarrow \beta_1 = \frac{dy/y}{dx/x}$

Therefore log coefficients can be interpreted as elasticities!

A 1% change in x-variable results in a  $\beta_1$  % change in the outcome variable

Here a 1% increase in displacement -> a
 0.56% decrease in highway mpg.

### Class 9: Outline

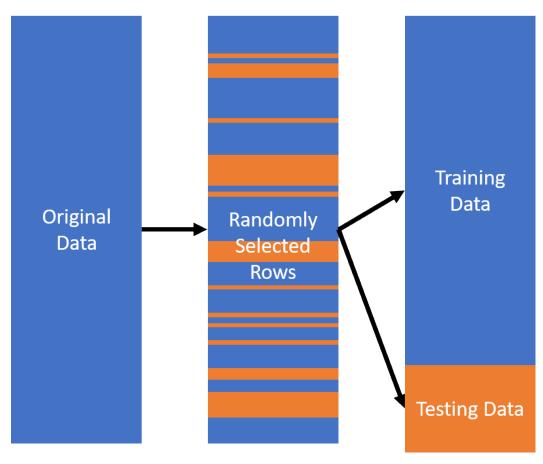
 Log Transformations and Interpreting log-log Regressions 6. Log Odds Ratio

#### 2. Model Evaluation

- Testing and Training Sets, RMSE, and R-Squared
- 3. Lab Class 9
- 4. Why Classification Models?
- 5. Logistic Function

### Recall: Training and Testing Sets

#### **Splitting Data for Machine Learning**



**Training set:** (observation-wise) subset of data used to develop models

**Test set:** subset of data used to evaluate final model performance

### Building Training and Testing Sets in R

```
> mpg_train <- training(mpg_split)
> mpg_test <- testing(mpg_split)
> # check the number of rows to ensure training
> # and testing split is correct
> nrow(mpg_train)
[1] 188
> nrow(mpg_test)
[1] 46
> |
```

- initial\_split() is a helper function to create testing and training sets
- Must specify the data frame to split
- Can also specify the % of data to use
   for training (defaults to 75%)
- The functions training() and testing()
  will create separate testing and
  training sets from the original data
  set

Always set seed before any randomize procedure to ensure code is reproducible

## Generating In-Sample (Training) and Out-of-Sample (Test) Predictions

- Estimate a model on the training set
- Never estimate a model using the test set
- In-sample predictions are the predicts using data in the training set
- Out-of-sample predictions are the predicts using data in the test set

### Quantitative Model Evaluation Using Yardstick

- The package 'yardstick' has several functions to quantitatively evaluate model performance
- We must first compile our model output in a 'results' data frame
- We include the predictions from the model
- True outcome values must exclude any missing values for Xs or Ys
- We must also do this for the test data set

```
library('yardstick')

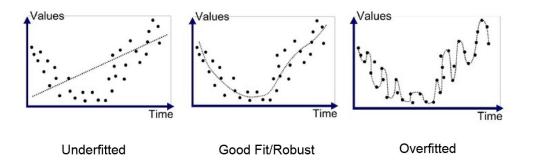
# create a

results_train <- data.frame(
   predicted = preds_train,
   actual = mpg_train %>%
   filter(complete.cases(hwy, year, displ)) %>%
   select(hwy),
   type = rep("train", length(preds_train))
) %>%
   rename(`predicted` = 1, `actual` = 2, `type` = 3)
```

```
results_test <- data.frame(
  predicted = preds_test,
  actual = mpg_test %>%
    filter(complete.cases(hwy, year, displ)) %>%
    select(hwy),
  type = rep("test", length(preds_test))
) %>%
  rename(`predicted` = 1, `actual` = 2, `type` = 3)
```

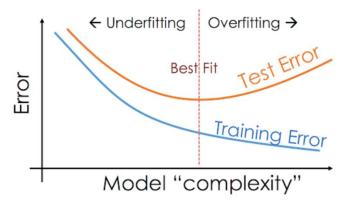
### Overfit Vs Underfit: Compare the Test and Training Error

- rmse() function computes root mean squared error (i.e. MSE<sup>(1/2)</sup>)
- Pass the data frame of results
- Also the column names (in the results DF) for the predicted and true values
- We compare across models by examining the same error metric
- Since the error in the test set is lower than error in the training set we conclude the model is underfit, meaning we can increase model complexity



### Other Functions for Evaluation: metrics() and mae()

```
> metrics(results_train, predicted, actual)
# A tibble: 3 x 3
  .metric .estimator .estimate
  <chr>
          <chr>
                           \langle db 1 \rangle
          standard
                           4.03
  rmse
          standard
                           0.563
2 rsq
          standard
                           2.93
  mae
> metrics(results_test, predicted, actual)
 A tibble: 3 x 3
  .metric .estimator .estimate
  <chr>
          <chr>
                           \langle db 1 \rangle
          standard
                           2.34
  rmse
                           0.820
          standard
  rsq
          standard
                           1.83
  mae
```



- metrics() function estimates a series of evaluation metrics
- mae is "mean absolute error"

$$MAE = \frac{1}{N} \sum_{i=1}^{N} |y_i - \hat{y}_i|$$

rsq is our friend R^2

$$R^{2} = 1 - \frac{\sum_{i} (y_{i} - \hat{y}_{i})^{2}}{\sum_{i} (y_{i} - \bar{y}_{i})^{2}}$$

$$= 1 - \frac{sum \ of \ squared \ residuals}{sum \ of \ total \ squares}$$

All tell the same story: model is underfit

### Lab Time!

```
lab_class_9_linear_regression_3_and_Cla...
                                 * - I
                                                                               Run 54
← ⇒ | I Source on Save | □
                                                                                           → Source →
                                                           Replace All
■ In selection ■ Match case ■ Whole word ■ Regex ✔ Wrap
 100
 101 - #-
 103 - #-
 104
 107
 108
 109
 110
 113
 116
 117
 118
 119
      library('tidyverse')
      library('forcats')
     set.seed(1818)
 123 movies <- read.csv(here::here("datasets", "IMDB_movies.csv"))
```

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- 6. Log Odds Ratio

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### Classification examples

cour criteria for acceptance.



### Credit Card Default Dataset

Default {ISLR}

R Documentation

#### Credit Card Default Data

#### **Description**

A simulated data set containing information on ten thousand customers. The aim here is to predict which customers will default on their credit card debt.

#### Usage

Default

#### **Format**

A data frame with 10000 observations on the following 4 variables.

default

A factor with levels No and Yes indicating whether the customer defaulted on their debt

student

A factor with levels No and Yes indicating whether the customer is a student

balance

The average balance that the customer has remaining on their credit card after making their monthly payment

income

Income of customer

#### **Source**

Simulated data

### Why not regression?

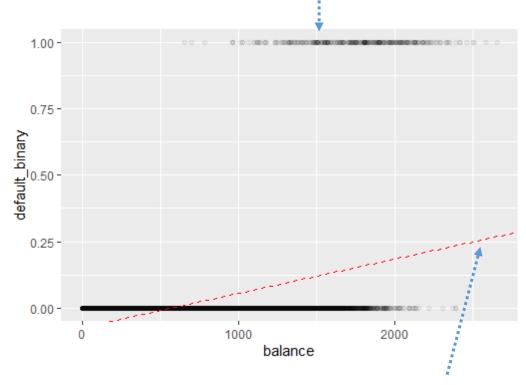
```
library(ISLR)
data(Default)
options(scipen = 3)
library(magrittr)
library(tidyverse)
library(ggExtra)
# create a binary version of default
Default %<>% mutate(default_binary =
                       ifelse(default == "Yes", 1,0))
summary(Default)
  variable as our dependent variable
mod1 <- lm(default_binary ~ balance,</pre>
            data = Default)
summary(mod1)
```

```
summary(mod1)
Call:
lm(formula = default_binary ~ balance, data = Default)
Residuals:
    Min
              10 Median
                                        Max
-0.23533 -0.06939 -0.02628 0.02004 0.99046
Coefficients:
               Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.075191959 0.003354360 -22.42
                                               <2e-16 ***
            0.000129872 0.000003475
                                       37.37
                                               <2e-16 ***
balance
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 0.1681 on 9998 degrees of freedom
Multiple R-squared: 0.1226,
                               Adjusted R-squared: 0.1225
F-statistic: 1397 on 1 and 9998 DF, p-value: < 2.2e-16
```

- Let's estimate a model predicting default based on credit card balance
- R2 looks low but otherwise this model looks perfectly fine

### Linear Model to Predict Default

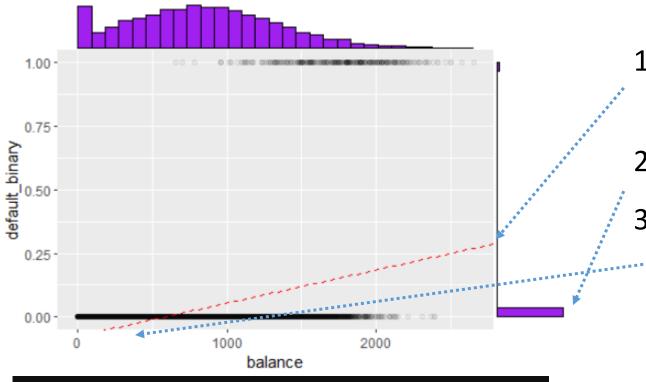
 Let's use the model to generate predictions of default (which is binary) Black dots show actual default behavior



Red line shows the predictions from the model

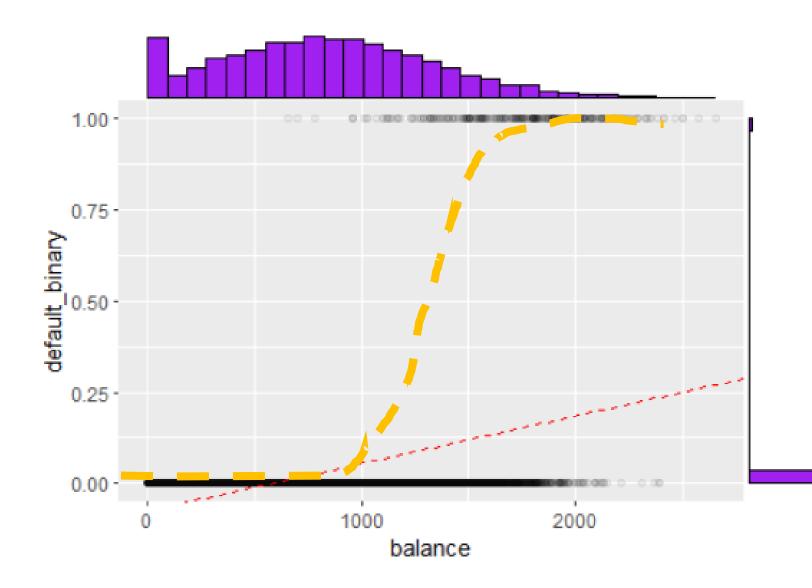
Why is the red line a bad prediction model for default?

### Why Is This a Bad Prediction Model?



- 1. We never predict more than 30% chance of default!
- 2. Most observations do not default!
  - We predict negative probability of default!

### One Way to Improve the Earlier Model: Squash Predictions



- Because probabilities are between 0 and 1 we want to compress red line to lie within 0 and 1 on the y axis
- i.e let p(X) = Pr(Y = 1|X)be the probability the event occurs
- We want our model to output:

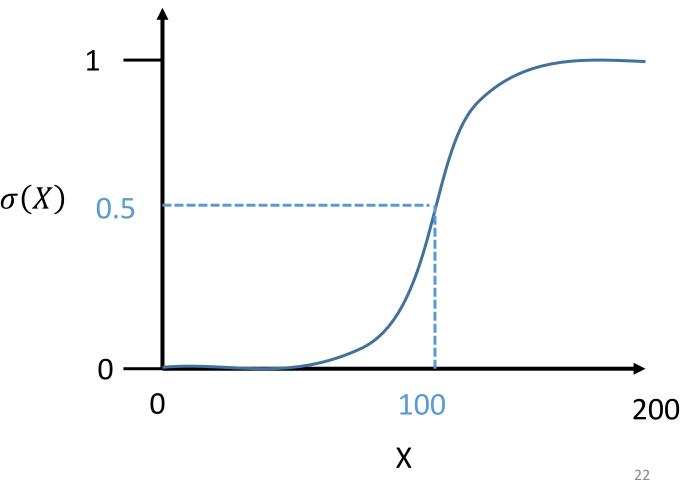
$$Pr(Y = 1|X) \in [0,1]$$

### What is The Logistic/Sigmoid Function

 Logisitic is a function that naturally takes inputs X and transforms between 0 and 1

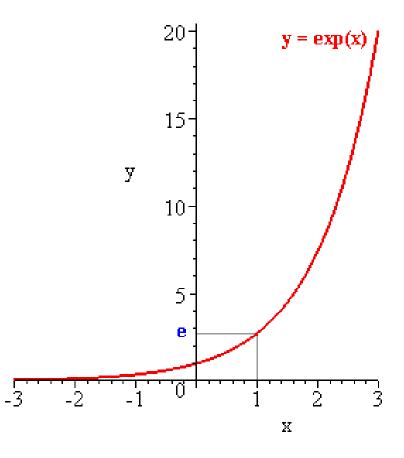
The logisitic is defined as

$$\sigma(X) = \frac{1}{1 + e^{-X}} = \frac{e^X}{e^X + 1}$$



### A note on $e^X = \exp(X)$

- Super spooky mathematical function
- $e = 2.718281828459045 \dots$
- $\frac{d}{dx}e^{X} = e^{X}$  and  $e^{0} = 1$
- e.g. rate of increase in function at
   X is equal to the function at X
   Many other ways to characterize function



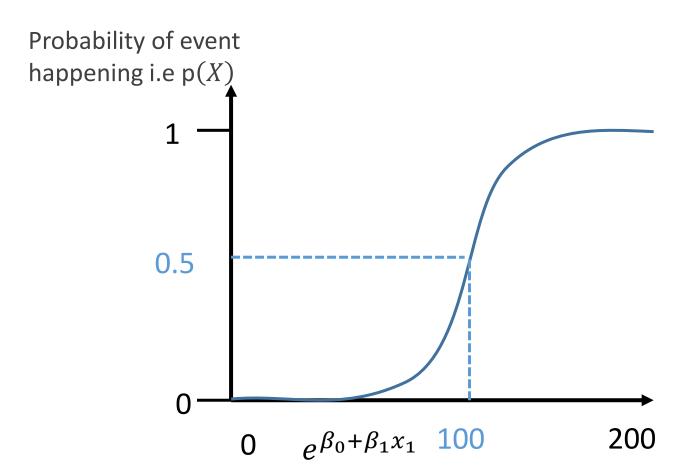
### Using the Logistic/Sigmoid Function to Generate Probabilities

- How do we generate probabilities from this function?
- We let  $X = \beta_0 + \beta_1 \cdot x_1 + \dots + \beta_k \cdot x_k$ and plug this into the logistic function

$$\sigma(X) = \frac{1}{1 + e^{-X}} = \frac{e^X}{e^X + 1}$$

$$Pr(Y = 1|X) = \frac{e^{\beta_0 + \beta_1 \cdot x_1}}{e^{\beta_0 + \beta_1 \cdot X} + 1}$$

$$Pr(Y = 1|X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x_1)}}$$



This is equivalent mathematically! I promise. Work it out on pen and paper if you don't believe me

### What is the "Odds Ratio"



- The outcome variable in a logit regression is the "odds ratio" (OR)
- In a deck of 52 cards there are 13 spades
- The probability of randomly drawing a spade is
   13/52 = 25%
- The probability of not drawing a spade is 39/52 = 75%
- Therefore the ratio of odds of drawing a spade vs not drawing a spade is

$$\frac{ratio\ of\ drawing\ a\ spade}{ratio\ of\ not\ drawing\ a\ spade} = \frac{13}{52} = \frac{13}{39/52} = \frac{13}{39} = 1:3 = 0.333$$

Log odds ratio is just log(0.333) = -0.4771...

### Logit Models Model the Outcome As a Log Odds Ratio

$$\frac{p(Y=1|X)}{p(Y=0|X)} = e^{\beta_0 + \beta_1 X}$$

$$log\left(\frac{p(Y=1|X)}{p(Y=0|X)}\right) = log(e^{\beta_0 + \beta_1 X})$$

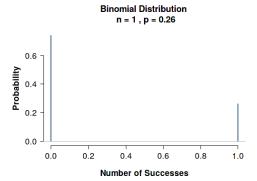
$$log\left(\frac{p(Y=1|X)}{p(Y=0|X)}\right) = \beta_0 + \beta_1 X$$

The outcome variable (Y) for a logistic regression is the log odds ratio

Log odds ratio is a linear expression of constants and coefficients of a nonlinear process!

All logistic coefficients can be interpreted as impact on log odds ratio

### Estimating Logit Models Using glm()



- Estimate logistic regression using the function glm() in R
- We still specify a formula in the usual manner
- glm() estimate a variety of "generalized linear models"
- To specific logit we must use the option "family = binomial"
- Binomial is a binary distribution aka the "link" function

### Estimating Impact of Being a Student on Default Probability using glm()

$$log\left(\frac{p(Y = default|X)}{p(Y = not \ default|X)}\right) = \beta_0 + \beta_1 \cdot student_i + \epsilon_i$$

$$\exp\left(\log\left(\frac{p(Y = default|X)}{p(Y = not \ default|X)}\right)\right) = \exp(\beta_0 + \beta_1 \cdot student_i + \epsilon_i)$$

$$\frac{p(Y = default|X)}{p(Y = not \ default|X)} = \exp(\beta_0 + \beta_1 \cdot student_i + \epsilon_i)$$

```
> exp(logit_fit1$coefficients)
(Intercept) studentYes
  0.03007299 1.49913321
```

- Remember the outcome variable in a logistic regression is the log odds ratio
- If we exponentiate the coefficients this tells us the impact of the variable on the unlogged odds ratio
- If we take our estimated logistic model we see  $\beta_1 = 0.40489$
- This means students have a 0.40489 higher log odd of defaulting
- Exponentiating the coefficients returns
  the impact of the X-variable on the odds
  ratio directly.
- Therefore the ratio of odds of default for student vs non-student is 1.49, or students have a 49% higher probability of default

### Lab Time!

```
#______# Lab 1
#_______# 1. Estimate a logistic regression model predicting
# default as a function of student, balance, and income
# and store this as 'logit_mod2'
# 2. Exponentiate the coefficient vector of logit_mod2
# 3. Interpret the impact of being a student on the probabiliy of default
# 4. Do students face a higher or lower risk of credit card default?
```

### Generating Predicted Probabilities from a Logit Model

 To generate predictions, we use the estimated coefficients in the logit equation

$$\hat{p}(X = 1000) = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 x_1}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 x_1}} =$$

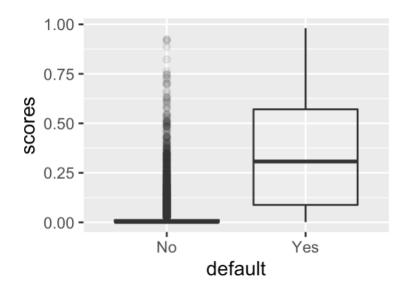
- The estimated probability of default with a balance of \$1,000 is given by
- The estimated probability of default with a balance of \$2,000 is given by
- To generate predicted probability for all observations in a dataset we use the predict function, but note type = "response"!
- This is also called "scoring" a dataset

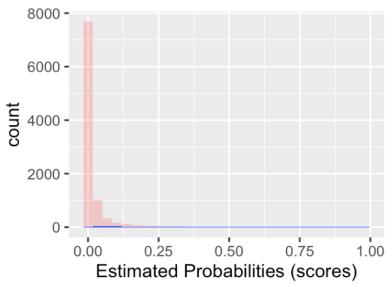
$$\hat{p}(X = 1000) = \frac{e^{-10.6513 + 0.0055 \cdot 1000}}{1 + e^{-10.6513 + 0.0055 \cdot 1000}} = 0.00575$$

$$\hat{p}(X = 2000) = \frac{e^{-10.6513 + 0.0055 \cdot 2000}}{1 + e^{-10.6513 + 0.0055 \cdot 2000}} = 0.05857$$

```
scores <- predict(logit_fit3,
type = "response")
```

#### What Do We Do With Scores or Estimated Probabilities?

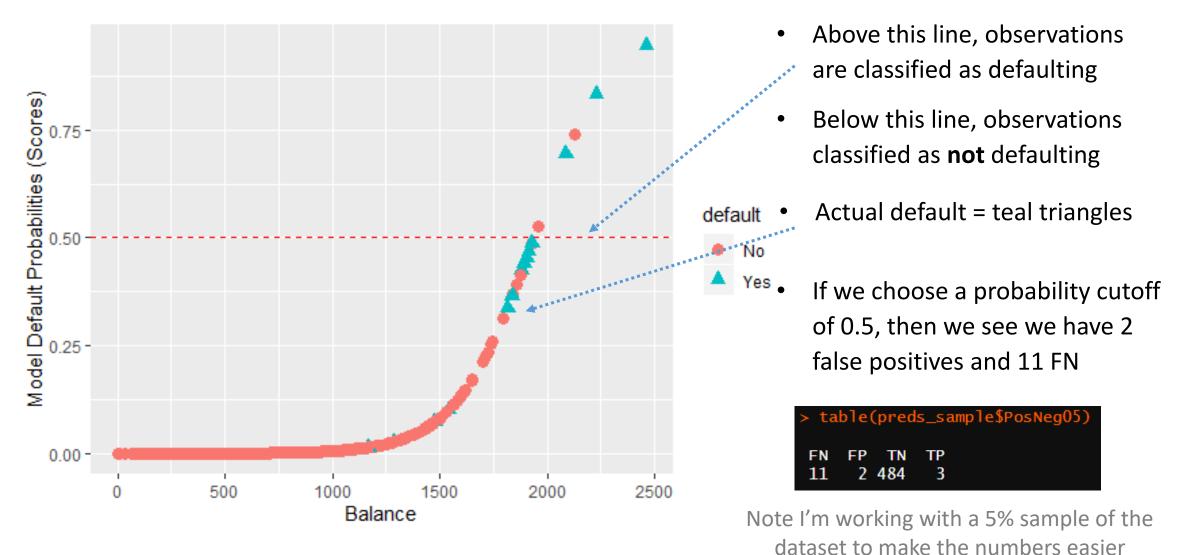


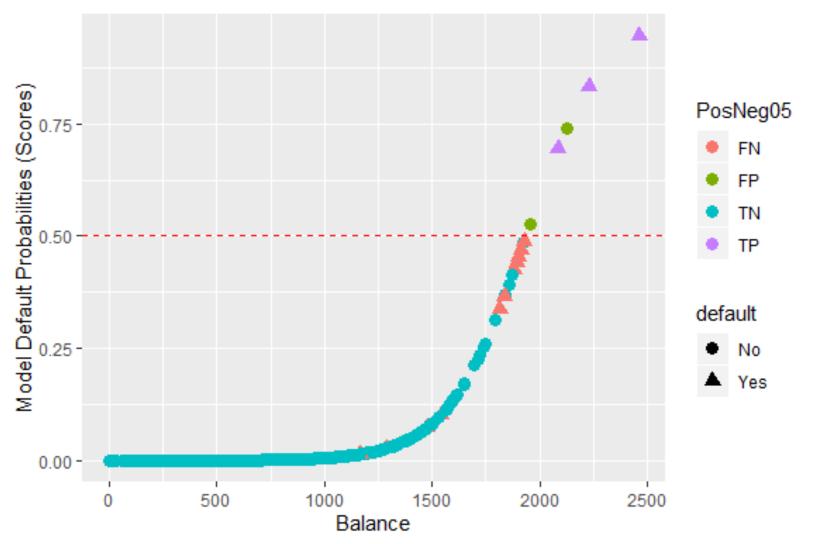


- Okay, so we have probabilities, what then?
- Note there is almost always some overlap between the probabilities of the classes
- We can't choose a probability such that above this all actual defaulters are correctly identified, and below this all non-defaulter are identified
- So we will always have some false positives and false negatives

# Confusion Matrix: Table of False/True Positives and False/True Negatives

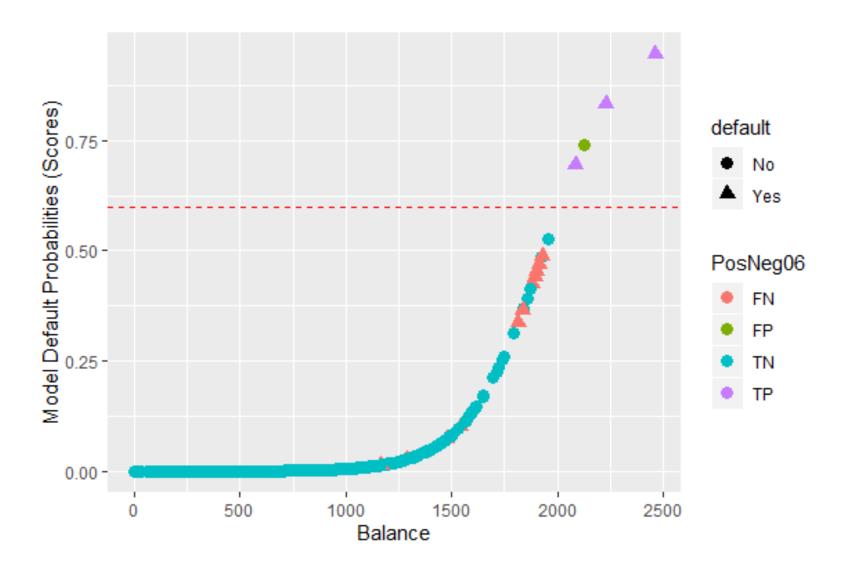
|                          |     | True default status |                     |
|--------------------------|-----|---------------------|---------------------|
|                          |     | No                  | Yes                 |
| Predicted default status | No  | True negative (TN)  | False Negative (FN) |
|                          | Yes | False Positive (FP) | True Positive (TP)  |





 If we choose a probability cutoff of 0.5, then we see we have 2 false positives and 11 FN

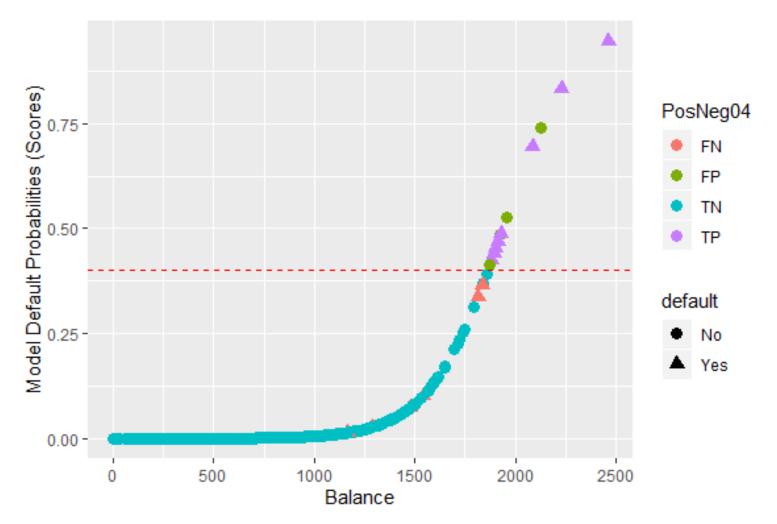
```
> table(preds_sample$PosNeg05)
FN FP TN TP
11 2 484 3
```



 Raising the cutoff to 0.6, then we see we have 1 false positives and 11 FN

```
> table(preds_sample$PosNeg06)

FN FP TN TP
11 1 485 3
```

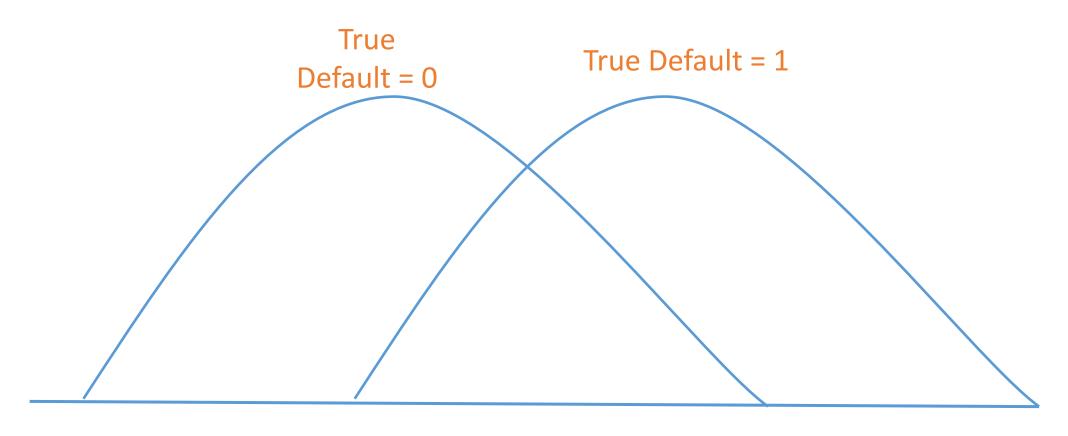


Lowering the cutoff to
0.4 results in more FPs
(4) but fewer FNs (6)

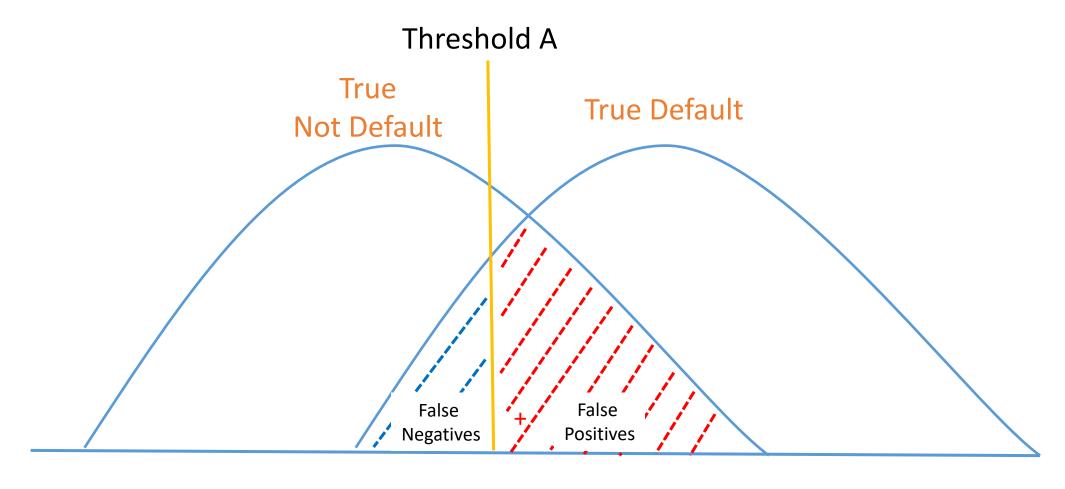
```
> table(preds_sample$PosNeg04)

FN FP TN TP
6 4 482 8
```

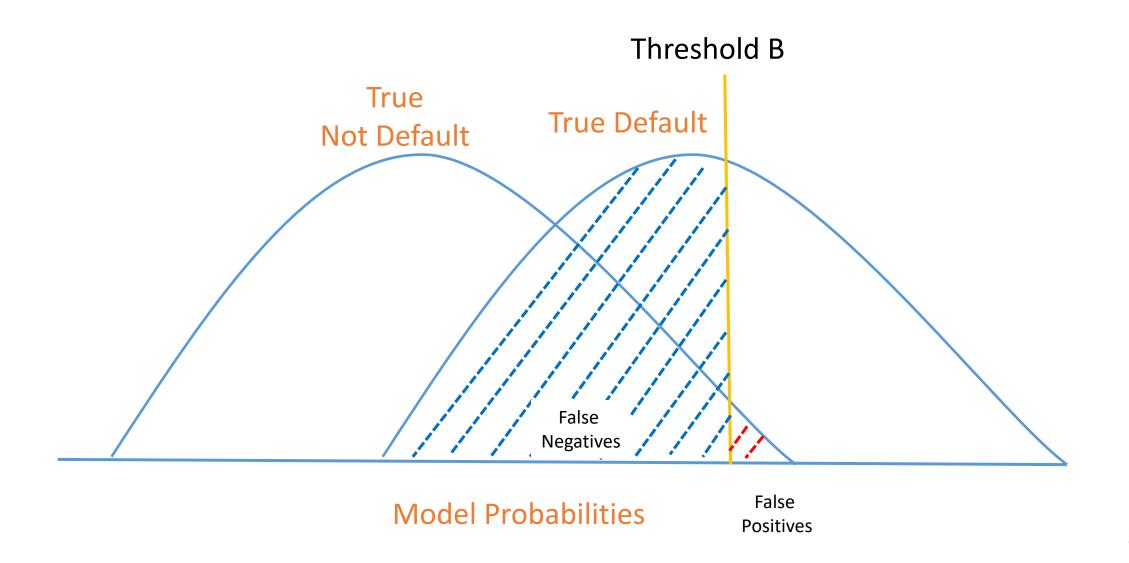
# Choosing Probability Cutoff to Assign Class



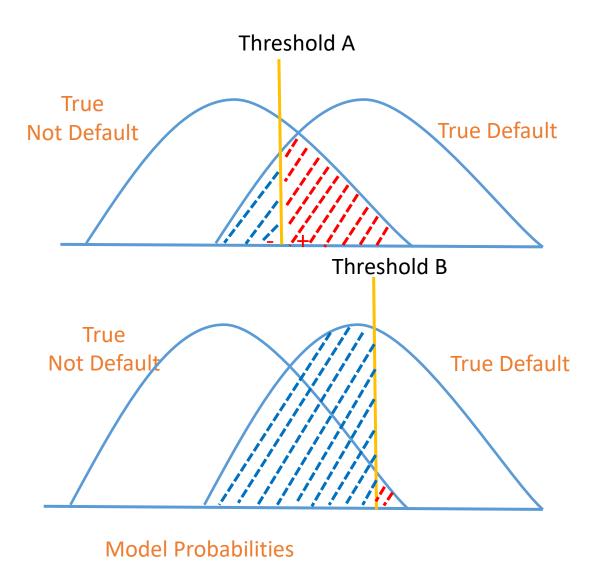
## Threshold A: Moderate Threshold



# Threshold B: Higher Threshold



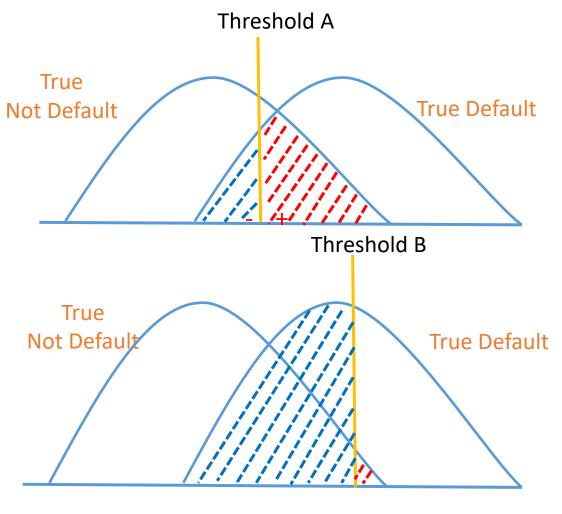
# Comparing cutoffs:



Many false positives

Few false positives

## Which Probability Cutoff To Use?



**Model Probabilities** 

- Threshold you choose should depend on relative costs of FPs and FN
  - e.g. screening at airport (cost of false neg high)
  - e.g. direct mail advertisement (cost of false positive low)
- Some common choices
  - Maximize Accuracy (equal weighting of FPs and FNs)
  - Threshold p\_hat > 0.5
  - Minimize cost: TC = costFP \*FPs + cost FN \* TNs

## Sensitivity and Specificity, Confusion Matrix at P Cutoff > 0.5

|   |     | True default status |         |          |
|---|-----|---------------------|---------|----------|
|   |     | No                  | Yes     |          |
| Predicted default status (cutoff p>0.5) | No  | TN = 484            | FN = 11 | N* = 495 |
|   | Yes | FP = 2              | TP = 3  | P*= 5    |
|   |     | N = 486             | P = 14  |          |

- Sensitivity: True positive rate (aka 1 power or recall)
  - TP/P = 3 / 14 = 21.4%
- **Specificity:** True <u>negative</u> rate
  - TN/N = 484 / 486= 99.5%
- False positive rate (aka Type I error, 1 Specificity)
  - FP/N = 2/486 = 0.004%

### Generating Confusion Matrices in R

- To produce a confusion matrix in R we will use the yardstick package
- The function conf\_mat() produces confusion matrices but we must format our data correctly
- We need to specify a data frame with
- Actual event (Y = 1) values
- Our estimated probabilities (scores)
- This example data frame shows how we need to structure our results data frame

```
Usage

conf_mat(data, ...)

## S3 method for class 'data.frame'
conf_mat(data, truth, estimate, dnn = c("Prediction", "Truth"), ...)

##.83 method for class 'conf_mat'
tidy(x, ...)

autoplot.conf_mat(object, type = "mosaic", ...)
```

```
> head(two_class_example)
   truth     Class1     Class2 predicted
1 Class2 0.003589243 0.9964107574     Class2
2 Class1 0.678621054 0.3213789460     Class1
3 Class2 0.110893522 0.8891064779     Class2
4 Class1 0.735161703 0.2648382969     Class1
5 Class2 0.016239960 0.9837600397     Class2
6 Class1 0.999275071 0.0007249286     Class1
```

yardstick

## Formatting Results Matrix for Confusion Matrix

- Let's store the model results in a data frame
- We must specify the actual default behavior
- And the probability of class1 (default) as well as probability of class2 (not default)
- We \*must\* specify a cutoff above which probabilities are classified as "class1" (or having the event) and below which they are not
- The cutoff probability is determined by the relative cost of false positives and false negatives! Do not use rules of thumb!

# Why Do So Many Practicing Data Scientists Not Understand Logistic Regression?

Posted on June 27, 2020 by W.D.

## Logistic Regression is Not Fundamentally a Classification Algorithm

Classification is when you make a concrete determination of what category something is a part of. Binary classification involves two categories, and by the law of the excluded middle, that means binary classification is for determining whether something "is" or "is not" part of a single category. There either are children playing in the park today (1), or there are not (0).

## Producing Confusion Matrix Using Formatted Results Data

- The conf\_mat() function shows the confusion matrix
- If we summarize the conf\_mat() object we see more binary metrics of classification (don't need to know all of these)
- **Sensitivity** is the true positive rate (TP/P) and here we identify of the true positives = 131/333 = 39.3%
- We may need to lower our threshold of cutoff probability

#### Continuous Cutoff: ROC Curve

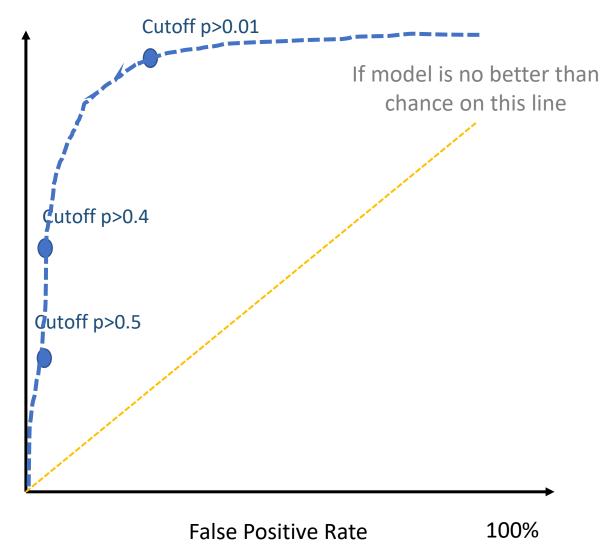
Can we show consequences
 of FPs and FNs as we vary the
 cutoff probability to assign
 classes?

True positive rate

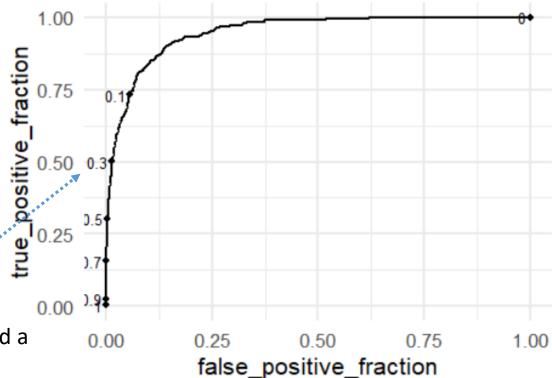
100%

Idea of a ROC (<u>Receiver</u>
 <u>Operator Curve</u>) plot

| Cutoff | TPR   | FPR    |
|--------|-------|--------|
| 0.01   | 100%  | 22.6%  |
| 0.4    | 57%   | 0.008  |
| 0.5    | 21.4% | 0.004% |
| 0.6    | 21.4% | 0.002% |



### ROC Curves in R



- At a cutoff of 0.3, we get a true positive fraction of 0.5 and a false positive fraction of a very low number
- Better models lie up and to the left in the ROC plot
- AUC calculates how much total area is under a particular curve
- AUC of 0.947 is pretty good

```
> calc_auc(p)
PANEL group AUC
1 1 -1 0.9479842
```

## Lab (time permitting)

```
Exercises
1. Generate predictions using your logit_mod2 model
   that predicts default as a function of
   student, balance, and income
2. Generate predicted probabilities (score the model)
3. Create a results data frame and print a confusion
   matrix using the results data
4. Plot a ROC curve using the results data
5. How well does the model perform?
```

## Class 5 Summary

- Log transformations of Y or X variables is useful when the data are "spread out"
- We interpret log-log regression coefficients as elasticities: a 1% change in the X variable leads to a coefficient % change in the Y variable
- We split data into testing and training sets, estimate a model on the training set and evaluate on the test set
- Logit functions compress predictions to lie between 0 and 1, which are valid probabilities
- The logistic model models the outcome (Y) as the log odds ratio!
- Confusion matrices show the true/false

positives/negatives.

- ROC plots measure the consequence on true positive fraction and false positive fraction for different cutoff probabilities
- Higher AUC scores mean a better ROC plot indicating a better model