Data Science Machine Learning

The textbook for the Data Science course series is freely available online.

Learning Objectives

- The basics of machine learning
- How to perform cross-validation to avoid overtraining
- Several popular machine learning algorithms
- How to build a recommendation system
- What regularization is and why it is useful

Course Overview

There are six major sections in this course: introduction to machine learning; machine learning basics; linear regression for prediction, smoothing, and working with matrices; distance, knn, cross validation, and generative models; classification with more than two classes and the caret package; and model fitting and recommendation systems.

Introduction to Machine Learning

In this section, you'll be introduced to some of the terminology and concepts you'll need going forward.

Machine Learning Basics

In this section, you'll learn how to start building a machine learning algorithm using training and test data sets and the importance of conditional probabilities for machine learning.

Linear Regression for Prediction, Smoothing, and Working with Matrices

In this section, you'll learn why linear regression is a useful baseline approach but is often insufficiently flexible for more complex analyses, how to smooth noisy data, and how to use matrices for machine learning.

Distance, Knn, Cross Validation, and Generative Models

In this section, you'll learn different types of discriminative and generative approaches for machine learning algorithms.

Classification with More than Two Classes and the Caret Package

In this section, you'll learn how to overcome the curse of dimensionality using methods that adapt to higher dimensions and how to use the caret package to implement many different machine learning algorithms.

Model Fitting and Recommendation Systems

In this section, you'll learn how to apply the machine learning algorithms you have learned.

Section 1 - Introduction to Machine Learning Overview

In the **Introduction to Machine Learning** section, you will be introduced to machine learning.

After completing this section, you will be able to:

- Explain the difference between the **outcome** and the **features**.
- Explain when to use **classification** and when to use **prediction**.
- Explain the importance of **prevalence**.
- Explain the difference between **sensitivity** and **specificity**.

This section has one part: **introduction to machine learning**.

Notation

There is a link to the relevant section of the textbook: Notation

Key points

- $X_1, ..., X_p$ denote the features, Y denotes the outcomes, and $\hat{Y}$ denotes the predictions.
- Machine learning prediction tasks can be divided into **categorical** and **continuous** outcomes. We refer to these as **classification** and **prediction**, respectively.

An Example

There is a link to the relevant section of the textbook: An Example

Key points

- Y_i = an outcome for observation or index i.
- We use boldface for $\mathbf{X_i}$ to distinguish the vector of predictors from the individual predictors $X_{i,1}, ..., X_{i,784}$.
- When referring to an arbitrary set of features and outcomes, we drop the index i and use Y and bold $\mathbf{X}$.
- Uppercase is used to refer to variables because we think of predictors as random variables.
- Lowercase is used to denote observed values. For example, $\mathbf{X} = \mathbf{x}$.

Comprehension Check - Introduction to Machine Learning

1. True or False: A key feature of machine learning is that the algorithms are built with data.

☒ A. True
☐ B. False

2. True or False: In machine learning, we build algorithms that take feature values (X) and train a model using known outcomes (Y) that is then used to predict outcomes when presented with features without known outcomes.

☒ A. True
☐ B. False

Section 2 - Machine Learning Basics Overview

In the **Machine Learning Basics** section, you will learn the basics of machine learning.

After completing this section, you will be able to:

- Start to use the **caret** package.
- Construct and interpret a **confusion matrix**.
- Use **conditional probabilities** in the context of machine learning.

This section has two parts: **basics of evaluating machine learning algorithms** and **conditional probabilities**.

Caret package, training and test sets, and overall accuracy

There is a link to the relevant sections of the textbook: Training and test sets and Overall accuracy

Key points

- Note: the `set.seed()` function is used to obtain reproducible results. If you have R 3.6 or later, please use the `sample.kind = "Rounding"` argument whenever you set the seed for this course.
- To mimic the ultimate evaluation process, we randomly split our data into two — a training set and a test set — and act as if we don't know the outcome of the test set. We develop algorithms using only the training set; the test set is used only for evaluation.
- The `createDataPartition()` function from the **caret** package can be used to generate indexes for randomly splitting data.
- Note: contrary to what the documentation says, this course will use the argument p as the percentage of data that goes to testing. The indexes made from `createDataPartition()` should be used to create the test set. Indexes should be created on the outcome and not a predictor.
- The simplest evaluation metric for categorical outcomes is overall accuracy: the proportion of cases that were correctly predicted in the test set.

Code

```
if(!require(tidyverse)) install.packages("tidyverse")
```

```
## Loading required package: tidyverse
```

```
## -- Attaching packages --------------------------------------- tidyverse 1.3.0 --
```

```
## v ggplot2 3.3.2     v purrr   0.3.4
## v tibble  3.0.4     v dplyr   1.0.2
## v tidyr   1.1.2     v stringr 1.4.0
## v readr   1.4.0     v forcats 0.5.0
```

```
## -- Conflicts ------------------------------------------ tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()
```

```r
if(!require(caret)) install.packages("caret")
```

```
## Loading required package: caret
```

```
## Loading required package: lattice
```

```
##
## Attaching package: 'caret'
```

```
## The following object is masked from 'package:purrr':
##
##     lift
```

```r
if(!require(dslabs)) install.packages("dslabs")
```

```
## Loading required package: dslabs
```

```r
library(tidyverse)
library(caret)
library(dslabs)
data(heights)

# define the outcome and predictors
y <- heights$sex
x <- heights$height

# generate training and test sets
set.seed(2, sample.kind = "Rounding") # if using R 3.5 or earlier, remove the sample.kind argument
```

```
## Warning in set.seed(2, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```r
test_index <- createDataPartition(y, times = 1, p = 0.5, list = FALSE)
test_set <- heights[test_index, ]
train_set <- heights[-test_index, ]

# guess the outcome
y_hat <- sample(c("Male", "Female"), length(test_index), replace = TRUE)
y_hat <- sample(c("Male", "Female"), length(test_index), replace = TRUE) %>%
  factor(levels = levels(test_set$sex))

# compute accuracy
mean(y_hat == test_set$sex)
```

```
## [1] 0.5238095
```

```r
heights %>% group_by(sex) %>% summarize(mean(height), sd(height))
```

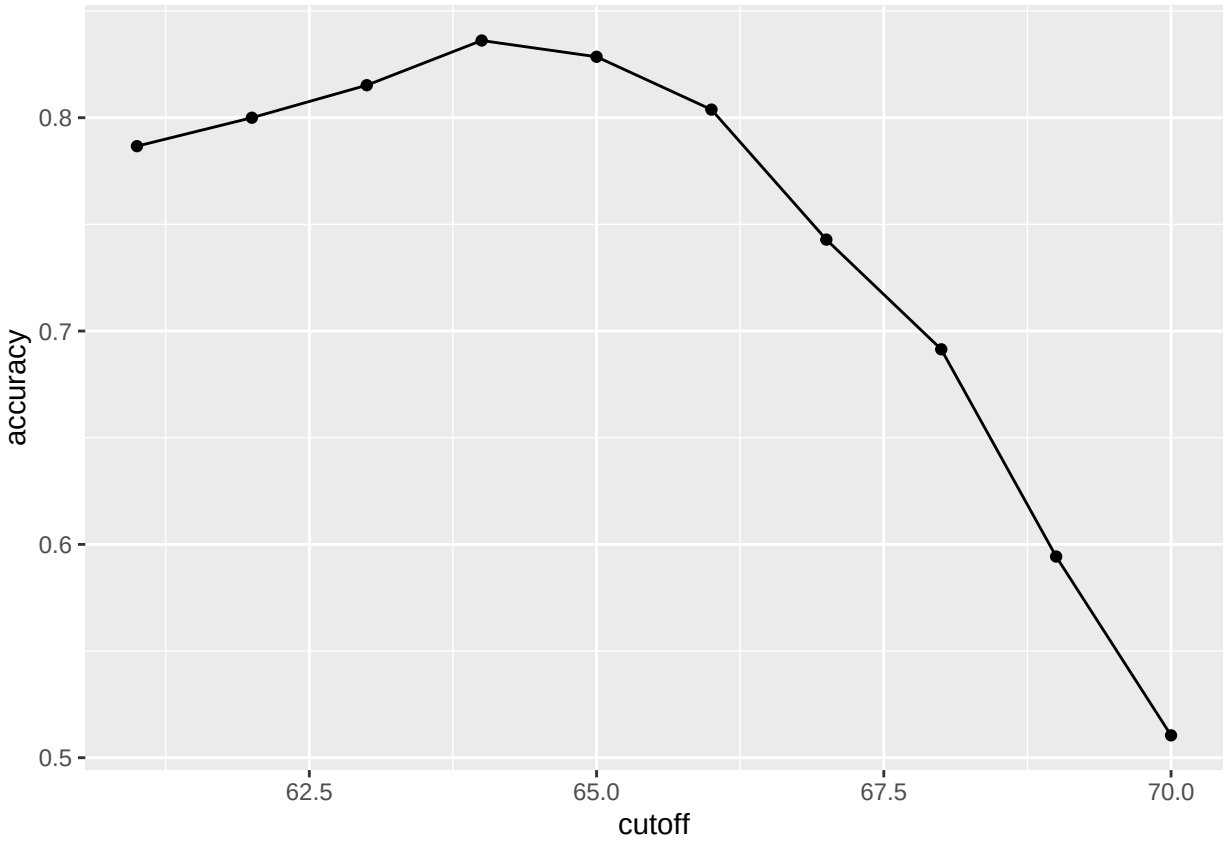
```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
## # A tibble: 2 x 3
##   sex    `mean(height)` `sd(height)`
##   <fct>           <dbl>        <dbl>
## 1 Female           64.9         3.76
## 2 Male             69.3         3.61
```

```
y_hat <- ifelse(x > 62, "Male", "Female") %>% factor(levels = levels(test_set$sex))
mean(y == y_hat)
```

```
## [1] 0.7933333
```

```
# examine the accuracy of 10 cutoffs
cutoff <- seq(61, 70)
accuracy <- map_dbl(cutoff, function(x){
  y_hat <- ifelse(train_set$height > x, "Male", "Female") %>%
    factor(levels = levels(test_set$sex))
  mean(y_hat == train_set$sex)
})
data.frame(cutoff, accuracy) %>%
  ggplot(aes(cutoff, accuracy)) +
  geom_point() +
  geom_line()
```




```
max(accuracy)
```

```
## [1] 0.8361905
```

```
best_cutoff <- cutoff[which.max(accuracy)]
best_cutoff
```

```
## [1] 64
```

```
y_hat <- ifelse(test_set$height > best_cutoff, "Male", "Female") %>%
  factor(levels = levels(test_set$sex))
y_hat <- factor(y_hat)
mean(y_hat == test_set$sex)
```

```
## [1] 0.8171429
```

Comprehension Check - Basics of Evaluating Machine Learning Algorithms

1. For each of the following, indicate whether the outcome is continuous or categorical.

- Digit reader - categorical
- Height - continuous

- Spam filter - categorical
- Stock prices - continuous
- Sex - categorical

2. How many features are available to us for prediction in the `mnist` digits dataset?

You can download the `mnist` dataset using the `read_mnist()` function from the **dslabs** package.

```
mnist <- read_mnist()
ncol(mnist$train$images)
```

```
## [1] 784
```

Confusion matrix

There is a link to the relevant section of the textbook: Confusion Matrix

Key points

- Overall accuracy can sometimes be a deceptive measure because of unbalanced classes.
- A general improvement to using overall accuracy is to study sensitivity and specificity separately. **Sensitivity**, also known as the true positive rate or recall, is the proportion of actual positive outcomes correctly identified as such. **Specificity**, also known as the true negative rate, is the proportion of actual negative outcomes that are correctly identified as such.
- A confusion matrix tabulates each combination of prediction and actual value. You can create a confusion matrix in R using the `table()` function or the `confusionMatrix()` function from the **caret** package.

Code

```r
# tabulate each combination of prediction and actual value
table(predicted = y_hat, actual = test_set$sex)
```

```
##          actual
## predicted Female Male
##    Female     50   27
##    Male       69  379
```

```r
test_set %>%
  mutate(y_hat = y_hat) %>%
  group_by(sex) %>%
  summarize(accuracy = mean(y_hat == sex))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
## # A tibble: 2 x 2
##   sex    accuracy
##   <fct>     <dbl>
## 1 Female    0.420
## 2 Male      0.933
```

```r
prev <- mean(y == "Male")

confusionMatrix(data = y_hat, reference = test_set$sex)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction Female Male
##     Female     50   27
##     Male       69  379
##
##                Accuracy : 0.8171
##                  95% CI : (0.7814, 0.8493)
##     No Information Rate : 0.7733
##     P-Value [Acc > NIR] : 0.008354
##
##                   Kappa : 0.4041
##
##  Mcnemar's Test P-Value : 2.857e-05
##
##             Sensitivity : 0.42017
##             Specificity : 0.93350
##          Pos Pred Value : 0.64935
##          Neg Pred Value : 0.84598
##              Prevalence : 0.22667
##          Detection Rate : 0.09524
##    Detection Prevalence : 0.14667
##       Balanced Accuracy : 0.67683
##
##        'Positive' Class : Female
##
```

Balanced accuracy and F1 score

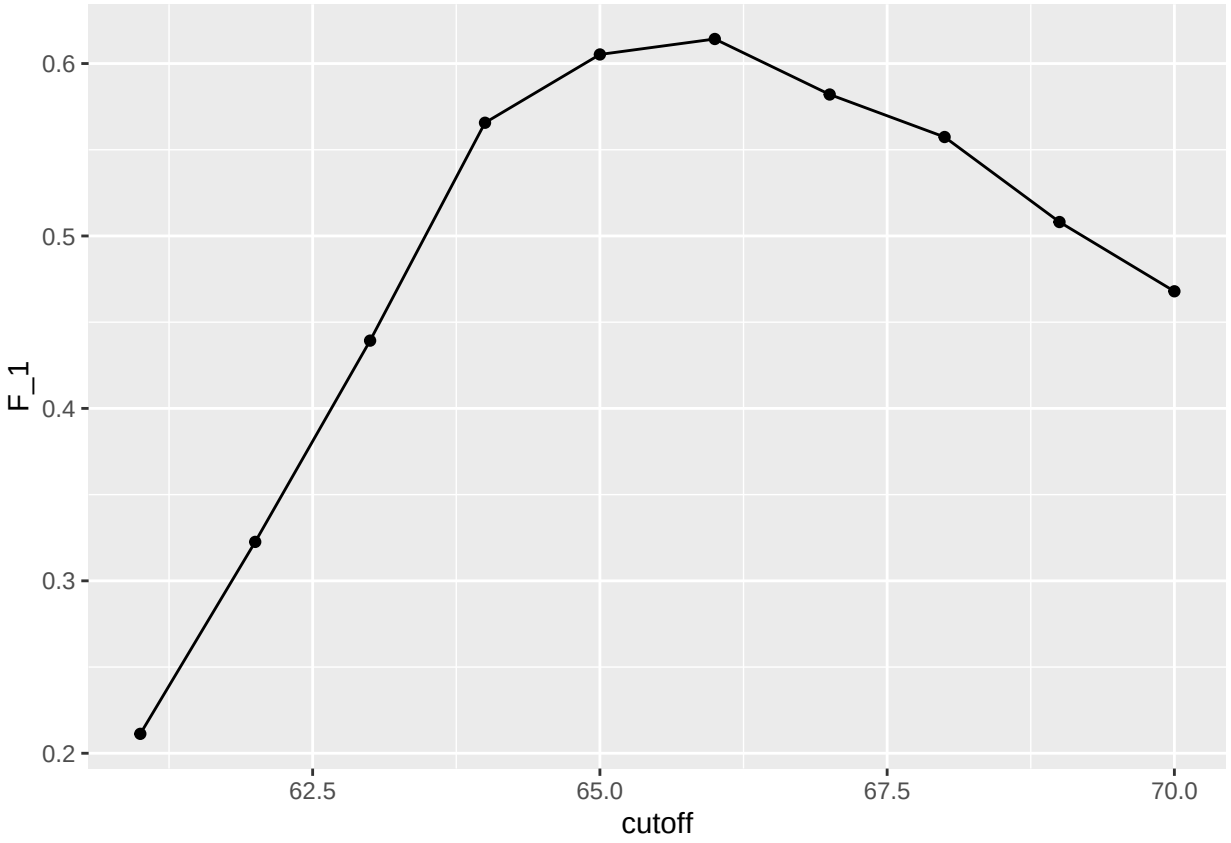
There is a link to the relevant section of the textbook: Balanced accuracy and F1 Score

Key points

- For optimization purposes, sometimes it is more useful to have a one number summary than studying both specificity and sensitivity. One preferred metric is **balanced accuracy**. Because specificity and sensitivity are rates, it is more appropriate to compute the *harmonic* average. In fact, the **F1-score**, a widely used one-number summary, is the harmonic average of precision and recall.
- Depending on the context, some type of errors are more costly than others. The **F1-score** can be adapted to weigh specificity and sensitivity differently.
- You can compute the **F1-score** using the `F_meas()` function in the **caret** package.

Code

```
# maximize F-score
cutoff <- seq(61, 70)
F_1 <- map_dbl(cutoff, function(x){
  y_hat <- ifelse(train_set$height > x, "Male", "Female") %>%
    factor(levels = levels(test_set$sex))
  F_meas(data = y_hat, reference = factor(train_set$sex))
})

data.frame(cutoff, F_1) %>%
  ggplot(aes(cutoff, F_1)) +
  geom_point() +
  geom_line()
```



```
max(F_1)
```

```
## [1] 0.6142322
```

```
best_cutoff <- cutoff[which.max(F_1)]
best_cutoff
```

```
## [1] 66
```

```
y_hat <- ifelse(test_set$height > best_cutoff, "Male", "Female") %>%
  factor(levels = levels(test_set$sex))
sensitivity(data = y_hat, reference = test_set$sex)
```

```
## [1] 0.6806723
```

```
specificity(data = y_hat, reference = test_set$sex)
```

```
## [1] 0.8349754
```

Prevalence matters in practice

There is a link to the relevant section of the textbook: Prevalence matters in practice

Key points

- A machine learning algorithm with very high sensitivity and specificity may not be useful in practice when prevalence is close to either 0 or 1. For example, if you develop an algorithm for disease diagnosis with very high sensitivity, but the prevalence of the disease is pretty low, then the precision of your algorithm is probably very low based on Bayes' theorem.

ROC and precision-recall curves

There is a link to the relevant section of the textbook: ROC and precision-recall curves

Key points

- A very common approach to evaluating accuracy and F1-score is to compare them graphically by plotting both. A widely used plot that does this is the **receiver operating characteristic (ROC) curve**. The ROC curve plots sensitivity (TPR) versus 1 - specificity or the false positive rate (FPR).
- However, ROC curves have one weakness and it is that neither of the measures plotted depend on prevalence. In cases in which prevalence matters, we may instead make a **precision-recall plot**, which has a similar idea with ROC curve.

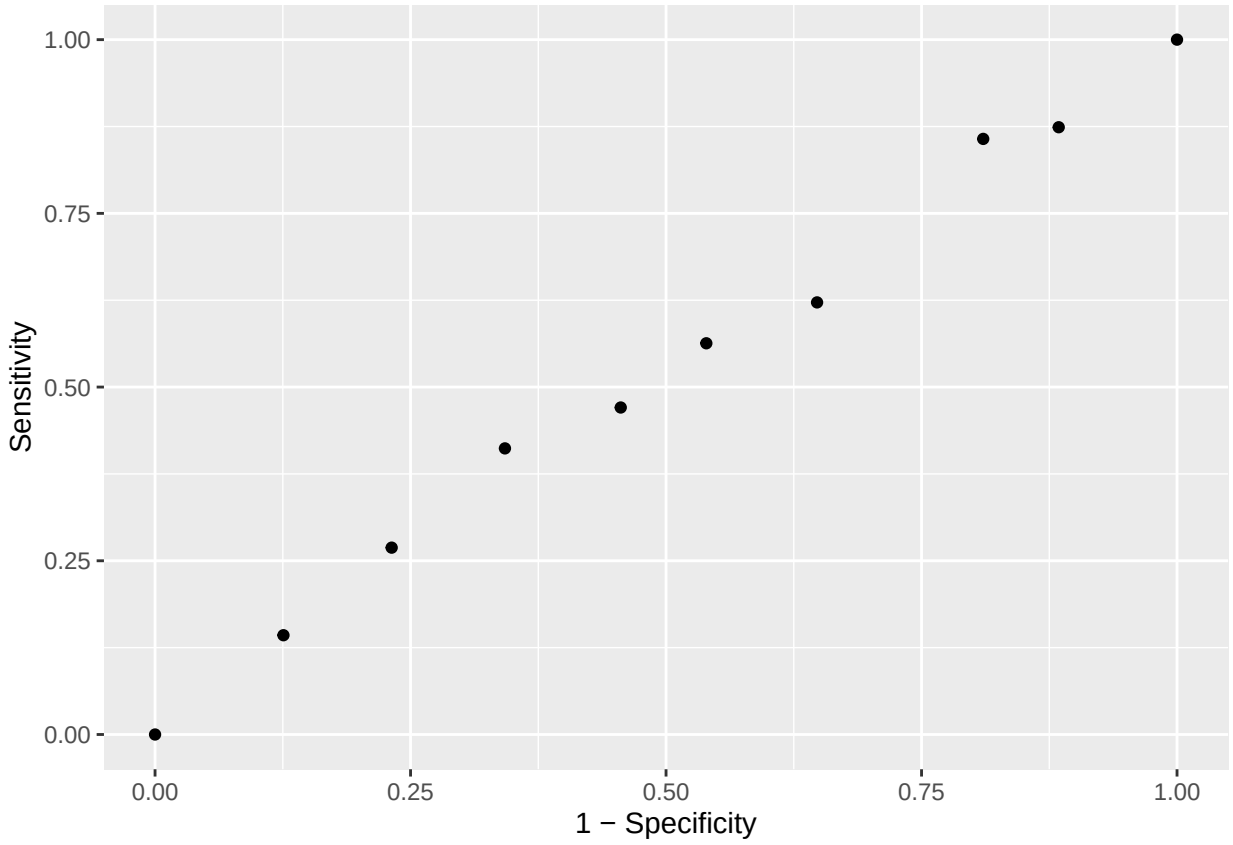
Code

Note: your results and plots may be slightly different.

```
p <- 0.9
n <- length(test_index)
y_hat <- sample(c("Male", "Female"), n, replace = TRUE, prob=c(p, 1-p)) %>%
  factor(levels = levels(test_set$sex))
mean(y_hat == test_set$sex)
```

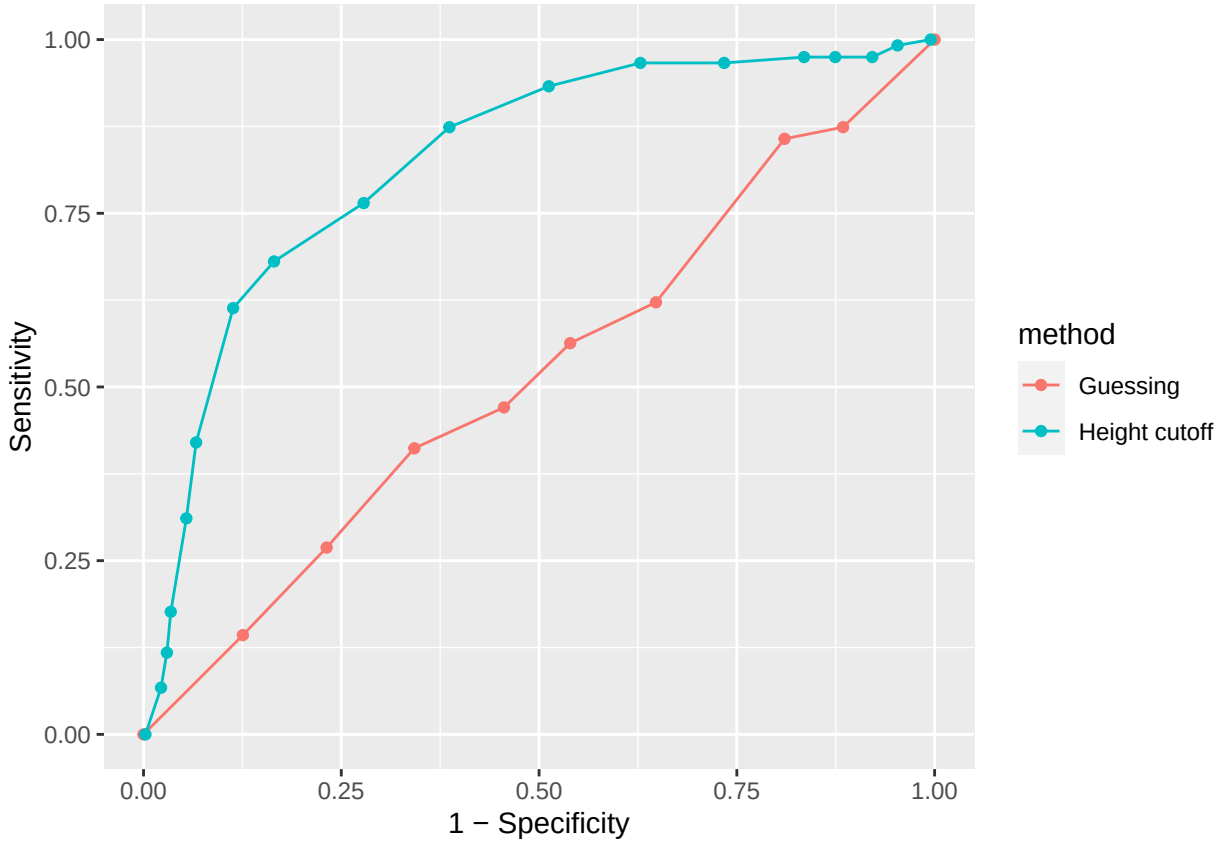
```
## [1] 0.7180952
```

```
# ROC curve
probs <- seq(0, 1, length.out = 10)
guessing <- map_df(probs, function(p){
  y_hat <-
    sample(c("Male", "Female"), n, replace = TRUE, prob=c(p, 1-p)) %>%
    factor(levels = c("Female", "Male"))
  list(method = "Guessing",
       FPR = 1 - specificity(y_hat, test_set$sex),
       TPR = sensitivity(y_hat, test_set$sex))
})
guessing %>% qplot(FPR, TPR, data =., xlab = "1 - Specificity", ylab = "Sensitivity")
```




```
cutoffs <- c(50, seq(60, 75), 80)
height_cutoff <- map_df(cutoffs, function(x){
  y_hat <- ifelse(test_set$height > x, "Male", "Female") %>%
    factor(levels = c("Female", "Male"))
   list(method = "Height cutoff",
        FPR = 1-specificity(y_hat, test_set$sex),
        TPR = sensitivity(y_hat, test_set$sex))
})

# plot both curves together
bind_rows(guessing, height_cutoff) %>%
  ggplot(aes(FPR, TPR, color = method)) +
```

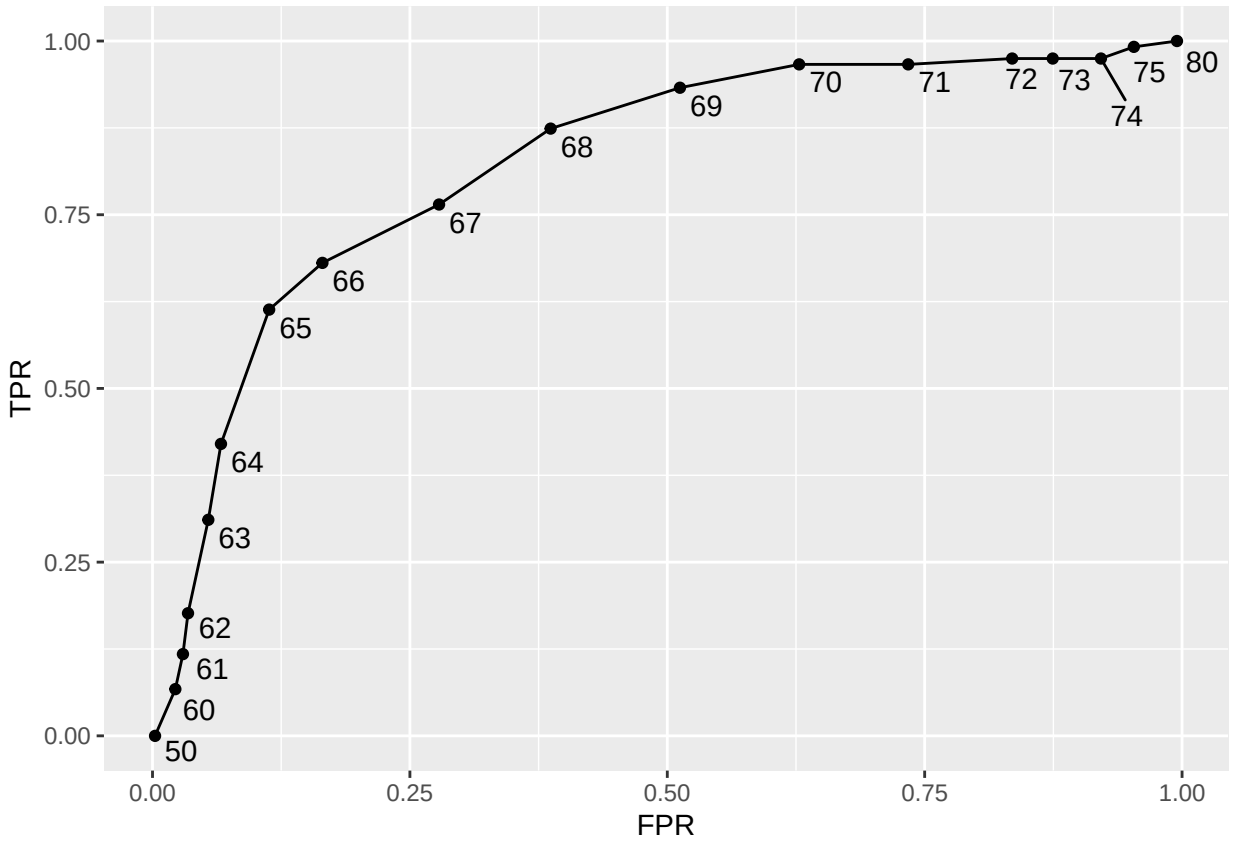
```
  geom_line() +
  geom_point() +
  xlab("1 - Specificity") +
  ylab("Sensitivity")
```




```
if(!require(ggrepel)) install.packages("ggrepel")
```

```
## Loading required package: ggrepel
```

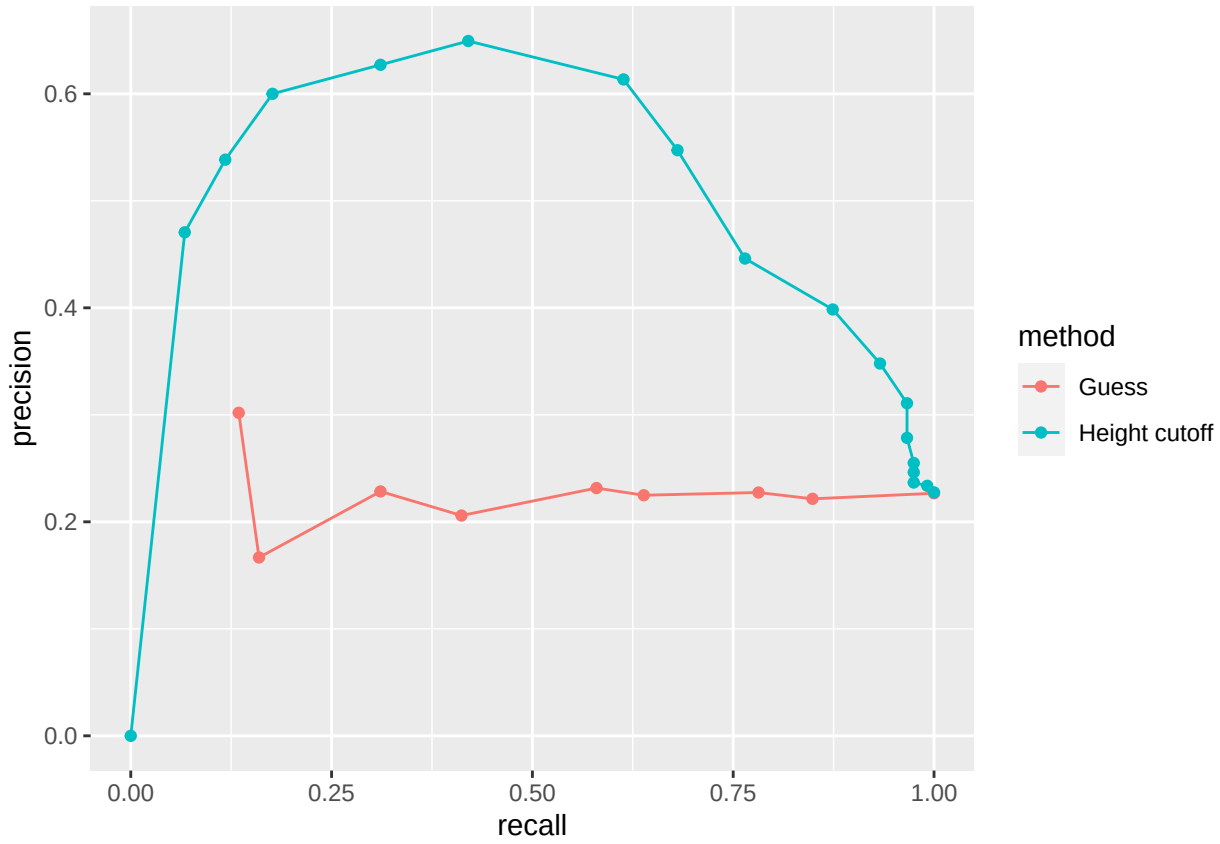
```
library(ggrepel)
map_df(cutoffs, function(x){
  y_hat <- ifelse(test_set$height > x, "Male", "Female") %>%
    factor(levels = c("Female", "Male"))
   list(method = "Height cutoff",
        cutoff = x,
        FPR = 1-specificity(y_hat, test_set$sex),
        TPR = sensitivity(y_hat, test_set$sex))
}) %>%
  ggplot(aes(FPR, TPR, label = cutoff)) +
  geom_line() +
  geom_point() +
  geom_text_repel(nudge_x = 0.01, nudge_y = -0.01)
```




```
# plot precision against recall
guessing <- map_df(probs, function(p){
  y_hat <- sample(c("Male", "Female"), length(test_index),
                  replace = TRUE, prob=c(p, 1-p)) %>%
    factor(levels = c("Female", "Male"))
  list(method = "Guess",
    recall = sensitivity(y_hat, test_set$sex),
    precision = precision(y_hat, test_set$sex))
})

height_cutoff <- map_df(cutoffs, function(x){
  y_hat <- ifelse(test_set$height > x, "Male", "Female") %>%
    factor(levels = c("Female", "Male"))
  list(method = "Height cutoff",
       recall = sensitivity(y_hat, test_set$sex),
    precision = precision(y_hat, test_set$sex))
})

bind_rows(guessing, height_cutoff) %>%
  ggplot(aes(recall, precision, color = method)) +
  geom_line() +
  geom_point()
```

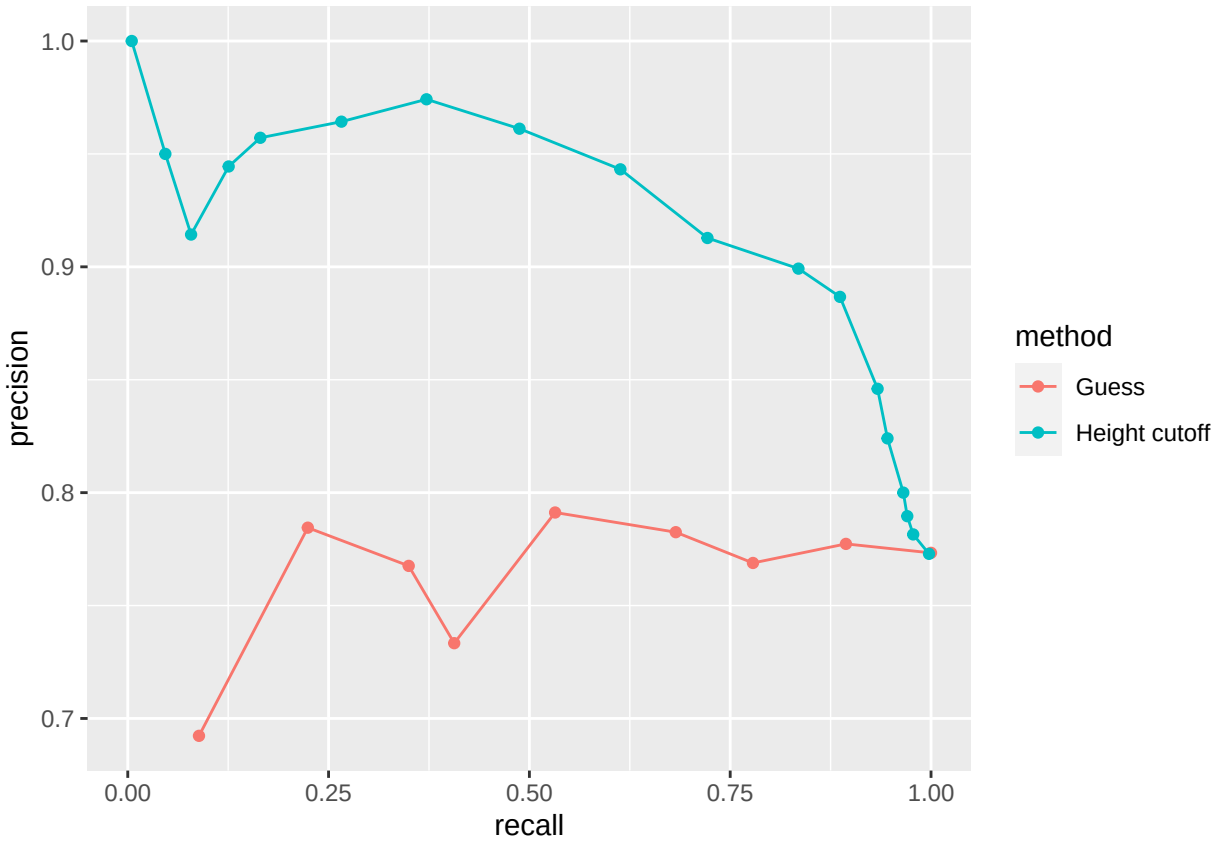
```
## Warning: Removed 1 row(s) containing missing values (geom_path).
```

```
## Warning: Removed 1 rows containing missing values (geom_point).
```




```
guessing <- map_df(probs, function(p){
  y_hat <- sample(c("Male", "Female"), length(test_index), replace = TRUE,
                  prob=c(p, 1-p)) %>%
    factor(levels = c("Male", "Female"))
  list(method = "Guess",
    recall = sensitivity(y_hat, relevel(test_set$sex, "Male", "Female")),
    precision = precision(y_hat, relevel(test_set$sex, "Male", "Female")))
})

height_cutoff <- map_df(cutoffs, function(x){
  y_hat <- ifelse(test_set$height > x, "Male", "Female") %>%
    factor(levels = c("Male", "Female"))
  list(method = "Height cutoff",
       recall = sensitivity(y_hat, relevel(test_set$sex, "Male", "Female")),
    precision = precision(y_hat, relevel(test_set$sex, "Male", "Female")))
})
bind_rows(guessing, height_cutoff) %>%
  ggplot(aes(recall, precision, color = method)) +
  geom_line() +
  geom_point()
```

```
## Warning: Removed 1 row(s) containing missing values (geom_path).

## Warning: Removed 1 rows containing missing values (geom_point).
```



Comprehension Check - Practice with Machine Learning, Part 1

The following questions all ask you to work with the dataset described below.

The `reported_heights` and `heights` datasets were collected from three classes taught in the Departments of Computer Science and Biostatistics, as well as remotely through the Extension School. The Biostatistics class was taught in 2016 along with an online version offered by the Extension School. On 2016-01-25 at 8:15 AM, during one of the lectures, the instructors asked student to fill in the sex and height questionnaire that populated the `reported_heights` dataset. The online students filled out the survey during the next few days, after the lecture was posted online. We can use this insight to define a variable which we will call `type`, to denote the type of student, `inclass` or `online`.

The code below sets up the dataset for you to analyze in the following exercises:

```
if(!require(dplyr)) install.packages("dplyr")
if(!require(lubridate)) install.packages("lubridate")
```

```
## Loading required package: lubridate
```

```
##
## Attaching package: 'lubridate'
```

```
## The following objects are masked from 'package:base':
##
##     date, intersect, setdiff, union
```

```
library(dplyr)
library(lubridate)
data(reported_heights)

dat <- mutate(reported_heights, date_time = ymd_hms(time_stamp)) %>%
  filter(date_time >= make_date(2016, 01, 25) & date_time < make_date(2016, 02, 1)) %>%
  mutate(type = ifelse(day(date_time) == 25 & hour(date_time) == 8 & between(minute(date_time), 15, 30)
  select(sex, type)

y <- factor(dat$sex, c("Female", "Male"))
x <- dat$type
```

1. The `type` column of `dat` indicates whether students took classes in person ("inclass") or online ("online"). What proportion of the inclass group is female? What proportion of the online group is female?

Enter your answer as a percentage or decimal (eg "50%" or "0.50") to at least the hundredths place.

```
dat %>% group_by(type) %>% summarize(prop_female = mean(sex == "Female"))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
## # A tibble: 2 x 2
##   type    prop_female
##   <chr>         <dbl>
## 1 inclass       0.667
## 2 online        0.378
```

2. In the course videos, height cutoffs were used to predict sex. Instead of height, use the `type` variable to predict sex. Assume that for each class type the students are either all male or all female, based on the most prevalent sex in each class type you calculated in Q1. Report the accuracy of your prediction of sex based on type. You do not need to split the data into training and test sets.

Enter your accuracy as a percentage or decimal (eg "50%" or "0.50") to at least the hundredths place.

```
y_hat <- ifelse(x == "online", "Male", "Female") %>%
      factor(levels = levels(y))
mean(y_hat==y)
```

```
## [1] 0.6333333
```

3. Write a line of code using the `table()` function to show the confusion matrix between `y_hat` and `y`. Use the **exact** format `function(a, b)` for your answer and do not name the columns and rows. Your answer should have exactly one space.

```
table(y_hat, y)
```

```
##         y
## y_hat    Female Male
##   Female     26   13
##   Male       42   69
```

4. What is the sensitivity of this prediction? You can use the `sensitivity()` function from the **caret** package. Enter your answer as a percentage or decimal (eg "50%" or "0.50") to at least the hundredths place.

```
sensitivity(y_hat, y)
```

```
## [1] 0.3823529
```

5. What is the specificity of this prediction? You can use the `specificity()` function from the **caret** package. Enter your answer as a percentage or decimal (eg "50%" or "0.50") to at least the hundredths place.

```
specificity(y_hat, y)
```

```
## [1] 0.8414634
```

6. What is the prevalence (% of females) in the `dat` dataset defined above? Enter your answer as a percentage or decimal (eg "50%" or "0.50") to at least the hundredths place.

```
mean(y == "Female")
```

```
## [1] 0.4533333
```

Comprehension Check - Practice with Machine Learning, Part 2

We will practice building a machine learning algorithm using a new dataset, `iris`, that provides multiple predictors for us to use to train. To start, we will remove the `setosa` species and we will focus on the `versicolor` and `virginica` iris species using the following code:

```
data(iris)
iris <- iris[-which(iris$Species=='setosa'),]
y <- iris$Species
```

The following questions all involve work with this dataset.

7. First let us create an even split of the data into `train` and `test` partitions using `createDataPartition()` from the **caret** package. The code with a missing line is given below:

```
# set.seed(2) # if using R 3.5 or earlier
set.seed(2, sample.kind="Rounding") # if using R 3.6 or later
# line of code
test <- iris[test_index,]
train <- iris[-test_index,]
```

Which code should be used in place of # line of code above?

- ☐ A. test_index <- createDataPartition(y,times=1,p=0.5)
- ☐ B. test_index <- sample(2,length(y),replace=FALSE)
- ☒ C. test_index <- createDataPartition(y,times=1,p=0.5,list=FALSE)
- ☐ D. test_index <- rep(1,length(y))

```
# set.seed(2) # if using R 3.5 or earlier
set.seed(2, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(2, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
test_index <- createDataPartition(y,times=1,p=0.5,list=FALSE)
```

```
## Warning in createDataPartition(y, times = 1, p = 0.5, list = FALSE): Some
## classes have no records ( setosa ) and these will be ignored
```

```
test <- iris[test_index,]
train <- iris[-test_index,]
```

8. Next we will figure out the singular feature in the dataset that yields the greatest overall accuracy when predicting species. You can use the code from the introduction and from Q7 to start your analysis.

Using only the `train` iris dataset, for each feature, perform a simple search to find the cutoff that produces the highest accuracy, predicting virginica if greater than the cutoff and versicolor otherwise. Use the `seq` function over the range of each feature by intervals of 0.1 for this search.

Which feature produces the highest accuracy?

```
foo <- function(x){
    rangedValues <- seq(range(x)[1],range(x)[2],by=0.1)
    sapply(rangedValues,function(i){
        y_hat <- ifelse(x>i,'virginica','versicolor')
        mean(y_hat==train$Species)
    })
}
predictions <- apply(train[,-5],2,foo)
sapply(predictions,max)
```

```
## Sepal.Length  Sepal.Width Petal.Length  Petal.Width
##         0.70         0.62         0.96         0.94
```

- ☐ A. Sepal.Length
- ☐ B. Sepal.Width
- ☒ C. Petal.Length
- ☐ D. Petal.Width

9. For the feature selected in Q8, use the smart cutoff value from the training data to calculate overall accuracy in the test data. What is the overall accuracy?

```
predictions <- foo(train[,3])
rangedValues <- seq(range(train[,3])[1],range(train[,3])[2],by=0.1)
cutoffs <-rangedValues[which(predictions==max(predictions))]

y_hat <- ifelse(test[,3]>cutoffs[1],'virginica','versicolor')
mean(y_hat==test$Species)
```

```
## [1] 0.9
```

10. Notice that we had an overall accuracy greater than 96% in the training data, but the overall accuracy was lower in the test data. This can happen often if we overtrain. In fact, it could be the case that a single feature is not the best choice. For example, a combination of features might be optimal. Using a single feature and optimizing the cutoff as we did on our training data can lead to overfitting.

Given that we know the test data, we can treat it like we did our training data to see if the same feature with a different cutoff will optimize our predictions.

Which feature best optimizes our overall accuracy?

```
foo <- function(x){
    rangedValues <- seq(range(x)[1],range(x)[2],by=0.1)
    sapply(rangedValues,function(i){
        y_hat <- ifelse(x>i,'virginica','versicolor')
        mean(y_hat==test$Species)
    })
}
predictions <- apply(test[,-5],2,foo)
sapply(predictions,max)
```

```
## Sepal.Length  Sepal.Width Petal.Length  Petal.Width
##         0.78         0.64         0.90         0.94
```

- ☐ A. Sepal.Length
- ☐ B. Sepal.Width
- ☐ C. Petal.Length
- ☒ D. Petal.Width

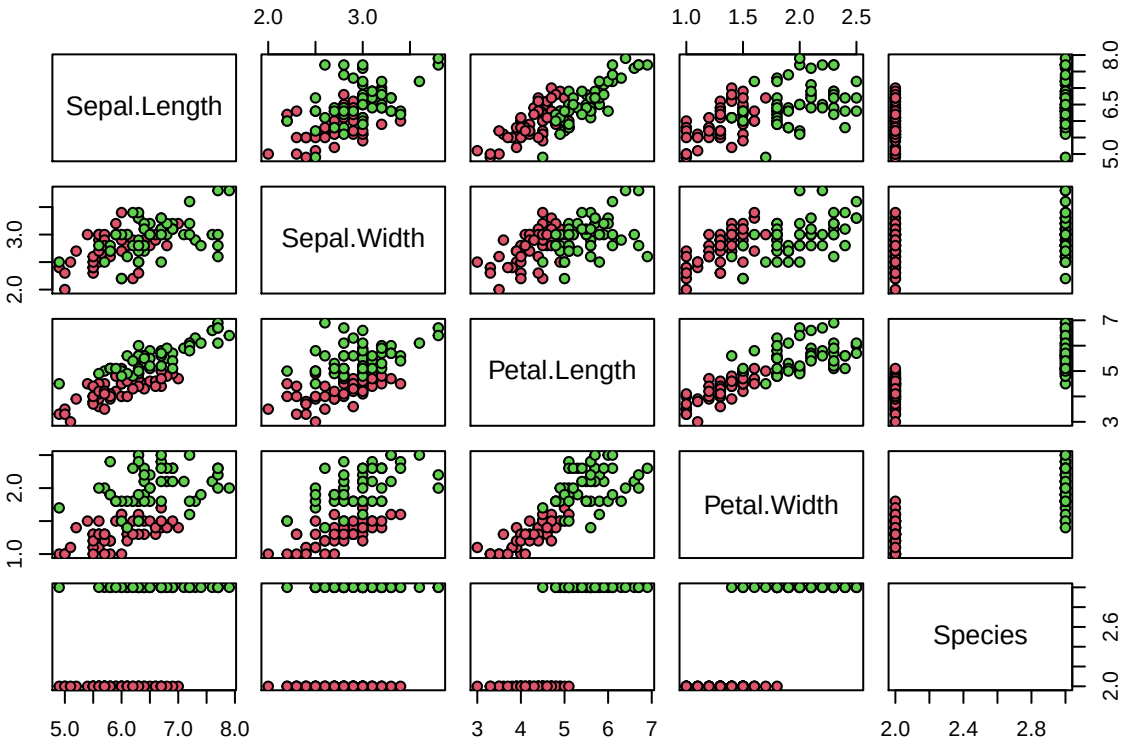
11. Now we will perform some exploratory data analysis on the data.

Notice that `Petal.Length` and `Petal.Width` in combination could potentially be more information than either feature alone.

Optimize the the cutoffs for `Petal.Length` and `Petal.Width` separately in the train dataset by using the `seq` function with increments of 0.1. Then, report the overall accuracy when applied to the test dataset by creating a rule that predicts virginica if `Petal.Length` is greater than the length cutoff OR `Petal.Width` is greater than the width cutoff, and versicolor otherwise.

What is the overall accuracy for the test data now?

```
data(iris)
iris <- iris[-which(iris$Species=='setosa'),]
y <- iris$Species

plot(iris,pch=21,bg=iris$Species)
```




```
# set.seed(2) # if using R 3.5 or earlier
set.seed(2, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(2, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
test_index <- createDataPartition(y,times=1,p=0.5,list=FALSE)
```

```
## Warning in createDataPartition(y, times = 1, p = 0.5, list = FALSE): Some
## classes have no records ( setosa ) and these will be ignored
```

```
test <- iris[test_index,]
train <- iris[-test_index,]

petalLengthRange <- seq(range(train$Petal.Length)[1],range(train$Petal.Length)[2],by=0.1)
petalWidthRange <- seq(range(train$Petal.Width)[1],range(train$Petal.Width)[2],by=0.1)

length_predictions <- sapply(petalLengthRange,function(i){
        y_hat <- ifelse(train$Petal.Length>i,'virginica','versicolor')
        mean(y_hat==train$Species)
    })
length_cutoff <- petalLengthRange[which.max(length_predictions)] # 4.7

width_predictions <- sapply(petalWidthRange,function(i){
        y_hat <- ifelse(train$Petal.Width>i,'virginica','versicolor')
        mean(y_hat==train$Species)
    })
width_cutoff <- petalWidthRange[which.max(width_predictions)] # 1.5
```

```
y_hat <- ifelse(test$Petal.Length>length_cutoff | test$Petal.Width>width_cutoff,'virginica','versicolor
mean(y_hat==test$Species)
```

```
## [1] 0.88
```

Conditional probabilities

There is a link to the relevant section of the textbook: Conditional probabilities

Key points

- Conditional probabilities for each class:

$p_k(x) = Pr(Y = k|X = x), for\, k = 1, ..., K$

- In machine learning, this is referred to as **Bayes' Rule**. This is a theoretical rule because in practice we don't know $p(x)$. Having a good estimate of the $p(x)$ will suffice for us to build optimal prediction models, since we can control the balance between specificity and sensitivity however we wish. In fact, estimating these conditional probabilities can be thought of as the main challenge of machine learning.

Conditional expectations and loss function

There is a link to the relevant sections of the textbook: Conditional expectations and Loss functions

Key points

- Due to the connection between **conditional probabilities** and **conditional expectations**:

$p_k(x) = Pr(Y = k|X = x)$, for $k = 1, ..., K$

we often only use the expectation to denote both the conditional probability and conditional expectation.

- For continuous outcomes, we define a loss function to evaluate the model. The most commonly used one is **MSE (Mean Squared Error)**. The reason why we care about the conditional expectation in machine learning is that the expected value minimizes the MSE:

$\hat{Y} = E(Y|X = x)$ minimizes $E\{(\hat{Y} - Y)^2|X = x\}$

Due to this property, a succinct description of the main task of machine learning is that we use data to estimate for any set of features. **The main way in which competing machine learning algorithms differ is in their approach to estimating this expectation**.

Comprehension Check - Conditional Probabilities, Part 1

1. In a previous module, we covered Bayes' theorem and the Bayesian paradigm. Conditional probabilities are a fundamental part of this previous covered rule.

$P(A|B) = P(B|A)\frac{P(A)}{P(B)}$

We first review a simple example to go over conditional probabilities.

Assume a patient comes into the doctor's office to test whether they have a particular disease.

- The test is positive 85% of the time when tested on a patient with the disease (high sensitivity): $P(\text{test}+|\text{disease}) = 0.85$
- The test is negative 90% of the time when tested on a healthy patient (high specificity): $P(\text{test}-|\text{heathy}) = 0.90$
- The disease is prevalent in about 2% of the community: $P(\text{disease}) = 0.02$

Using Bayes' theorem, calculate the probability that you have the disease if the test is positive.

$P(\text{disease}|\text{test}+) = P(\text{test}+|\text{disease}) \times \frac{P(\text{disease})}{P(\text{test}+)} = \frac{P(\text{test}+|\text{disease})P(\text{disease})}{P(\text{test}+|\text{disease})P(\text{disease})+P(\text{test}+|\text{healthy})P(\text{healthy})]} = \frac{0.85 \times 0.02}{0.85 \times 0.02 + 0.1 \times 0.98} = 0.1478261$

The following 4 questions (Q2-Q5) all relate to implementing this calculation using R.

We have a hypothetical population of 1 million individuals with the following conditional probabilities as described below:

- The test is positive 85% of the time when tested on a patient with the disease (high sensitivity): $P(\text{test}+|\text{disease}) = 0.85$
- The test is negative 90% of the time when tested on a healthy patient (high specificity): $P(\text{test}-|\text{heathy}) = 0.90$
- The disease is prevalent in about 2% of the community: $P(\text{disease}) = 0.02$

Here is some sample code to get you started:

```
# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
disease <- sample(c(0,1), size=1e6, replace=TRUE, prob=c(0.98,0.02))
test <- rep(NA, 1e6)
test[disease==0] <- sample(c(0,1), size=sum(disease==0), replace=TRUE, prob=c(0.90,0.10))
test[disease==1] <- sample(c(0,1), size=sum(disease==1), replace=TRUE, prob=c(0.15, 0.85))
```

2. What is the probability that a test is positive?

```
mean(test)
```

```
## [1] 0.114509
```

3. What is the probability that an individual has the disease if the test is negative?

```
mean(disease[test==0])
```

```
## [1] 0.003461356
```

4. What is the probability that you have the disease if the test is positive? Remember: calculate the conditional probability the disease is positive assuming a positive test.

```
mean(disease[test==1]==1)
```

```
## [1] 0.1471762
```

5. Compare the prevalence of disease in people who test positive to the overall prevalence of disease.

If a patient's test is positive, by how many times does that increase their risk of having the disease? First calculate the probability of having the disease given a positive test, then divide by the probability of having the disease.

```
mean(disease[test==1]==1)/mean(disease==1)
```

```
## [1] 7.389106
```

Comprehension Check - Conditional Probabilities, Part 2

6. We are now going to write code to compute conditional probabilities for being male in the heights dataset. Round the heights to the closest inch. Plot the estimated conditional probability $P(x) = \Pr(\text{Male}|\text{height} = x)$.

Part of the code is provided here:

```
data("heights")
# MISSING CODE
    qplot(height, p, data =.)
```

Which of the following blocks of code can be used to replace **# MISSING CODE** to make the correct plot?

☐ A.

```
heights %>%
    group_by(height) %>%
    summarize(p = mean(sex == "Male")) %>%
```

☐ B.

```
heights %>%
    mutate(height = round(height)) %>%
    group_by(height) %>%
    summarize(p = mean(sex == "Female")) %>%
```

☐ C.

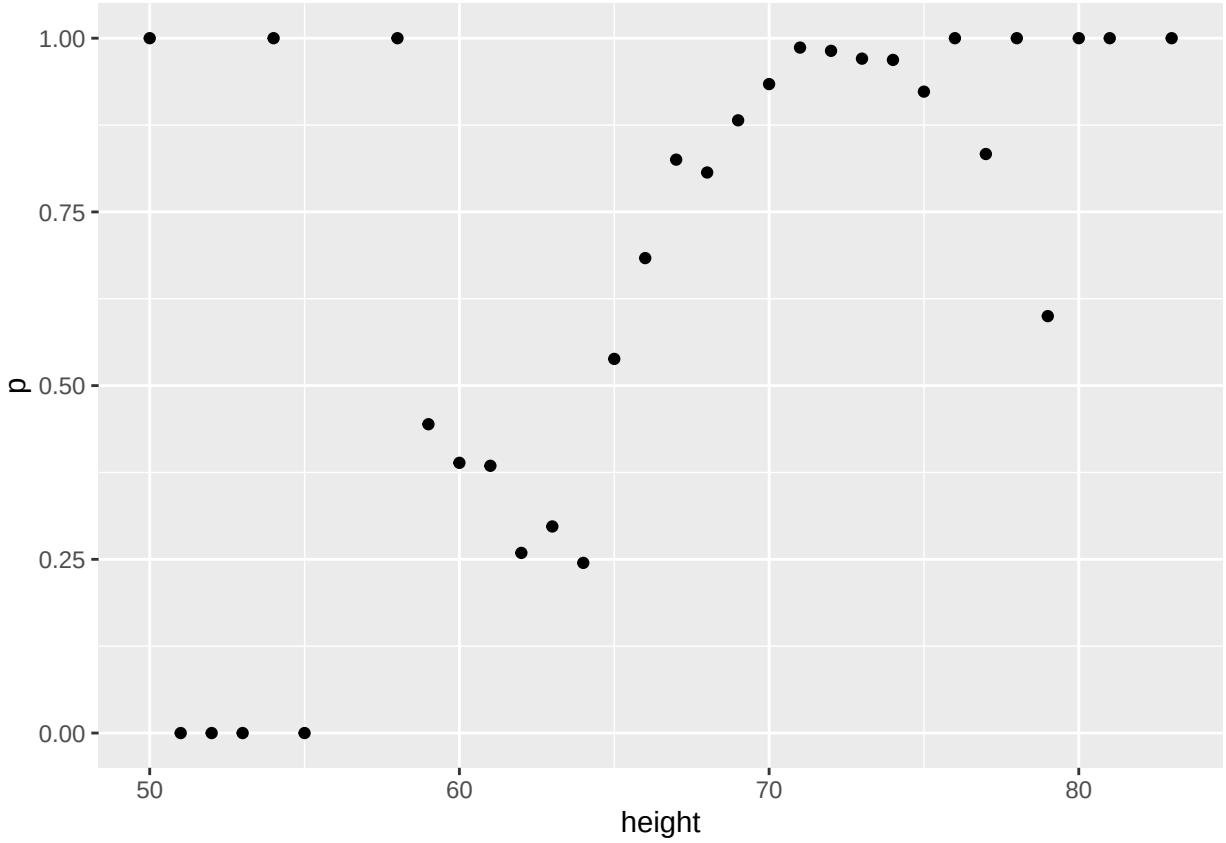
```
heights %>%
    mutate(height = round(height)) %>%
    summarize(p = mean(sex == "Male")) %>%
```

☒ D.

```
heights %>%
    mutate(height = round(height)) %>%
    group_by(height) %>%
    summarize(p = mean(sex == "Male")) %>%
```

```
data("heights")
heights %>%
    mutate(height = round(height)) %>%
    group_by(height) %>%
    summarize(p = mean(sex == "Male")) %>%
    qplot(height, p, data =.)
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```



7. In the plot we just made in Q6 we see high variability for low values of height. This is because we have few data points. This time use the quantile $0.1, 0.2, \ldots, 0.9$ and the `cut()` function to assure each group has the same number of points. Note that for any numeric vector `x`, you can create groups based on quantiles like this: `cut(x, quantile(x, seq(0, 1, 0.1)), include.lowest = TRUE)`.

Part of the code is provided here:

```
ps <- seq(0, 1, 0.1)
heights %>%
    # MISSING CODE
```

```
    group_by(g) %>%
    summarize(p = mean(sex == "Male"), height = mean(height)) %>%
    qplot(height, p, data =.)
```

Which of the following lines of code can be used to replace # **MISSING CODE** to make the correct plot?

☐ A.

```
mutate(g = cut(male, quantile(height, ps), include.lowest = TRUE)) %>%
```

☒ B.

```
mutate(g = cut(height, quantile(height, ps), include.lowest = TRUE)) %>%
```

☐ C.

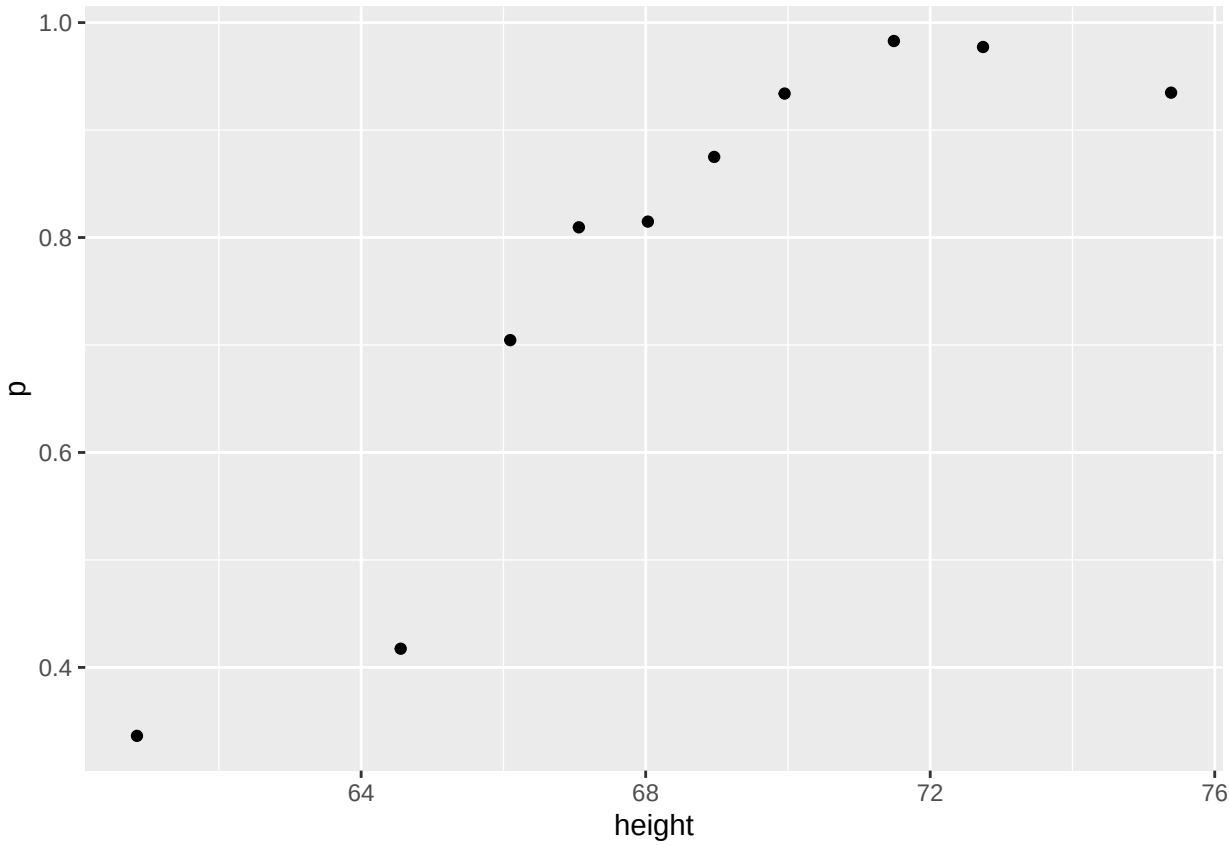
```
mutate(g = cut(female, quantile(height, ps), include.lowest = TRUE)) %>%
```

☐ D.

```
mutate(g = cut(height, quantile(height, ps))) %>%
```

```
ps <- seq(0, 1, 0.1)
heights %>%
    mutate(g = cut(height, quantile(height, ps), include.lowest = TRUE)) %>%
    group_by(g) %>%
    summarize(p = mean(sex == "Male"), height = mean(height)) %>%
    qplot(height, p, data =.)
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```



8. You can generate data from a bivariate normal distrubution using the **MASS** package using the following code:

```
if(!require(MASS)) install.packages("MASS")
```

```
## Loading required package: MASS
```

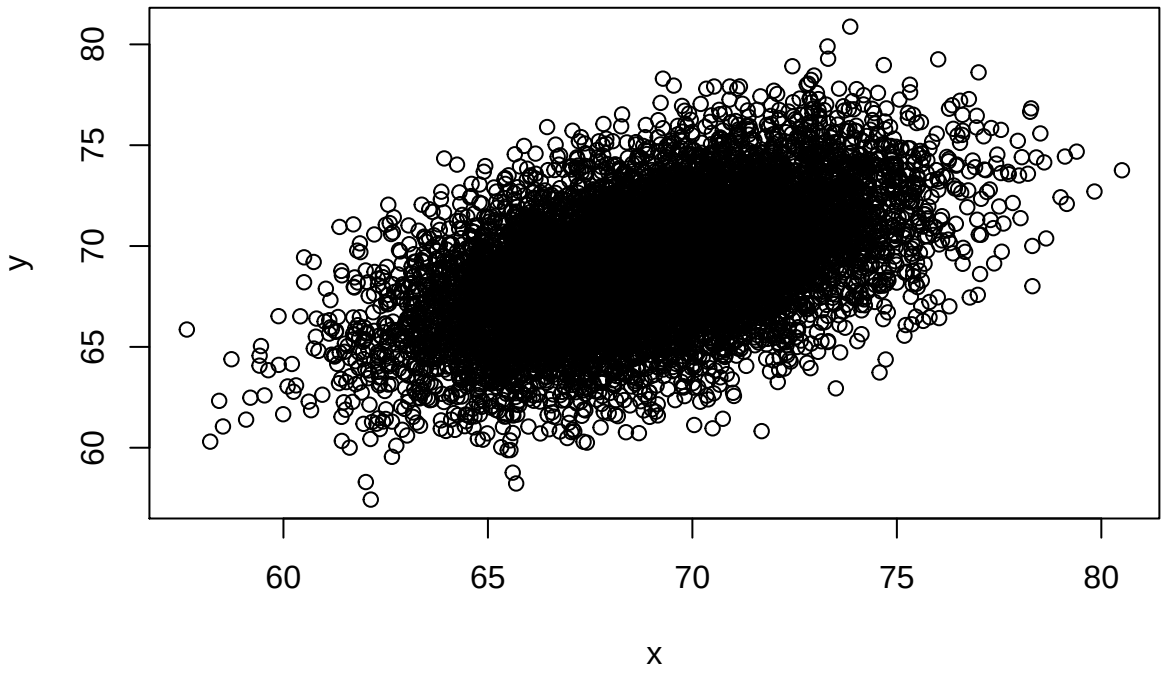
```
##
## Attaching package: 'MASS'
```

```
## The following object is masked from 'package:dplyr':
##
##     select
```

```
Sigma <- 9*matrix(c(1,0.5,0.5,1), 2, 2)
dat <- MASS::mvrnorm(n = 10000, c(69, 69), Sigma) %>%
    data.frame() %>% setNames(c("x", "y"))
```

And you can make a quick plot using `plot(dat)`.

```
plot(dat)
```



Using an approach similar to that used in the previous exercise, let's estimate the conditional expectations and make a plot. Part of the code has again been provided for you:

```
ps <- seq(0, 1, 0.1)
dat %>%
    # MISSING CODE
    qplot(x, y, data =.)
```

Which of the following blocks of code can be used to replace # **MISSING CODE** to make the correct plot?

☒ A.

```
mutate(g = cut(x, quantile(x, ps), include.lowest = TRUE)) %>%
group_by(g) %>%
summarize(y = mean(y), x = mean(x)) %>%
```

☐ B.

```
mutate(g = cut(x, quantile(x, ps))) %>%
group_by(g) %>%
summarize(y = mean(y), x = mean(x)) %>%
```

☐ C.

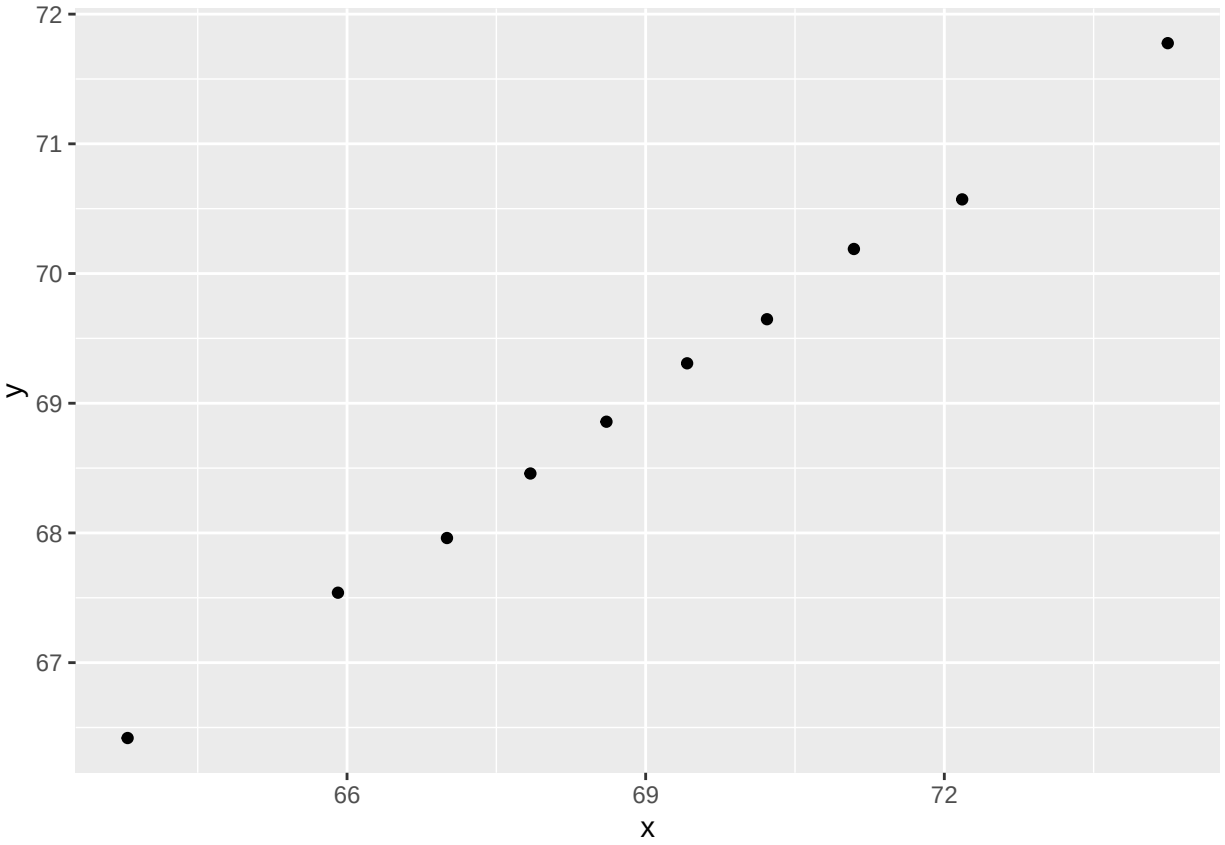
```
mutate(g = cut(x, quantile(x, ps), include.lowest = TRUE)) %>%
summarize(y = mean(y), x = mean(x)) %>%
```

☐ D.

```
mutate(g = cut(x, quantile(x, ps), include.lowest = TRUE)) %>%
group_by(g) %>%
summarize(y =(y), x =(x)) %>%
```

```
ps <- seq(0, 1, 0.1)
dat %>%
    mutate(g = cut(x, quantile(x, ps), include.lowest = TRUE)) %>%
    group_by(g) %>%
    summarize(y = mean(y), x = mean(x)) %>%
    qplot(x, y, data =.)
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```



Section 3 - Linear Regression for Prediction, Smoothing, and Working with Matrices Overview

In the **Linear Regression for Prediction, Smoothing, and Working with Matrices Overview** section, you will learn why linear regression is a useful baseline approach but is often insufficiently flexible for more complex analyses, how to smooth noisy data, and how to use matrices for machine learning.

After completing this section, you will be able to:

- Use **linear regression for prediction** as a baseline approach.

- Use **logistic regression** for categorical data.
- Detect trends in noisy data using **smoothing** (also known as **curve fitting** or **low pass filtering**).
- Convert predictors to **matrices** and outcomes to **vectors** when all predictors are numeric (or can be converted to numerics in a meaningful way).
- Perform basic **matrix algebra** calculations.

This section has three parts: **linear regression for prediction**, **smoothing**, and **working with matrices**.

Linear Regression for Prediction

There is a link to the relevant section of the textbook: Linear regression for prediction

Key points

- Linear regression can be considered a machine learning algorithm. Although it can be too rigid to be useful, it works rather well for some challenges. It also serves as a baseline approach: if you can't beat it with a more complex approach, you probably want to stick to linear regression.

Code

Note: the seed was not set before `createDataPartition` so your results may be different.

```
if(!require(HistData)) install.packages("HistData")
```

```
## Loading required package: HistData
```

```
library(HistData)

galton_heights <- GaltonFamilies %>%
  filter(childNum == 1 & gender == "male") %>%
  dplyr::select(father, childHeight) %>%
  rename(son = childHeight)

y <- galton_heights$son
test_index <- createDataPartition(y, times = 1, p = 0.5, list = FALSE)

train_set <- galton_heights %>% slice(-test_index)
test_set <- galton_heights %>% slice(test_index)

avg <- mean(train_set$son)
avg
```

```
## [1] 70.50114
```

```
mean((avg - test_set$son)^2)
```

```
## [1] 6.034931
```

```
# fit linear regression model
fit <- lm(son ~ father, data = train_set)
fit$coef
```

```
## (Intercept)      father
##  34.8934373   0.5170499
```

```
y_hat <- fit$coef[1] + fit$coef[2]*test_set$father
mean((y_hat - test_set$son)^2)
```

```
## [1] 4.632629
```

Predict Function

There is a link to the relevant section of the textbook: Predict function

Key points

- The `predict()` function takes a fitted object from functions such as `lm()` or `glm()` and a data frame with the new predictors for which to predict. We can use predict like this:

```
y_hat <- predict(fit, test_set)
```

- `predict()` is a generic function in R that calls other functions depending on what kind of object it receives. To learn about the specifics, you can read the help files using code like this:

```
?predict.lm    # or ?predict.glm
```

Code

```
y_hat <- predict(fit, test_set)
mean((y_hat - test_set$son)^2)
```

```
## [1] 4.632629
```

```
# read help files
?predict.lm
?predict.glm
```

Comprehension Check - Linear Regression

1. Create a data set using the following code:

```
# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
n <- 100
Sigma <- 9*matrix(c(1.0, 0.5, 0.5, 1.0), 2, 2)
dat <- MASS::mvrnorm(n = 100, c(69, 69), Sigma) %>%
      data.frame() %>% setNames(c("x", "y"))
```

We will build 100 linear models using the data above and calculate the mean and standard deviation of the combined models. First, set the seed to 1 again (make sure to use `sample.kind="Rounding"` if your R is version 3.6 or later). Then, within a `replicate()` loop, (1) partition the dataset into test and training sets with `p = 0.5` and using `dat$y` to generate your indices, (2) train a linear model predicting `y` from `x`, (3) generate predictions on the test set, and (4) calculate the RMSE of that model. Then, report the mean and standard deviation (SD) of the RMSEs from all 100 models.

Report all answers to at least 3 significant digits.

```
# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
rmse <- replicate(100, {
    test_index <- createDataPartition(dat$y, times = 1, p = 0.5, list = FALSE)
    train_set <- dat %>% slice(-test_index)
    test_set <- dat %>% slice(test_index)
    fit <- lm(y ~ x, data = train_set)
    y_hat <- predict(fit, newdata = test_set)
    sqrt(mean((y_hat-test_set$y)^2))
})

mean(rmse)
```

```
## [1] 2.488661
```

```
sd(rmse)
```

```
## [1] 0.1243952
```

2. Now we will repeat the exercise above but using larger datasets. Write a function that takes a size `n`, then (1) builds a dataset using the code provided at the top of Q1 but with `n` observations instead of 100 and without the `set.seed(1)`, (2) runs the `replicate()` loop that you wrote to answer Q1, which builds 100 linear models and returns a vector of RMSEs, and (3) calculates the mean and standard deviation of the 100 RMSEs.

Set the seed to 1 (if using R 3.6 or later, use the argument `sample.kind="Rounding"`) and then use `sapply()` or `map()` to apply your new function to `n <- c(100, 500, 1000, 5000, 10000)`.

Hint: You only need to set the seed once before running your function; do not set a seed within your function. Also be sure to use `sapply()` or `map()` as you will get different answers running the simulations individually due to setting the seed.

```
# set.seed(1) # if R 3.5 or earlier
set.seed(1, sample.kind="Rounding") # if R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
n <- c(100, 500, 1000, 5000, 10000)
res <- sapply(n, function(n){
    Sigma <- 9*matrix(c(1.0, 0.5, 0.5, 1.0), 2, 2)
    dat <- MASS::mvrnorm(n, c(69, 69), Sigma) %>%
        data.frame() %>% setNames(c("x", "y"))
    rmse <- replicate(100, {
        test_index <- createDataPartition(dat$y, times = 1, p = 0.5, list = FALSE)
        train_set <- dat %>% slice(-test_index)
        test_set <- dat %>% slice(test_index)
        fit <- lm(y ~ x, data = train_set)
        y_hat <- predict(fit, newdata = test_set)
        sqrt(mean((y_hat-test_set$y)^2))
    })
    c(avg = mean(rmse), sd = sd(rmse))
})

res
```

```
##          [,1]       [,2]       [,3]       [,4]       [,5]
## avg 2.4977540 2.72095125 2.55554451 2.62482800 2.61844227
## sd  0.1180821 0.08002108 0.04560258 0.02309673 0.01689205
```

3. What happens to the RMSE as the size of the dataset becomes larger?

☒ A. On average, the RMSE does not change much as n gets larger, but the variability of the RMSE decreases.
☐ B. Because of the law of large numbers the RMSE decreases; more data means more precise estimates.
☐ C. n = 10000 is not sufficiently large. To see a decrease in the RMSE we would need to make it larger.
☐ D. The RMSE is not a random variable.

4. Now repeat the exercise from Q1, this time making the correlation between `x` and `y` larger, as in the following code:

```
# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
n <- 100
Sigma <- 9*matrix(c(1.0, 0.95, 0.95, 1.0), 2, 2)
dat <- MASS::mvrnorm(n = 100, c(69, 69), Sigma) %>%
    data.frame() %>% setNames(c("x", "y"))
```

Note what happens to RMSE - set the seed to 1 as before.

```
# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
rmse <- replicate(100, {
    test_index <- createDataPartition(dat$y, times = 1, p = 0.5, list = FALSE)
    train_set <- dat %>% slice(-test_index)
    test_set <- dat %>% slice(test_index)
    fit <- lm(y ~ x, data = train_set)
    y_hat <- predict(fit, newdata = test_set)
    sqrt(mean((y_hat-test_set$y)^2))
})

mean(rmse)
```

```
## [1] 0.9099808
```

```
sd(rmse)
```

```
## [1] 0.06244347
```

5. Which of the following best explains why the RMSE in question 4 is so much lower than the RMSE in question 1?

☐ A. It is just luck. If we do it again, it will be larger.
☐ B. The central limit theorem tells us that the RMSE is normal.
☒ C. When we increase the correlation between x and y, x has more predictive power and thus provides a better estimate of y.
☐ D. These are both examples of regression so the RMSE has to be the same.

6. Create a data set using the following code.

```
# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
Sigma <- matrix(c(1.0, 0.75, 0.75, 0.75, 1.0, 0.25, 0.75, 0.25, 1.0), 3, 3)
dat <- MASS::mvrnorm(n = 100, c(0, 0, 0), Sigma) %>%
    data.frame() %>% setNames(c("y", "x_1", "x_2"))
```

Note that `y` is correlated with both `x_1` and `x_2` but the two predictors are independent of each other, as seen by `cor(dat)`.

Set the seed to 1, then use the **caret** package to partition into test and training sets with `p = 0.5`. Compare the RMSE when using just `x_1`, just `x_2` and both `x_1` and `x_2`. Train a single linear model for each (not 100 like in the previous questions).

Which of the three models performs the best (has the lowest RMSE)?

```
# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
test_index <- createDataPartition(dat$y, times = 1, p = 0.5, list = FALSE)
train_set <- dat %>% slice(-test_index)
test_set <- dat %>% slice(test_index)

fit <- lm(y ~ x_1, data = train_set)
y_hat <- predict(fit, newdata = test_set)
sqrt(mean((y_hat-test_set$y)^2))
```

```
## [1] 0.600666
```

```
fit <- lm(y ~ x_2, data = train_set)
y_hat <- predict(fit, newdata = test_set)
sqrt(mean((y_hat-test_set$y)^2))
```

```
## [1] 0.630699
```

```
fit <- lm(y ~ x_1 + x_2, data = train_set)
y_hat <- predict(fit, newdata = test_set)
sqrt(mean((y_hat-test_set$y)^2))
```

```
## [1] 0.3070962
```

- ☐ A. x_1
- ☐ B. x_2
- ☒ C. x_1 and x_2

7. Report the lowest RMSE of the three models tested in Q6.

```
fit <- lm(y ~ x_1 + x_2, data = train_set)
y_hat <- predict(fit, newdata = test_set)
sqrt(mean((y_hat-test_set$y)^2))
```

```
## [1] 0.3070962
```

8. Repeat the exercise from Q6 but now create an example in which `x_1` and `x_2` are highly correlated.

```
# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
Sigma <- matrix(c(1.0, 0.75, 0.75, 0.75, 1.0, 0.95, 0.75, 0.95, 1.0), 3, 3)
dat <- MASS::mvrnorm(n = 100, c(0, 0, 0), Sigma) %>%
    data.frame() %>% setNames(c("y", "x_1", "x_2"))
```

Set the seed to 1, then use the **caret** package to partition into a test and training set of equal size. Compare the RMSE when using just `x_1`, just `x_2`, and both `x_1` and `x_2`.

Compare the results from Q6 and Q8. What can you conclude?

```r
# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```r
test_index <- createDataPartition(dat$y, times = 1, p = 0.5, list = FALSE)
train_set <- dat %>% slice(-test_index)
test_set <- dat %>% slice(test_index)

fit <- lm(y ~ x_1, data = train_set)
y_hat <- predict(fit, newdata = test_set)
sqrt(mean((y_hat-test_set$y)^2))
```

```
## [1] 0.6592608
```

```r
fit <- lm(y ~ x_2, data = train_set)
y_hat <- predict(fit, newdata = test_set)
sqrt(mean((y_hat-test_set$y)^2))
```

```
## [1] 0.640081
```

```r
fit <- lm(y ~ x_1 + x_2, data = train_set)
y_hat <- predict(fit, newdata = test_set)
sqrt(mean((y_hat-test_set$y)^2))
```

```
## [1] 0.6597865
```

- ☐ A. Unless we include all predictors we have no predictive power.
- ☐ B. Adding extra predictors improves RMSE regardless of whether the added predictors are correlated with other predictors or not.
- ☐ C. Adding extra predictors results in over fitting.
- ☒ D. Adding extra predictors can improve RMSE substantially, but not when the added predictors are highly correlated with other predictors.

Regression for a Categorical Outcome

There is a link to the relevant section of the textbook: Regression for a categorical outcome

Key points

- The regression approach can be extended to categorical data. For example, we can try regression to estimate the conditional probability:

$p(x) = Pr(Y = 1|X = x) = \beta_0 + \beta_1 x$

- Once we have estimates β_0 and β_1, we can obtain an actual prediction $p(x)$. Then we can define a specific decision rule to form a prediction.

Code

```r
data("heights")
y <- heights$height

set.seed(2) #if you are using R 3.5 or earlier
set.seed(2, sample.kind = "Rounding") #if you are using R 3.6 or later
```

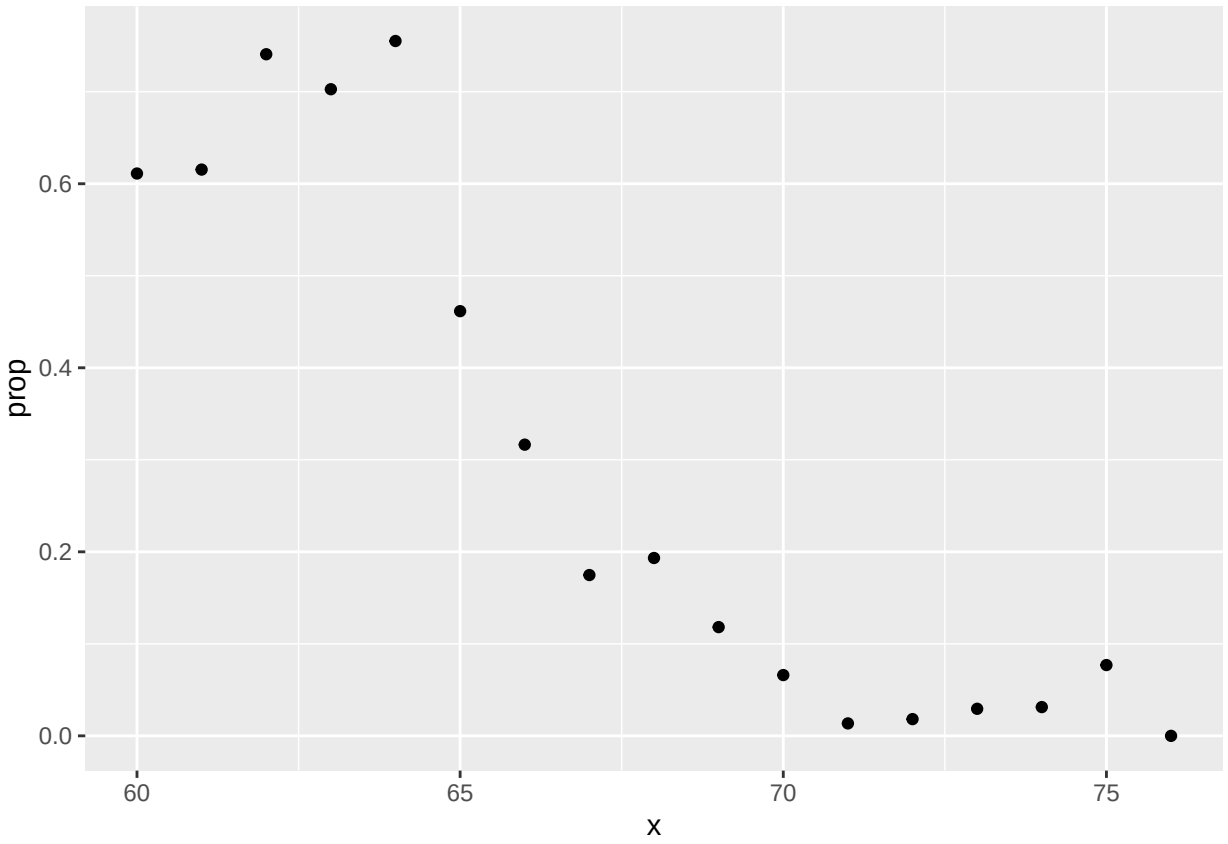
```
## Warning in set.seed(2, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```r
test_index <- createDataPartition(y, times = 1, p = 0.5, list = FALSE)
train_set <- heights %>% slice(-test_index)
test_set <- heights %>% slice(test_index)

train_set %>%
  filter(round(height)==66) %>%
  summarize(y_hat = mean(sex=="Female"))
```

```
##       y_hat
## 1 0.2424242
```

```r
heights %>%
  mutate(x = round(height)) %>%
  group_by(x) %>%
  filter(n() >= 10) %>%
  summarize(prop = mean(sex == "Female")) %>%
  ggplot(aes(x, prop)) +
  geom_point()
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```




```
lm_fit <- mutate(train_set, y = as.numeric(sex == "Female")) %>% lm(y ~ height, data = .)
p_hat <- predict(lm_fit, test_set)
y_hat <- ifelse(p_hat > 0.5, "Female", "Male") %>% factor()
confusionMatrix(y_hat, test_set$sex)$overall["Accuracy"]
```

```
##  Accuracy
## 0.7851711
```

Logistic Regression

There is a link to the relevant section of the textbook: Logistic regression

Key points

- **Logistic regression** is an extension of linear regression that assures that the estimate of conditional probability $Pr(Y = 1|X = x)$ is between 0 and 1. This approach makes use of the logistic transformation:

$g(p) = log\frac{p}{1-p}$

- With logistic regression, we model the conditional probability directly with:

$g\{Pr(Y = 1|X = x)\} = \beta_0 + \beta_1 x$

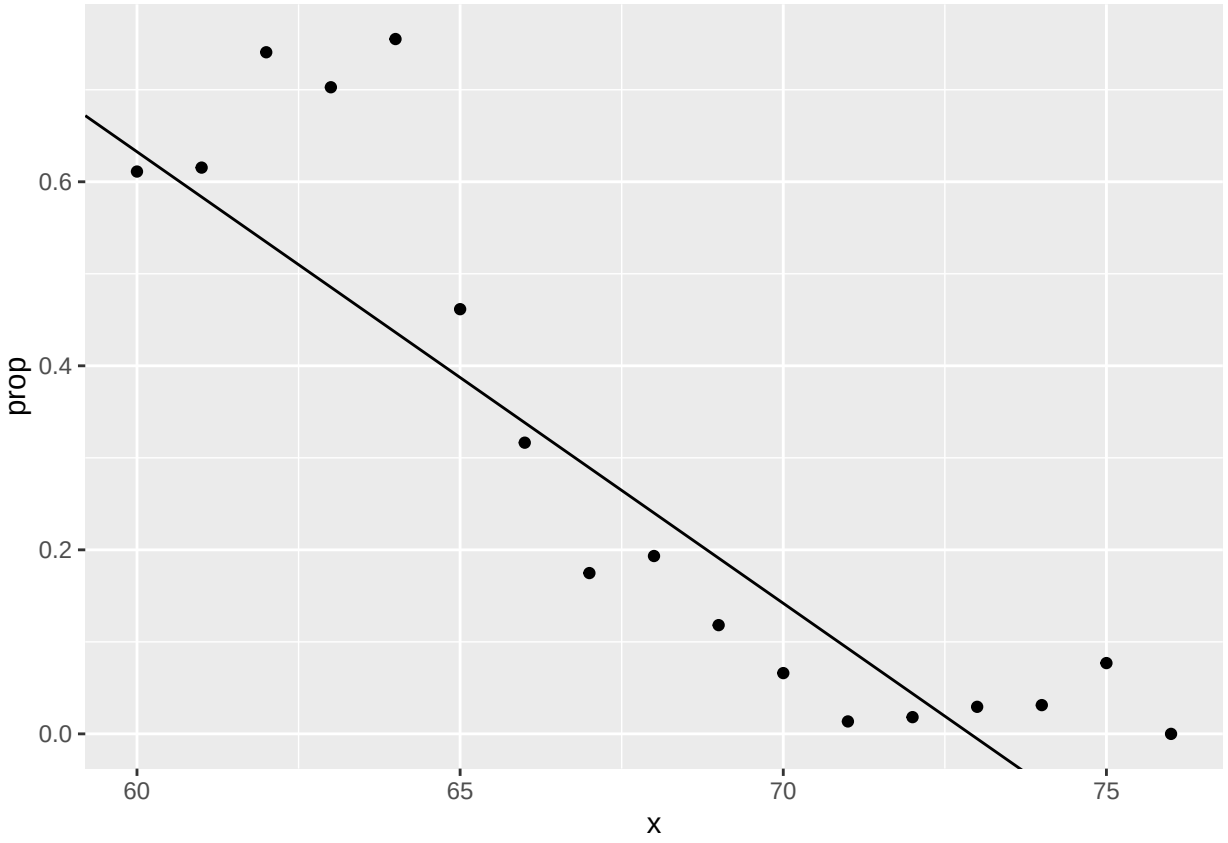
- Note that with this model, we can no longer use least squares. Instead we compute the **maximum likelihood estimate (MLE)**.

- In R, we can fit the logistic regression model with the function `glm()` (generalized linear models). If we want to compute the conditional probabilities, we want `type="response"` since the default is to return the logistic transformed values.

Code

```
heights %>%
  mutate(x = round(height)) %>%
  group_by(x) %>%
  filter(n() >= 10) %>%
  summarize(prop = mean(sex == "Female")) %>%
  ggplot(aes(x, prop)) +
  geom_point() +
  geom_abline(intercept = lm_fit$coef[1], slope = lm_fit$coef[2])
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```




```
range(p_hat)
```

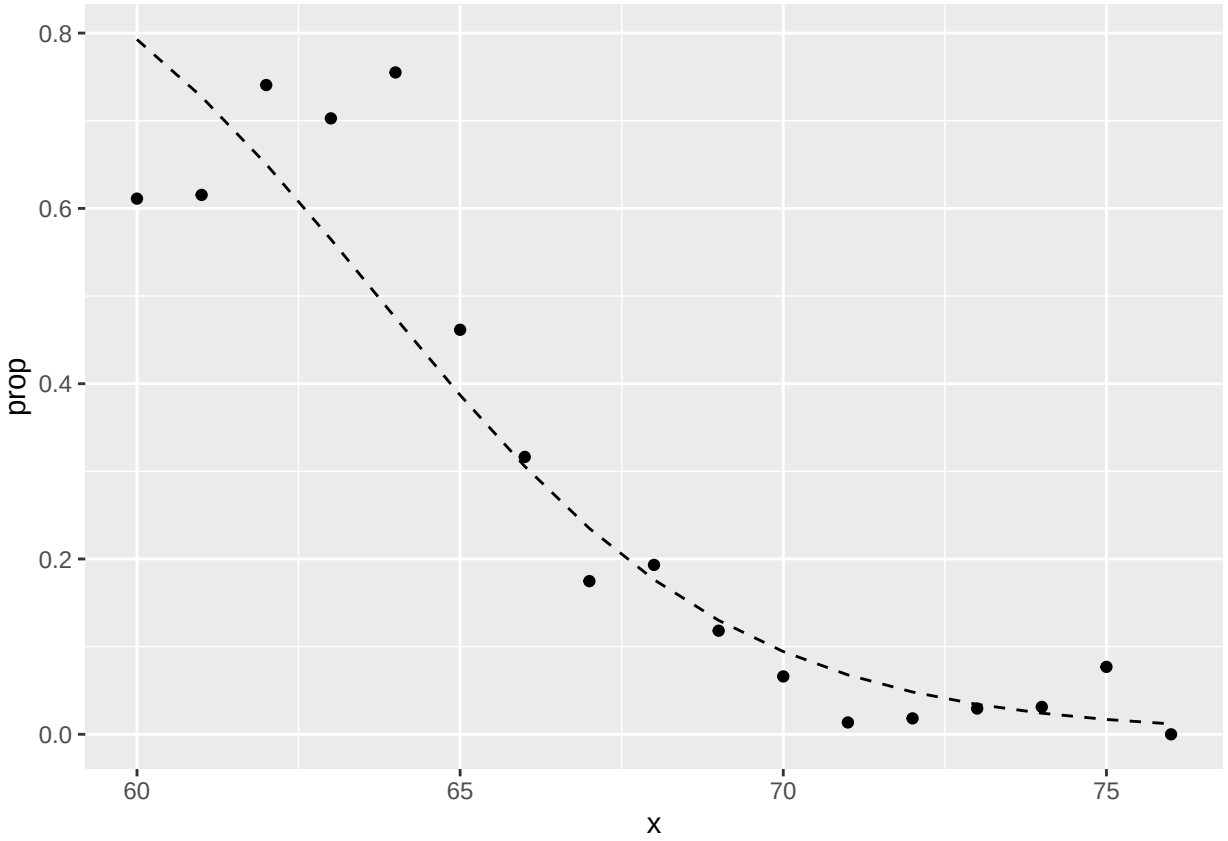
```
## [1] -0.397868  1.123309
```

```
# fit logistic regression model
glm_fit <- train_set %>%
  mutate(y = as.numeric(sex == "Female")) %>%
  glm(y ~ height, data=., family = "binomial")
```

```
p_hat_logit <- predict(glm_fit, newdata = test_set, type = "response")

tmp <- heights %>%
  mutate(x = round(height)) %>%
  group_by(x) %>%
  filter(n() >= 10) %>%
  summarize(prop = mean(sex == "Female"))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
logistic_curve <- data.frame(x = seq(min(tmp$x), max(tmp$x))) %>%
  mutate(p_hat = plogis(glm_fit$coef[1] + glm_fit$coef[2]*x))
tmp %>%
  ggplot(aes(x, prop)) +
  geom_point() +
  geom_line(data = logistic_curve, mapping = aes(x, p_hat), lty = 2)
```




```
y_hat_logit <- ifelse(p_hat_logit > 0.5, "Female", "Male") %>% factor
confusionMatrix(y_hat_logit, test_set$sex)$overall[["Accuracy"]]
```

```
## [1] 0.7984791
```

Case Study: 2 or 7

There is a link to the relevant section of the textbook: Case study: 2 or 7

Key points

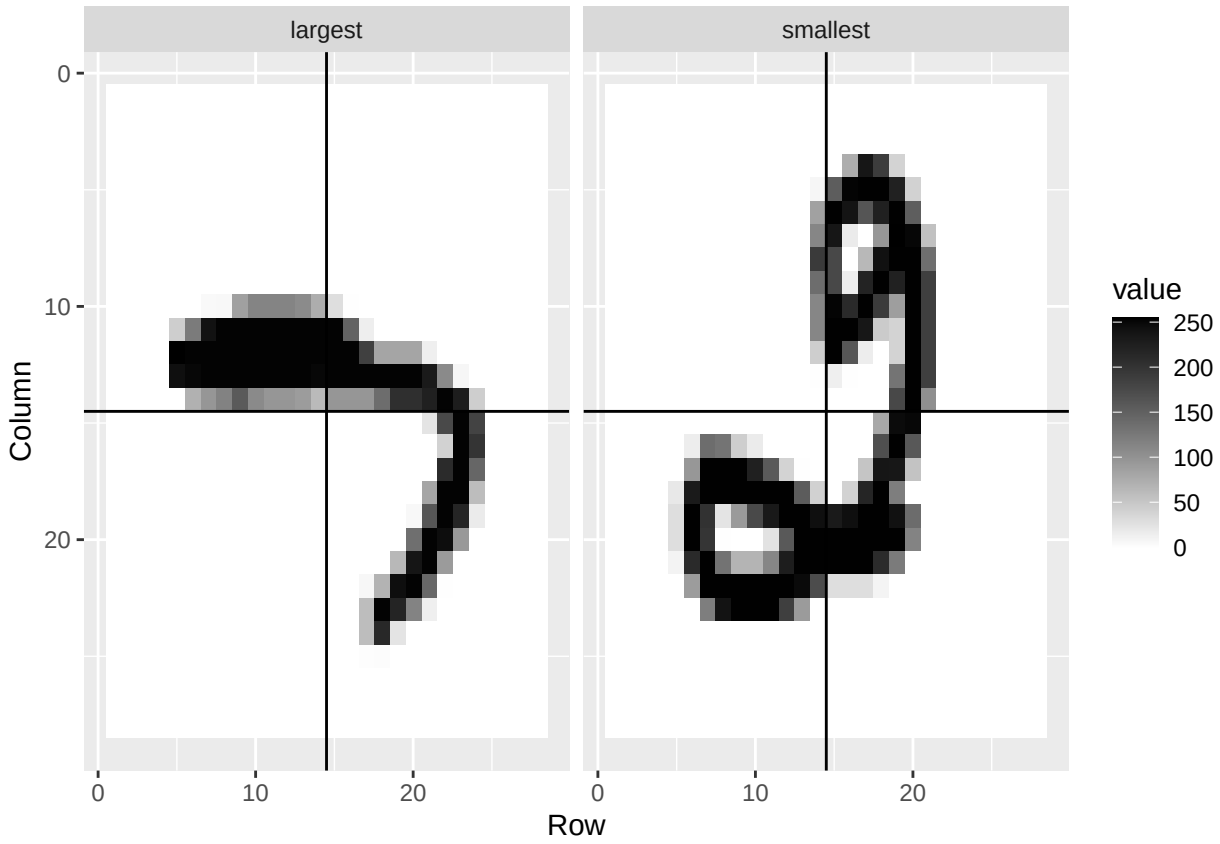
- In this case study we apply logistic regression to classify whether a digit is two or seven. We are interested in estimating a conditional probability that depends on two variables:

$$g\{p(x_1, x_2\} = g\{Pr(Y = 1|X_1 = x_1, X_2 = x_2)\} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

- Through this case, we know that logistic regression forces our estimates to be a **plane** and our boundary to be a **line**. This implies that a logistic regression approach has no chance of capturing the **non-linear** nature of the true $p(x_1, x_2)$. Therefore, we need other more flexible methods that permit other shapes.

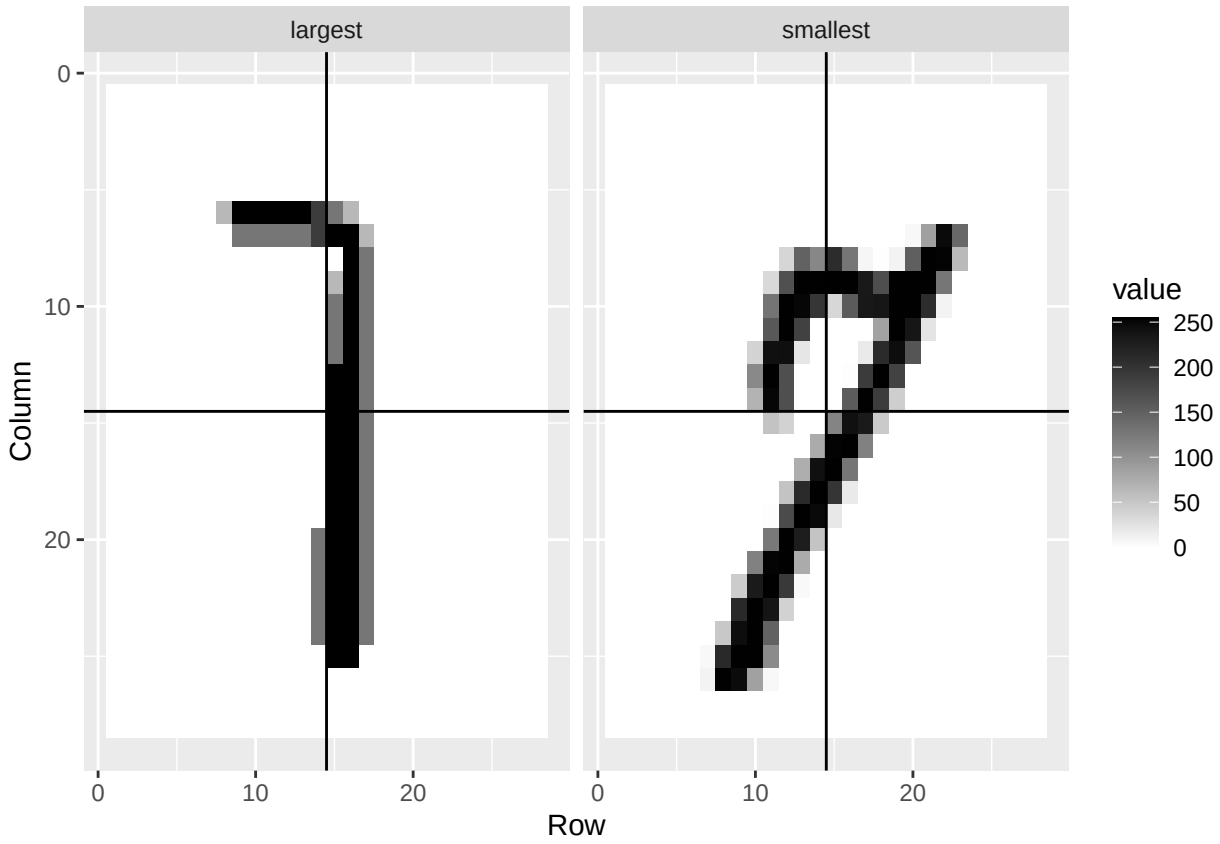
Code

```
mnist <- read_mnist()
is <- mnist_27$index_train[c(which.min(mnist_27$train$x_1), which.max(mnist_27$train$x_1))]
titles <- c("smallest","largest")
tmp <- lapply(1:2, function(i){
    expand.grid(Row=1:28, Column=1:28) %>%
        mutate(label=titles[i],
               value = mnist$train$images[is[i],])
})
tmp <- Reduce(rbind, tmp)
tmp %>% ggplot(aes(Row, Column, fill=value)) +
    geom_raster() +
    scale_y_reverse() +
    scale_fill_gradient(low="white", high="black") +
    facet_grid(.~label) +
    geom_vline(xintercept = 14.5) +
    geom_hline(yintercept = 14.5)
```




```
data("mnist_27")
mnist_27$train %>% ggplot(aes(x_1, x_2, color = y)) + geom_point()
```

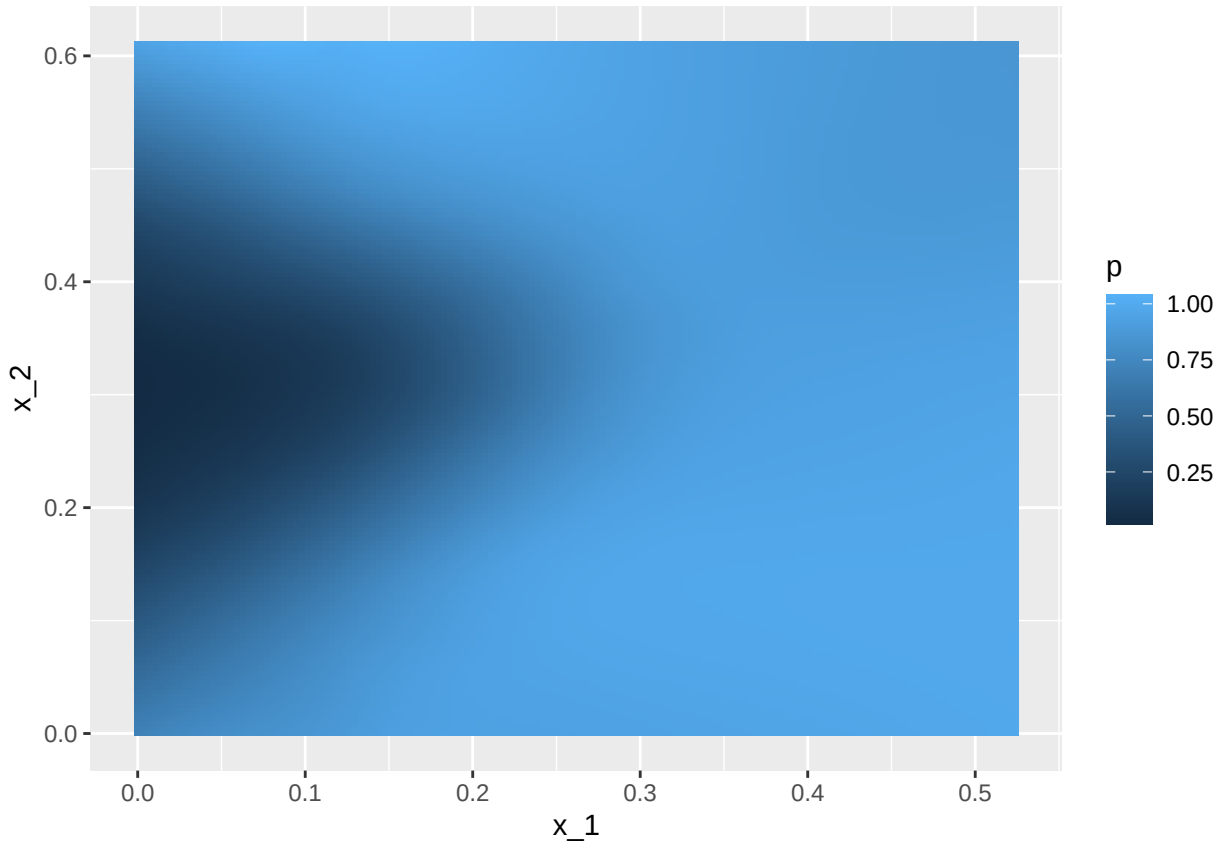

```
is <- mnist_27$index_train[c(which.min(mnist_27$train$x_2), which.max(mnist_27$train$x_2))]
titles <- c("smallest","largest")
tmp <- lapply(1:2, function(i){
    expand.grid(Row=1:28, Column=1:28) %>%
        mutate(label=titles[i],
               value = mnist$train$images[is[i],])
})
tmp <- Reduce(rbind, tmp)
tmp %>% ggplot(aes(Row, Column, fill=value)) +
    geom_raster() +
    scale_y_reverse() +
    scale_fill_gradient(low="white", high="black") +
    facet_grid(.~label) +
    geom_vline(xintercept = 14.5) +
    geom_hline(yintercept = 14.5)
```



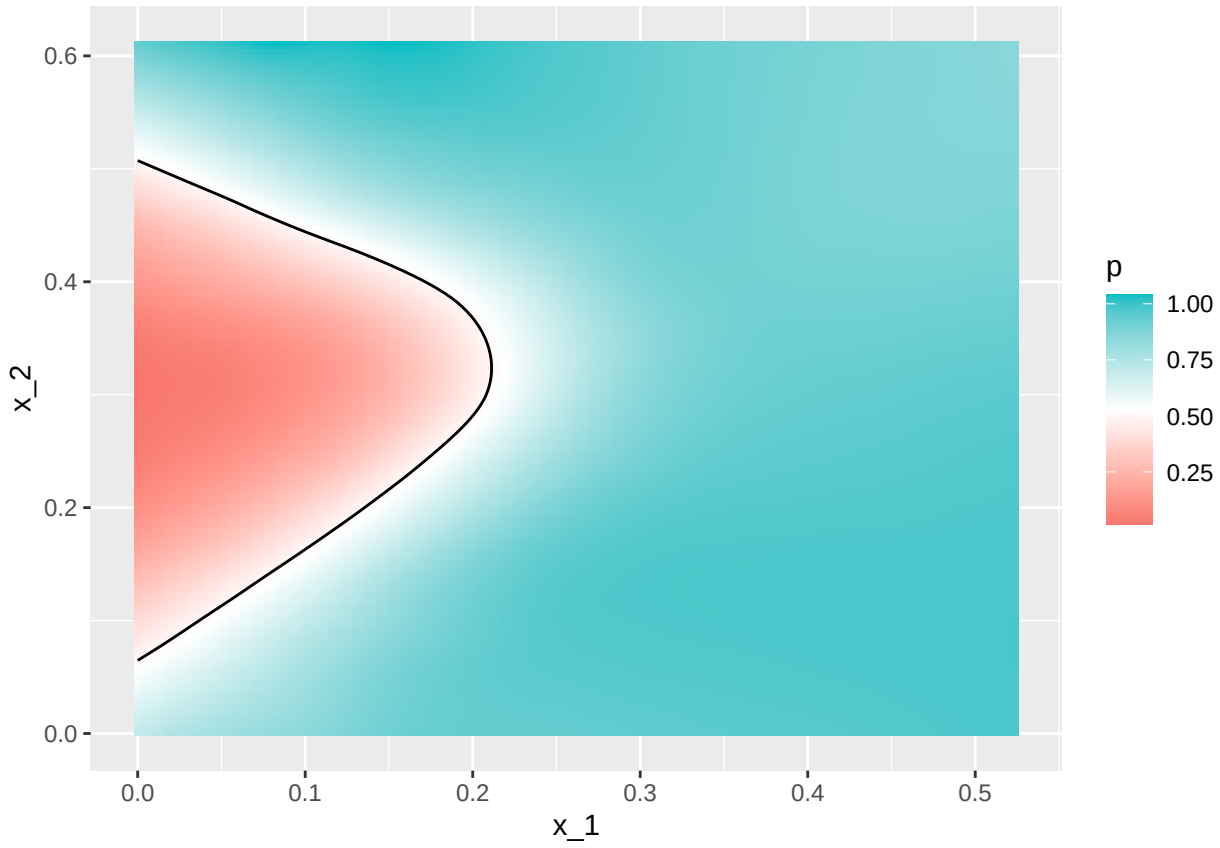

```
fit_glm <- glm(y ~ x_1 + x_2, data=mnist_27$train, family = "binomial")
p_hat_glm <- predict(fit_glm, mnist_27$test)
y_hat_glm <- factor(ifelse(p_hat_glm > 0.5, 7, 2))
confusionMatrix(data = y_hat_glm, reference = mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##     0.76
```

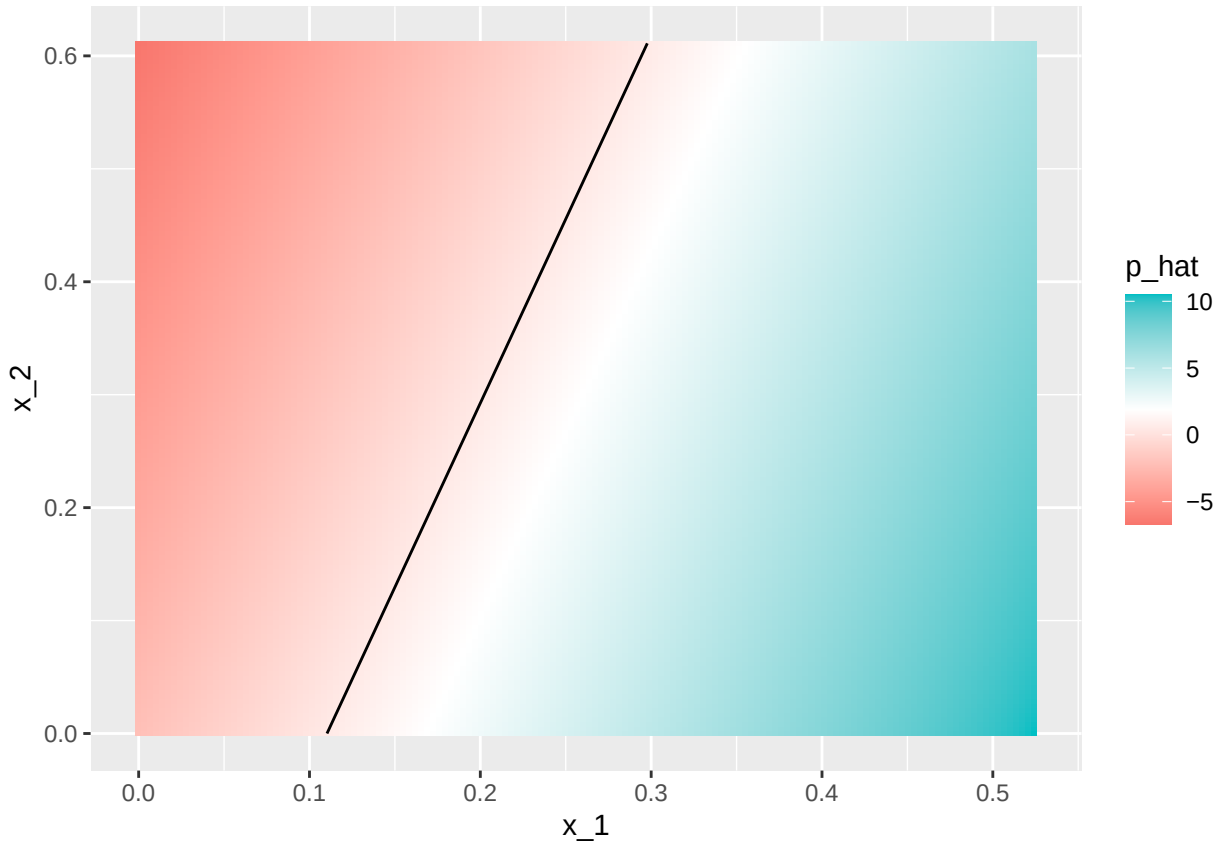
```
mnist_27$true_p %>% ggplot(aes(x_1, x_2, fill=p)) +
    geom_raster()
```



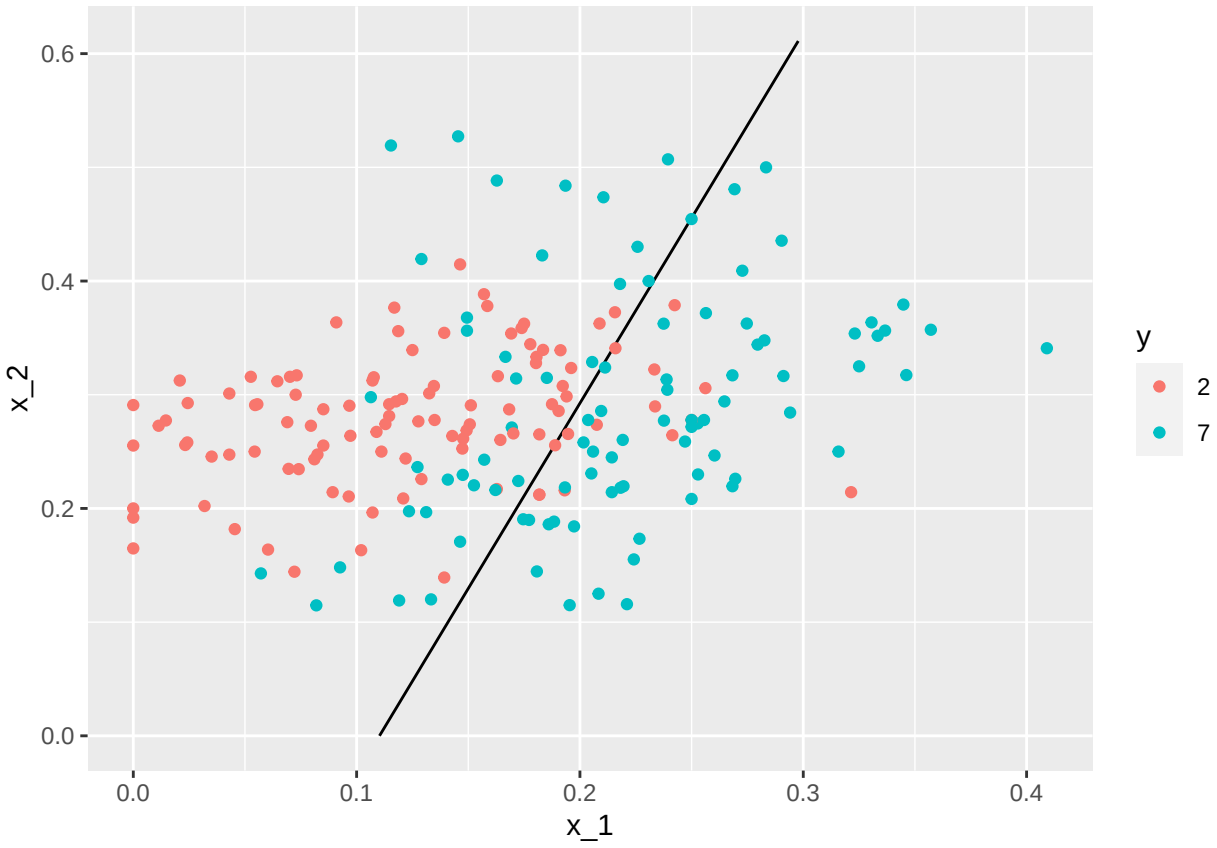

```
mnist_27$true_p %>% ggplot(aes(x_1, x_2, z=p, fill=p)) +
    geom_raster() +
    scale_fill_gradientn(colors=c("#F8766D","white","#00BFC4")) +
    stat_contour(breaks=c(0.5), color="black")
```




```
p_hat <- predict(fit_glm, newdata = mnist_27$true_p)
mnist_27$true_p %>%
    mutate(p_hat = p_hat) %>%
    ggplot(aes(x_1, x_2,  z=p_hat, fill=p_hat)) +
    geom_raster() +
    scale_fill_gradientn(colors=c("#F8766D","white","#00BFC4")) +
    stat_contour(breaks=c(0.5),color="black")
```




```
p_hat <- predict(fit_glm, newdata = mnist_27$true_p)
mnist_27$true_p %>%
    mutate(p_hat = p_hat) %>%
    ggplot() +
    stat_contour(aes(x_1, x_2, z=p_hat), breaks=c(0.5), color="black") +
    geom_point(mapping = aes(x_1, x_2, color=y), data = mnist_27$test)
```



Comprehension Check - Logistic Regression

1. Define a dataset using the following code:

```
# set.seed(2) #if you are using R 3.5 or earlier
set.seed(2, sample.kind="Rounding") #if you are using R 3.6 or later
```

```
## Warning in set.seed(2, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
make_data <- function(n = 1000, p = 0.5,
                mu_0 = 0, mu_1 = 2,
                sigma_0 = 1,  sigma_1 = 1){

y <- rbinom(n, 1, p)
f_0 <- rnorm(n, mu_0, sigma_0)
f_1 <- rnorm(n, mu_1, sigma_1)
x <- ifelse(y == 1, f_1, f_0)

test_index <- createDataPartition(y, times = 1, p = 0.5, list = FALSE)

list(train = data.frame(x = x, y = as.factor(y)) %>% slice(-test_index),
    test = data.frame(x = x, y = as.factor(y)) %>% slice(test_index))
}
dat <- make_data()
```

Note that we have defined a variable `x` that is predictive of a binary outcome `y`:

`dat$train %>% ggplot(aes(x, color = y)) + geom_density()`.

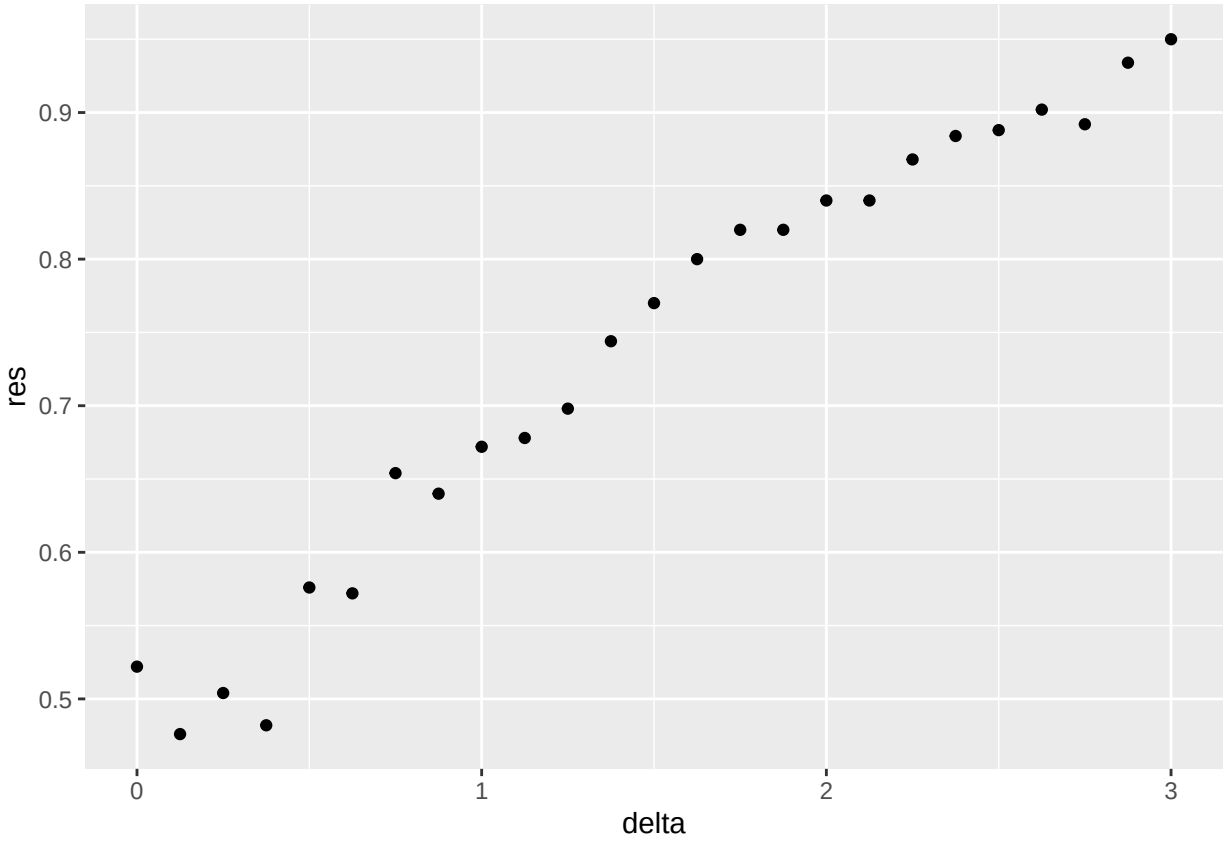
Set the seed to 1, then use the `make_data()` function defined above to generate 25 different datasets with `mu_1 <- seq(0, 3, len=25)`. Perform logistic regression on each of the 25 different datasets (predict 1 if $p > 0.5$) and plot accuracy (`res` in the figures) vs mu_1 (`delta` in the figures).

Which is the correct plot?

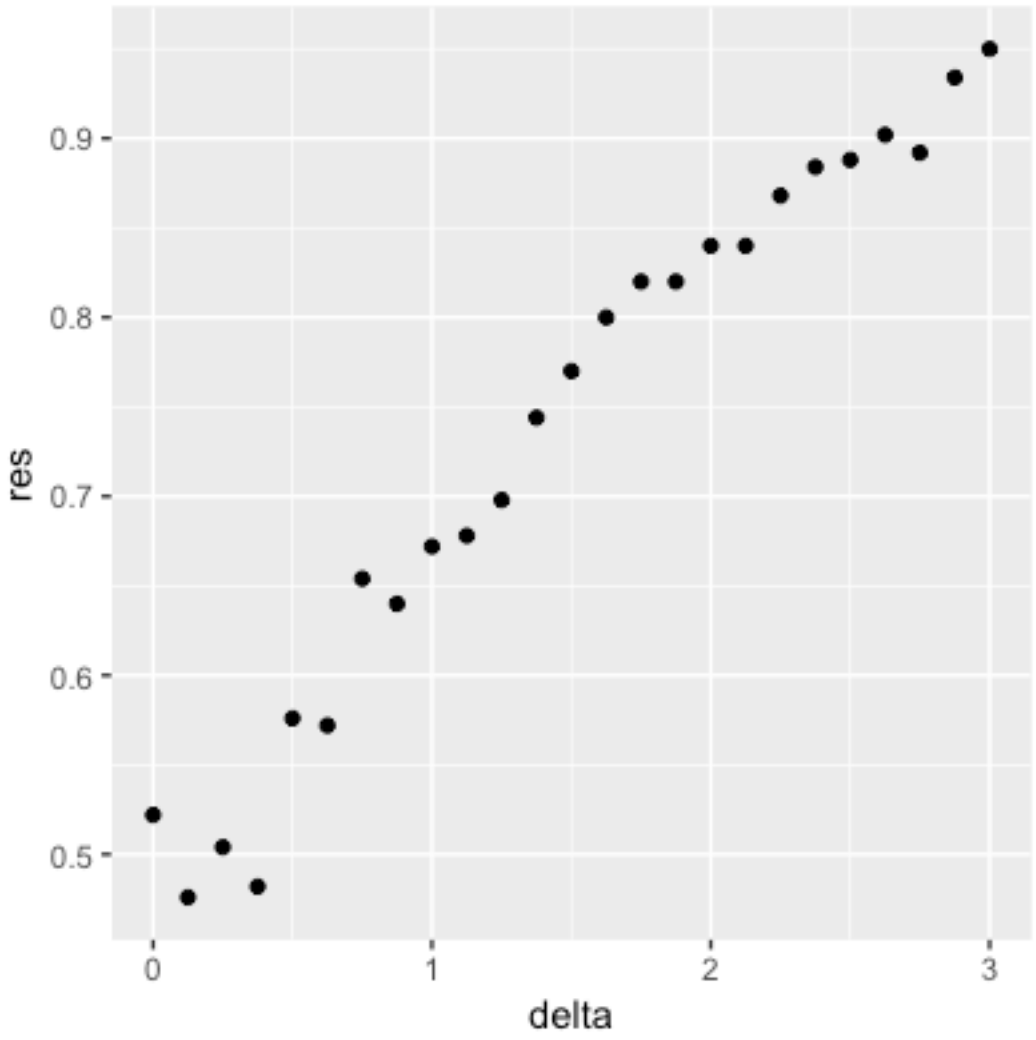
```
set.seed(1) #if you are using R 3.5 or earlier
set.seed(1, sample.kind="Rounding") #if you are using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

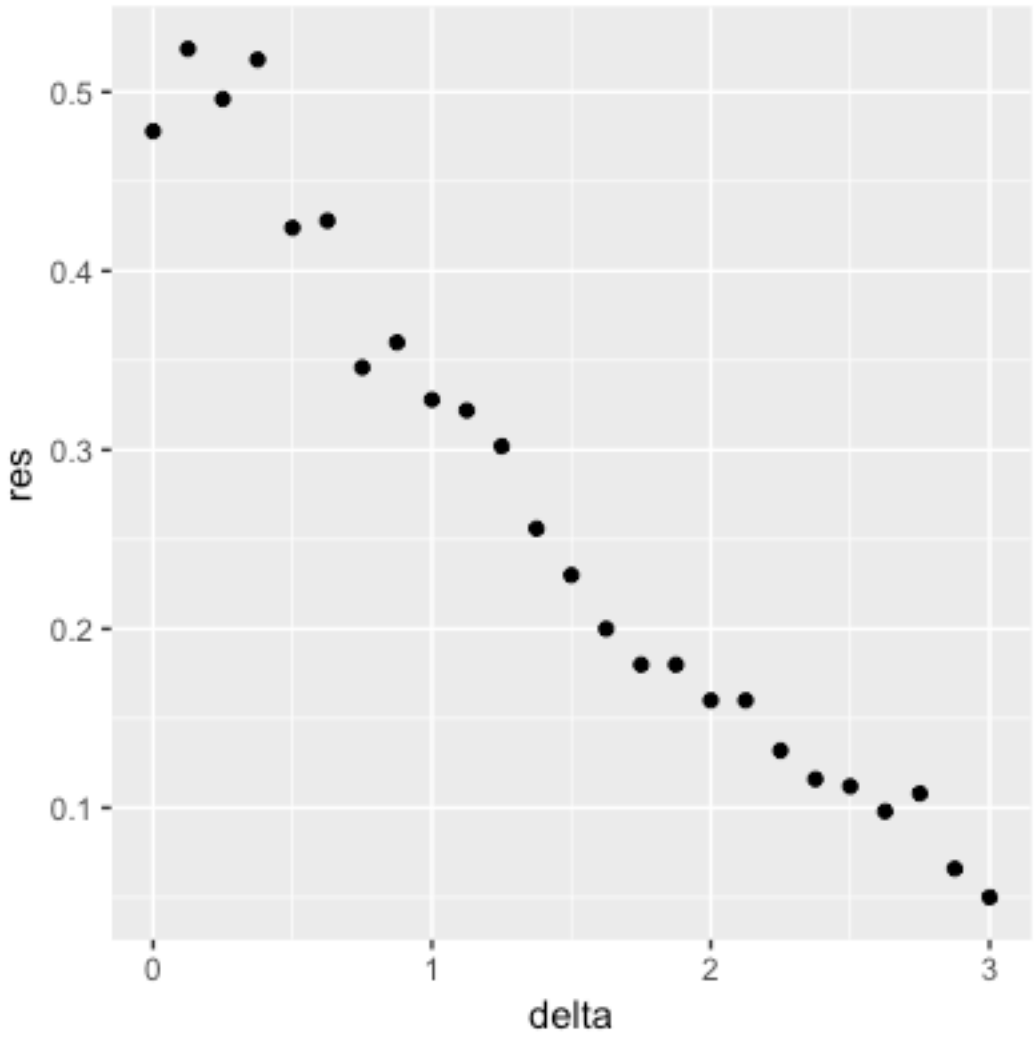
```
delta <- seq(0, 3, len = 25)
res <- sapply(delta, function(d){
    dat <- make_data(mu_1 = d)
    fit_glm <- dat$train %>% glm(y ~ x, family = "binomial", data = .)
    y_hat_glm <- ifelse(predict(fit_glm, dat$test) > 0.5, 1, 0) %>% factor(levels = c(0, 1))
    mean(y_hat_glm == dat$test$y)
})
qplot(delta, res)
```



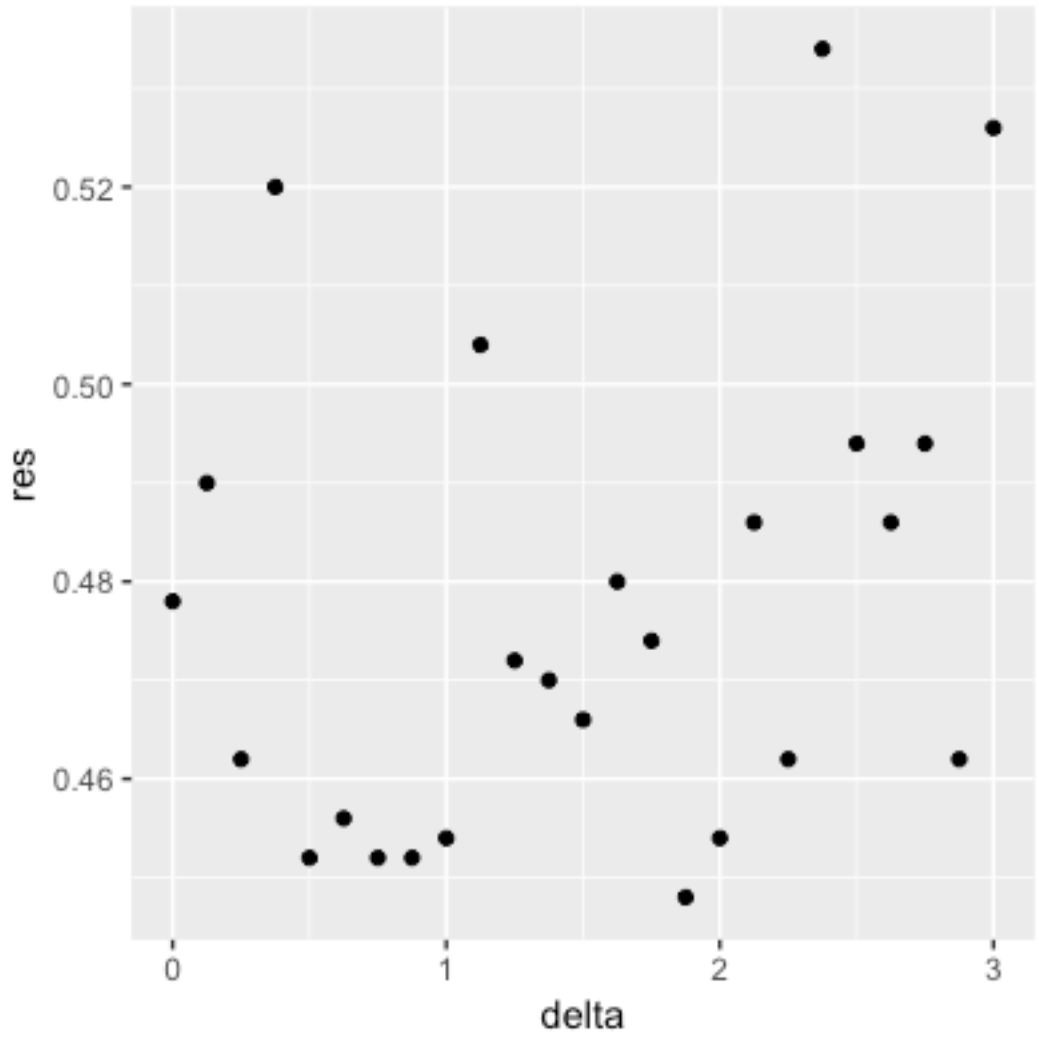
☒ A.



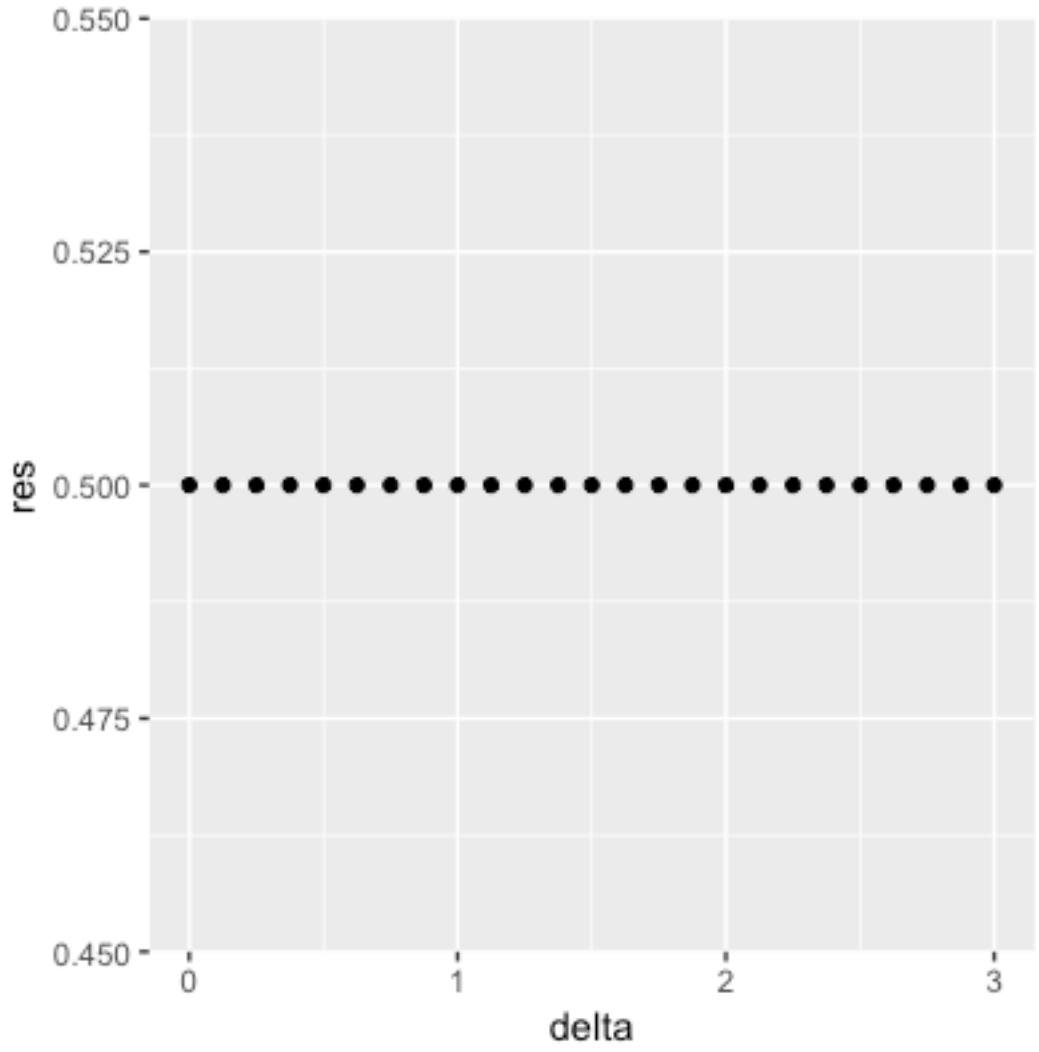
☐ B.



□ C.



□ D.



Introduction to Smoothing

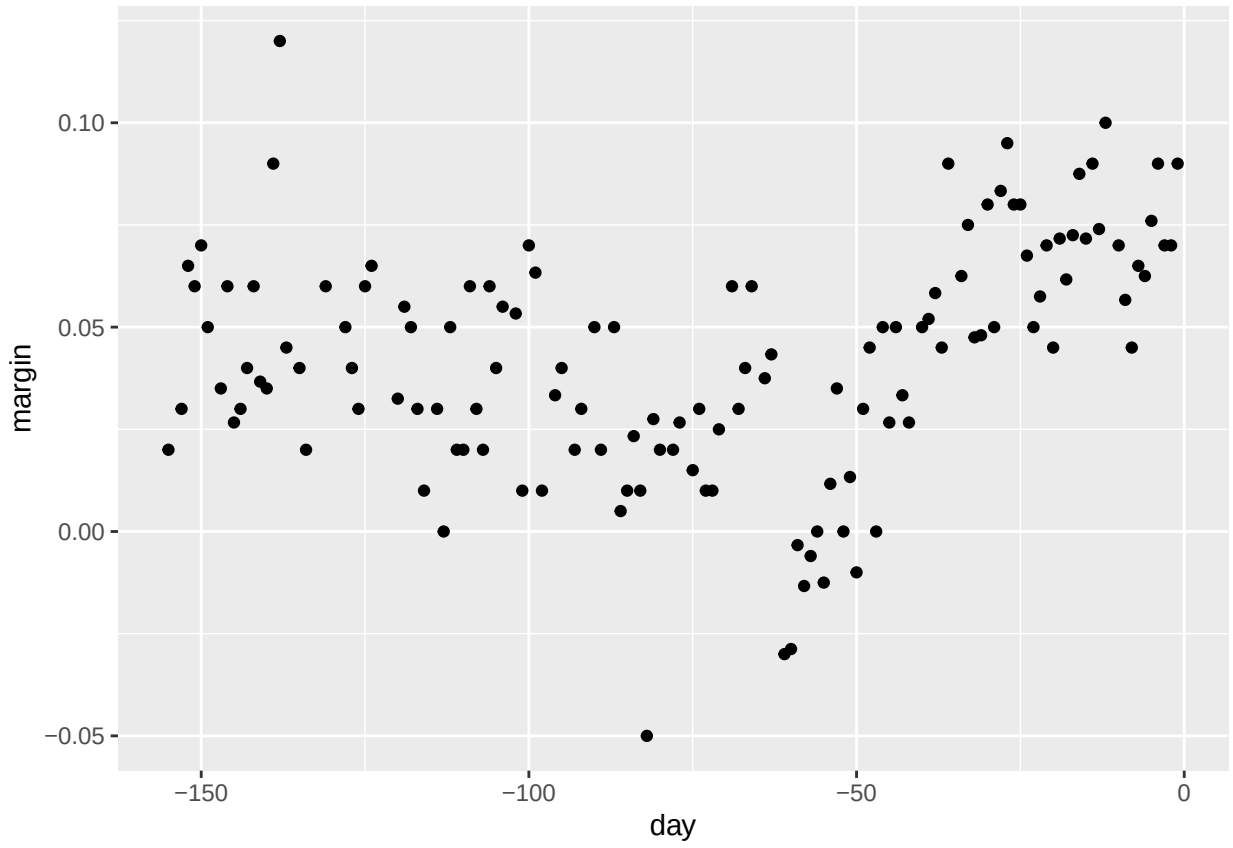
There is a link to the relevant section of the textbook: Smoothing

Key points

- **Smoothing** is a very powerful technique used all across data analysis. It is designed to detect trends in the presence of noisy data in cases in which the shape of the trend is unknown.
- The concepts behind smoothing techniques are extremely useful in machine learning because **conditional expectations/probabilities** can be thought of as **trends** of unknown shapes that we need to estimate in the presence of uncertainty.

Code

```
data("polls_2008")
qplot(day, margin, data = polls_2008)
```



Bin Smoothing and Kernels

There is a link to the relevant sections of the textbook: Bin smoothing and Kernels

Key points

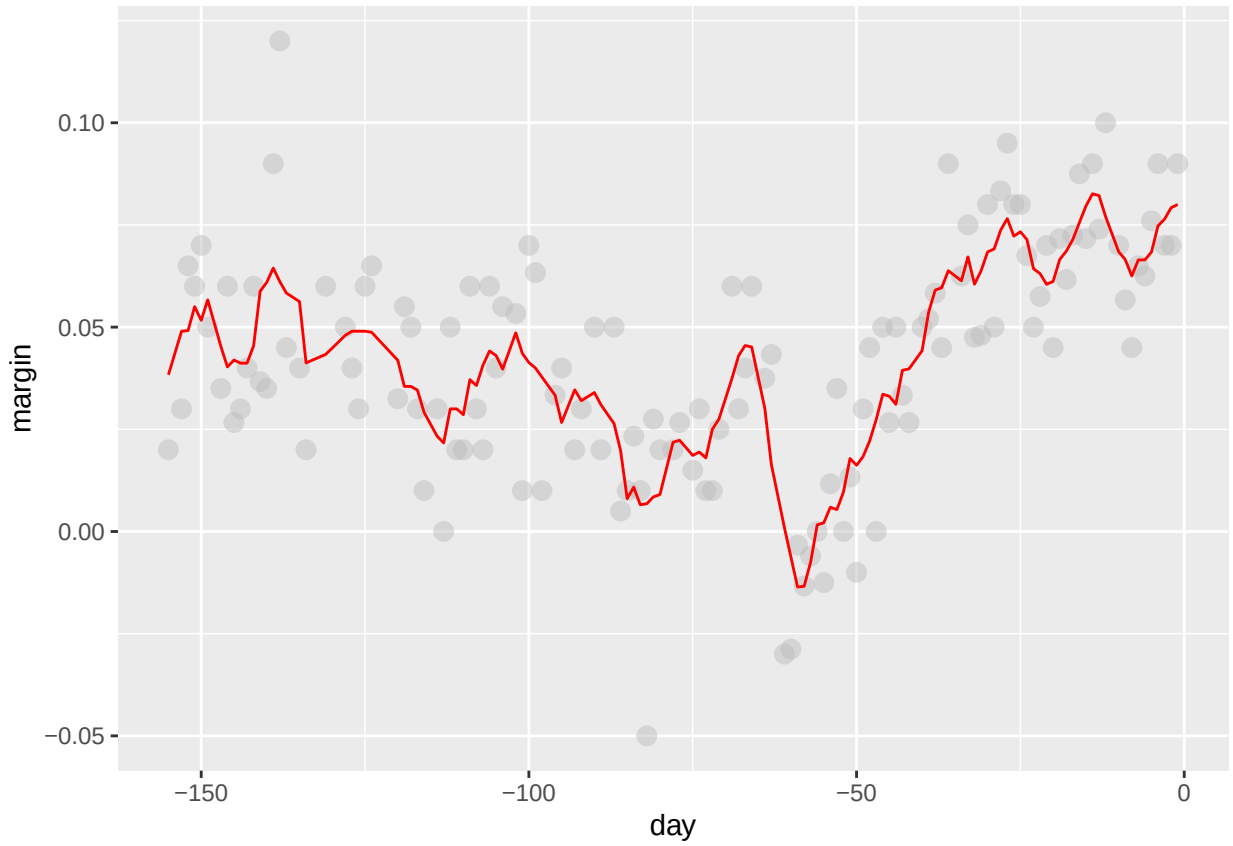
- The general idea of smoothing is to group data points into strata in which the value of $f(x)$ can be assumed to be constant. We can make this assumption because we think $f(x)$ changes slowly and, as a result, $f(x)$ is almost constant in small windows of time.
- This assumption implies that a good estimate for $f(x)$ is the average of the Y_i values in the window. The estimate is:

$\hat{f}(x_0) = \frac{1}{N_0} \sum_{i \in A_0} Y_i$

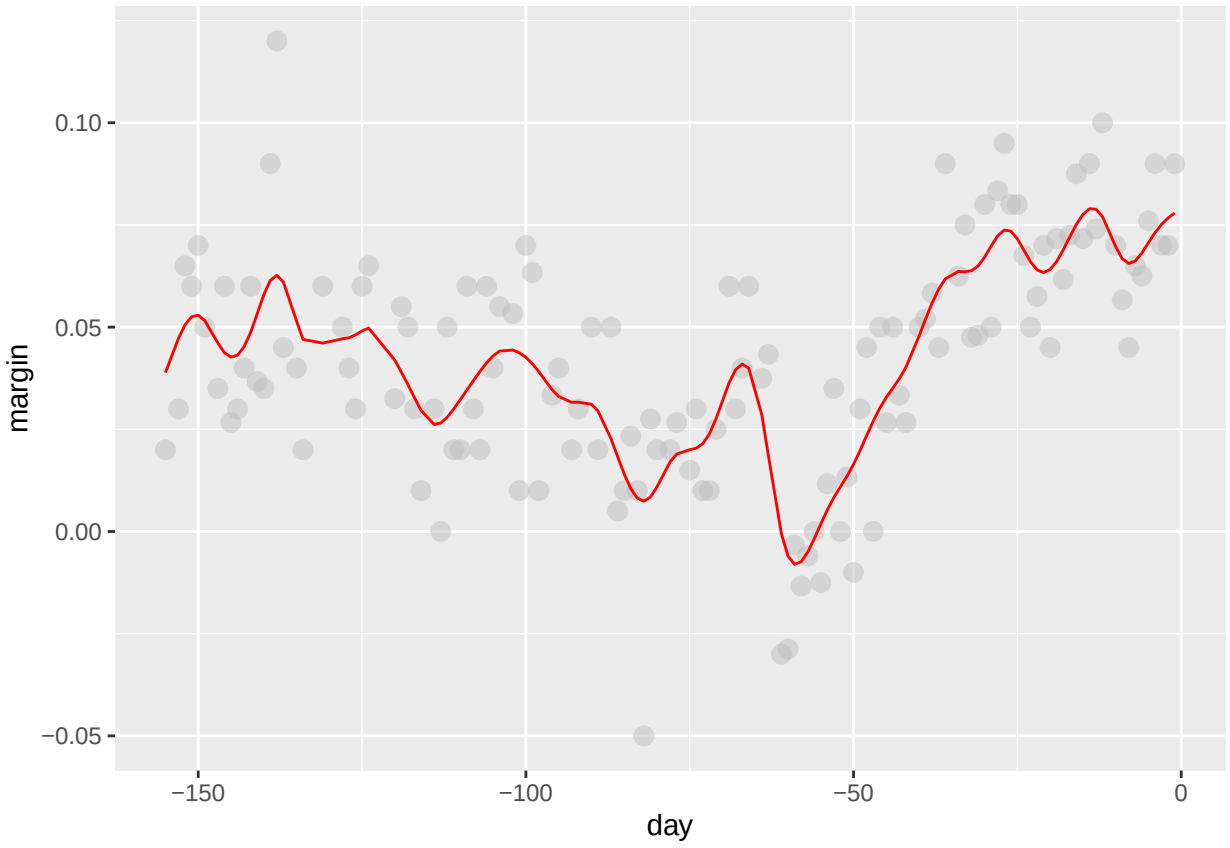
- In smoothing, we call the size of the interval $|x - x_0|$ satisfying the particular condition the window size, bandwidth or span.

Code

```
# bin smoothers
span <- 7
fit <- with(polls_2008,ksmooth(day, margin, x.points = day, kernel="box", bandwidth =span))
polls_2008 %>% mutate(smooth = fit$y) %>%
    ggplot(aes(day, margin)) +
    geom_point(size = 3, alpha = .5, color = "grey") +
    geom_line(aes(day, smooth), color="red")
```




```
# kernel
span <- 7
fit <- with(polls_2008, ksmooth(day, margin,  x.points = day, kernel="normal", bandwidth = span))
polls_2008 %>% mutate(smooth = fit$y) %>%
  ggplot(aes(day, margin)) +
  geom_point(size = 3, alpha = .5, color = "grey") +
  geom_line(aes(day, smooth), color="red")
```



Local Weighted Regression (loess)

There is a link to the relevant section of the textbook: Local weighted regression

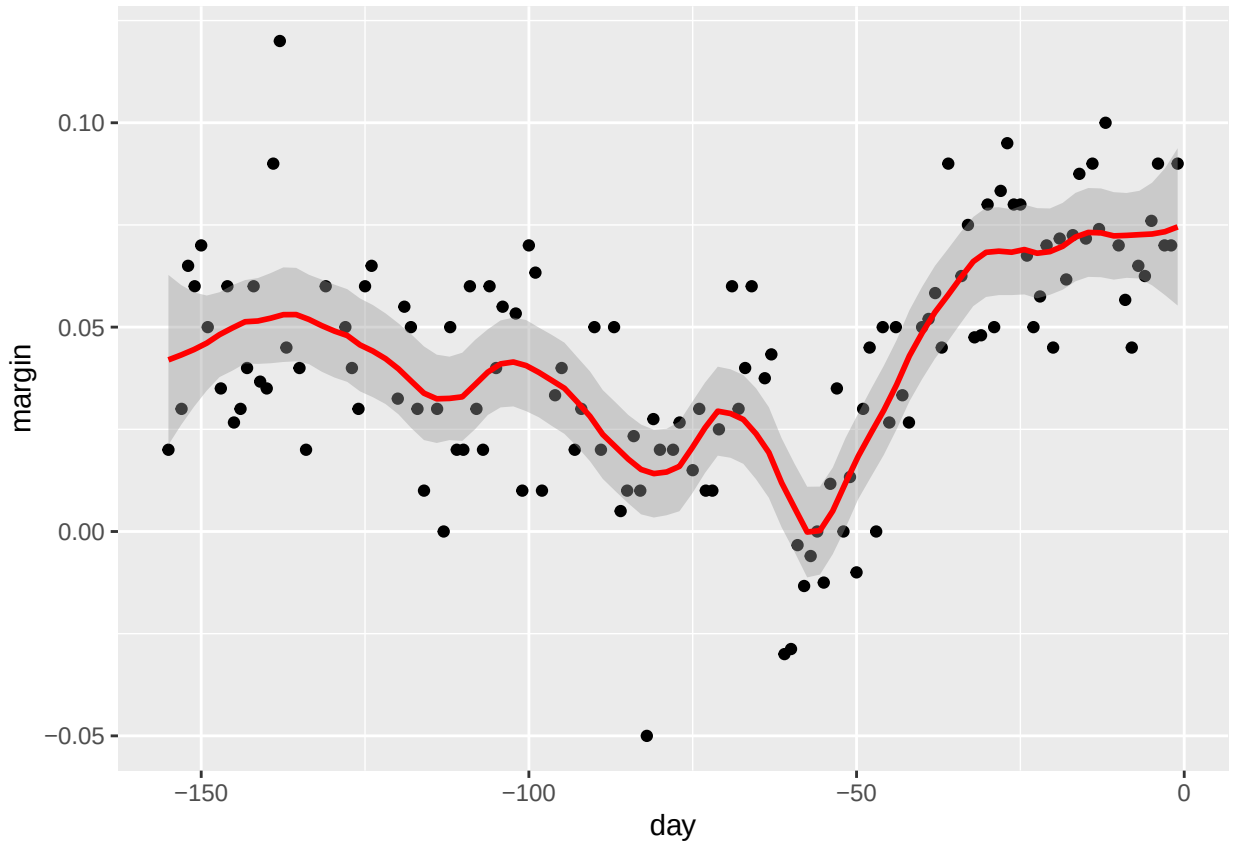
Key points

- A limitation of the bin smoothing approach is that we need small windows for the approximately constant assumptions to hold which may lead to imprecise estimates of $f(x)$. **Local weighted regression (loess)** permits us to consider larger window sizes.
- One important difference between loess and bin smoother is that we assume the smooth function is locally **linear** in a window instead of constant.
- The result of loess is a smoother fit than bin smoothing because we use larger sample sizes to estimate our local parameters.

Code

```
polls_2008 %>% ggplot(aes(day, margin)) +
  geom_point() +
  geom_smooth(color="red", span = 0.15, method = "loess", method.args = list(degree=1))
```

```
## `geom_smooth()` using formula 'y ~ x'
```



Comprehension Check - Smoothing

1. In the Wrangling course of this series, PH125.6x, we used the following code to obtain mortality counts for Puerto Rico for 2015-2018:

```
if(!require(purrr)) install.packages("purrr")
if(!require(pdftools)) install.packages("pdftools")
```

```
## Loading required package: pdftools
```

```
## Using poppler version 0.73.0
```

```
library(tidyverse)
library(lubridate)
library(purrr)
library(pdftools)

fn <- system.file("extdata", "RD-Mortality-Report_2015-18-180531.pdf", package="dslabs")
dat <- map_df(str_split(pdf_text(fn), "\n"), function(s){
    s <- str_trim(s)
    header_index <- str_which(s, "2015")[1]
    tmp <- str_split(s[header_index], "\\s+", simplify = TRUE)
    month <- tmp[1]
    header <- tmp[-1]
```

```
    tail_index  <- str_which(s, "Total")
    n <- str_count(s, "\\d+")
    out <- c(1:header_index, which(n==1), which(n>=28), tail_index:length(s))
    s[-out] %>%
        str_remove_all("[^\\d\\s]") %>%
        str_trim() %>%
        str_split_fixed("\\s+", n = 6) %>%
        .[,1:5] %>%
        as_data_frame() %>%
        setNames(c("day", header)) %>%
        mutate(month = month,
            day = as.numeric(day)) %>%
        gather(year, deaths, -c(day, month)) %>%
        mutate(deaths = as.numeric(deaths))
}) %>%
    mutate(month = recode(month, "JAN" = 1, "FEB" = 2, "MAR" = 3, "APR" = 4, "MAY" = 5, "JUN" = 6,
                          "JUL" = 7, "AGO" = 8, "SEP" = 9, "OCT" = 10, "NOV" = 11, "DEC" = 12)) %>%
    mutate(date = make_date(year, month, day)) %>%
        dplyr::filter(date <= "2018-05-01")
```

```
## Warning: `as_data_frame()` is deprecated as of tibble 2.0.0.
## Please use `as_tibble()` instead.
## The signature and semantics have changed, see `?as_tibble`.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_warnings()` to see where this warning was generated.
```

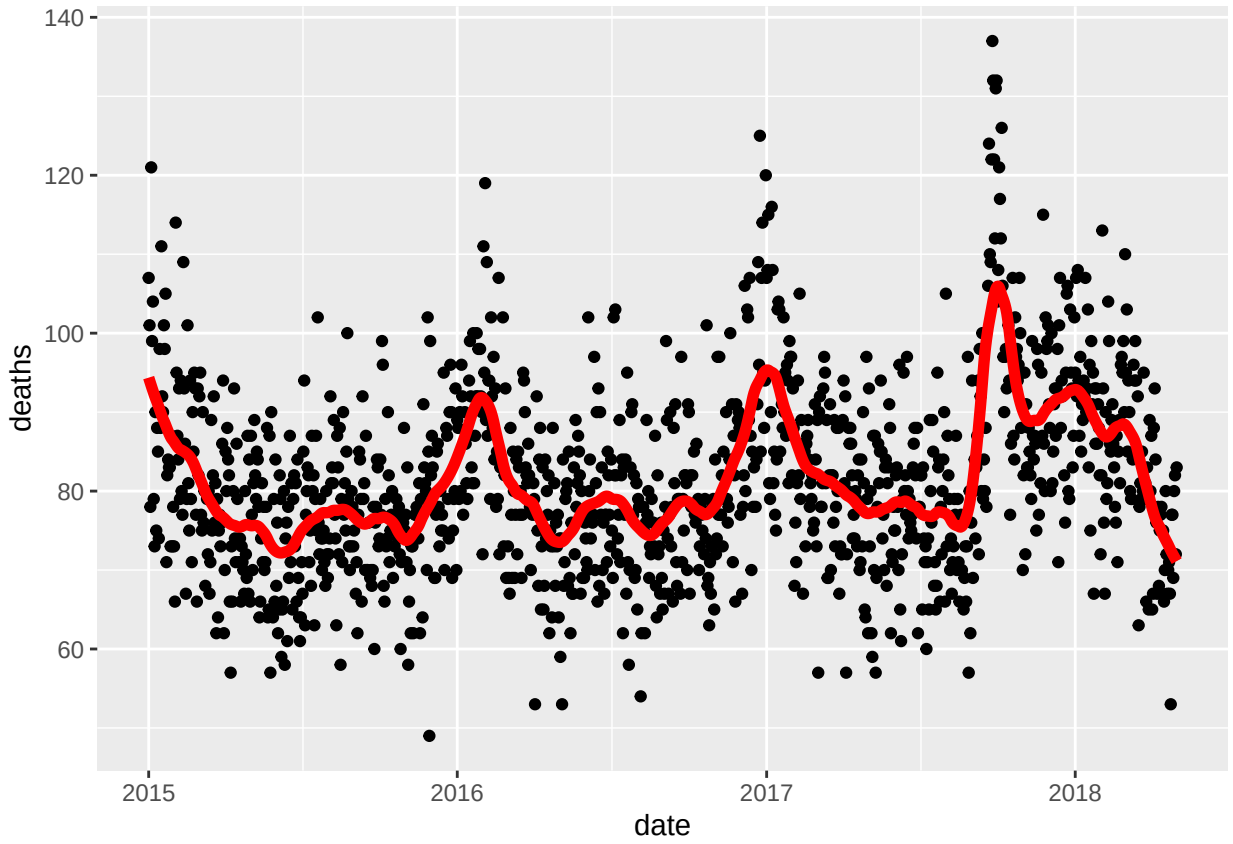
```
## Warning: The `x` argument of `as_tibble.matrix()` must have unique column names if `.name_repair` is
## Using compatibility `.name_repair`.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_warnings()` to see where this warning was generated.
```

Use the `loess()` function to obtain a smooth estimate of the expected number of deaths as a function of date. Plot this resulting smooth function. Make the span about two months long.

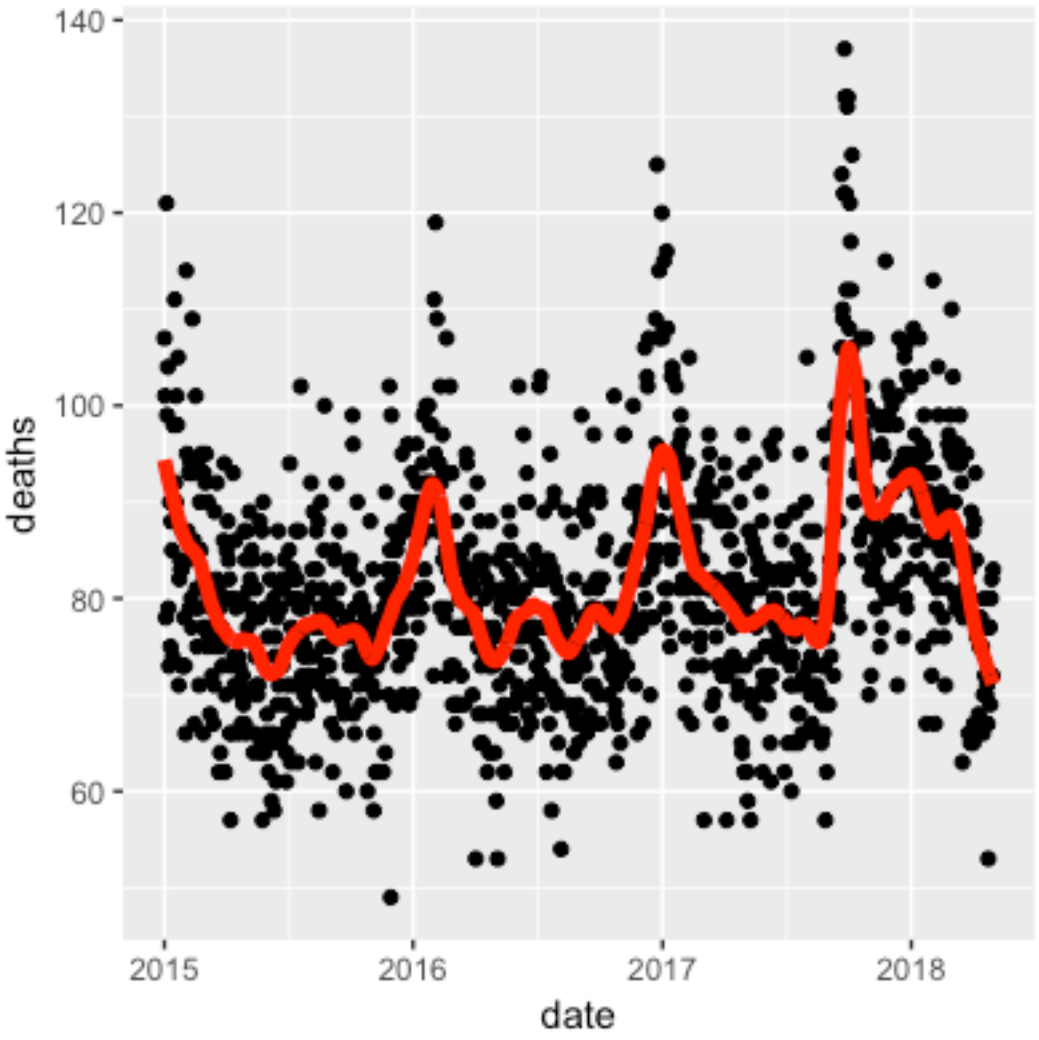
Which of the following plots is correct?

```
span <- 60 / as.numeric(diff(range(dat$date)))
fit <- dat %>% mutate(x = as.numeric(date)) %>% loess(deaths ~ x, data = ., span = span, degree = 1)
dat %>% mutate(smooth = predict(fit, as.numeric(date))) %>%
    ggplot() +
    geom_point(aes(date, deaths)) +
    geom_line(aes(date, smooth), lwd = 2, col = "red")
```

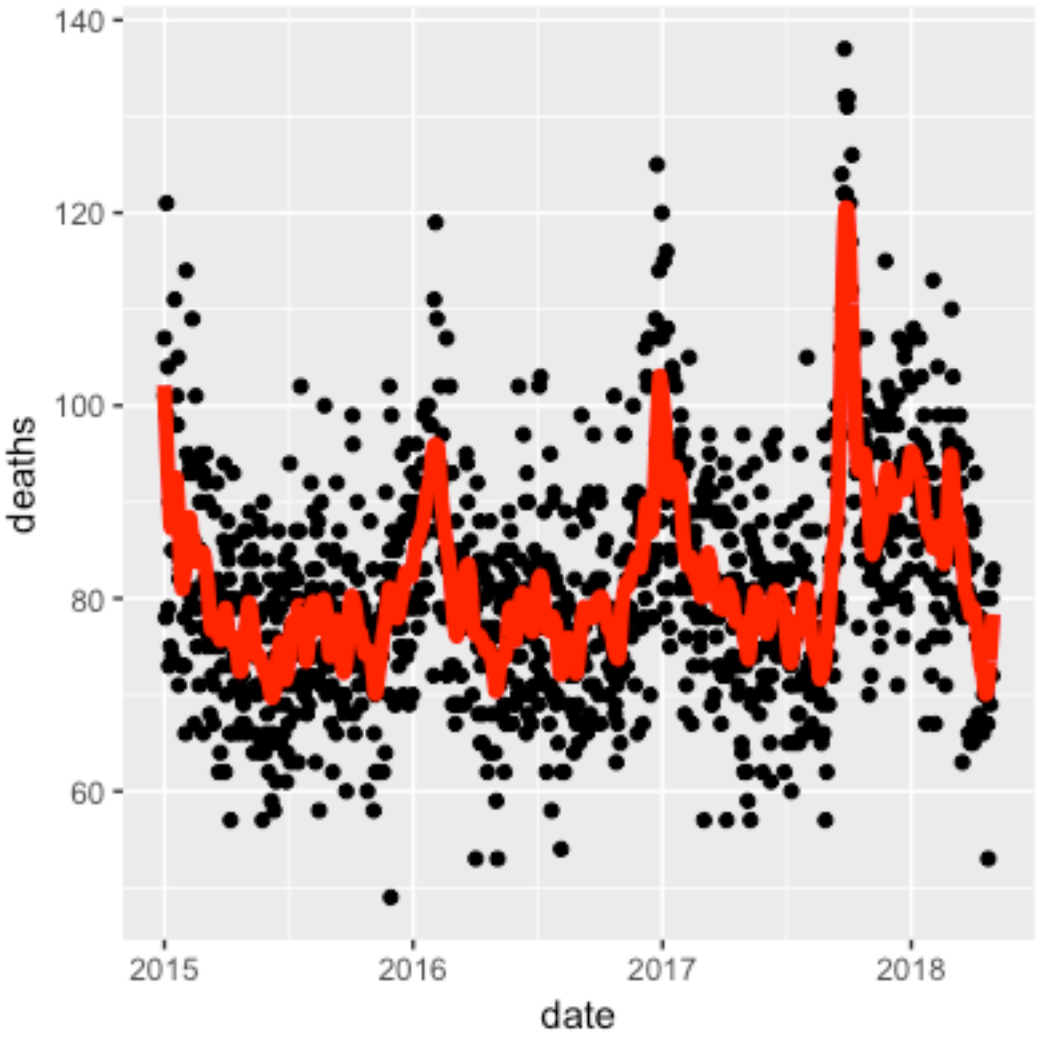
```
## Warning: Removed 1 rows containing missing values (geom_point).
```



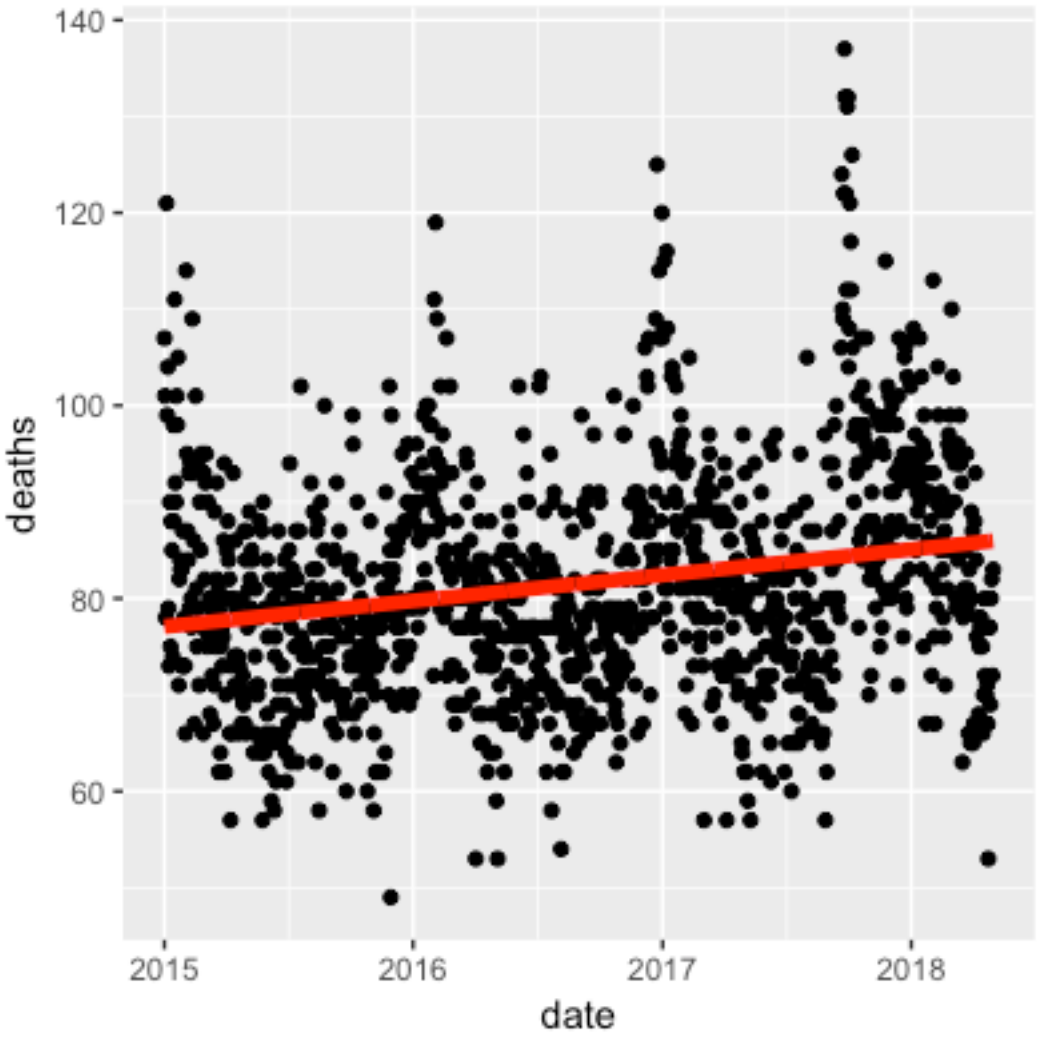
☒ A.



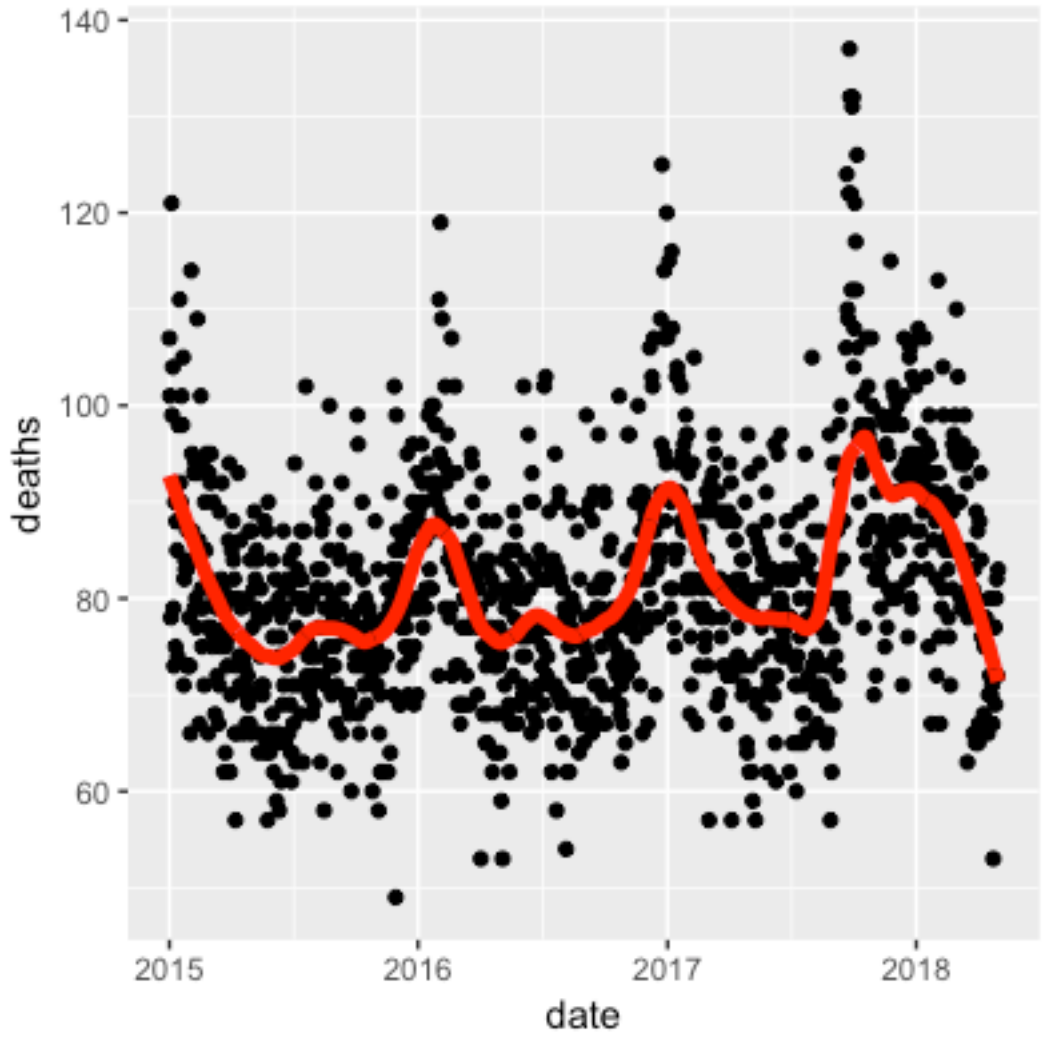
☐ B.



□ C.



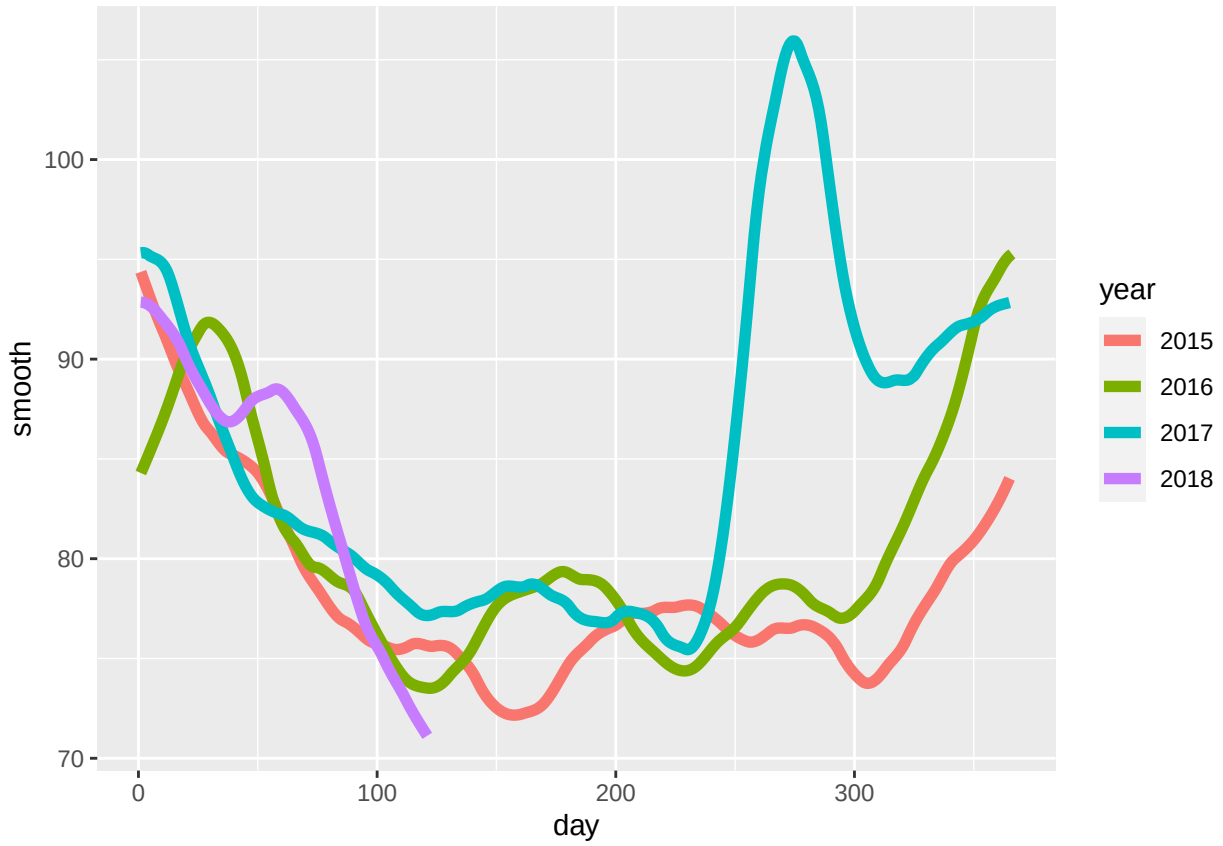
□ D.



2. Work with the same data as in Q1 to plot smooth estimates against day of the year, all on the same plot, but with different colors for each year.

Which code produces the desired plot?

```
dat %>%
    mutate(smooth = predict(fit, as.numeric(date)), day = yday(date), year = as.character(year(date))) %
    ggplot(aes(day, smooth, col = year)) +
    geom_line(lwd = 2)
```



☐ A.

```
dat %>%
    mutate(smooth = predict(fit), day = yday(date), year = as.character(year(date))) %>%
    ggplot(aes(day, smooth, col = year)) +
    geom_line(lwd = 2)
```

☐ B.

```
dat %>%
    mutate(smooth = predict(fit, as.numeric(date)), day = mday(date), year = as.character(year(date))) %
    ggplot(aes(day, smooth, col = year)) +
    geom_line(lwd = 2)
```

☐ C.

```
 dat %>%
    mutate(smooth = predict(fit, as.numeric(date)), day = yday(date), year = as.character(year(date))) %
    ggplot(aes(day, smooth)) +
    geom_line(lwd = 2)
```

☒ D.

```
dat %>%
    mutate(smooth = predict(fit, as.numeric(date)), day = yday(date), year = as.character(year(date))) %
    ggplot(aes(day, smooth, col = year)) +
    geom_line(lwd = 2)
```

3. Suppose we want to predict 2s and 7s in the `mnist_27` dataset with just the second covariate. Can we do this? On first inspection it appears the data does not have much predictive power.

In fact, if we fit a regular logistic regression the coefficient for `x_2` is not significant!

This can be seen using this code:

```
if(!require(broom)) install.packages("broom")
```

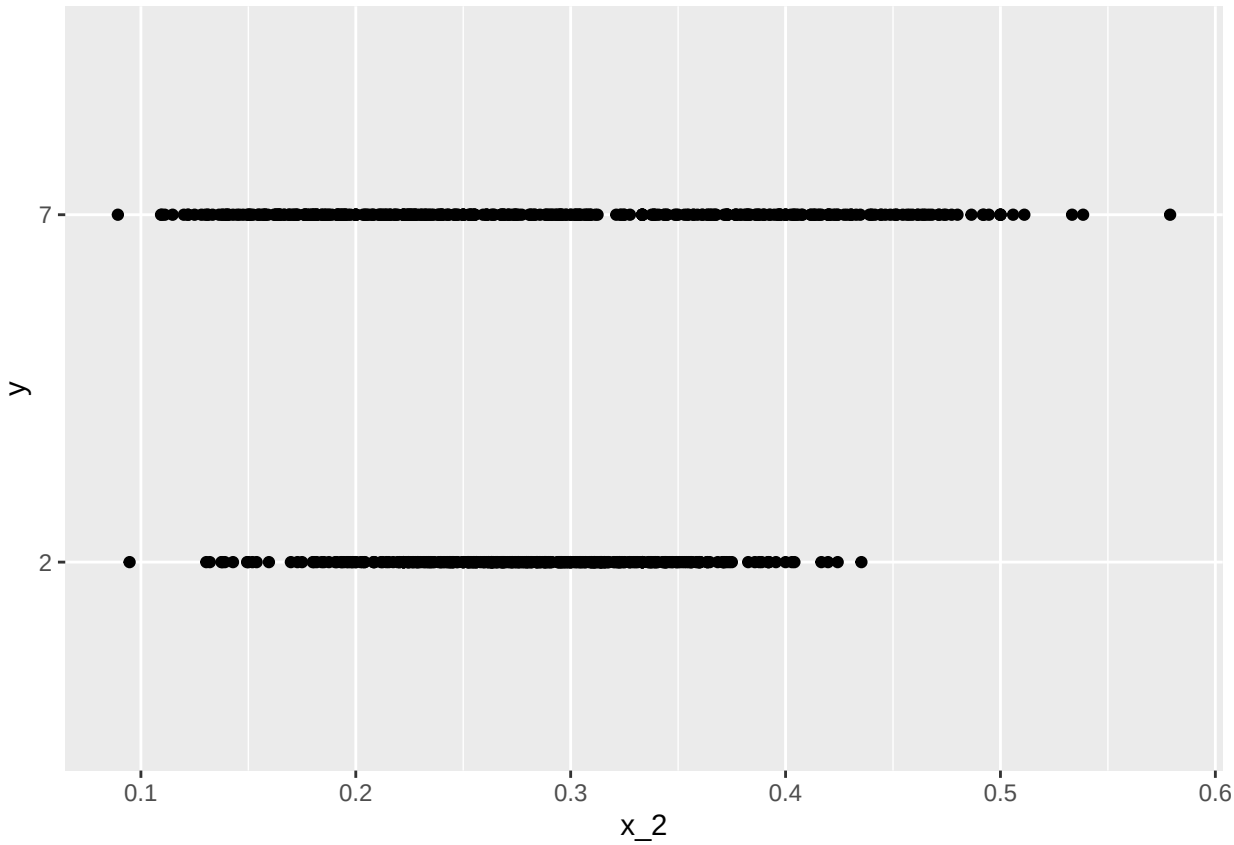
```
## Loading required package: broom
```

```
library(broom)
mnist_27$train %>% glm(y ~ x_2, family = "binomial", data = .) %>% tidy()
```

```
## # A tibble: 2 x 5
##   term        estimate std.error statistic p.value
##   <chr>          <dbl>     <dbl>     <dbl>   <dbl>
## 1 (Intercept)  -0.0907     0.247    -0.368   0.713
## 2 x_2           0.685      0.827     0.829   0.407
```

Plotting a scatterplot here is not useful since `y` is binary:

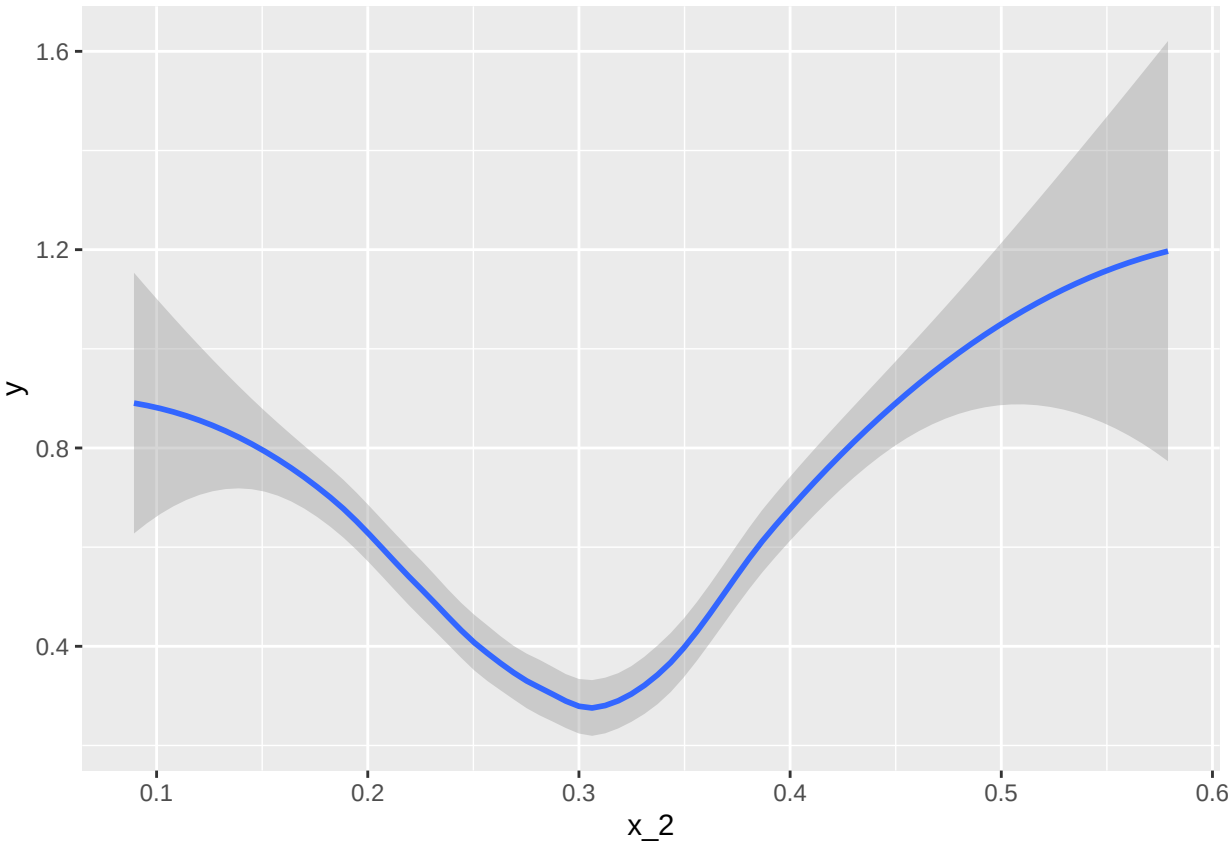
```
qplot(x_2, y, data = mnist_27$train)
```



Fit a loess line to the data above and plot the results. What do you observe?

```
mnist_27$train %>%
    mutate(y = ifelse(y=="7", 1, 0)) %>%
    ggplot(aes(x_2, y)) +
    geom_smooth(method = "loess")
```

```
## `geom_smooth()` using formula 'y ~ x'
```



☐ A. There is no predictive power and the conditional probability is linear.
☐ B. There is no predictive power and the conditional probability is non-linear.
☐ C. There is predictive power and the conditional probability is linear.
☒ D. There is predictive power and the conditional probability is non-linear.

Matrices

There is a link to the relevant section of the textbook: Matrices

Key points

- The main reason for using matrices is that certain mathematical operations needed to develop efficient code can be performed using techniques from a branch of mathematics called **linear algebra**.
- **Linear algebra** and **matrix notation** are key elements of the language used in academic papers describing machine learning techniques.

Code

```
if(!exists("mnist")) mnist <- read_mnist()

class(mnist$train$images)
```

```
## [1] "matrix" "array"
```

```
x <- mnist$train$images[1:1000,]
y <- mnist$train$labels[1:1000]
```

Matrix Notation

There is a link to the relevant section of the textbook: Matrix notation

Key points

- In matrix algebra, we have three main types of objects: **scalars**, **vectors**, and **matrices**.
  - **Scalar:** $\alpha = 1$
  - **Vector:** $X_1 = \begin{pmatrix} x_{1,1} \\ \vdots \\ x_{N,1} \end{pmatrix}$
  - **Matrix:** $X = [X_1 X_2] = \begin{pmatrix} x_{1,1} & x_{1,2} \\ \vdots & \vdots \\ x_{N,1} & x_{N,2} \end{pmatrix}$
- In R, we can extract the dimension of a matrix with the function `dim()`. We can convert a vector into a matrix using the function `as.matrix()`.

Code

```
length(x[,1])
```

```
## [1] 1000
```

```
x_1 <- 1:5
x_2 <- 6:10
cbind(x_1, x_2)
```

```
##      x_1 x_2
## [1,]   1   6
## [2,]   2   7
## [3,]   3   8
## [4,]   4   9
## [5,]   5  10
```

```
dim(x)
```

```
## [1] 1000  784
```

```
dim(x_1)
```

```
## NULL
```

```
dim(as.matrix(x_1))
```

```
## [1] 5 1
```

```
dim(x)
```

```
## [1] 1000  784
```

Converting a Vector to a Matrix

There is a link to the relevant section of the textbook: Converting a vector to a matrix

Key points

- In R, we can **convert a vector into a matrix** with the `matrix()` function. The matrix is filled in by column, but we can fill by row by using the `byrow` argument. The function `t()` can be used to directly transpose a matrix.
- Note that the matrix function **recycles values in the vector** without warning if the product of columns and rows does not match the length of the vector.

Code

```
my_vector <- 1:15

# fill the matrix by column
mat <- matrix(my_vector, 5, 3)
mat
```

```
##      [,1] [,2] [,3]
## [1,]    1    6   11
## [2,]    2    7   12
## [3,]    3    8   13
## [4,]    4    9   14
## [5,]    5   10   15
```

```
# fill by row
mat_t <- matrix(my_vector, 3, 5, byrow = TRUE)
mat_t
```

```
##      [,1] [,2] [,3] [,4] [,5]
## [1,]    1    2    3    4    5
## [2,]    6    7    8    9   10
## [3,]   11   12   13   14   15
```

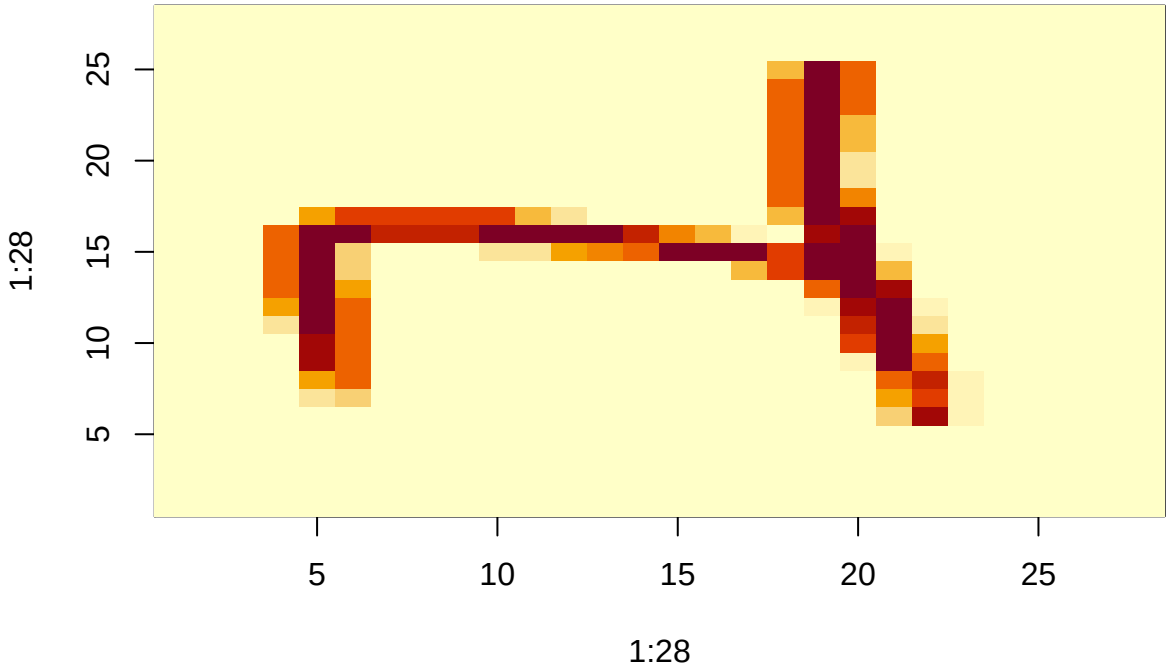
```
identical(t(mat), mat_t)
```

```
## [1] TRUE
```

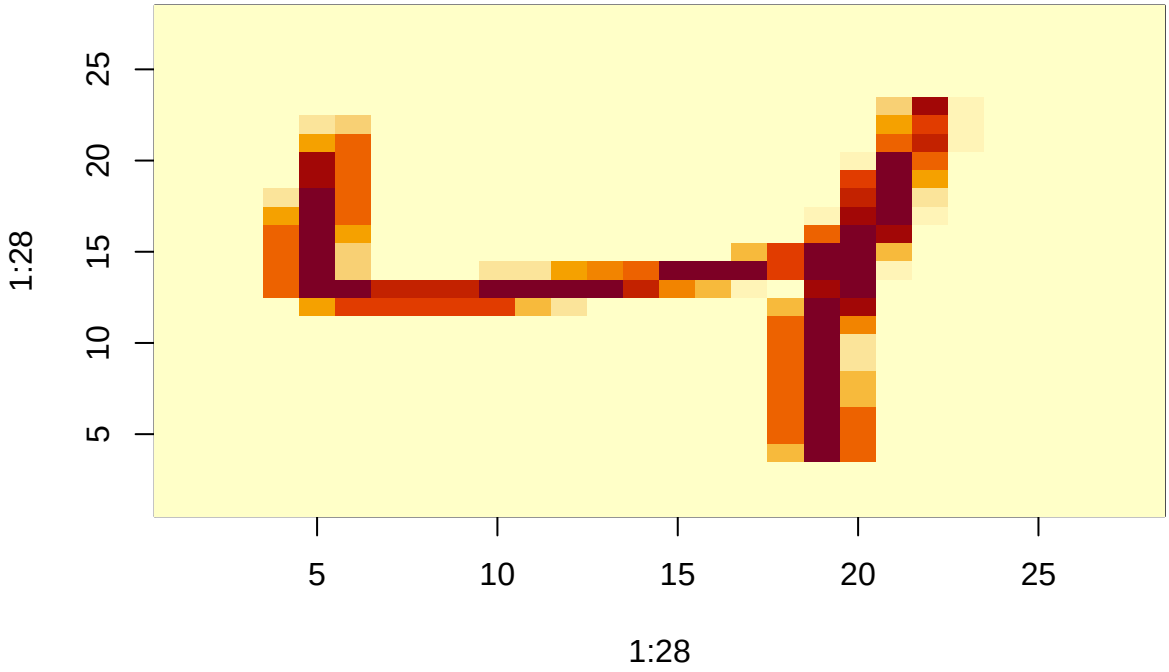
```
matrix(my_vector, 5, 5)
```

```
##      [,1] [,2] [,3] [,4] [,5]
## [1,]    1    6   11    1    6
## [2,]    2    7   12    2    7
## [3,]    3    8   13    3    8
## [4,]    4    9   14    4    9
## [5,]    5   10   15    5   10
```

```
grid <- matrix(x[3,], 28, 28)
image(1:28, 1:28, grid)
```




```
# flip the image back
image(1:28, 1:28, grid[, 28:1])
```



Row and Column Summaries and Apply

There is a link to the relevant section of the textbook: Row and column summaries

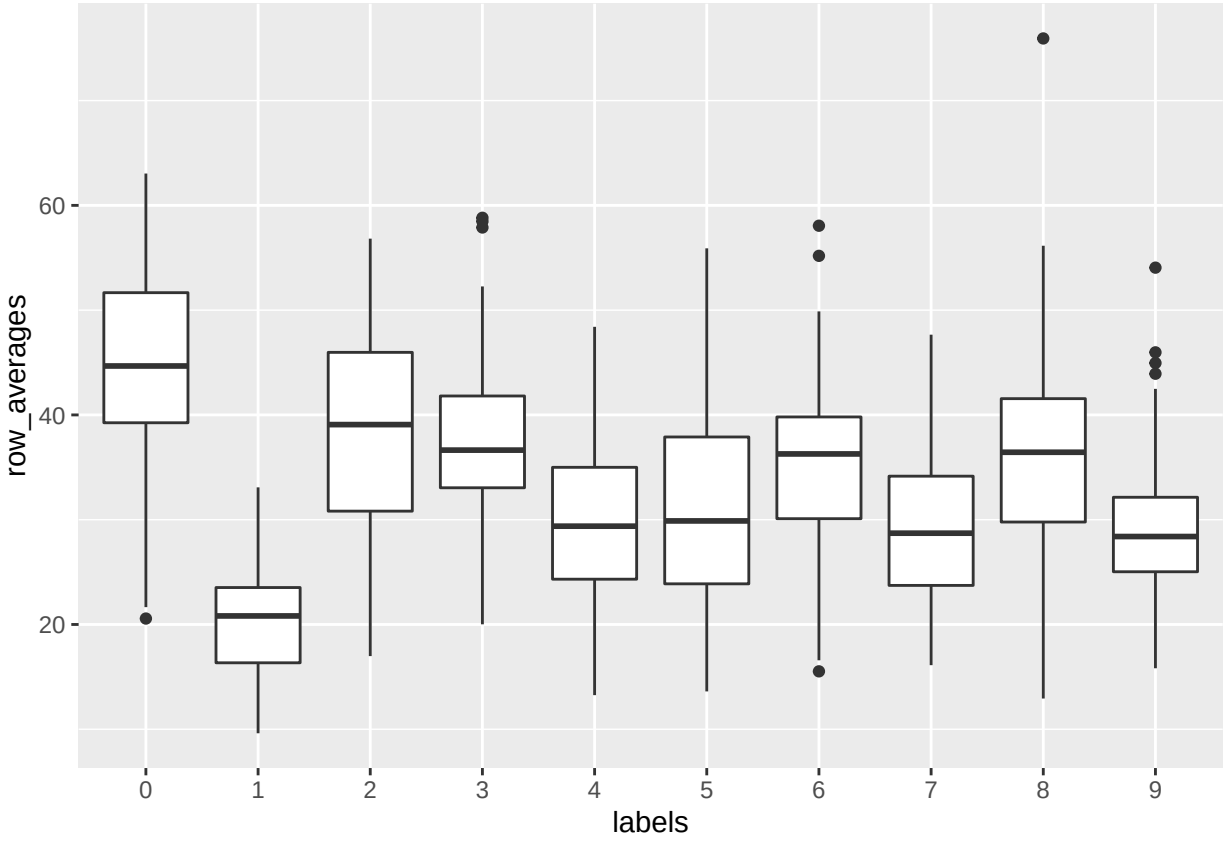
Key points

- The function `rowSums()` computes the sum of each row.
- The function `rowMeans()` computes the average of each row.
- We can compute the column sums and averages using the functions `colSums()` and `colMeans()`.
- The **matrixStats** package adds functions that performs operations on each row or column very efficiently, including the functions `rowSds()` and `colSds()`.
- The `apply()` function lets you apply any function to a matrix. The first argument is the **matrix**, the second is the **dimension** (1 for rows, 2 for columns), and the third is the **function**.

Code

```
sums <- rowSums(x)
avg <- rowMeans(x)

data_frame(labels = as.factor(y), row_averages = avg) %>%
    qplot(labels, row_averages, data = ., geom = "boxplot")
```

```
## Warning: `data_frame()` is deprecated as of tibble 1.1.0.
## Please use `tibble()` instead.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_warnings()` to see where this warning was generated.
```




```
avgs <- apply(x, 1, mean)
sds <- apply(x, 2, sd)
```

Filtering Columns Based on Summaries

There is a link to the relevant section of the textbook: Filtering columns based on summaries

Key points

- The operations used to extract columns: `x[,c(351,352)]`.
- The operations used to extract rows: `x[c(2,3),]`.
- We can also use logical indexes to determine which columns or rows to keep: `new_x <- x[ ,colSds(x) > 60]`.
- **Important note:** if you select only one column or only one row, the result is no longer a matrix but a **vector**. We can **preserve the matrix class** by using the argument `drop=FALSE`.

Code

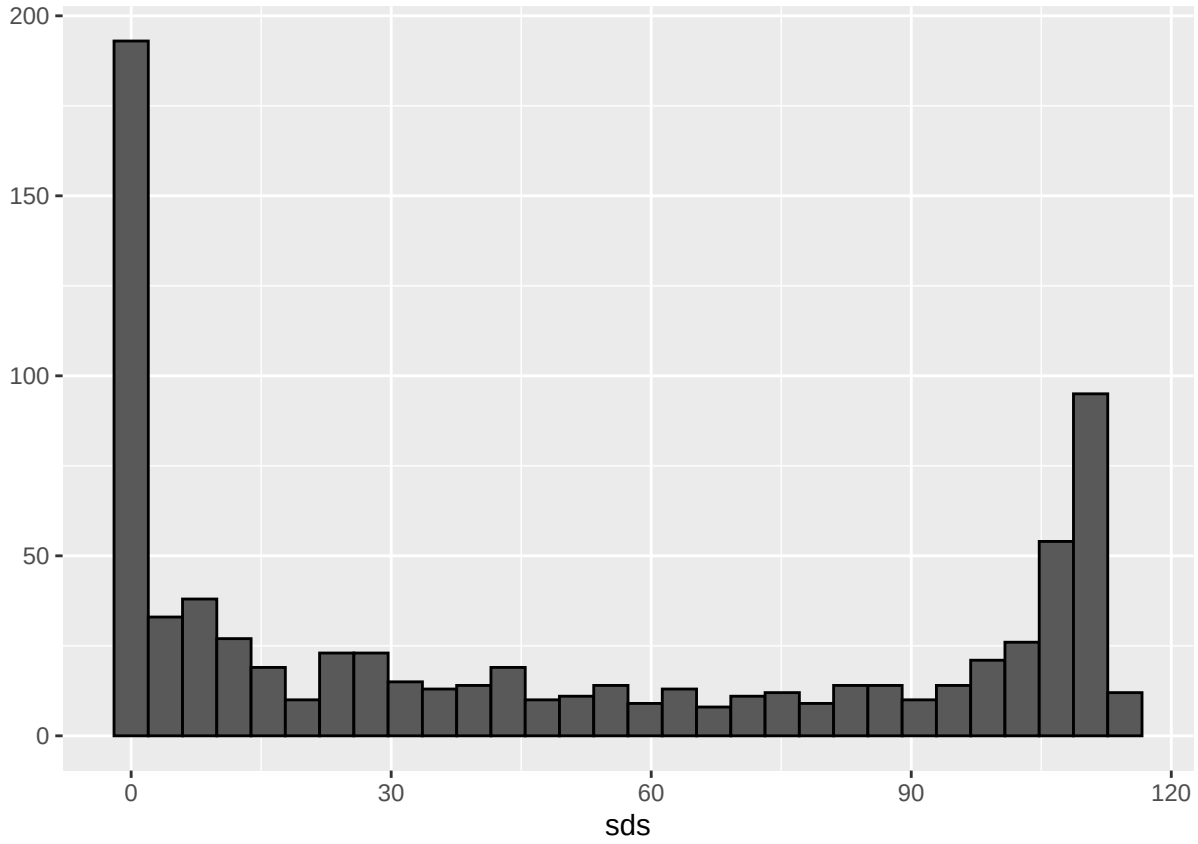
```
if(!require(matrixStats)) install.packages("matrixStats")
```

```
## Loading required package: matrixStats
```

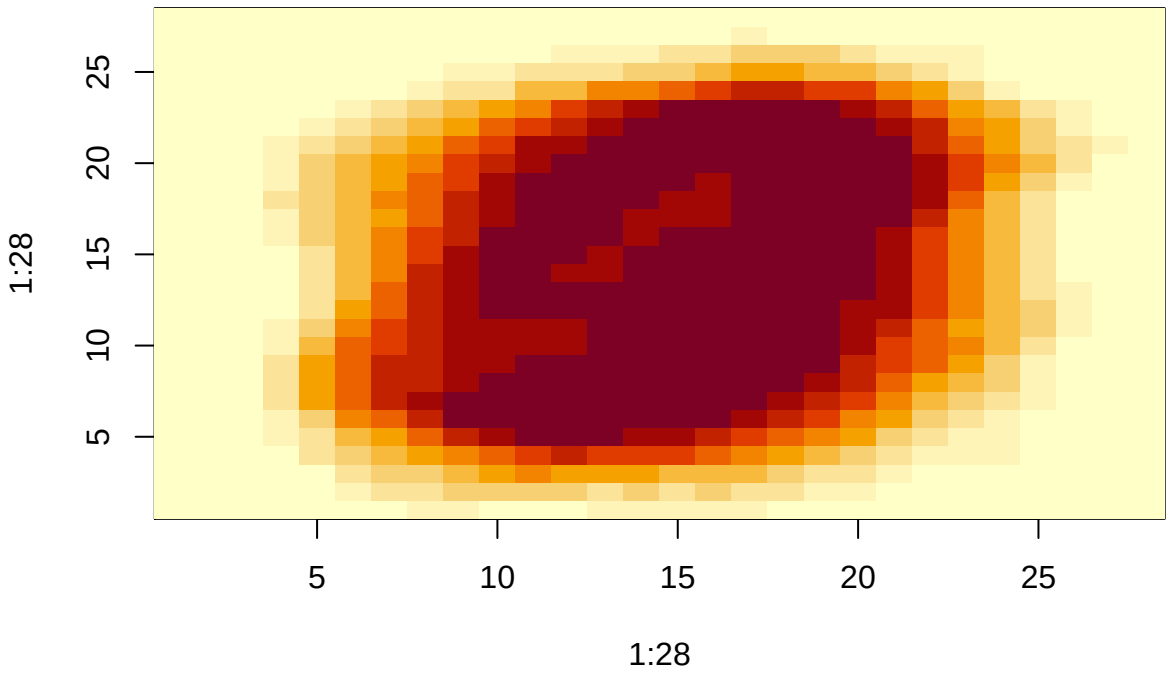
```
##
## Attaching package: 'matrixStats'
```

```
## The following object is masked from 'package:dplyr':
##
##     count
```

```
library(matrixStats)

sds <- colSds(x)
qplot(sds, bins = "30", color = I("black"))
```




```
image(1:28, 1:28, matrix(sds, 28, 28)[, 28:1])
```




```
#extract columns and rows
x[ ,c(351,352)]
```

```
##         [,1] [,2]
##    [1,]   70    0
##    [2,]    0    0
##    [3,]    0    0
##    [4,]  205  253
##    [5,]    8   78
##    [6,]    0    0
##    [7,]  253  253
##    [8,]   91  212
##    [9,]  254  143
##   [10,]    0    0
##   [11,]  254  254
##   [12,]   78   79
##   [13,]  254  248
##   [14,]    0  114
##   [15,]  254  109
##   [16,]    0    0
##   [17,]    0    0
##   [18,]   80  223
##   [19,]    0    0
##   [20,]    8   43
##   [21,]  109  109
##   [22,]   96  204
##   [23,]    0    0
##   [24,]  142  255
##   [25,]   32  254
##   [26,]  250  253
##   [27,]    0    0
##   [28,]  253  253
##   [29,]    0    0
##   [30,]    2    0
##   [31,]  253  253
##   [32,]  253  253
##   [33,]    0    0
##   [34,]  228  216
##   [35,]  225    0
##   [36,]  141   86
##   [37,]  107    0
##   [38,]    0    0
##   [39,]    0   15
##   [40,]    0    0
##   [41,]  253  253
##   [42,]  232  233
##   [43,]    0  182
##   [44,]   71  173
##   [45,]  253  203
##   [46,]   44  199
##   [47,]    0  154
##   [48,]    0    0
##   [49,]  169  254
##   [50,]  252  176
##   [51,]  254  254
##   [52,]    0    0
##   [53,]    0    0
```

```
##   [54,]   24  242
##   [55,]   71  122
##   [56,]    0  186
##   [57,]    0    0
##   [58,]    0    0
##   [59,]  111  189
##   [60,]  229  254
##   [61,]    0    0
##   [62,]    0  227
##   [63,]    0    0
##   [64,]  253  251
##   [65,]    0    0
##   [66,]  216  151
##   [67,]  128  128
##   [68,]  254  254
##   [69,]    0    0
##   [70,]   29    0
##   [71,]  253  122
##   [72,]   69    0
##   [73,]  254  204
##   [74,]   17  179
##   [75,]  253  252
##   [76,]  182   15
##   [77,]  254  254
##   [78,]  251  253
##   [79,]  173  253
##   [80,]   10    0
##   [81,]  252  253
##   [82,]    0    0
##   [83,]    0    0
##   [84,]    0  128
##   [85,]    0    0
##   [86,]  253  253
##   [87,]  253  253
##   [88,]   21   52
##   [89,]    0    0
##   [90,]    0    0
##   [91,]    0    0
##   [92,]   53   53
##   [93,]    0    0
##   [94,]   70  236
##   [95,]   38    0
##   [96,]    0    0
##   [97,]    0   26
##   [98,]   38   38
##   [99,]  253  240
##  [100,]   69  253
##  [101,]    0    0
##  [102,]   66    0
##  [103,]  254   95
##  [104,]    0    0
##  [105,]  251    0
##  [106,]  253  253
##  [107,]    0    0
```

```
##  [108,]  191  255
##  [109,]    0    0
##  [110,]  163    8
##  [111,]   78  253
##  [112,]   55  139
##  [113,]  252  253
##  [114,]  252  252
##  [115,]    0    0
##  [116,]    0    0
##  [117,]    0   15
##  [118,]  253  253
##  [119,]    0    0
##  [120,]   14    0
##  [121,]    0    0
##  [122,]    0    0
##  [123,]    0  150
##  [124,]    0    0
##  [125,]  253  233
##  [126,]  254  178
##  [127,]    0    0
##  [128,]   61    1
##  [129,]  253  253
##  [130,]  192  252
##  [131,]  254  247
##  [132,]    0    5
##  [133,]  253  253
##  [134,]  141  240
##  [135,]  253  251
##  [136,]  252  252
##  [137,]  254  179
##  [138,]  255  255
##  [139,]  244  253
##  [140,]    0    0
##  [141,]    0    0
##  [142,]  131   44
##  [143,]    0    0
##  [144,]  162  255
##  [145,]   72  142
##  [146,]    0    0
##  [147,]    0   34
##  [148,]    0    0
##  [149,]    0    0
##  [150,]  252  252
##  [151,]  221  254
##  [152,]    0    0
##  [153,]  232  254
##  [154,]    5   89
##  [155,]  253  213
##  [156,]    0   36
##  [157,]    0    0
##  [158,]  179  242
##  [159,]   50   50
##  [160,]    0   90
##  [161,]  254  254
```

```
##  [162,]  229  254
##  [163,]    0    0
##  [164,]   76  243
##  [165,]    0    0
##  [166,]   63  167
##  [167,]    0    0
##  [168,]    0    0
##  [169,]  253  252
##  [170,]  105    4
##  [171,]   37  168
##  [172,]   69  168
##  [173,]  255  152
##  [174,]  170    0
##  [175,]  252  253
##  [176,]  185    8
##  [177,]  254  253
##  [178,]  251  253
##  [179,]    0    0
##  [180,]   59  106
##  [181,]    0  178
##  [182,]    0    0
##  [183,]  176  253
##  [184,]    0   64
##  [185,]  253  226
##  [186,]    0    0
##  [187,]    0    0
##  [188,]  254  254
##  [189,]    0    0
##  [190,]  252  252
##  [191,]  167  254
##  [192,]    0    0
##  [193,]    0    0
##  [194,]   32   32
##  [195,]    0    0
##  [196,]  148  149
##  [197,]    0    0
##  [198,]  250  225
##  [199,]  104  252
##  [200,]    0   11
##  [201,]  253  169
##  [202,]  157  252
##  [203,]  100  247
##  [204,]  162  216
##  [205,]    0    0
##  [206,]  253  251
##  [207,]    0    0
##  [208,]    0    0
##  [209,]  253  253
##  [210,]    0    0
##  [211,]    0    0
##  [212,]  253  254
##  [213,]  199  253
##  [214,]    0   20
##  [215,]    0    0
```

```
##  [216,]  253  253
##  [217,]    0    0
##  [218,]    0    0
##  [219,]  106  239
##  [220,]  181   84
##  [221,]    0    0
##  [222,]    0   31
##  [223,]  152  244
##  [224,]    0    0
##  [225,]    0   61
##  [226,]  253  227
##  [227,]    0  136
##  [228,]    0    0
##  [229,]    0    0
##  [230,]    0    0
##  [231,]    0    0
##  [232,]  253  251
##  [233,]    0    0
##  [234,]    0    0
##  [235,]    0    2
##  [236,]  253  253
##  [237,]    0    0
##  [238,]    0    0
##  [239,]    0    0
##  [240,]   98   88
##  [241,]  253  252
##  [242,]    0    0
##  [243,]  254  254
##  [244,]    0    0
##  [245,]    0  169
##  [246,]  255  255
##  [247,]    0    0
##  [248,]    0    2
##  [249,]  254  252
##  [250,]    0    0
##  [251,]    0    1
##  [252,]  253  253
##  [253,]  253  252
##  [254,]    0    0
##  [255,]  254  254
##  [256,]  253  253
##  [257,]  253  171
##  [258,]    0    0
##  [259,]    0    0
##  [260,]  254  231
##  [261,]    0    0
##  [262,]    0    0
##  [263,]    0    0
##  [264,]    0    0
##  [265,]    0    0
##  [266,]  236   62
##  [267,]   77    0
##  [268,]    0   90
##  [269,]    0   93
```

```
##  [270,]  253  253
##  [271,]  251   57
##  [272,]    0    0
##  [273,]  125  168
##  [274,]  127  127
##  [275,]  232    8
##  [276,]    0    0
##  [277,]  191  254
##  [278,]    0    0
##  [279,]  245  254
##  [280,]    0  128
##  [281,]    0   51
##  [282,]  253  255
##  [283,]    0    0
##  [284,]    0    0
##  [285,]  253  253
##  [286,]    0    0
##  [287,]  253  253
##  [288,]  254  251
##  [289,]    0    0
##  [290,]    0    0
##  [291,]  252  253
##  [292,]  253  253
##  [293,]    2   45
##  [294,]    0    0
##  [295,]    0    0
##  [296,]  133  160
##  [297,]    0    0
##  [298,]    0    0
##  [299,]  253  253
##  [300,]    0  155
##  [301,]   42  235
##  [302,]    0    0
##  [303,]    0    0
##  [304,]    0    0
##  [305,]   29   29
##  [306,]    0    0
##  [307,]  100  176
##  [308,]    0    0
##  [309,]    0    0
##  [310,]  232  253
##  [311,]  235  254
##  [312,]    0    0
##  [313,]  183  102
##  [314,]    0   35
##  [315,]    0    0
##  [316,]  243  253
##  [317,]  255  255
##  [318,]    0    0
##  [319,]  241  224
##  [320,]    0    5
##  [321,]    0    0
##  [322,]  230  253
##  [323,]    0    0
```

```
##  [324,]    0    0
##  [325,]    0    0
##  [326,]    0    0
##  [327,]    0    0
##  [328,]  253  253
##  [329,]   45    0
##  [330,]    0    0
##  [331,]   70   70
##  [332,]    0    0
##  [333,]    0    0
##  [334,]  184  184
##  [335,]    0  183
##  [336,]  211   86
##  [337,]    0    0
##  [338,]    0    0
##  [339,]    0    0
##  [340,]    0    0
##  [341,]    0   64
##  [342,]  253  255
##  [343,]  132  152
##  [344,]  252  241
##  [345,]    0    0
##  [346,]  158  254
##  [347,]    8  134
##  [348,]    0    0
##  [349,]  205  254
##  [350,]    0    0
##  [351,]    0    3
##  [352,]  180  253
##  [353,]  253  207
##  [354,]    0    0
##  [355,]    0  102
##  [356,]  254  254
##  [357,]  253  253
##  [358,]  211  253
##  [359,]  254   95
##  [360,]    0    0
##  [361,]  253  253
##  [362,]  160  252
##  [363,]    0    0
##  [364,]    0   96
##  [365,]    0    0
##  [366,]    0    0
##  [367,]  253  217
##  [368,]    0    0
##  [369,]  254  254
##  [370,]    0    0
##  [371,]  253  253
##  [372,]    0    0
##  [373,]    0   43
##  [374,]    0    0
##  [375,]  121  252
##  [376,]    0    0
##  [377,]    0    0
```

```
##  [378,]    0    0
##  [379,]    0    0
##  [380,]    0    3
##  [381,]    0    0
##  [382,]    0    0
##  [383,]  254   84
##  [384,]    0    0
##  [385,]    0   56
##  [386,]    0   52
##  [387,]  252  240
##  [388,]    0    0
##  [389,]    0    0
##  [390,]    0    0
##  [391,]   38  233
##  [392,]  197  173
##  [393,]   53  232
##  [394,]   64   64
##  [395,]  181    0
##  [396,]    0    0
##  [397,]    0    0
##  [398,]  207  252
##  [399,]  253  158
##  [400,]   27    0
##  [401,]    0    0
##  [402,]    0    0
##  [403,]    0    0
##  [404,]  105    0
##  [405,]  253  253
##  [406,]   93  239
##  [407,]  253   58
##  [408,]   42   27
##  [409,]  254  195
##  [410,]    0    0
##  [411,]  229  253
##  [412,]    0    0
##  [413,]    0  100
##  [414,]    0    0
##  [415,]    0   70
##  [416,]    0    0
##  [417,]  253  251
##  [418,]   58    0
##  [419,]    7  221
##  [420,]    0   45
##  [421,]  252  253
##  [422,]    0    0
##  [423,]    0   77
##  [424,]    0    0
##  [425,]  253  253
##  [426,]   23   29
##  [427,]  252  252
##  [428,]    0    0
##  [429,]  135  246
##  [430,]    0    0
##  [431,]    0    0
```

```
##  [432,]    0    0
##  [433,]    0    0
##  [434,]  253  253
##  [435,]    0    0
##  [436,]    0    0
##  [437,]    0    0
##  [438,]   40    8
##  [439,]    0   34
##  [440,]  254  254
##  [441,]    0    0
##  [442,]    0   47
##  [443,]    0    0
##  [444,]   99  253
##  [445,]  222  246
##  [446,]  252  209
##  [447,]    0    0
##  [448,]  172  253
##  [449,]   12  161
##  [450,]    0    0
##  [451,]  251  180
##  [452,]    0    0
##  [453,]  254  253
##  [454,]    0    0
##  [455,]  254  223
##  [456,]  237  252
##  [457,]  252  252
##  [458,]    0    0
##  [459,]    0    0
##  [460,]   49  159
##  [461,]    0    0
##  [462,]    0    0
##  [463,]    0    0
##  [464,]    0    0
##  [465,]    0    0
##  [466,]    0    0
##  [467,]   98  254
##  [468,]    0    0
##  [469,]    0    0
##  [470,]    0    0
##  [471,]    0    0
##  [472,]   51   51
##  [473,]  154  250
##  [474,]    0    0
##  [475,]    0    0
##  [476,]  211  253
##  [477,]    0    0
##  [478,]    0    0
##  [479,]  114  253
##  [480,]  254  253
##  [481,]    0    0
##  [482,]    0    0
##  [483,]    0    0
##  [484,]    0    0
##  [485,]  253  132
```

```
##  [486,]    0    0
##  [487,]   67    0
##  [488,]    0    9
##  [489,]  254  255
##  [490,]    0    0
##  [491,]  253  250
##  [492,]    0  255
##  [493,]  252  250
##  [494,]    0    0
##  [495,]    0    0
##  [496,]  253  253
##  [497,]  202  203
##  [498,]    0    0
##  [499,]    0    0
##  [500,]  130   76
##  [501,]    0    0
##  [502,]    0    0
##  [503,]    0    0
##  [504,]  115   34
##  [505,]  105    0
##  [506,]    0    0
##  [507,]    0    0
##  [508,]  143  253
##  [509,]  254  254
##  [510,]  160  253
##  [511,]  253  224
##  [512,]   12  118
##  [513,]    0    0
##  [514,]    0    0
##  [515,]  148  237
##  [516,]    0    0
##  [517,]    0    0
##  [518,]   24    0
##  [519,]    0    7
##  [520,]    0    0
##  [521,]    0    0
##  [522,]  128   25
##  [523,]    0    0
##  [524,]    0    0
##  [525,]    0    0
##  [526,]    0    0
##  [527,]    0    0
##  [528,]   12    0
##  [529,]  221   62
##  [530,]    0   51
##  [531,]    0    0
##  [532,]    0    0
##  [533,]  253  253
##  [534,]   18  246
##  [535,]  204  252
##  [536,]  128  253
##  [537,]    0    0
##  [538,]  156  127
##  [539,]  254  254
```

```
##  [540,]    0   42
##  [541,]  114    0
##  [542,]    0    0
##  [543,]  151    0
##  [544,]    0    0
##  [545,]  189  112
##  [546,]    0  164
##  [547,]  252  253
##  [548,]    0   15
##  [549,]    0    0
##  [550,]   82  202
##  [551,]    0    8
##  [552,]    0    0
##  [553,]  215  254
##  [554,]  206  252
##  [555,]  251  253
##  [556,]    0    0
##  [557,]  253  253
##  [558,]  253  253
##  [559,]  115    0
##  [560,]  110  231
##  [561,]    0  136
##  [562,]  254  254
##  [563,]    0    0
##  [564,]    0   23
##  [565,]    0    0
##  [566,]  113  206
##  [567,]    0   71
##  [568,]    0    0
##  [569,]    0    0
##  [570,]    0   22
##  [571,]    0    0
##  [572,]   25  119
##  [573,]  255  255
##  [574,]  246  253
##  [575,]  253  128
##  [576,]   21   22
##  [577,]  194  113
##  [578,]    0    0
##  [579,]    0    0
##  [580,]    0    0
##  [581,]   43  225
##  [582,]  253  253
##  [583,]    0    0
##  [584,]  112  166
##  [585,]    0    0
##  [586,]    0    0
##  [587,]    0    0
##  [588,]  253  253
##  [589,]   70  254
##  [590,]    0    0
##  [591,]    0  157
##  [592,]    0    0
##  [593,]    0    6
```

```
##  [594,]  179  253
##  [595,]  221  253
##  [596,]    0   32
##  [597,]    0    0
##  [598,]  252   82
##  [599,]    0    0
##  [600,]    0    0
##  [601,]  111  245
##  [602,]    0    0
##  [603,]  253   65
##  [604,]   64    0
##  [605,]   47  254
##  [606,]    0   14
##  [607,]   10  168
##  [608,]    7  160
##  [609,]    0    0
##  [610,]  252  252
##  [611,]    0    0
##  [612,]   23  172
##  [613,]    0    0
##  [614,]  253  247
##  [615,]    0    0
##  [616,]    0    0
##  [617,]    0    0
##  [618,]    0    0
##  [619,]  253    0
##  [620,]    0    0
##  [621,]  252  253
##  [622,]    0    0
##  [623,]  253  255
##  [624,]   50    7
##  [625,]    0    0
##  [626,]    0    0
##  [627,]    0    0
##  [628,]    0    0
##  [629,]  182  253
##  [630,]  206  253
##  [631,]   68   41
##  [632,]    0    0
##  [633,]   47    5
##  [634,]   18    0
##  [635,]    0   80
##  [636,]    0    0
##  [637,]    0    0
##  [638,]  193  254
##  [639,]  254  177
##  [640,]    0    0
##  [641,]   84   19
##  [642,]  236  253
##  [643,]    0    0
##  [644,]  253  253
##  [645,]  254  254
##  [646,]  253  253
##  [647,]  164  253
```

```
##  [648,]    0    0
##  [649,]  229  254
##  [650,]    5    0
##  [651,]   88  211
##  [652,]    0    0
##  [653,]  252  229
##  [654,]    0    0
##  [655,]    0    9
##  [656,]    0    0
##  [657,]    5    0
##  [658,]    0    0
##  [659,]    0    0
##  [660,]    8  128
##  [661,]   25    0
##  [662,]    0   29
##  [663,]   19    0
##  [664,]    0    0
##  [665,]    0   10
##  [666,]  235  239
##  [667,]    0    0
##  [668,]  255  128
##  [669,]    0    0
##  [670,]    0    0
##  [671,]   14   51
##  [672,]  253  253
##  [673,]    0    0
##  [674,]    0    0
##  [675,]  244   89
##  [676,]  253  253
##  [677,]  254  230
##  [678,]   20    0
##  [679,]  253  253
##  [680,]  239  249
##  [681,]    0    0
##  [682,]    0    0
##  [683,]    0    0
##  [684,]    0    0
##  [685,]    0    0
##  [686,]  254  254
##  [687,]    0    0
##  [688,]    0    0
##  [689,]   13  221
##  [690,]    0    0
##  [691,]    0    0
##  [692,]  206  253
##  [693,]  131  178
##  [694,]   57  144
##  [695,]   73  253
##  [696,]  252  252
##  [697,]    0   47
##  [698,]    0    0
##  [699,]  253  253
##  [700,]  237  165
##  [701,]    0    0
```

```
##  [702,]    0    0
##  [703,]    0    0
##  [704,]    0    0
##  [705,]   17   65
##  [706,]  253  253
##  [707,]   49  189
##  [708,]   51   92
##  [709,]  133  254
##  [710,]    0    0
##  [711,]  253   72
##  [712,]  252  252
##  [713,]  180    0
##  [714,]    0   55
##  [715,]  113  254
##  [716,]  254  253
##  [717,]  249  127
##  [718,]    0    0
##  [719,]  253  254
##  [720,]  251  253
##  [721,]  253  246
##  [722,]    0    0
##  [723,]    8    0
##  [724,]    0    0
##  [725,]    0    0
##  [726,]  252  252
##  [727,]  254  218
##  [728,]    0    0
##  [729,]    0   51
##  [730,]    0    0
##  [731,]    0    0
##  [732,]  253  253
##  [733,]  209  253
##  [734,]    0    0
##  [735,]  122  198
##  [736,]    0    0
##  [737,]  255   29
##  [738,]   32    0
##  [739,]  254   59
##  [740,]    0    5
##  [741,]  254  139
##  [742,]    0    0
##  [743,]    0    0
##  [744,]    7    0
##  [745,]  226  226
##  [746,]   73    0
##  [747,]    0  219
##  [748,]  176  253
##  [749,]  194   71
##  [750,]    9    0
##  [751,]    0   29
##  [752,]  253  254
##  [753,]  252  252
##  [754,]    0    0
##  [755,]    0    0
```

```
##  [756,]    0    0
##  [757,]  208  208
##  [758,]  246  230
##  [759,]  251  252
##  [760,]    0    0
##  [761,]  243   40
##  [762,]  177    8
##  [763,]    0    0
##  [764,]    0    0
##  [765,]    0   57
##  [766,]  253  253
##  [767,]  203  204
##  [768,]  254  200
##  [769,]  208  199
##  [770,]  252  253
##  [771,]    0    0
##  [772,]  110  110
##  [773,]   15  178
##  [774,]    0    0
##  [775,]    0    0
##  [776,]   60  100
##  [777,]    0    0
##  [778,]  241  101
##  [779,]    0    0
##  [780,]  253  252
##  [781,]  253  252
##  [782,]    7    0
##  [783,]    0    0
##  [784,]  253  253
##  [785,]  224  252
##  [786,]    0    0
##  [787,]    0    0
##  [788,]    0    0
##  [789,]    0    0
##  [790,]  254  254
##  [791,]    0    0
##  [792,]  218  253
##  [793,]  242   78
##  [794,]    0    0
##  [795,]    7    0
##  [796,]    0   54
##  [797,]   24    0
##  [798,]    0   10
##  [799,]    0    0
##  [800,]  253  254
##  [801,]    0  103
##  [802,]  132  253
##  [803,]    0   78
##  [804,]    0    6
##  [805,]    0    0
##  [806,]  254  254
##  [807,]    0   15
##  [808,]  144  254
##  [809,]  252  154
```

```
##  [810,]  253  252
##  [811,]  116  137
##  [812,]  253  253
##  [813,]    0   54
##  [814,]    0  131
##  [815,]  141  210
##  [816,]  203  223
##  [817,]    0    0
##  [818,]  254  254
##  [819,]    0    0
##  [820,]    0    0
##  [821,]    0    0
##  [822,]  253  253
##  [823,]    2   41
##  [824,]   13  126
##  [825,]    0  135
##  [826,]    0    0
##  [827,]    0    0
##  [828,]    0    0
##  [829,]    0    0
##  [830,]    5    0
##  [831,]  252  253
##  [832,]  137  184
##  [833,]  255  253
##  [834,]  253  252
##  [835,]    0    0
##  [836,]  253  252
##  [837,]   82  223
##  [838,]  254  254
##  [839,]  252  253
##  [840,]    0    0
##  [841,]  253  204
##  [842,]    0    0
##  [843,]  253  253
##  [844,]  254  253
##  [845,]    0    0
##  [846,]  249  253
##  [847,]    0    0
##  [848,]    0    0
##  [849,]    0    0
##  [850,]   64    0
##  [851,]    0    0
##  [852,]    0    0
##  [853,]   59    0
##  [854,]    0    0
##  [855,]    0    0
##  [856,]    0    0
##  [857,]  254  253
##  [858,]  252  252
##  [859,]    0    0
##  [860,]    0    0
##  [861,]    0    0
##  [862,]  253  134
##  [863,]    0  190
```

```
##  [864,]   77  254
##  [865,]  159  254
##  [866,]  242  253
##  [867,]    0    0
##  [868,]  253  253
##  [869,]    0    0
##  [870,]    8    0
##  [871,]  253  253
##  [872,]  240  254
##  [873,]    0    0
##  [874,]    0    0
##  [875,]  253  253
##  [876,]  253  253
##  [877,]   44  249
##  [878,]    0    0
##  [879,]  243  174
##  [880,]   97   97
##  [881,]    0    0
##  [882,]    6   86
##  [883,]    0    0
##  [884,]    0    0
##  [885,]   82  253
##  [886,]  197  253
##  [887,]  114    0
##  [888,]    1   25
##  [889,]    0    0
##  [890,]    0    0
##  [891,]  252  253
##  [892,]  240  253
##  [893,]  181   20
##  [894,]    0    0
##  [895,]  203  254
##  [896,]  254  253
##  [897,]    0    0
##  [898,]    0    0
##  [899,]    0    0
##  [900,]   24    0
##  [901,]    6  191
##  [902,]    0    0
##  [903,]    0    0
##  [904,]    0    0
##  [905,]    0    0
##  [906,]  104  254
##  [907,]    0  152
##  [908,]    0    8
##  [909,]   67  160
##  [910,]  253  253
##  [911,]    0    0
##  [912,]    0    0
##  [913,]    0    0
##  [914,]   37  167
##  [915,]    0    0
##  [916,]   35    0
##  [917,]    7  108
```

```
##  [918,]    0    0
##  [919,]   71  241
##  [920,]  254  254
##  [921,]  253  253
##  [922,]    0    0
##  [923,]    1    0
##  [924,]    0   64
##  [925,]  198  198
##  [926,]    0  170
##  [927,]    0    0
##  [928,]    0    0
##  [929,]    0    0
##  [930,]    0    0
##  [931,]    0    0
##  [932,]    0    0
##  [933,]  123  254
##  [934,]  251  225
##  [935,]    0    0
##  [936,]   14   69
##  [937,]   89  253
##  [938,]    0    0
##  [939,]  190  252
##  [940,]   94    0
##  [941,]    0    0
##  [942,]  150  254
##  [943,]  163  238
##  [944,]    7    0
##  [945,]  168  169
##  [946,]    0    0
##  [947,]   75  231
##  [948,]    1    0
##  [949,]  128  254
##  [950,]    0    0
##  [951,]  116  253
##  [952,]  241  254
##  [953,]    0    0
##  [954,]  254  254
##  [955,]    0    0
##  [956,]    0    0
##  [957,]   74   53
##  [958,]    8    0
##  [959,]  253  253
##  [960,]  253  253
##  [961,]    0    0
##  [962,]  234  254
##  [963,]    0    0
##  [964,]   98  253
##  [965,]  222   25
##  [966,]    0    0
##  [967,]  241  189
##  [968,]    0    0
##  [969,]    0   46
##  [970,]    0    0
##  [971,]    6    6
```

```
##  [972,]    0    0
##  [973,]    0    0
##  [974,]   23    0
##  [975,]  231  254
##  [976,]  254  254
##  [977,]    0   32
##  [978,]   15    0
##  [979,]  155    0
##  [980,]    6    0
##  [981,]  135  243
##  [982,]    0    0
##  [983,]  253  201
##  [984,]  198  254
##  [985,]    0    0
##  [986,]   22    0
##  [987,]    3  171
##  [988,]    0    0
##  [989,]    0    0
##  [990,]    0    0
##  [991,]    0    0
##  [992,]  221  151
##  [993,]  254  172
##  [994,]  156  253
##  [995,]    0    0
##  [996,]  254  254
##  [997,]    0    0
##  [998,]    0    0
##  [999,]  103   64
## [1000,]  139    0
```

```
x[c(2,3),]
```

```
##      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10] [,11] [,12] [,13] [,14]
## [1,]    0    0    0    0    0    0    0    0    0     0     0     0     0     0
## [2,]    0    0    0    0    0    0    0    0    0     0     0     0     0     0
##      [,15] [,16] [,17] [,18] [,19] [,20] [,21] [,22] [,23] [,24] [,25] [,26]
## [1,]     0     0     0     0     0     0     0     0     0     0     0     0
## [2,]     0     0     0     0     0     0     0     0     0     0     0     0
##      [,27] [,28] [,29] [,30] [,31] [,32] [,33] [,34] [,35] [,36] [,37] [,38]
## [1,]     0     0     0     0     0     0     0     0     0     0     0     0
## [2,]     0     0     0     0     0     0     0     0     0     0     0     0
##      [,39] [,40] [,41] [,42] [,43] [,44] [,45] [,46] [,47] [,48] [,49] [,50]
## [1,]     0     0     0     0     0     0     0     0     0     0     0     0
## [2,]     0     0     0     0     0     0     0     0     0     0     0     0
##      [,51] [,52] [,53] [,54] [,55] [,56] [,57] [,58] [,59] [,60] [,61] [,62]
## [1,]     0     0     0     0     0     0     0     0     0     0     0     0
## [2,]     0     0     0     0     0     0     0     0     0     0     0     0
##      [,63] [,64] [,65] [,66] [,67] [,68] [,69] [,70] [,71] [,72] [,73] [,74]
## [1,]     0     0     0     0     0     0     0     0     0     0     0     0
## [2,]     0     0     0     0     0     0     0     0     0     0     0     0
##      [,75] [,76] [,77] [,78] [,79] [,80] [,81] [,82] [,83] [,84] [,85] [,86]
## [1,]     0     0     0     0     0     0     0     0     0     0     0     0
## [2,]     0     0     0     0     0     0     0     0     0     0     0     0
##      [,87] [,88] [,89] [,90] [,91] [,92] [,93] [,94] [,95] [,96] [,97] [,98]
```

```
## [1,]     0     0     0     0     0     0     0     0     0     0     0     0
## [2,]     0     0     0     0     0     0     0     0     0     0     0     0
##      [,99] [,100] [,101] [,102] [,103] [,104] [,105] [,106] [,107] [,108]
## [1,]     0      0      0      0      0      0      0      0      0      0
## [2,]     0      0      0      0      0      0      0      0      0      0
##      [,109] [,110] [,111] [,112] [,113] [,114] [,115] [,116] [,117] [,118]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,119] [,120] [,121] [,122] [,123] [,124] [,125] [,126] [,127] [,128]
## [1,]      0      0      0      0      0      0      0      0      0     51
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,129] [,130] [,131] [,132] [,133] [,134] [,135] [,136] [,137] [,138]
## [1,]    159    253    159     50      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,139] [,140] [,141] [,142] [,143] [,144] [,145] [,146] [,147] [,148]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,149] [,150] [,151] [,152] [,153] [,154] [,155] [,156] [,157] [,158]
## [1,]      0      0      0      0      0      0     48    238    252    252
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,159] [,160] [,161] [,162] [,163] [,164] [,165] [,166] [,167] [,168]
## [1,]    252    237      0      0      0      0      0      0      0      0
## [2,]      0      0     67    232     39      0      0      0      0      0
##      [,169] [,170] [,171] [,172] [,173] [,174] [,175] [,176] [,177] [,178]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0     62     81      0      0      0      0
##      [,179] [,180] [,181] [,182] [,183] [,184] [,185] [,186] [,187] [,188]
## [1,]      0      0      0     54    227    253    252    239    233    252
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,189] [,190] [,191] [,192] [,193] [,194] [,195] [,196] [,197] [,198]
## [1,]     57      6      0      0      0      0      0      0      0      0
## [2,]    120    180     39      0      0      0      0      0      0      0
##      [,199] [,200] [,201] [,202] [,203] [,204] [,205] [,206] [,207] [,208]
## [1,]      0      0      0      0      0      0      0      0      0     10
## [2,]      0      0    126    163      0      0      0      0      0      0
##      [,209] [,210] [,211] [,212] [,213] [,214] [,215] [,216] [,217] [,218]
## [1,]     60    224    252    253    252    202     84    252    253    122
## [2,]      0      0      0      0      0      0      0      2    153    210
##      [,219] [,220] [,221] [,222] [,223] [,224] [,225] [,226] [,227] [,228]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]     40      0      0      0      0      0      0      0      0      0
##      [,229] [,230] [,231] [,232] [,233] [,234] [,235] [,236] [,237] [,238]
## [1,]      0      0      0      0      0      0      0    163    252    252
## [2,]    220    163      0      0      0      0      0      0      0      0
##      [,239] [,240] [,241] [,242] [,243] [,244] [,245] [,246] [,247] [,248]
## [1,]    252    253    252    252     96    189    253    167      0      0
## [2,]      0      0      0      0      0     27    254    162      0      0
##      [,249] [,250] [,251] [,252] [,253] [,254] [,255] [,256] [,257] [,258]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0    222    163
##      [,259] [,260] [,261] [,262] [,263] [,264] [,265] [,266] [,267] [,268]
## [1,]      0      0      0      0     51    238    253    253    190    114
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,269] [,270] [,271] [,272] [,273] [,274] [,275] [,276] [,277] [,278]
```

```
## [1,]    253    228     47     79    255    168      0      0      0      0
## [2,]      0      0      0    183    254    125      0      0      0      0
##      [,279] [,280] [,281] [,282] [,283] [,284] [,285] [,286] [,287] [,288]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0     46    245    163      0      0
##      [,289] [,290] [,291] [,292] [,293] [,294] [,295] [,296] [,297] [,298]
## [1,]      0     48    238    252    252    179     12     75    121     21
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,299] [,300] [,301] [,302] [,303] [,304] [,305] [,306] [,307] [,308]
## [1,]      0      0    253    243     50      0      0      0      0      0
## [2,]      0    198    254     56      0      0      0      0      0      0
##      [,309] [,310] [,311] [,312] [,313] [,314] [,315] [,316] [,317] [,318]
## [1,]      0      0      0      0      0      0      0      0     38    165
## [2,]      0      0      0    120    254    163      0      0      0      0
##      [,319] [,320] [,321] [,322] [,323] [,324] [,325] [,326] [,327] [,328]
## [1,]    253    233    208     84      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0     23    231
##      [,329] [,330] [,331] [,332] [,333] [,334] [,335] [,336] [,337] [,338]
## [1,]    253    252    165      0      0      0      0      0      0      0
## [2,]    254     29      0      0      0      0      0      0      0      0
##      [,339] [,340] [,341] [,342] [,343] [,344] [,345] [,346] [,347] [,348]
## [1,]      0      0      0      0      0      7    178    252    240     71
## [2,]      0    159    254    120      0      0      0      0      0      0
##      [,349] [,350] [,351] [,352] [,353] [,354] [,355] [,356] [,357] [,358]
## [1,]     19     28      0      0      0      0      0      0    253    252
## [2,]      0      0      0      0      0      0    163    254    216     16
##      [,359] [,360] [,361] [,362] [,363] [,364] [,365] [,366] [,367] [,368]
## [1,]    195      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0    159
##      [,369] [,370] [,371] [,372] [,373] [,374] [,375] [,376] [,377] [,378]
## [1,]      0      0      0     57    252    252     63      0      0      0
## [2,]    254     67      0      0      0      0      0      0      0      0
##      [,379] [,380] [,381] [,382] [,383] [,384] [,385] [,386] [,387] [,388]
## [1,]      0      0      0      0      0      0    253    252    195      0
## [2,]      0     14     86    178    248    254     91      0      0      0
##      [,389] [,390] [,391] [,392] [,393] [,394] [,395] [,396] [,397] [,398]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0    159    254     85
##      [,399] [,400] [,401] [,402] [,403] [,404] [,405] [,406] [,407] [,408]
## [1,]      0    198    253    190      0      0      0      0      0      0
## [2,]      0      0      0     47     49    116    144    150    241    243
##      [,409] [,410] [,411] [,412] [,413] [,414] [,415] [,416] [,417] [,418]
## [1,]      0      0      0      0    255    253    196      0      0      0
## [2,]    234    179    241    252     40      0      0      0      0      0
##      [,419] [,420] [,421] [,422] [,423] [,424] [,425] [,426] [,427] [,428]
## [1,]      0      0      0      0      0      0      0      0     76    246
## [2,]      0      0      0      0      0    150    253    237    207    207
##      [,429] [,430] [,431] [,432] [,433] [,434] [,435] [,436] [,437] [,438]
## [1,]    252    112      0      0      0      0      0      0      0      0
## [2,]    207    253    254    250    240    198    143     91     28      5
##      [,439] [,440] [,441] [,442] [,443] [,444] [,445] [,446] [,447] [,448]
## [1,]      0      0    253    252    148      0      0      0      0      0
## [2,]    233    250      0      0      0      0      0      0      0      0
##      [,449] [,450] [,451] [,452] [,453] [,454] [,455] [,456] [,457] [,458]
```

```
## [1,]      0      0      0      0      0      0     85    252    230     25
## [2,]      0      0      0      0    119    177    177    177    177    177
##      [,459] [,460] [,461] [,462] [,463] [,464] [,465] [,466] [,467] [,468]
## [1,]      0      0      0      0      0      0      0      0      7    135
## [2,]     98     56      0      0      0      0      0    102    254    220
##      [,469] [,470] [,471] [,472] [,473] [,474] [,475] [,476] [,477] [,478]
## [1,]    253    186     12      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,479] [,480] [,481] [,482] [,483] [,484] [,485] [,486] [,487] [,488]
## [1,]      0      0      0      0     85    252    223      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,489] [,490] [,491] [,492] [,493] [,494] [,495] [,496] [,497] [,498]
## [1,]      0      0      0      0      0      7    131    252    225     71
## [2,]      0      0      0      0      0    169    254    137      0      0
##      [,499] [,500] [,501] [,502] [,503] [,504] [,505] [,506] [,507] [,508]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,509] [,510] [,511] [,512] [,513] [,514] [,515] [,516] [,517] [,518]
## [1,]      0      0     85    252    145      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,519] [,520] [,521] [,522] [,523] [,524] [,525] [,526] [,527] [,528]
## [1,]      0      0     48    165    252    173      0      0      0      0
## [2,]      0      0      0    169    254     57      0      0      0      0
##      [,529] [,530] [,531] [,532] [,533] [,534] [,535] [,536] [,537] [,538]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,539] [,540] [,541] [,542] [,543] [,544] [,545] [,546] [,547] [,548]
## [1,]     86    253    225      0      0      0      0      0      0    114
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,549] [,550] [,551] [,552] [,553] [,554] [,555] [,556] [,557] [,558]
## [1,]    238    253    162      0      0      0      0      0      0      0
## [2,]      0    169    254     57      0      0      0      0      0      0
##      [,559] [,560] [,561] [,562] [,563] [,564] [,565] [,566] [,567] [,568]
## [1,]      0      0      0      0      0      0      0      0     85    252
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,569] [,570] [,571] [,572] [,573] [,574] [,575] [,576] [,577] [,578]
## [1,]    249    146     48     29     85    178    225    253    223    167
## [2,]      0      0      0      0      0      0      0      0      0    169
##      [,579] [,580] [,581] [,582] [,583] [,584] [,585] [,586] [,587] [,588]
## [1,]     56      0      0      0      0      0      0      0      0      0
## [2,]    255     94      0      0      0      0      0      0      0      0
##      [,589] [,590] [,591] [,592] [,593] [,594] [,595] [,596] [,597] [,598]
## [1,]      0      0      0      0      0      0     85    252    252    252
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,599] [,600] [,601] [,602] [,603] [,604] [,605] [,606] [,607] [,608]
## [1,]    229    215    252    252    252    196    130      0      0      0
## [2,]      0      0      0      0      0      0      0    169    254     96
##      [,609] [,610] [,611] [,612] [,613] [,614] [,615] [,616] [,617] [,618]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,619] [,620] [,621] [,622] [,623] [,624] [,625] [,626] [,627] [,628]
## [1,]      0      0      0      0     28    199    252    252    253    252
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,629] [,630] [,631] [,632] [,633] [,634] [,635] [,636] [,637] [,638]
```

```
## [1,]    252    233    145      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0    169    254    153      0      0
##      [,639] [,640] [,641] [,642] [,643] [,644] [,645] [,646] [,647] [,648]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,649] [,650] [,651] [,652] [,653] [,654] [,655] [,656] [,657] [,658]
## [1,]      0      0      0     25    128    252    253    252    141     37
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,659] [,660] [,661] [,662] [,663] [,664] [,665] [,666] [,667] [,668]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0    169    255    153      0      0      0      0
##      [,669] [,670] [,671] [,672] [,673] [,674] [,675] [,676] [,677] [,678]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,679] [,680] [,681] [,682] [,683] [,684] [,685] [,686] [,687] [,688]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,689] [,690] [,691] [,692] [,693] [,694] [,695] [,696] [,697] [,698]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0     96    254    153      0      0      0      0      0      0
##      [,699] [,700] [,701] [,702] [,703] [,704] [,705] [,706] [,707] [,708]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,709] [,710] [,711] [,712] [,713] [,714] [,715] [,716] [,717] [,718]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,719] [,720] [,721] [,722] [,723] [,724] [,725] [,726] [,727] [,728]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,729] [,730] [,731] [,732] [,733] [,734] [,735] [,736] [,737] [,738]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,739] [,740] [,741] [,742] [,743] [,744] [,745] [,746] [,747] [,748]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,749] [,750] [,751] [,752] [,753] [,754] [,755] [,756] [,757] [,758]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,759] [,760] [,761] [,762] [,763] [,764] [,765] [,766] [,767] [,768]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,769] [,770] [,771] [,772] [,773] [,774] [,775] [,776] [,777] [,778]
## [1,]      0      0      0      0      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0      0      0      0      0
##      [,779] [,780] [,781] [,782] [,783] [,784]
## [1,]      0      0      0      0      0      0
## [2,]      0      0      0      0      0      0
```

```
new_x <- x[ ,colSds(x) > 60]
dim(new_x)
```

```
## [1] 1000  314
```

```
class(x[,1])
```

```
## [1] "integer"
```

```
dim(x[1,])
```

```
## NULL
```

```
#preserve the matrix class
class(x[ , 1, drop=FALSE])
```

```
## [1] "matrix" "array"
```

```
dim(x[, 1, drop=FALSE])
```

```
## [1] 1000    1
```

Indexing with Matrices and Binarizing the Data

There is a link to the relevant sections of the textbook: Indexing with matrices and Binarizing the data

Key points

- We can use logical operations with matrices:

```
mat <- matrix(1:15, 5, 3)
mat[mat > 6 & mat < 12] <- 0
```

- We can also binarize the data using just matrix operations:

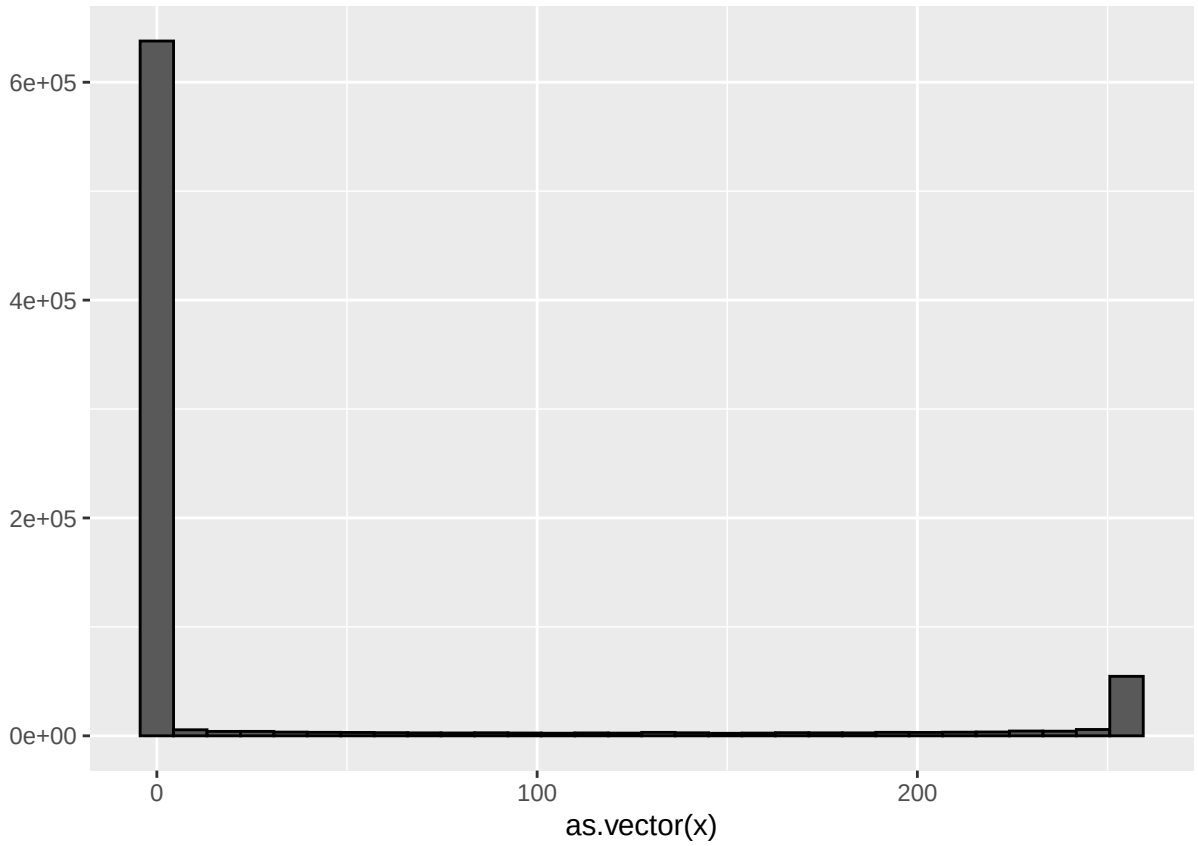
```
bin_x <- x
bin_x[bin_x < 255/2] <- 0
bin_x[bin_x > 255/2] <- 1
```

Code

```
#index with matrices
mat <- matrix(1:15, 5, 3)
as.vector(mat)
```

```
##  [1]  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15
```

```
qplot(as.vector(x), bins = 30, color = I("black"))
```




```
new_x <- x
new_x[new_x < 50] <- 0

mat <- matrix(1:15, 5, 3)
mat[mat < 3] <- 0
mat
```

```
##      [,1] [,2] [,3]
## [1,]    0    6   11
## [2,]    0    7   12
## [3,]    3    8   13
## [4,]    4    9   14
## [5,]    5   10   15
```

```
mat <- matrix(1:15, 5, 3)
mat[mat > 6 & mat < 12] <- 0
mat
```

```
##      [,1] [,2] [,3]
## [1,]    1    6    0
## [2,]    2    0   12
## [3,]    3    0   13
## [4,]    4    0   14
## [5,]    5    0   15
```

```r
#binarize the data
bin_x <- x
bin_x[bin_x < 255/2] <- 0
bin_x[bin_x > 255/2] <- 1
bin_X <- (x > 255/2)*1
```

Vectorization for Matrices and Matrix Algebra Operations

There is a link to the relevant sections of the textbook: Vectorization for matrices and Matrix algebra operations

Key points

- We can scale each row of a matrix using this line of code:

```r
(x - rowMeans(x)) / rowSds(x)
```

- To scale each column of a matrix, we use this code:

```r
t(t(X) - colMeans(X))
```

- We can also use a function called `sweep()` that works similarly to `apply()`. It takes each entry of a vector and subtracts it from the corresponding row or column:

```r
X_mean_0 <- sweep(x, 2, colMeans(x))
```

- Matrix multiplication: `t(x) %*% x`
- The cross product: `crossprod(x)`
- The inverse of a function: `solve(crossprod(x))`
- The QR decomposition: `qr(x)`

Code

```r
#scale each row of a matrix
(x - rowMeans(x)) / rowSds(x)

#scale each column
t(t(x) - colMeans(x))
```

```r
#take each entry of a vector and subtracts it from the corresponding row or column
x_mean_0 <- sweep(x, 2, colMeans(x))

#divide by the standard deviation
x_mean_0 <- sweep(x, 2, colMeans(x))
x_standardized <- sweep(x_mean_0, 2, colSds(x), FUN = "/")
```

Comprehension Check - Working with Matrices

1. Which line of code correctly creates a 100 by 10 matrix of randomly generated normal numbers and assigns it to `x`?

☐ A. `x <- matrix(rnorm(1000), 100, 100)`

☒ B. `x <- matrix(rnorm(100*10), 100, 10)`

☐ C. `x <- matrix(rnorm(100*10), 10, 10)`

☐ D. `x <- matrix(rnorm(100*10), 10, 100)`

2. Write the line of code that would give you the specified information about the matrix `x` that you generated in q1. Do not include any spaces in your line of code.

Dimension of x: `dim(x)`

Number of rows of x: `nrow(x)` or `dim(x)[1]` or `length(x[,1])`

Number of columns of x: `ncol(x)` or `dim(x)[2]` or `length(x[1,])`

3. Which of the following lines of code would add the scalar 1 to row 1, the scalar 2 to row 2, and so on, for the matrix `x`? Select ALL that apply.

☒ A. `x <- x + seq(nrow(x))`

☐ B. `x <- 1:nrow(x)`

☐ C. `x <- sweep(x, 2, 1:nrow(x),"+")`

☒ D. `x <- sweep(x, 1, 1:nrow(x),"+")`

4. Which of the following lines of code would add the scalar 1 to column 1, the scalar 2 to column 2, and so on, for the matrix `x`? Select ALL that apply.

☐ A. `x <- 1:ncol(x)`

☐ B. `x <- 1:col(x)`

☒ C. `x <- sweep(x, 2, 1:ncol(x), FUN = "+")`

☐ D. `x <- -x`

5. Which code correctly computes the average of each row of x?

☐ A. `mean(x)`

☐ B. `rowMedians(x)`

☐ C. `sapply(x,mean)`

☐ D. `rowSums(x)`

☒ E. `rowMeans(x)`

Which code correctly computes the average of each column of x?

☐ A. `mean(x)`

☐ B. `sapply(x,mean)`

☒ C. `colMeans(x)`

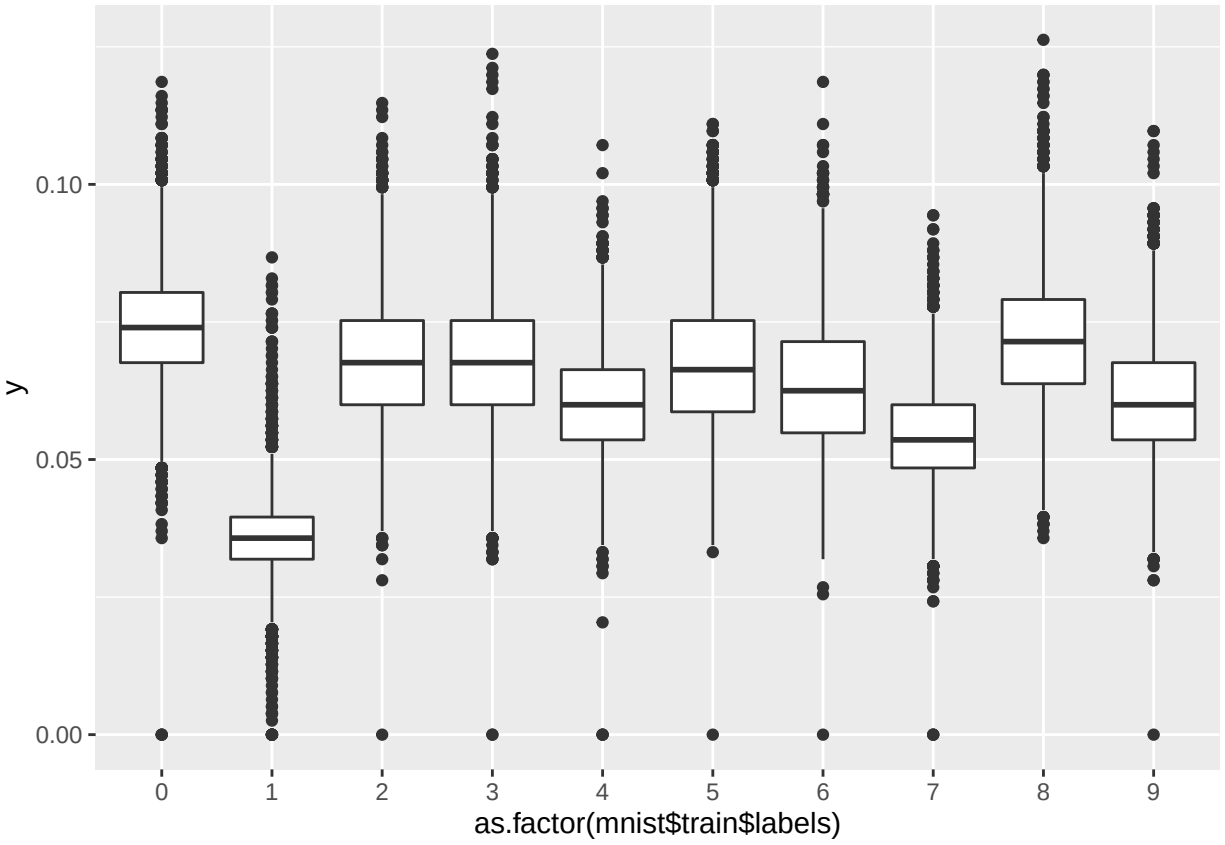
☐ D. `colMedians(x)`

☐ C. `colSums(x)`

6. For each observation in the mnist training data, compute the proportion of pixels that are in the **grey area**, defined as values between 50 and 205 (but not including 50 and 205). (To visualize this, you can make a boxplot by digit class.)

What proportion of the 60000*784 pixels in the mnist training data are in the grey area overall, defined as values between 50 and 205? Report your answer to at least 3 significant digits.

```
mnist <- read_mnist()
y <- rowMeans(mnist$train$images>50 & mnist$train$images<205)
qplot(as.factor(mnist$train$labels), y, geom = "boxplot")
```




```
mean(y) # proportion of pixels
```

```
## [1] 0.06183703
```

Section 4 - Distance, Knn, Cross Validation, and Generative Models

In the **Distance, kNN, Cross Validation, and Generative Models** section, you will learn about different types of discriminative and generative approaches for machine learning algorithms.

After completing this section, you will be able to:

- Use the **k-nearest neighbors (kNN)** algorithm.
- Understand the problems of **overtraining** and **oversmoothing**.
- Use **cross-validation** to reduce the **true error** and the **apparent error**.
- Use **generative models** such as **naive Bayes, quadratic discriminant analysis (qda),** and **linear discriminant analysis (lda)** for machine learning.

This section has three parts: **nearest neighbors, cross-validation,** and **generative models**.

Distance

There is a link to the relevant section of the textbook: Distance

Key points

- Most clustering and machine learning techniques rely on being able to define distance between observations, using features or predictors.
- With high dimensional data, a quick way to compute all the distances at once is to use the function `dist()`, which computes the distance between each row and produces an object of class `dist()`:

```
d <- dist(x)
```

- We can also compute distances between predictors. If N is the number of observations, the distance between two predictors, say 1 and 2, is:

$$\text{dist}(1,2) = \sqrt{\sum_{i=1}^{N}(x_{i,1} - x_{i,2})^2}$$

- To compute the distance between all pairs of the 784 predictors, we can transpose the matrix first and then use dist():

```
d <- dist(t(x))
```

Code

```
if(!exists("mnist")) mnist <- read_mnist()
set.seed(0) # if using R 3.5 or earlier
set.seed(0, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(0, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
ind <- which(mnist$train$labels %in% c(2,7)) %>% sample(500)

#the predictors are in x and the labels in y
x <- mnist$train$images[ind,]
y <- mnist$train$labels[ind]

y[1:3]
```

```
## [1] 7 7 2
```

```
x_1 <- x[1,]
x_2 <- x[2,]
x_3 <- x[3,]

#distance between two numbers
sqrt(sum((x_1 - x_2)^2))
```

```
## [1] 2079.753
```

```
sqrt(sum((x_1 - x_3)^2))
```

```
## [1] 2252.129
```

```
sqrt(sum((x_2 - x_3)^2))
```

```
## [1] 2642.906
```

```
#compute distance using matrix algebra
sqrt(crossprod(x_1 - x_2))
```

```
##          [,1]
## [1,] 2079.753
```

```
sqrt(crossprod(x_1 - x_3))
```

```
##          [,1]
## [1,] 2252.129
```

```
sqrt(crossprod(x_2 - x_3))
```

```
##          [,1]
## [1,] 2642.906
```

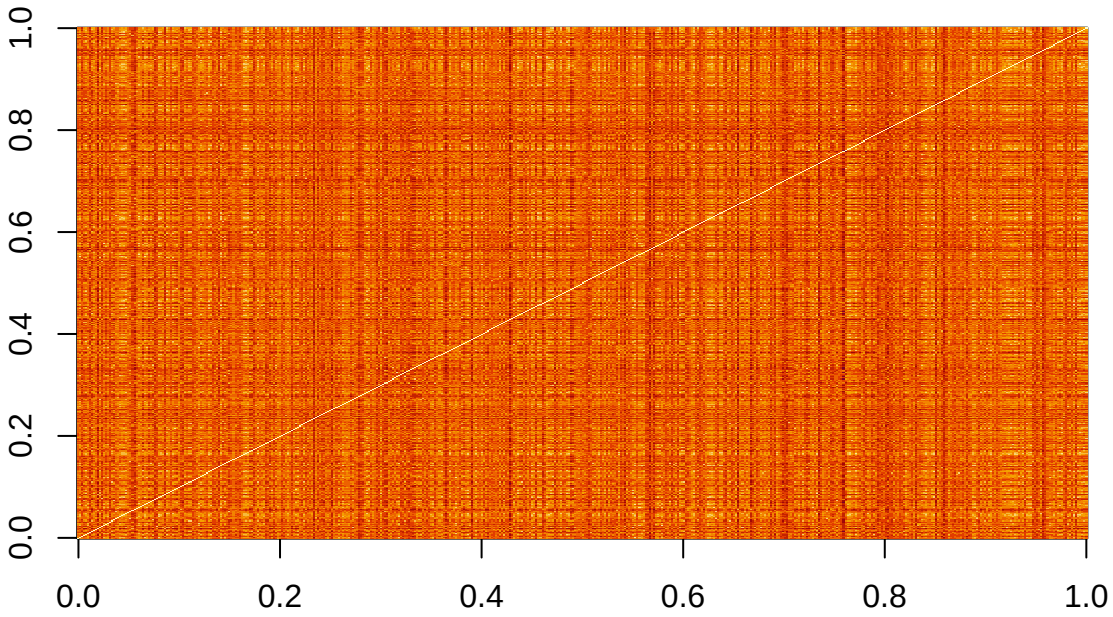
```
#compute distance between each row
d <- dist(x)
class(d)
```

```
## [1] "dist"
```

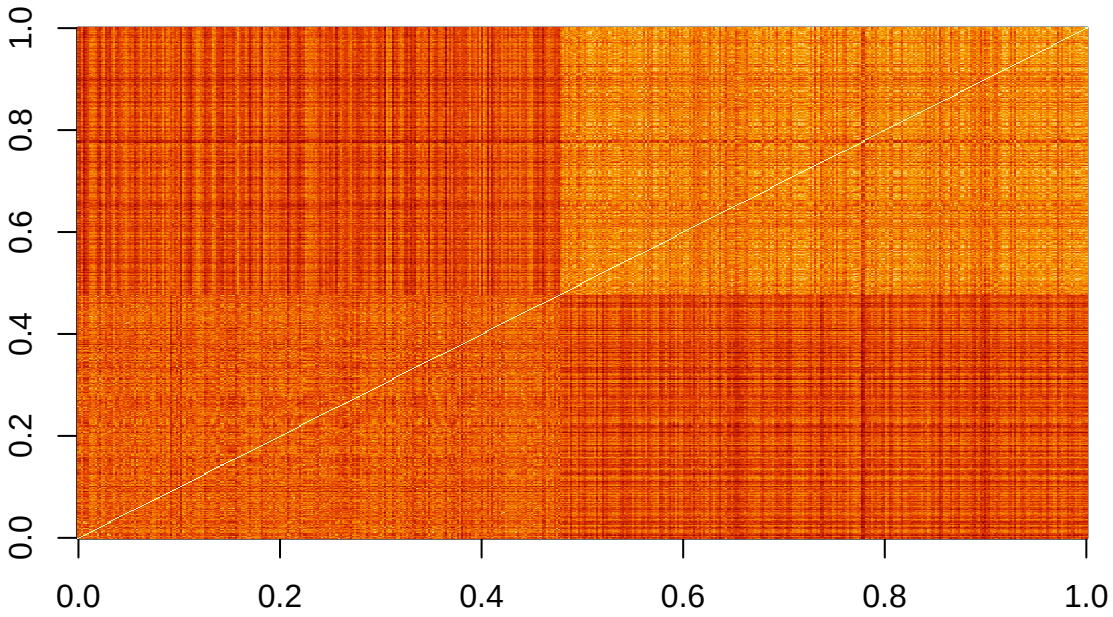
```r
as.matrix(d)[1:3,1:3]
```

```
##          1        2        3
## 1    0.000 2079.753 2252.129
## 2 2079.753    0.000 2642.906
## 3 2252.129 2642.906    0.000
```

```r
#visualize these distances
image(as.matrix(d))
```



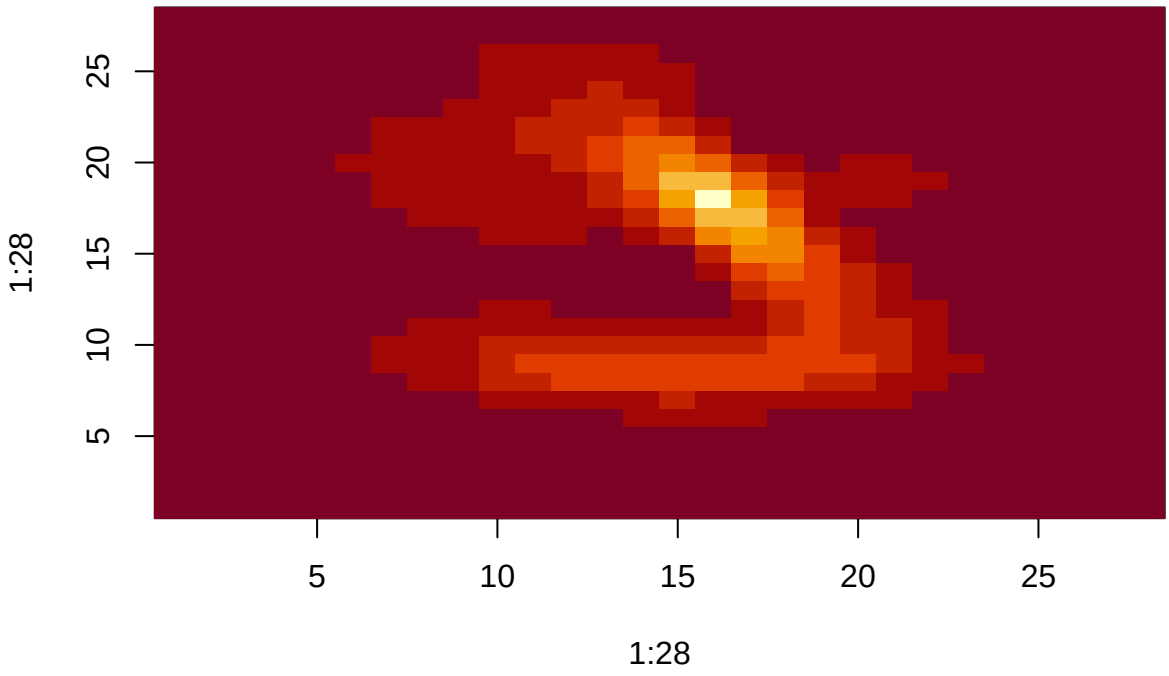

```r
#order the distance by labels
image(as.matrix(d)[order(y), order(y)])
```



```
#compute distance between predictors
d <- dist(t(x))
dim(as.matrix(d))
```

```
## [1] 784 784
```

```
d_492 <- as.matrix(d)[492,]

image(1:28, 1:28, matrix(d_492, 28, 28))
```



Comprehension Check - Distance

1. Load the following dataset:

```
data(tissue_gene_expression)
```

This dataset includes a matrix `x`:

```
dim(tissue_gene_expression$x)
```

```
## [1] 189 500
```

This matrix has the gene expression levels of 500 genes from 189 biological samples representing seven different tissues. The tissue type is stored in `y`:

```
table(tissue_gene_expression$y)
```

```
##
##  cerebellum       colon endometrium hippocampus      kidney       liver
##          38          34          15          31          39          26
##    placenta
##           6
```

Which of the following lines of code computes the Euclidean distance between each observation and stores it in the object `d`?

```
d <- dist(tissue_gene_expression$x)
```

- ☐ A. `d <- dist(tissue_gene_expression$x, distance='maximum')`
- ☐ B. `d <- dist(tissue_gene_expression)`
- ☒ C. `d <- dist(tissue_gene_expression$x)`
- ☐ D. `d <- cor(tissue_gene_expression$x)`

2. Using the dataset from Q1, compare the distances between observations 1 and 2 (both cerebellum), observations 39 and 40 (both colon), and observations 73 and 74 (both endometrium).

Distance-wise, are samples from tissues of the same type closer to each other than tissues of different type?

```
ind <- c(1, 2, 39, 40, 73, 74)
as.matrix(d)[ind,ind]
```

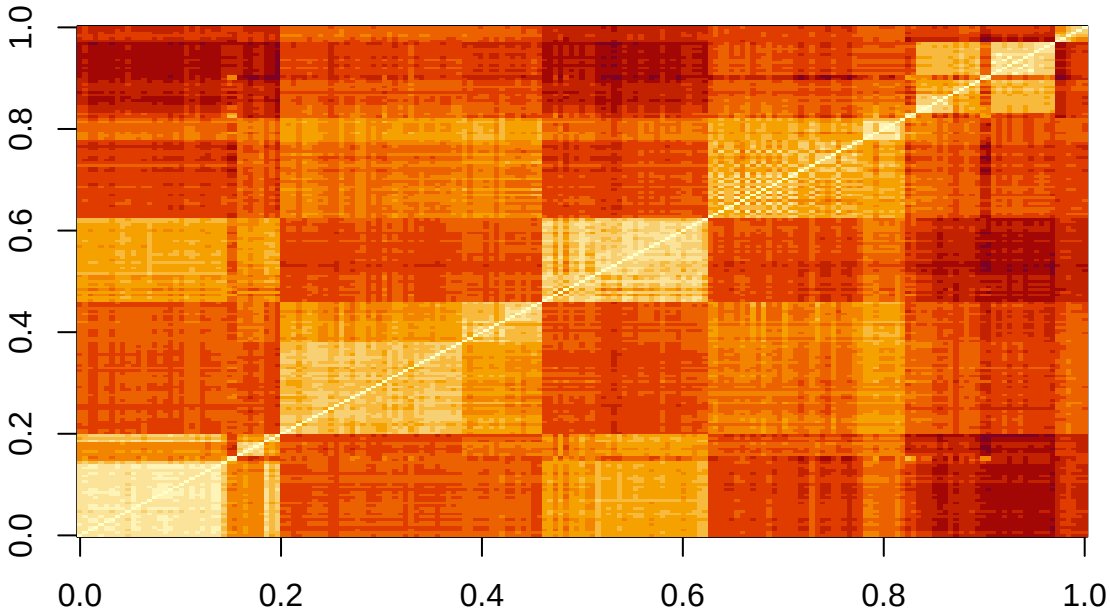
```
##               cerebellum_1 cerebellum_2   colon_1   colon_2 endometrium_1
## cerebellum_1      0.000000     7.005922 22.694801 22.699755      21.12763
## cerebellum_2      7.005922     0.000000 22.384821 22.069557      20.87910
## colon_1          22.694801    22.384821  0.000000  8.191935      14.99672
## colon_2          22.699755    22.069557  8.191935  0.000000      14.80355
## endometrium_1    21.127629    20.879099 14.996715 14.803545       0.00000
## endometrium_2    21.780792    20.674802 18.089213 17.004456      14.29405
##               endometrium_2
## cerebellum_1       21.78079
## cerebellum_2       20.67480
## colon_1            18.08921
## colon_2            17.00446
## endometrium_1      14.29405
## endometrium_2       0.00000
```

- ☐ A. No, the samples from the same tissue type are not necessarily closer.
- ☐ B. The two colon samples are close to each other, but the samples from the other two tissues are not.
- ☐ C. The two cerebellum samples are close to each other, but the samples from the other two tissues are not.
- ☒ D. Yes, the samples from the same tissue type are closer to each other.

3. Make a plot of all the distances using the image() function to see if the pattern you observed in Q2 is general.

Which code would correctly make the desired plot?

```
image(as.matrix(d))
```



☐ A. `image(d)`

☒ B. `image(as.matrix(d))`

☐ C. `d`

☐ D. `image()`

Knn

There is a link to the relevant section of the textbook: k-nearest neighbors

Key points

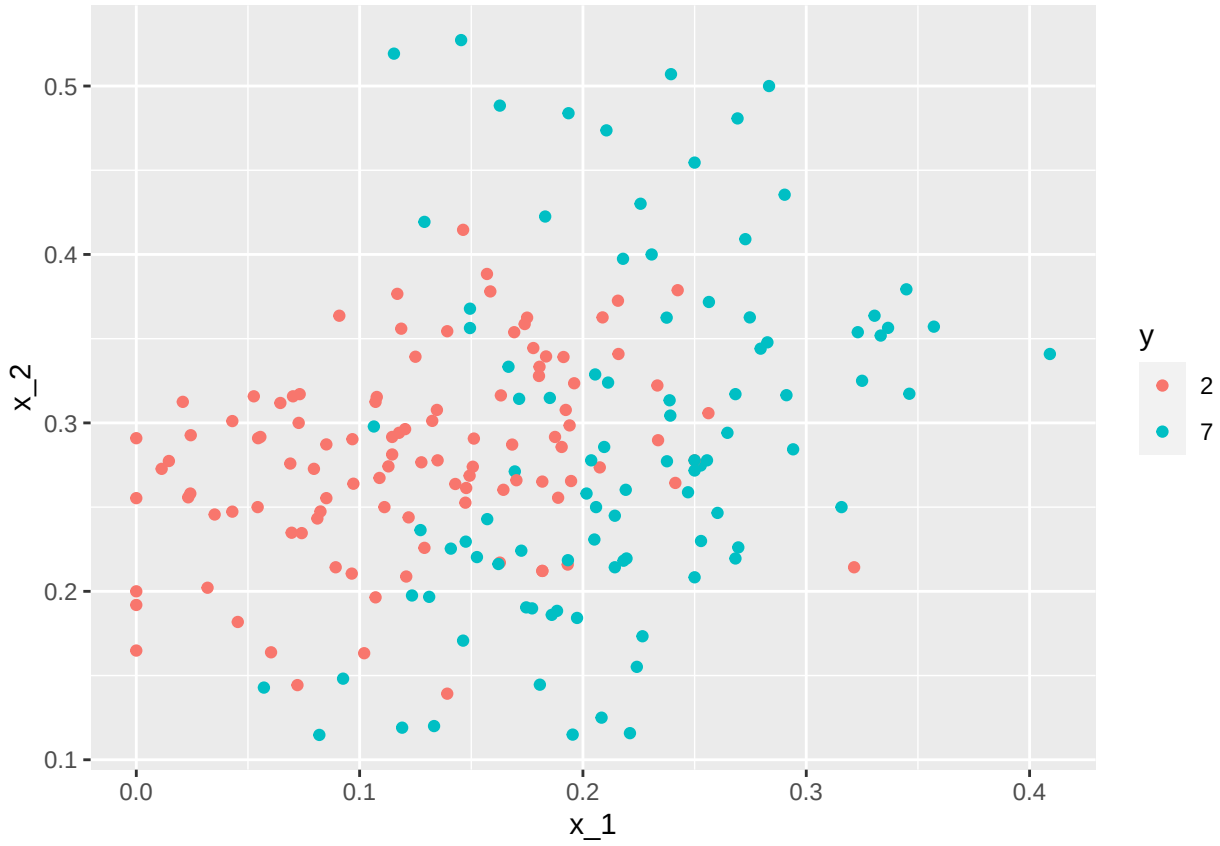
- **K-nearest neighbors (kNN)** estimates the conditional probabilities in a similar way to bin smoothing. However, kNN is easier to adapt to multiple dimensions.
- Using kNN, for any point (x_1, x_2) for which we want an estimate of $p(x_1, x_2)$, we look for the **k nearest points** to (x_1, x_2) and take an average of the 0s and 1s associated with these points. We refer to the set of points used to compute the average as the **neighborhood**. Larger values of k result in smoother estimates, while smaller values of k result in more flexible and more wiggly estimates.
- To implement the algorithm, we can use the `knn3()` function from the **caret** package. There are two ways to call this function:

1. We need to specify a formula and a data frame. The formula looks like this: outcome $\sim$ predictor$_1$ + predictor$_2$ + predictor$_3$. The `predict()` function for `knn3` produces a probability for each class.
2. We can also call the function with the first argument being the matrix predictors and the second a vector of outcomes, like this:

```
x <- as.matrix(mnist_27$train[,2:3])
y <- mnist_27$train$y
knn_fit <- knn3(x,y)
```

Code

```
data("mnist_27")
mnist_27$test %>% ggplot(aes(x_1, x_2, color = y)) + geom_point()
```




```
#logistic regression
library(caret)
fit_glm <- glm(y~x_1+x_2, data=mnist_27$train, family="binomial")
p_hat_logistic <- predict(fit_glm, mnist_27$test)
y_hat_logistic <- factor(ifelse(p_hat_logistic > 0.5, 7, 2))
confusionMatrix(data = y_hat_logistic, reference = mnist_27$test$y)$overall[1]
```

```
## Accuracy
##     0.76
```

```
#fit knn model
knn_fit <- knn3(y ~ ., data = mnist_27$train)

x <- as.matrix(mnist_27$train[,2:3])
y <- mnist_27$train$y
knn_fit <- knn3(x, y)

knn_fit <- knn3(y ~ ., data = mnist_27$train, k=5)

y_hat_knn <- predict(knn_fit, mnist_27$test, type = "class")
confusionMatrix(data = y_hat_knn, reference = mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##    0.815
```

Over-training and Over-smoothing

There is a link to the relevant sections of the textbook: Over-training and Over-smoothing

Key points

- **Over-training** is the reason that we have higher accuracy in the train set compared to the test set. Over-training is at its worst when we set $k = 1$. With $k = 1$, the estimate for each (x_1, x_2) in the training set is obtained with just the y corresponding to that point.
- When we try a larger k, the k might be so large that it does not permit enough flexibility. We call this **over-smoothing**.
- Note that if we use the test set to pick this k, we should not expect the accompanying accuracy estimate to extrapolate to the real world. This is because even here we broke a golden rule of machine learning: **we selected the k using the test set. Cross validation** also provides an estimate that takes this into account.

Code

```
y_hat_knn <- predict(knn_fit, mnist_27$train, type = "class")
confusionMatrix(data = y_hat_knn, reference = mnist_27$train$y)$overall["Accuracy"]
```

```
## Accuracy
##   0.8825
```

```
y_hat_knn <- predict(knn_fit, mnist_27$test, type = "class")
confusionMatrix(data = y_hat_knn, reference = mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##    0.815
```

```
#fit knn with k=1
knn_fit_1 <- knn3(y ~ ., data = mnist_27$train, k = 1)
y_hat_knn_1 <- predict(knn_fit_1, mnist_27$train, type = "class")
confusionMatrix(data=y_hat_knn_1, reference=mnist_27$train$y)$overall[["Accuracy"]]
```

```
## [1] 0.995
```

```
y_hat_knn_1 <- predict(knn_fit_1, mnist_27$test, type = "class")
confusionMatrix(data=y_hat_knn_1, reference=mnist_27$test$y)$overall[["Accuracy"]]
```

```
## [1] 0.74
```

```
#fit knn with k=401
knn_fit_401 <- knn3(y ~ ., data = mnist_27$train, k = 401)
y_hat_knn_401 <- predict(knn_fit_401, mnist_27$test, type = "class")
confusionMatrix(data=y_hat_knn_401, reference=mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##     0.79
```

```
#pick the k in knn
ks <- seq(3, 251, 2)
library(purrr)
accuracy <- map_df(ks, function(k){
    fit <- knn3(y ~ ., data = mnist_27$train, k = k)
    y_hat <- predict(fit, mnist_27$train, type = "class")
    cm_train <- confusionMatrix(data = y_hat, reference = mnist_27$train$y)
    train_error <- cm_train$overall["Accuracy"]
    y_hat <- predict(fit, mnist_27$test, type = "class")
    cm_test <- confusionMatrix(data = y_hat, reference = mnist_27$test$y)
    test_error <- cm_test$overall["Accuracy"]

tibble(train = train_error, test = test_error)
})


#pick the k that maximizes accuracy using the estimates built on the test data
ks[which.max(accuracy$test)]
```

```
## [1] 41
```

```
max(accuracy$test)
```

```
## [1] 0.86
```

Comprehension Check - Nearest Neighbors

1. Previously, we used logistic regression to predict sex based on height. Now we are going to use knn to do the same. Set the seed to 1, then use the **caret** package to partition the **dslabs** `heights` data into a training and test set of equal size. Use the `sapply()` function to perform knn with `k` values of `seq(1, 101, 3)` and calculate F1 scores with the `F_meas()` function using the default value of the relevant argument.

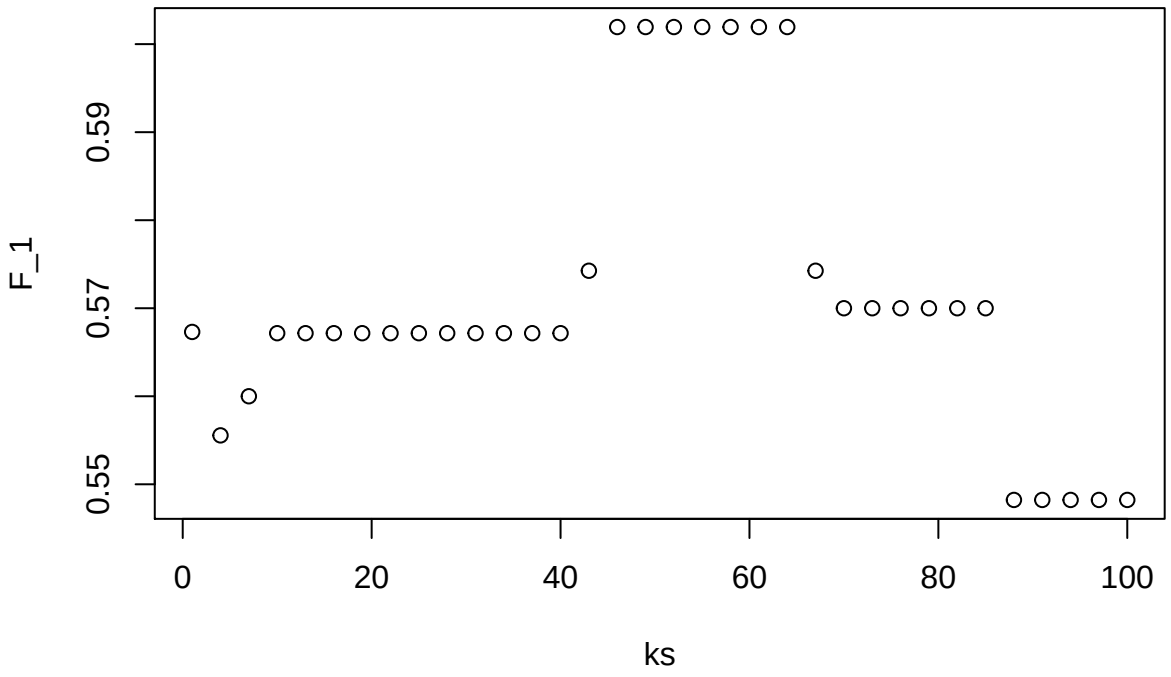
What is the max value of `F_1`?

At what value of `k` does the max occur?

```
data("heights")

# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
test_index <- createDataPartition(heights$sex, times = 1, p = 0.5, list = FALSE)
test_set <- heights[test_index, ]
train_set <- heights[-test_index, ]

ks <- seq(1, 101, 3)
F_1 <- sapply(ks, function(k){
    fit <- knn3(sex ~ height, data = train_set, k = k)
    y_hat <- predict(fit, test_set, type = "class") %>%
        factor(levels = levels(train_set$sex))
    F_meas(data = y_hat, reference = test_set$sex)
})
plot(ks, F_1)
```




```
max(F_1)
```

```
## [1] 0.6019417
```

```
ks[which.max(F_1)]
```

```
## [1] 46
```

2. Next we will use the same gene expression example used in the Comprehension Check: Distance exercises. You can load it like this:

```
library(dslabs)
library(caret)
data("tissue_gene_expression")
```

First, set the seed to 1 and split the data into training and test sets with `p = 0.5`. Then, report the accuracy you obtain from predicting tissue type using KNN with `k = seq(1, 11, 2)` using `sapply()` or `map_df()`. Note: use the `createDataPartition()` function outside of `sapply()` or `map_df()`.

```
# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
y <- tissue_gene_expression$y
x <- tissue_gene_expression$x
test_index <- createDataPartition(y, list = FALSE)
sapply(seq(1, 11, 2), function(k){
    fit <- knn3(x[-test_index,], y[-test_index], k = k)
    y_hat <- predict(fit, newdata = data.frame(x=x[test_index,]),
                type = "class")
mean(y_hat == y[test_index])
})
```

```
## [1] 0.9895833 0.9687500 0.9479167 0.9166667 0.9166667 0.9062500
```

K-fold cross validation

There is a link to the relevant section of the textbook: K-fold cross validation

Key points

- For k**-fold cross validation**, we divide the dataset into a training set and a test set. We train our algorithm exclusively on the training set and use the test set only for evaluation purposes.
- For each set of algorithm parameters being considered, we want an **estimate of the MSE and then we will choose the parameters with the smallest MSE**. In k-fold cross validation, we randomly split the observations into k non-overlapping sets, and repeat the calculation for MSE for each of these sets. Then, we compute the average MSE and obtain an estimate of our loss. Finally, we can select the optimal parameter that minimized the MSE.
- In terms of how to select k for cross validation, **larger values of** k **are preferable but they will also take much more** computational time. For this reason, the choices of $k = 5$ and $k = 10$ are common.

Comprehension Check - Cross-validation

1. Generate a set of random predictors and outcomes using the following code:

```
# set.seed(1996) #if you are using R 3.5 or earlier
set.seed(1996, sample.kind="Rounding") #if you are using R 3.6 or later
```

```
## Warning in set.seed(1996, sample.kind = "Rounding"): non-uniform 'Rounding'
## sampler used
```

```
n <- 1000
p <- 10000
x <- matrix(rnorm(n*p), n, p)
colnames(x) <- paste("x", 1:ncol(x), sep = "_")
y <- rbinom(n, 1, 0.5) %>% factor()

x_subset <- x[ ,sample(p, 100)]
```

Because `x` and `y` are completely independent, you should not be able to predict `y` using `x` with accuracy greater than 0.5. Confirm this by running cross-validation using logistic regression to fit the model. Because we have so many predictors, we selected a random sample `x_subset`. Use the subset when training the model.

Which code correctly performs this cross-validation?

```
fit <- train(x_subset, y, method = "glm")
fit$results
```

```
##   parameter  Accuracy      Kappa AccuracySD    KappaSD
## 1      none 0.5078406 0.01318925 0.02336971 0.04626366
```

☐ A.

```
fit <- train(x_subset, y)
fit$results
```

☒ B.

```
fit <- train(x_subset, y, method = "glm")
fit$results
```

☐ C.

```
fit <- train(y, x_subset, method = "glm")
fit$results
```

☐ D.

```
fit <- test(x_subset, y, method = "glm")
fit$results
```

2. Now, instead of using a random selection of predictors, we are going to search for those that are most predictive of the outcome. We can do this by comparing the values for the $y = 1$ group to those in the $y = 0$ group, for each predictor, using a t-test. You can do perform this step like this:

```
if(!require(BiocManager)) install.packages("BiocManager")
```

```
## Loading required package: BiocManager
```

```
## Bioconductor version 3.11 (BiocManager 1.30.10), ?BiocManager::install for help
```

```
## Bioconductor version '3.11' is out-of-date; the current release version '3.12'
##   is available with R version '4.0'; see https://bioconductor.org/install
```

```
BiocManager::install("genefilter")
```

```
## Bioconductor version 3.11 (BiocManager 1.30.10), R 4.0.2 (2020-06-22)
```

```
## Installing package(s) 'genefilter'

##
## The downloaded binary packages are in
##  /var/folders/6m/nz2p76pn679b692c99t644bm0000gn/T//RtmpUgisOW/downloaded_packages
```

```
library(genefilter)
```

```
##
## Attaching package: 'genefilter'

## The following objects are masked from 'package:matrixStats':
##
##     rowSds, rowVars

## The following object is masked from 'package:MASS':
##
##     area

## The following object is masked from 'package:readr':
##
##     spec
```

```
tt <- colttests(x, y)
```

Which of the following lines of code correctly creates a vector of the p-values called pvals?

```
pvals <- tt$p.value
```

- ☐ A. `pvals <- tt$dm`
- ☐ B. `pvals <- tt$statistic`
- ☐ C. `pvals <- tt`
- ☒ D. `pvals <- tt$p.value`

3. Create an index `ind` with the column numbers of the predictors that were "statistically significantly" associated with `y`. Use a p-value cutoff of 0.01 to define "statistically significantly."

How many predictors survive this cutoff?

```
ind <- which(pvals <= 0.01)
length(ind)
```

```
## [1] 108
```

4. Now re-run the cross-validation after redefinining `x_subset` to be the subset of `x` defined by the columns showing "statistically significant" association with `y`.

What is the accuracy now?

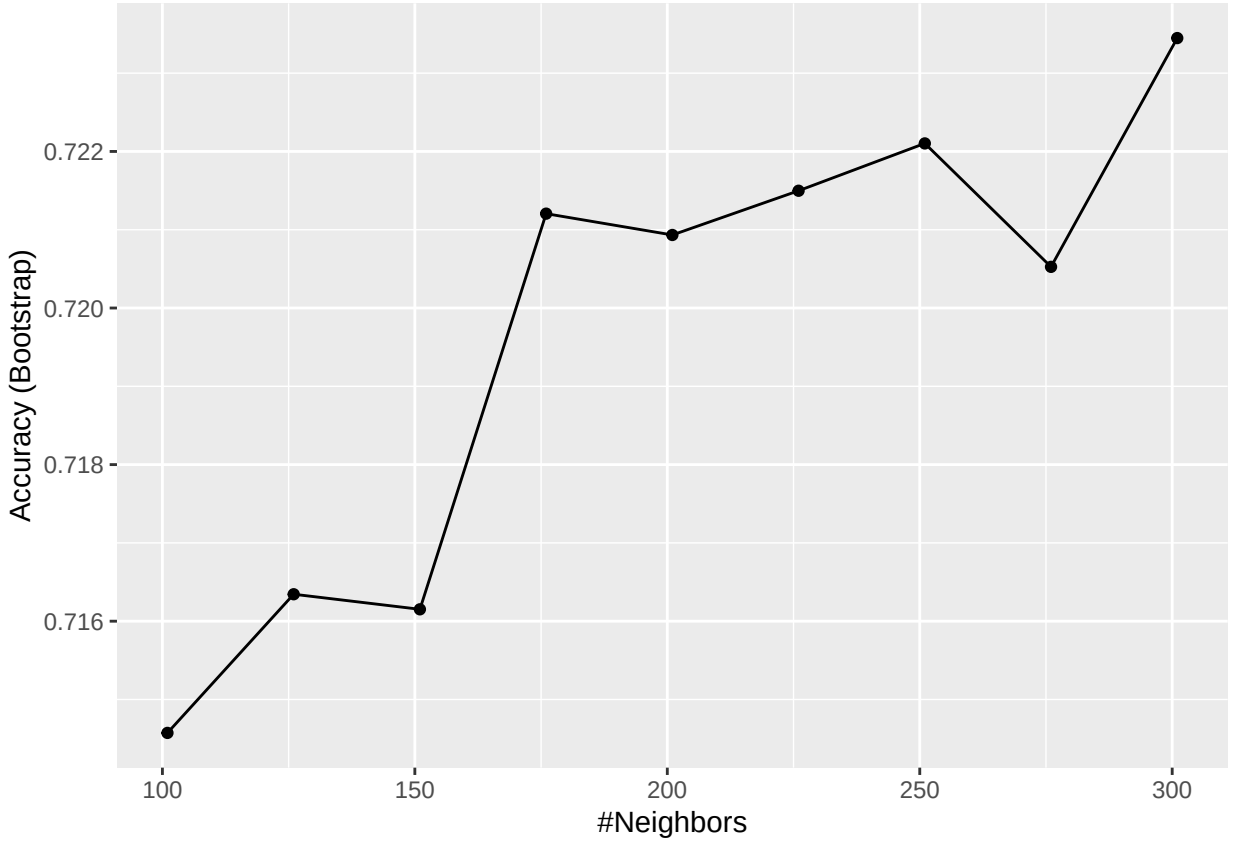
```
x_subset <- x[,ind]
fit <- train(x_subset, y, method = "glm")
fit$results
```

```
##   parameter  Accuracy     Kappa AccuracySD    KappaSD
## 1      none 0.7571395 0.5134142 0.01922097 0.03805696
```

5. Re-run the cross-validation again, but this time using kNN. Try out the following grid `k = seq(101, 301, 25)` of tuning parameters. Make a plot of the resulting accuracies.

Which code is correct?

```
fit <- train(x_subset, y, method = "knn", tuneGrid = data.frame(k = seq(101, 301, 25)))
ggplot(fit)
```



☒ A.

```
fit <- train(x_subset, y, method = "knn", tuneGrid = data.frame(k = seq(101, 301, 25)))
ggplot(fit)
```

☐ B.

```
fit <- train(x_subset, y, method = "knn")
ggplot(fit)
```

☐ C.

```
fit <- train(x_subset, y, method = "knn", tuneGrid = data.frame(k = seq(103, 301, 25)))
ggplot(fit)
```

☐ D.

```
fit <- train(x_subset, y, method = "knn", tuneGrid = data.frame(k = seq(101, 301, 5)))
ggplot(fit)
```

6. In the previous exercises, we see that despite the fact that `x` and `y` are completely independent, we were able to predict `y` with accuracy higher than 70%. We must be doing something wrong then.

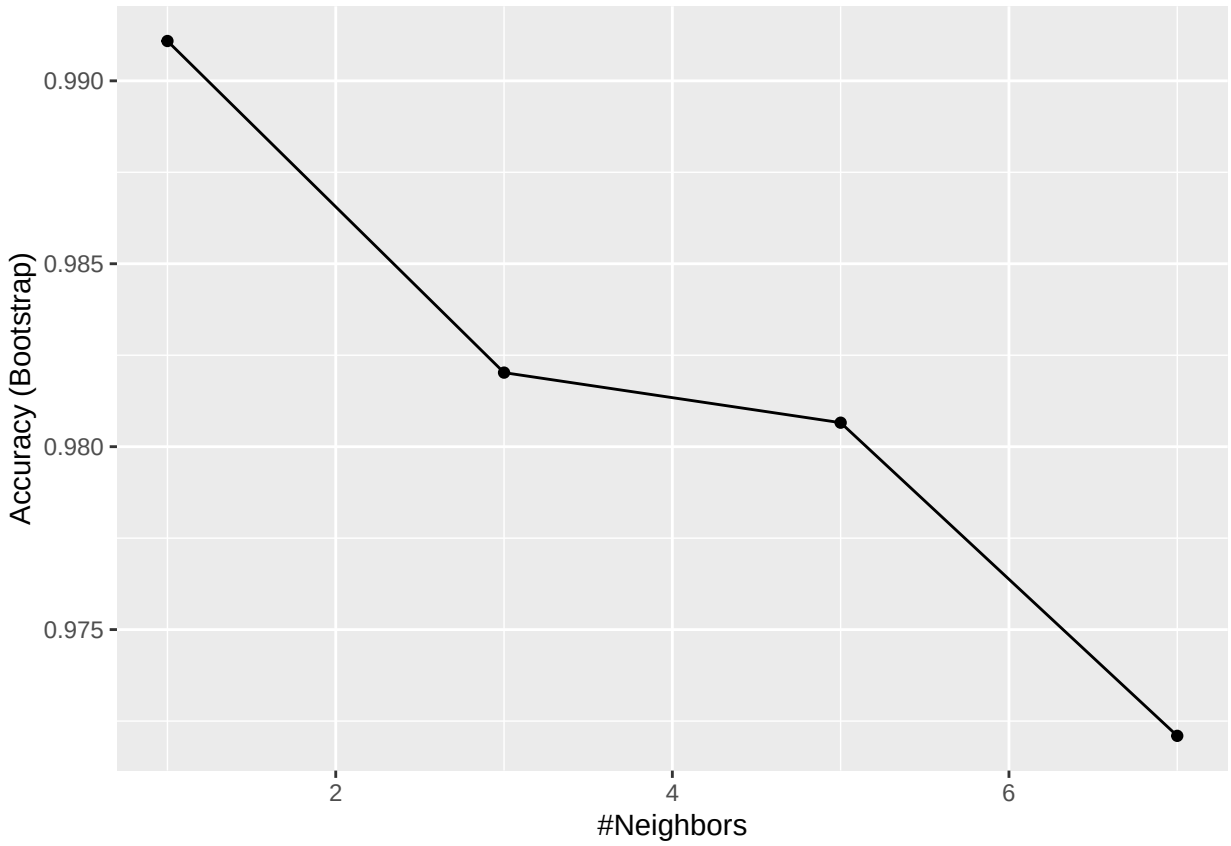
What is it?

☐ A. The function `train()` estimates accuracy on the same data it uses to train the algorithm.
☐ B. We are overfitting the model by including 100 predictors.
☒ C. We used the entire dataset to select the columns used in the model.
☐ D. The high accuracy is just due to random variability.

7. Use the `train()` function with kNN to select the best `k` for predicting tissue from gene expression on the `tissue_gene_expression` dataset from **dslabs**. Try `k = seq(1,7,2)` for tuning parameters. For this question, do not split the data into test and train sets (understand this can lead to overfitting, but ignore this for now).

What value of `k` results in the highest accuracy?

```
data("tissue_gene_expression")
fit <- with(tissue_gene_expression, train(x, y, method = "knn", tuneGrid = data.frame( k = seq(1, 7, 2))
ggplot(fit)
```




```
fit$results
```

```
##   k  Accuracy     Kappa AccuracySD    KappaSD
## 1 1 0.9910881 0.9892456 0.01127300 0.01349575
## 2 3 0.9820243 0.9781738 0.01389797 0.01683721
## 3 5 0.9806558 0.9765964 0.02484299 0.02995977
## 4 7 0.9720962 0.9660514 0.03007035 0.03650127
```

Bootstrap

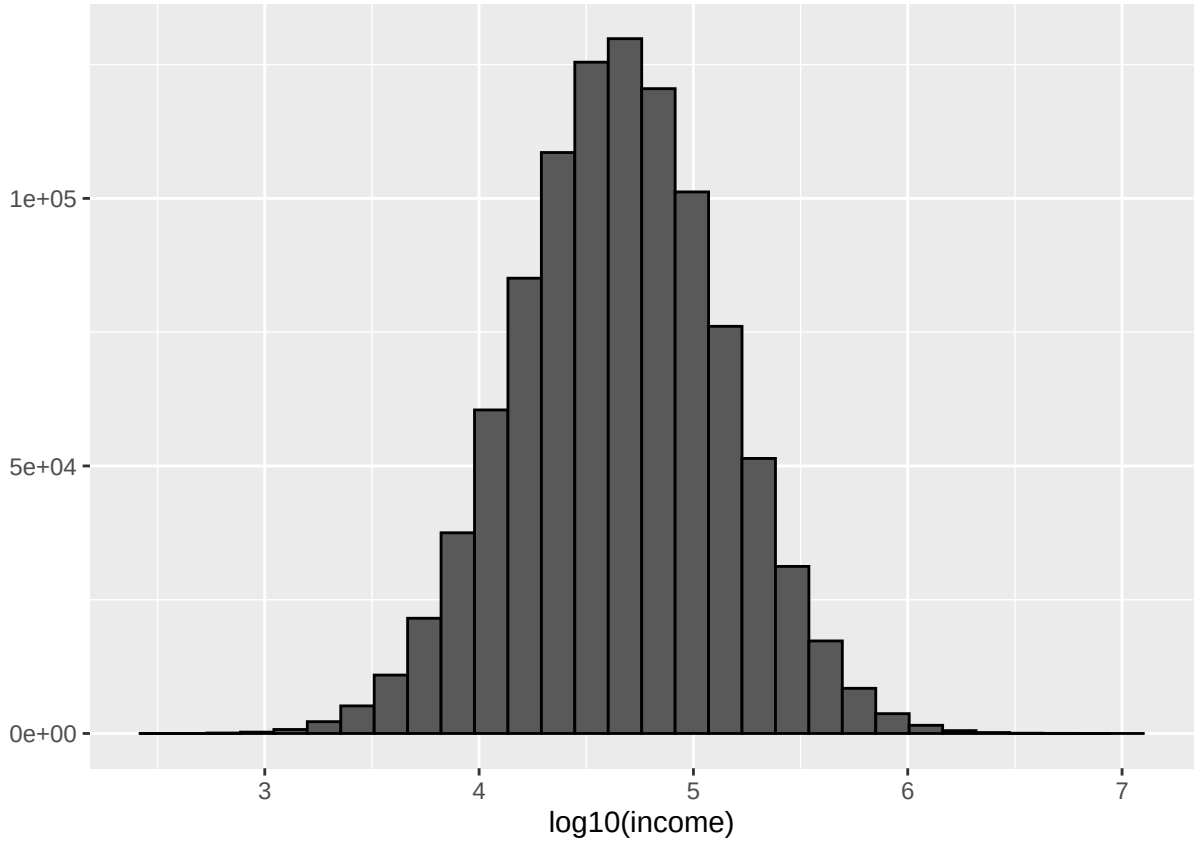
There is a link to the relevant section of the textbook: Bootstrap

Key points

- When we don't have access to the entire population, we can use **bootstrap** to estimate the population median m.
- The bootstrap permits us to **approximate a Monte Carlo simulation** without access to the entire distribution. The general idea is relatively simple. We act as if the observed sample is the population. We then sample datasets (with replacement) of the same sample size as the original dataset. Then we compute the summary statistic, in this case the median, on this bootstrap sample.
- Note that we can use ideas similar to those used in the bootstrap in **cross validation**: instead of dividing the data into equal partitions, we simply bootstrap many times.

Code

```
n <- 10^6
income <- 10^(rnorm(n, log10(45000), log10(3)))
qplot(log10(income), bins = 30, color = I("black"))
```




```
m <- median(income)
m
```

```
## [1] 44986.86
```

```
set.seed(1)
#use set.seed(1, sample.kind="Rounding") instead if using R 3.6 or later
N <- 250
X <- sample(income, N)
M<- median(X)
M
```

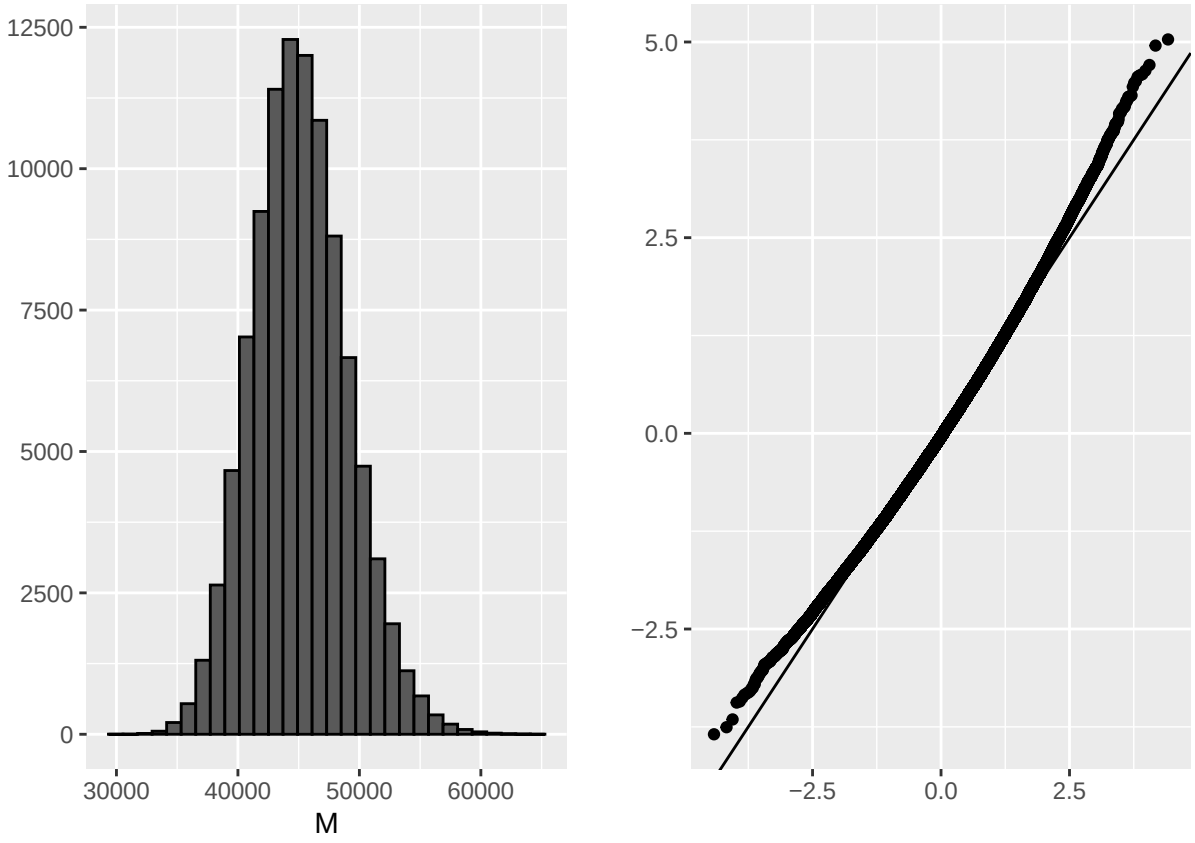
```
## [1] 47024.18
```

```
library(gridExtra)
```

```
##
## Attaching package: 'gridExtra'
```

```
## The following object is masked from 'package:dplyr':
##
##     combine
```

```
B <- 10^5
M <- replicate(B, {
    X <- sample(income, N)
    median(X)
})
p1 <- qplot(M, bins = 30, color = I("black"))
p2 <- qplot(sample = scale(M)) + geom_abline()
grid.arrange(p1, p2, ncol = 2)
```



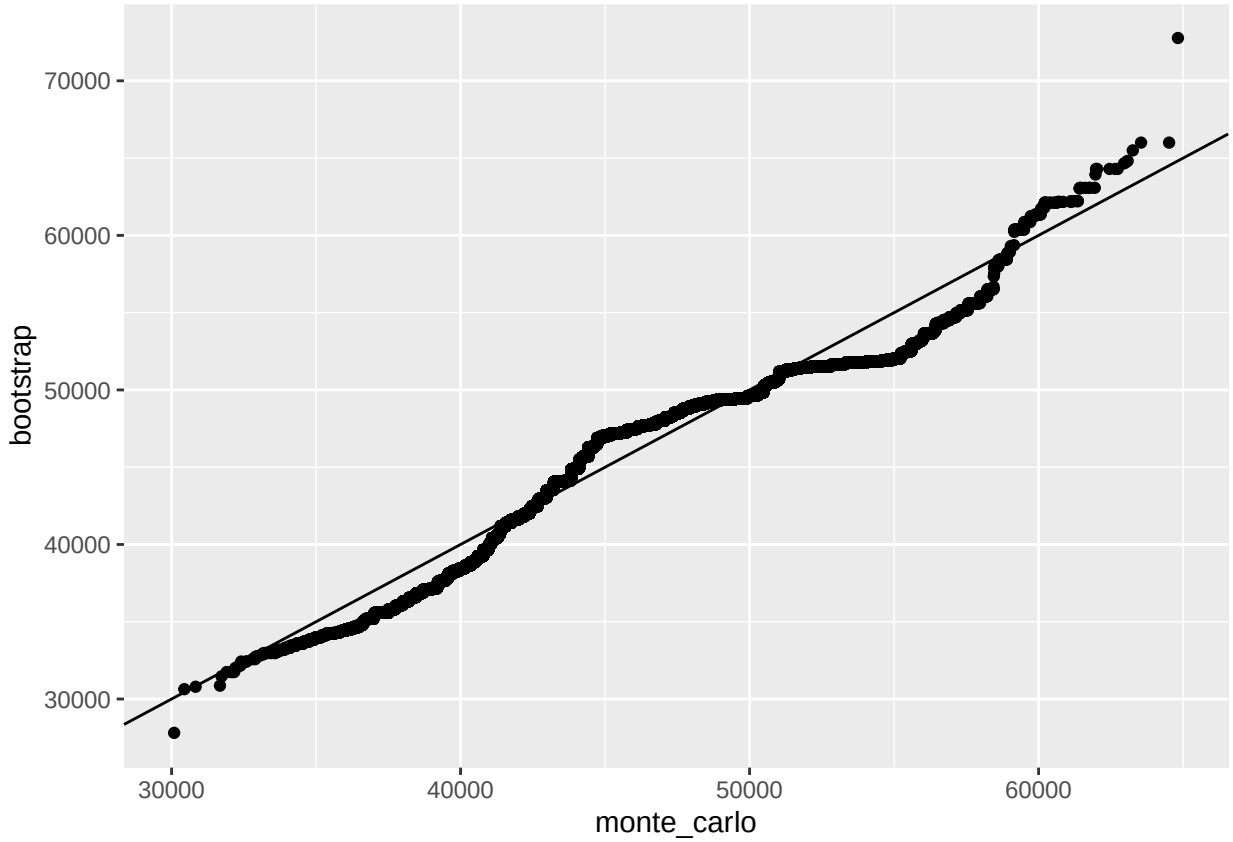

```
mean(M)
```

```
## [1] 45132.14
```

```
sd(M)
```

```
## [1] 3912.368
```

```
B <- 10^5
M_star <- replicate(B, {
    X_star <- sample(X, N, replace = TRUE)
    median(X_star)
})

tibble(monte_carlo = sort(M), bootstrap = sort(M_star)) %>%
    qplot(monte_carlo, bootstrap, data = .) +
    geom_abline()
```




```
quantile(M, c(0.05, 0.95))
```

```
##       5%      95%
## 38996.50 51811.42
```

```
quantile(M_star, c(0.05, 0.95))
```

```
##       5%      95%
## 37112.39 51462.43
```

```
median(X) + 1.96 * sd(X) / sqrt(N) * c(-1, 1)
```

```
## [1] 33154.08 60894.28
```

```
mean(M) + 1.96 * sd(M) * c(-1,1)
```

```
## [1] 37463.90 52800.38
```

```
mean(M_star) + 1.96 * sd(M_star) * c(-1, 1)
```

```
## [1] 36913.52 53897.73
```

Comprehension Check - Bootstrap

1. The `createResample()` function can be used to create bootstrap samples. For example, we can create the indexes for 10 bootstrap samples for the `mnist_27` dataset like this:

```
data(mnist_27)
# set.seed(1995) # if R 3.5 or earlier
set.seed(1995, sample.kind="Rounding") # if R 3.6 or later
```

```
## Warning in set.seed(1995, sample.kind = "Rounding"): non-uniform 'Rounding'
## sampler used
```

```
indexes <- createResample(mnist_27$train$y, 10)
```

How many times do 3, 4, and 7 appear in the first resampled index?

```
sum(indexes[[1]] == 3)
```

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

```
sum(indexes[[1]] == 4)
```

```
## [1] 4
```

```
sum(indexes[[1]] == 7)
```

```
## [1] 0
```

2. We see that some numbers appear more than once and others appear no times. This has to be this way for each dataset to be independent. Repeat the exercise for all the resampled indexes.

What is the total number of times that 3 appears in all of the resampled indexes?

```
x=sapply(indexes, function(ind){
    sum(ind == 3)
})
sum(x)
```

```
## [1] 11
```

3. Generate a random dataset using the following code:

```
y <- rnorm(100, 0, 1)
```

Estimate the 75th quantile, which we know is `qnorm(0.75)`, with the sample quantile: `quantile(y, 0.75)`.

Now, set the seed to 1 and perform a Monte Carlo simulation with 10,000 repetitions, generating the random dataset and estimating the 75th quantile each time. What is the expected value and standard error of the 75th quantile?

Report all answers to at least 3 decimal digits.

```r
# set.seed(1) # # if R 3.5 or earlier
set.seed(1, sample.kind = "Rounding") # if R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```r
B <- 10000
q_75 <- replicate(B, {
    y <- rnorm(100, 0, 1)
    quantile(y, 0.75)
})

mean(q_75)
```

```
## [1] 0.6656107
```

```r
sd(q_75)
```

```
## [1] 0.1353809
```

4. In practice, we can't run a Monte Carlo simulation. Use the sample:

```r
# set.seed(1) # if R 3.5 or earlier
set.seed(1, sample.kind = "Rounding") # if R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```r
y <- rnorm(100, 0, 1)
```

Set the seed to 1 again after generating `y` and use 10 bootstrap samples to estimate the expected value and standard error of the 75th quantile.

```r
# set.seed(1) # if R 3.5 or earlier
set.seed(1, sample.kind = "Rounding") # if R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```r
y <- rnorm(100, 0, 1)

# set.seed(1) # if R 3.5 or earlier
set.seed(1, sample.kind="Rounding") # if R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
indexes <- createResample(y, 10)
q_75_star <- sapply(indexes, function(ind){
    y_star <- y[ind]
    quantile(y_star, 0.75)
})
mean(q_75_star)
```

```
## [1] 0.7312648
```

```
sd(q_75_star)
```

```
## [1] 0.07419278
```

5. Repeat the exercise from Q4 but with 10,000 bootstrap samples instead of 10. Set the seed to 1 first.

```
# set.seed(1) # # if R 3.5 or earlier
set.seed(1, sample.kind = "Rounding") # if R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
indexes <- createResample(y, 10000)
q_75_star <- sapply(indexes, function(ind){
    y_star <- y[ind]
    quantile(y_star, 0.75)
})
mean(q_75_star)
```

```
## [1] 0.6737512
```

```
sd(q_75_star)
```

```
## [1] 0.0930575
```

6. When doing bootstrap sampling, the simulated samples are drawn from the empirical distribution of the original data.

True or False: The bootstrap is particularly useful in situations when we do not have access to the distribution or it is unknown.

☒ A. True
☐ B. False

Generative Models

There is a link to the relevant section of the textbook: Generative models

**Key points

- **Discriminative approaches** estimate the conditional probability directly and do not consider the distribution of the predictors.
- **Generative models** are methods that model the joint distribution and X (we model how the entire data, X and Y, are generated).

Naive Bayes

There is a link to the relevant section of the textbook: Naive Bayes

Key points

- Bayes' rule:

$p(x) = Pr(Y = 1|X = x) = \frac{f_{X|Y=1}(X)Pr(Y=1)}{f_{X|Y=0}(X)Pr(Y=0)+f_{X|Y=1}(X)Pr(Y=1)}$

with $f_{X|Y=1}$ and $f_{X|Y=0}$ representing the distribution functions of the predictor X for the two classes $Y = 1$ and $Y = 0$.

- The **Naive Bayes** approach is similar to the logistic regression prediction mathematically. However, we leave the demonstration to a more advanced text, such as The Elements of Statistical Learning by Hastie, Tibshirani, and Friedman.

Code

```
# Generating train and test set
data("heights")
y <- heights$height
set.seed(2)
test_index <- createDataPartition(y, times = 1, p = 0.5, list = FALSE)
train_set <- heights %>% slice(-test_index)
test_set <- heights %>% slice(test_index)

# Estimating averages and standard deviations
params <- train_set %>%
 group_by(sex) %>%
 summarize(avg = mean(height), sd = sd(height))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
params
```

```
## # A tibble: 2 x 3
##   sex      avg    sd
##   <fct>  <dbl> <dbl>
## 1 Female  64.5  4.02
## 2 Male    69.3  3.52
```

```
# Estimating the prevalence
pi <- train_set %>% summarize(pi=mean(sex=="Female")) %>% pull(pi)
pi
```

```
## [1] 0.2290076
```

```
# Getting an actual rule
x <- test_set$height
f0 <- dnorm(x, params$avg[2], params$sd[2])
f1 <- dnorm(x, params$avg[1], params$sd[1])
p_hat_bayes <- f1*pi / (f1*pi + f0*(1 - pi))
```

Controlling Prevalence

There is a link to the relevant section of the textbook: Controlling prevalence

Key points

- The Naive Bayes approach includes a **parameter to account for differences in prevalence** $\pi = Pr(Y = 1)$. If we use hats to denote the estimates, we can write $p(\widehat{x})$ as:

$$\hat{p}(x) = \frac{\hat{f}_{X|Y=1}(x)\hat{\pi}}{\hat{f}_{X|Y=0}(x)(1-\hat{\pi}) + \hat{f}_{X|Y=1}(x)\hat{\pi}}$$

- The Naive Bayes approach gives us a direct way to correct the imbalance between sensitivity and specificity by simply forcing $\hat{\pi}$ to be whatever value we want it to be in order to better **balance specificity and sensitivity**.

Code

```
# Computing sensitivity
y_hat_bayes <- ifelse(p_hat_bayes > 0.5, "Female", "Male")
sensitivity(data = factor(y_hat_bayes), reference = factor(test_set$sex))
```

```
## [1] 0.2627119
```

```
# Computing specificity
specificity(data = factor(y_hat_bayes), reference = factor(test_set$sex))
```

```
## [1] 0.9534314
```

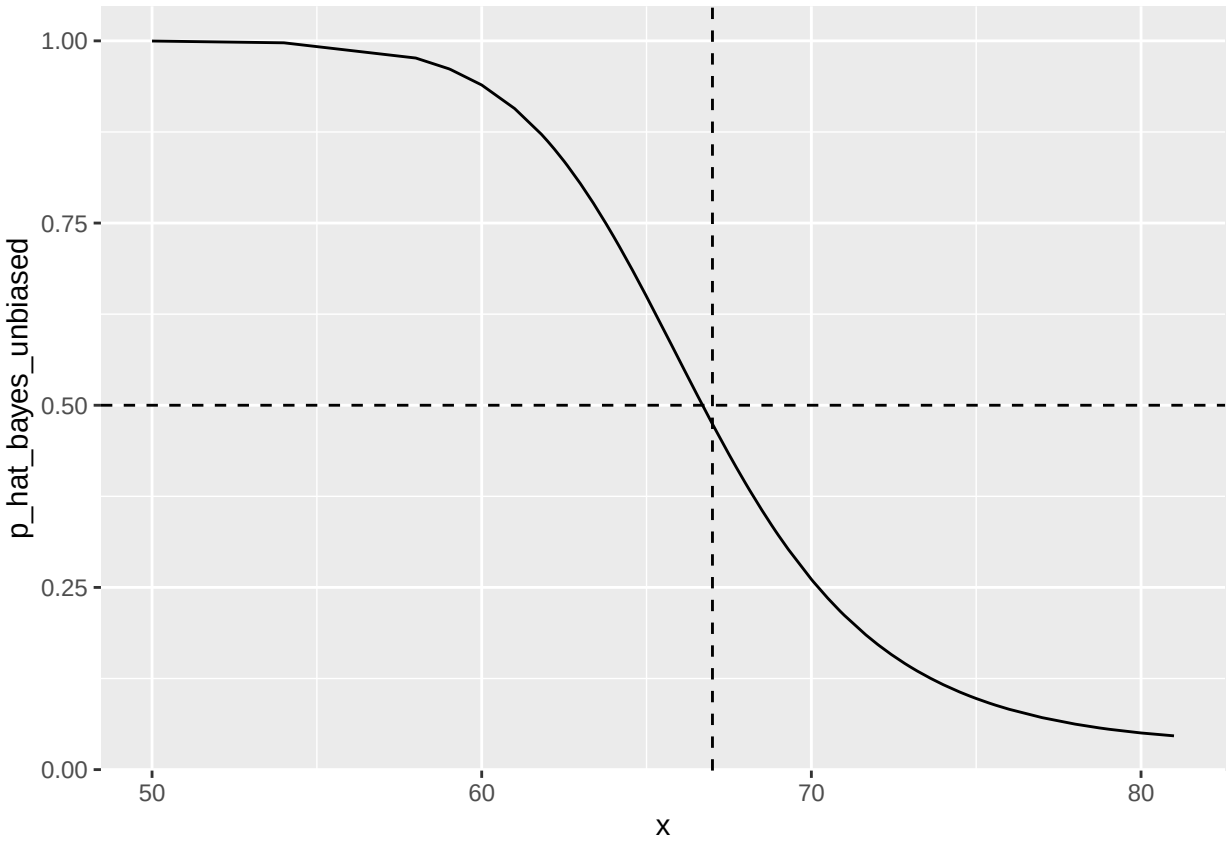
```
# Changing the cutoff of the decision rule
p_hat_bayes_unbiased <- f1 * 0.5 / (f1 * 0.5 + f0 * (1 - 0.5))
y_hat_bayes_unbiased <- ifelse(p_hat_bayes_unbiased > 0.5, "Female", "Male")
sensitivity(data = factor(y_hat_bayes_unbiased), reference = factor(test_set$sex))
```

```
## [1] 0.7118644
```

```
specificity(data = factor(y_hat_bayes_unbiased), reference = factor(test_set$sex))
```

```
## [1] 0.8210784
```

```
# Draw plot
qplot(x, p_hat_bayes_unbiased, geom = "line") +
 geom_hline(yintercept = 0.5, lty = 2) +
 geom_vline(xintercept = 67, lty = 2)
```



qda and lda

There is a link to the relevant sections of the textbook: Quadratic discriminant analysis and Linear discriminant analysis

Key points

- **Quadratic discriminant analysis (QDA)** is a version of Naive Bayes in which we assume that the distributions $p_{X|Y=1}(x)$ and $p_{X|Y=0}(x)$ are multivariate normal.
- QDA can work well with a few predictors, but it becomes **harder to use as the number of predictors increases**. Once the number of parameters approaches the size of our data, the method becomes impractical due to overfitting.
- Forcing the assumption that all predictors share the same standard deviations and correlations, the boundary will be a line, just as with logistic regression. For this reason, we call the method **linear discriminant analysis (LDA)**.
- In the case of LDA, the lack of flexibility **does not permit us to capture the non-linearity** in the true conditional probability function.

Code

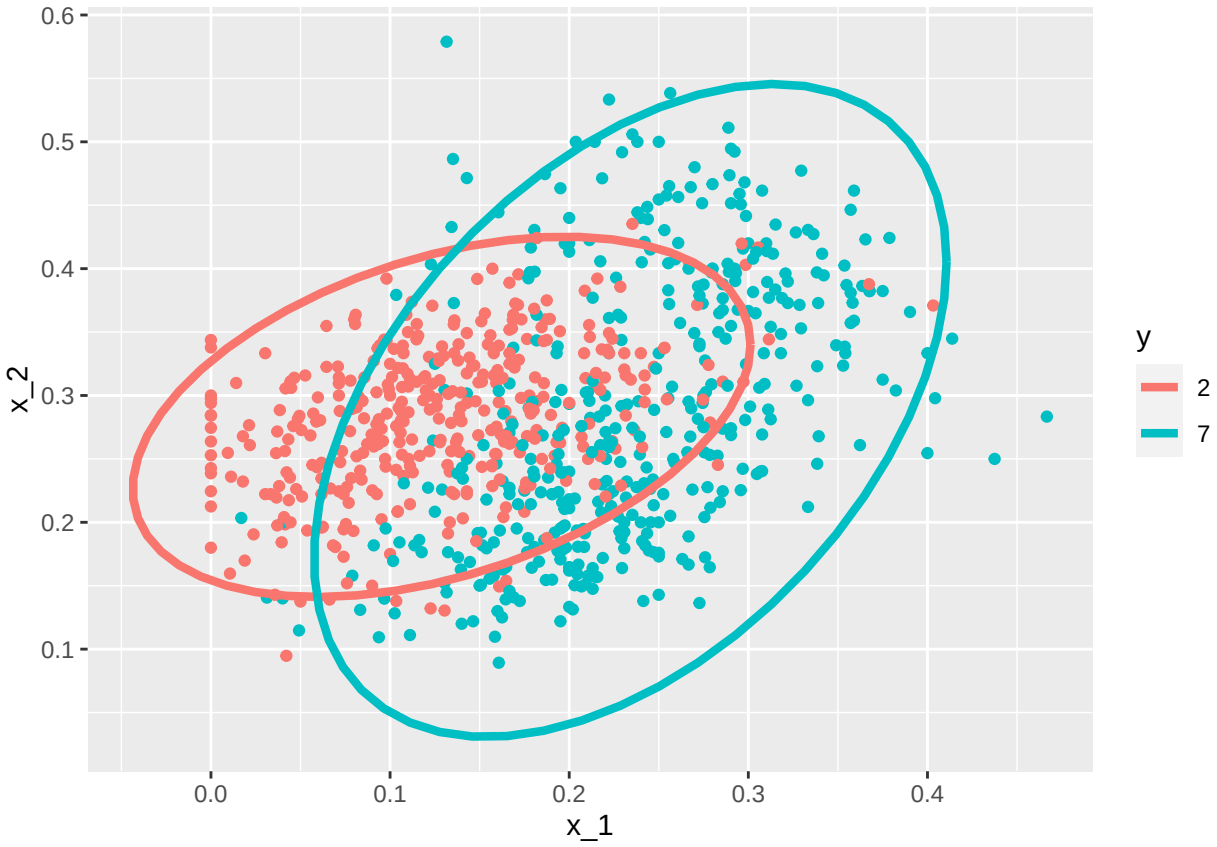
QDA

```
# Load data
data("mnist_27")

# Estimate parameters from the data
```

```
params <- mnist_27$train %>%
 group_by(y) %>%
 summarize(avg_1 = mean(x_1), avg_2 = mean(x_2),
        sd_1 = sd(x_1), sd_2 = sd(x_2),
        r = cor(x_1, x_2))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

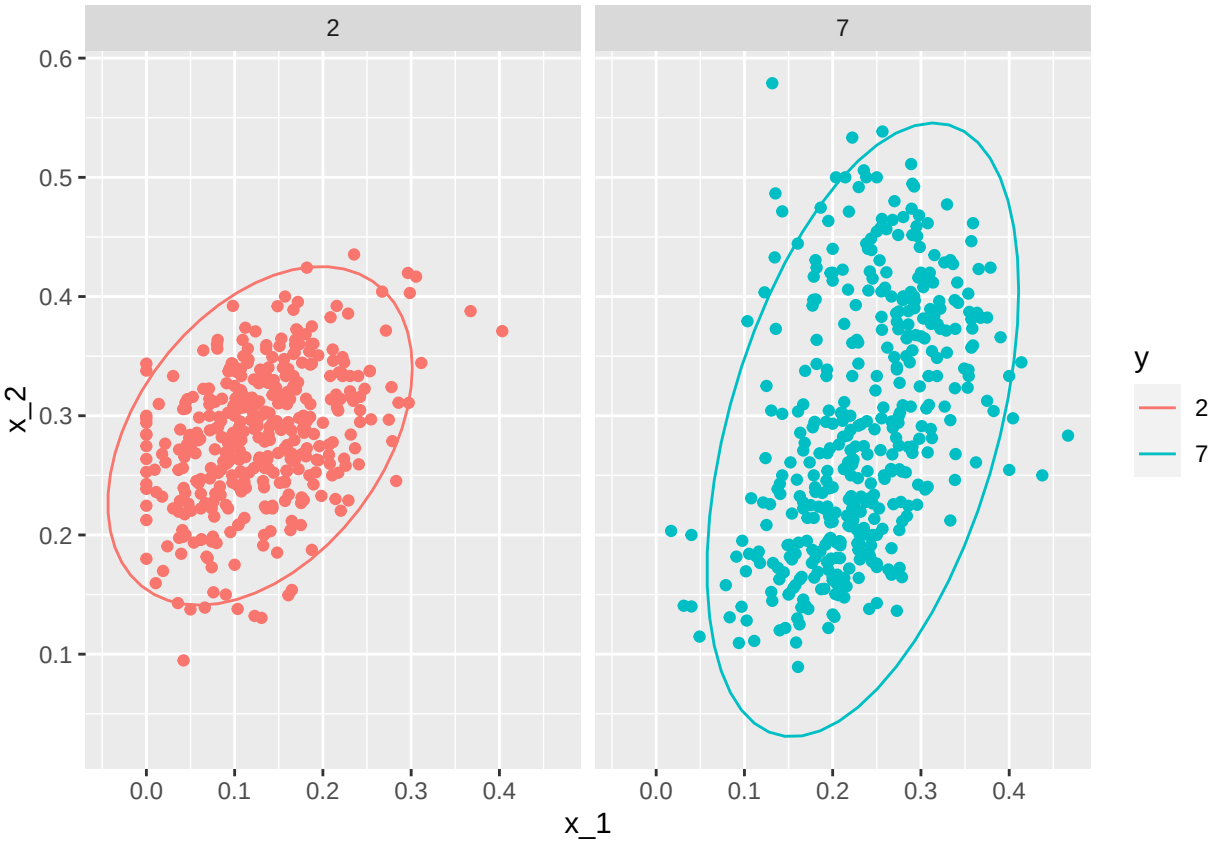
```
# Contour plots
mnist_27$train %>% mutate(y = factor(y)) %>%
 ggplot(aes(x_1, x_2, fill = y, color = y)) +
 geom_point(show.legend = FALSE) +
 stat_ellipse(type="norm", lwd = 1.5)
```




```
# Fit model
library(caret)
train_qda <- train(y ~., method = "qda", data = mnist_27$train)
# Obtain predictors and accuracy
y_hat <- predict(train_qda, mnist_27$test)
confusionMatrix(data = y_hat, reference = mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##     0.82
```

```
# Draw separate plots for 2s and 7s
mnist_27$train %>% mutate(y = factor(y)) %>%
 ggplot(aes(x_1, x_2, fill = y, color = y)) +
 geom_point(show.legend = FALSE) +
 stat_ellipse(type="norm") +
 facet_wrap(~y)
```



LDA

```
params <- mnist_27$train %>%
 group_by(y) %>%
 summarize(avg_1 = mean(x_1), avg_2 = mean(x_2),
        sd_1 = sd(x_1), sd_2 = sd(x_2),
        r = cor(x_1, x_2))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
params <- params %>% mutate(sd_1 = mean(sd_1), sd_2 = mean(sd_2), r = mean(r))
train_lda <- train(y ~., method = "lda", data = mnist_27$train)
y_hat <- predict(train_lda, mnist_27$test)
confusionMatrix(data = y_hat, reference = mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##     0.75
```

Case Study - More than Three Classes

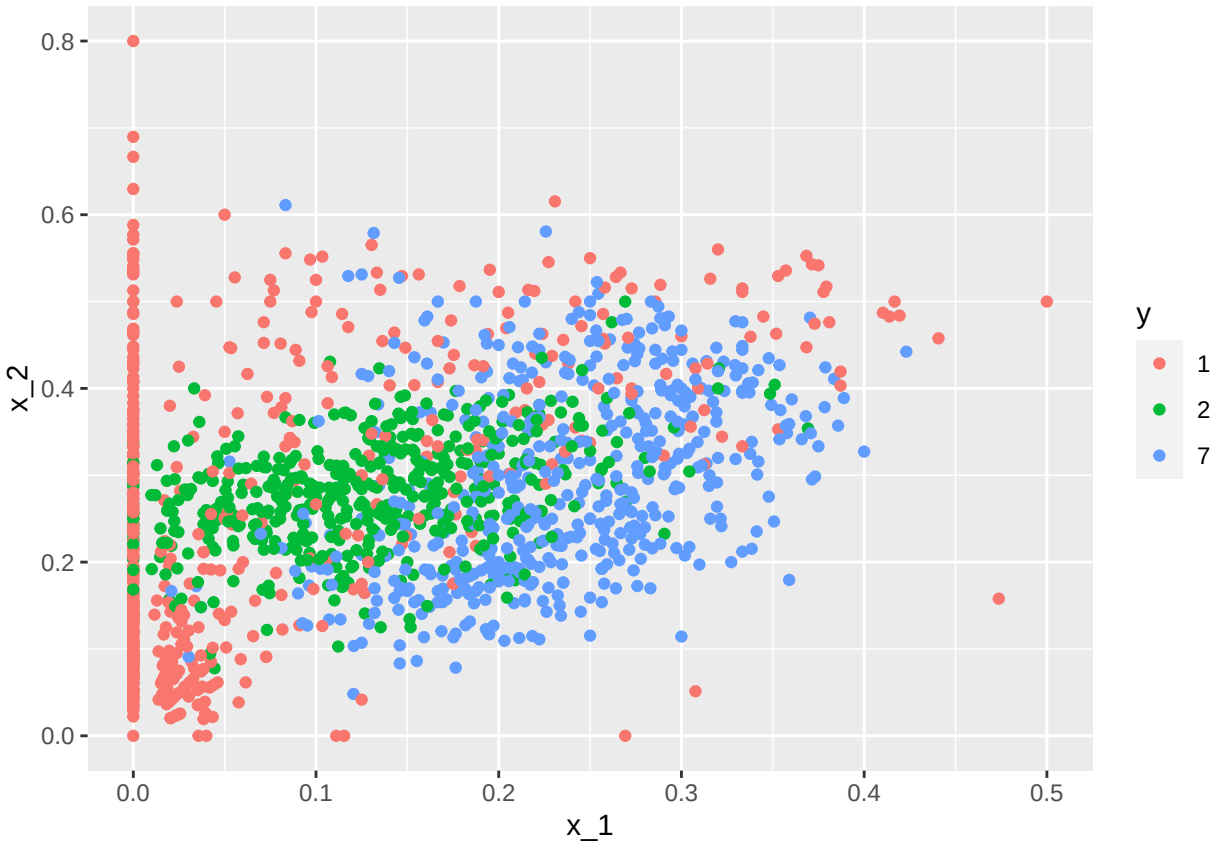
There is a link to the relevant section of the textbook: Case study: more than three classes

Key points

- In this case study, we will briefly give a slightly more complex example: one with **3 classes instead of 2**. Then we will fit QDA, LDA, and KNN models for prediction.
- Generative models can be very powerful, but only when we are able to **successfully approximate the joint distribution** of predictors conditioned on each class.

Code

```
if(!exists("mnist"))mnist <- read_mnist()

set.seed(3456)    #use set.seed(3456, sample.kind="Rounding") in R 3.6 or later
index_127 <- sample(which(mnist$train$labels %in% c(1,2,7)), 2000)
y <- mnist$train$labels[index_127]
x <- mnist$train$images[index_127,]
index_train <- createDataPartition(y, p=0.8, list = FALSE)

# get the quadrants
# temporary object to help figure out the quadrants
row_column <- expand.grid(row=1:28, col=1:28)
upper_left_ind <- which(row_column$col <= 14 & row_column$row <= 14)
lower_right_ind <- which(row_column$col > 14 & row_column$row > 14)

# binarize the values. Above 200 is ink, below is no ink
x <- x > 200

# cbind proportion of pixels in upper right quadrant and proportion of pixels in lower right quadrant
x <- cbind(rowSums(x[ ,upper_left_ind])/rowSums(x),
           rowSums(x[ ,lower_right_ind])/rowSums(x))

train_set <- data.frame(y = factor(y[index_train]),
                        x_1 = x[index_train,1],
                        x_2 = x[index_train,2])

test_set <- data.frame(y = factor(y[-index_train]),
                       x_1 = x[-index_train,1],
                       x_2 = x[-index_train,2])

train_set %>%  ggplot(aes(x_1, x_2, color=y)) + geom_point()
```




```
train_qda <- train(y ~ ., method = "qda", data = train_set)
predict(train_qda, test_set, type = "prob") %>% head()
```

```
##            1         2          7
## 1 0.22232613 0.6596410 0.11803290
## 2 0.19256640 0.4535212 0.35391242
## 3 0.62749331 0.3220448 0.05046191
## 4 0.04623381 0.1008304 0.85293583
## 5 0.21671529 0.6229295 0.16035523
## 6 0.12669776 0.3349700 0.53833219
```

```
predict(train_qda, test_set) %>% head()
```

```
## [1] 2 2 1 7 2 7
## Levels: 1 2 7
```

```
confusionMatrix(predict(train_qda, test_set), test_set$y)$table
```

```
##            Reference
## Prediction   1   2   7
##          1 111  17   7
##          2  14  80  17
##          7  19  25 109
```

```
confusionMatrix(predict(train_qda, test_set), test_set$y)$overall["Accuracy"]
```

```
##  Accuracy
## 0.7518797
```

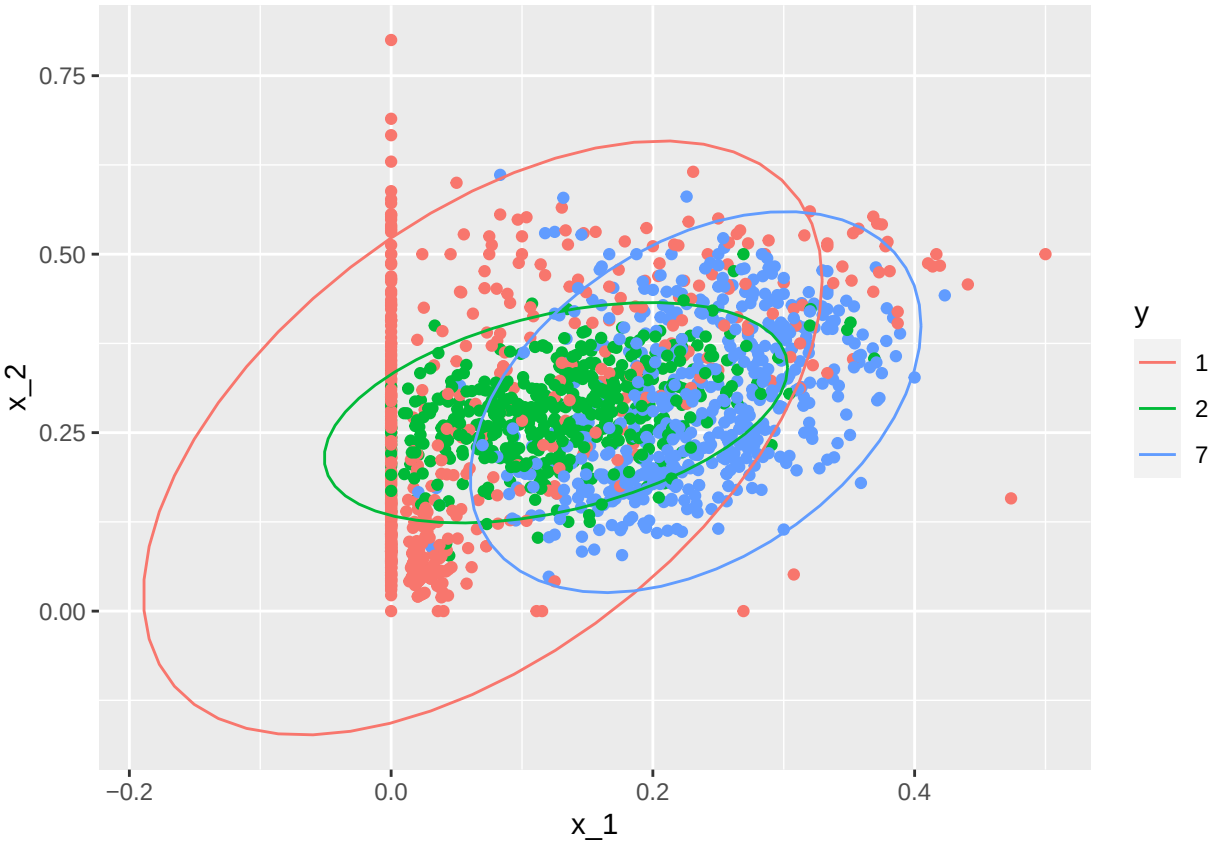
```
train_lda <- train(y ~ ., method = "lda", data = train_set)
confusionMatrix(predict(train_lda, test_set), test_set$y)$overall["Accuracy"]
```

```
##  Accuracy
## 0.6641604
```

```
train_knn <- train(y ~ ., method = "knn", tuneGrid = data.frame(k = seq(15, 51, 2)),
    data = train_set)
confusionMatrix(predict(train_knn, test_set), test_set$y)$overall["Accuracy"]
```

```
##  Accuracy
## 0.7719298
```

```
train_set %>% mutate(y = factor(y)) %>% ggplot(aes(x_1, x_2, fill = y, color=y)) + geom_point(show.lege
```



Comprehension Check - Generative Models

In the following exercises, we are going to apply LDA and QDA to the `tissue_gene_expression` dataset from **dslabs**. We will start with simple examples based on this dataset and then develop a realistic example.

1. Create a dataset of samples from just cerebellum and hippocampus, two parts of the brain, and a predictor matrix with 10 randomly selected columns using the following code:

```
data("tissue_gene_expression")

# set.seed(1993) #if using R 3.5 or earlier
set.seed(1993, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1993, sample.kind = "Rounding"): non-uniform 'Rounding'
## sampler used
```

```
ind <- which(tissue_gene_expression$y %in% c("cerebellum", "hippocampus"))
y <- droplevels(tissue_gene_expression$y[ind])
x <- tissue_gene_expression$x[ind, ]
x <- x[, sample(ncol(x), 10)]
```

Use the `train()` function to estimate the accuracy of LDA. For this question, use the version of `x` and `y` created with the code above: do not split them or `tissue_gene_expression` into training and test sets (understand this can lead to overfitting). Report the accuracy from the `train()` results (do not make predictions).

What is the accuracy? Enter your answer as a percentage or decimal (eg "50%" or "0.50") to at least the thousandths place.

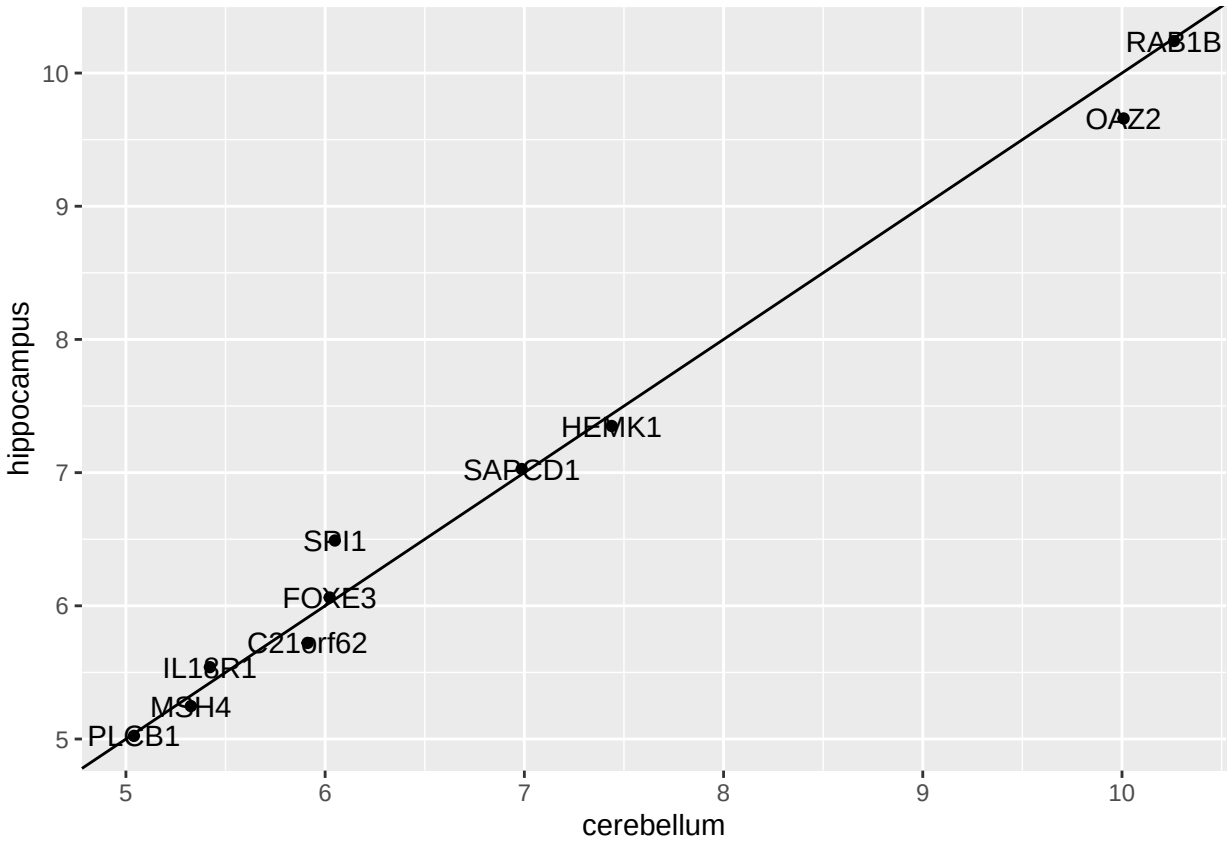
```
fit_lda <- train(x, y, method = "lda")
fit_lda$results["Accuracy"]
```

```
##    Accuracy
## 1 0.8707879
```

2. In this case, LDA fits two 10-dimensional normal distributions. Look at the fitted model by looking at the `finalModel` component of the result of `train()`. Notice there is a component called `means` that includes the estimated means of both distributions. Plot the mean vectors against each other and determine which predictors (genes) appear to be driving the algorithm.

Which TWO genes appear to be driving the algorithm (i.e. the two genes with the highest means)?

```
t(fit_lda$finalModel$means) %>% data.frame() %>%
    mutate(predictor_name = rownames(.)) %>%
    ggplot(aes(cerebellum, hippocampus, label = predictor_name)) +
    geom_point() +
    geom_text() +
    geom_abline()
```



☐ A. PLCB1
☒ B. RAB1B
☐ C. MSH4
☒ D. OAZ2
☐ E. SPI1
☐ F. SAPCD1
☐ G. HEMK1

3. Repeat the exercise in Q1 with QDA.

Create a dataset of samples from just cerebellum and hippocampus, two parts of the brain, and a predictor matrix with 10 randomly selected columns using the following code:

```
data("tissue_gene_expression")

set.seed(1993) #set.seed(1993, sample.kind="Rounding") if using R 3.6 or later
ind <- which(tissue_gene_expression$y %in% c("cerebellum", "hippocampus"))
y <- droplevels(tissue_gene_expression$y[ind])
x <- tissue_gene_expression$x[ind, ]
x <- x[, sample(ncol(x), 10)]
```

Use the `train()` function to estimate the accuracy of QDA. For this question, use the version of `x` and `y` created above instead of the default from `tissue_gene_expression`. Do not split them into training and test sets (understand this can lead to overfitting).

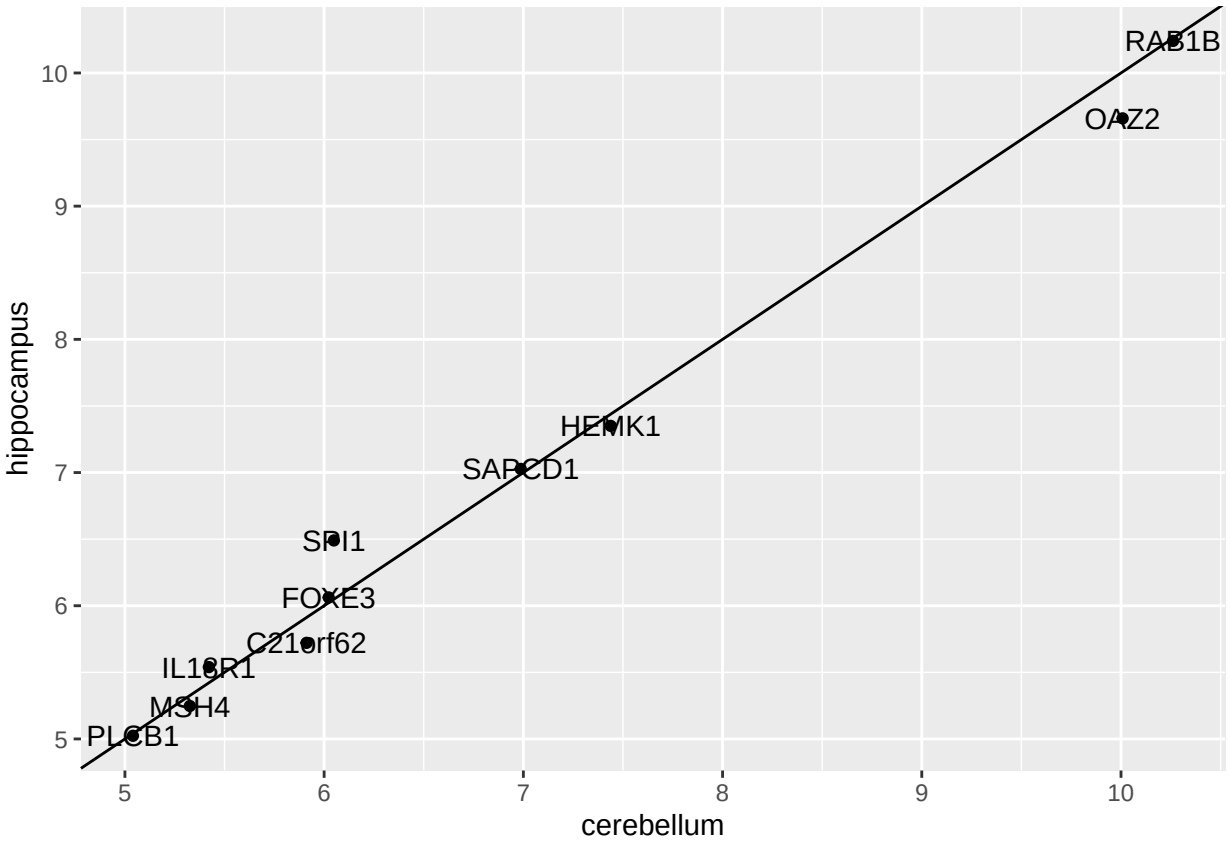
What is the accuracy?

```
fit_qda <- train(x, y, method = "qda")
fit_qda$results["Accuracy"]
```

```
##    Accuracy
## 1 0.8147954
```

4. Which TWO genes drive the algorithm when using QDA instead of LDA (i.e. the two genes with the highest means)?

```
t(fit_qda$finalModel$means) %>% data.frame() %>%
    mutate(predictor_name = rownames(.)) %>%
    ggplot(aes(cerebellum, hippocampus, label = predictor_name)) +
    geom_point() +
    geom_text() +
    geom_abline()
```



☐ A. PLCB1
☒ B. RAB1B
☐ C. MSH4
☒ D. OAZ2
☐ E. SPI1
☐ F. SAPCD1
☐ G. HEMK1

5. One thing we saw in the previous plots is that the values of the predictors correlate in both groups: some predictors are low in both groups and others high in both groups. The mean value of each

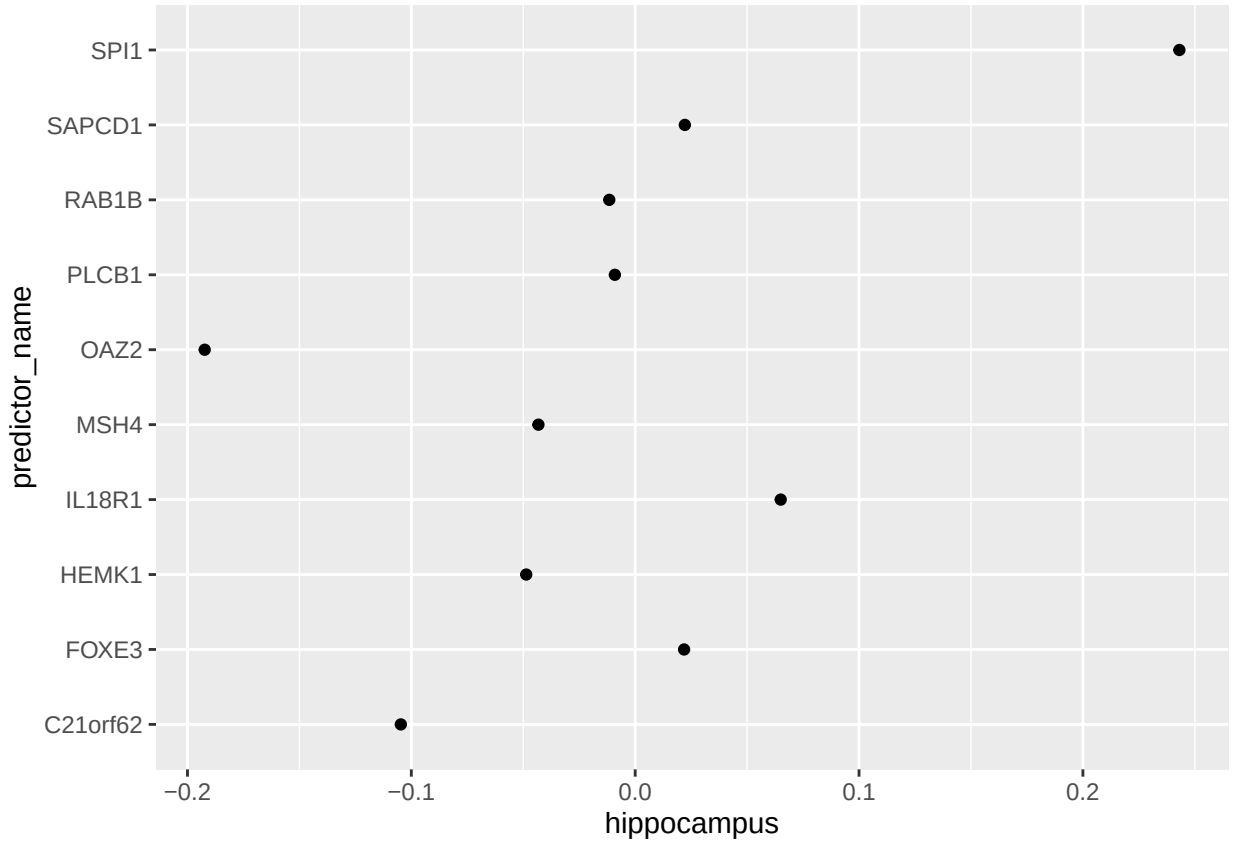
predictor found in `colMeans(x)` is not informative or useful for prediction and often for purposes of interpretation, it is useful to center or scale each column. This can be achieved with the `preProcess` argument in `train()`. Re-run LDA with `preProcess = "center"`. Note that accuracy does not change, but it is now easier to identify the predictors that differ more between groups than based on the plot made in Q2.

Which TWO genes drive the algorithm after performing the scaling?

```
fit_lda <- train(x, y, method = "lda", preProcess = "center")
fit_lda$results["Accuracy"]
```

```
##    Accuracy
## 1 0.8595389
```

```
t(fit_lda$finalModel$means) %>% data.frame() %>%
    mutate(predictor_name = rownames(.)) %>%
    ggplot(aes(predictor_name, hippocampus)) +
    geom_point() +
    coord_flip()
```

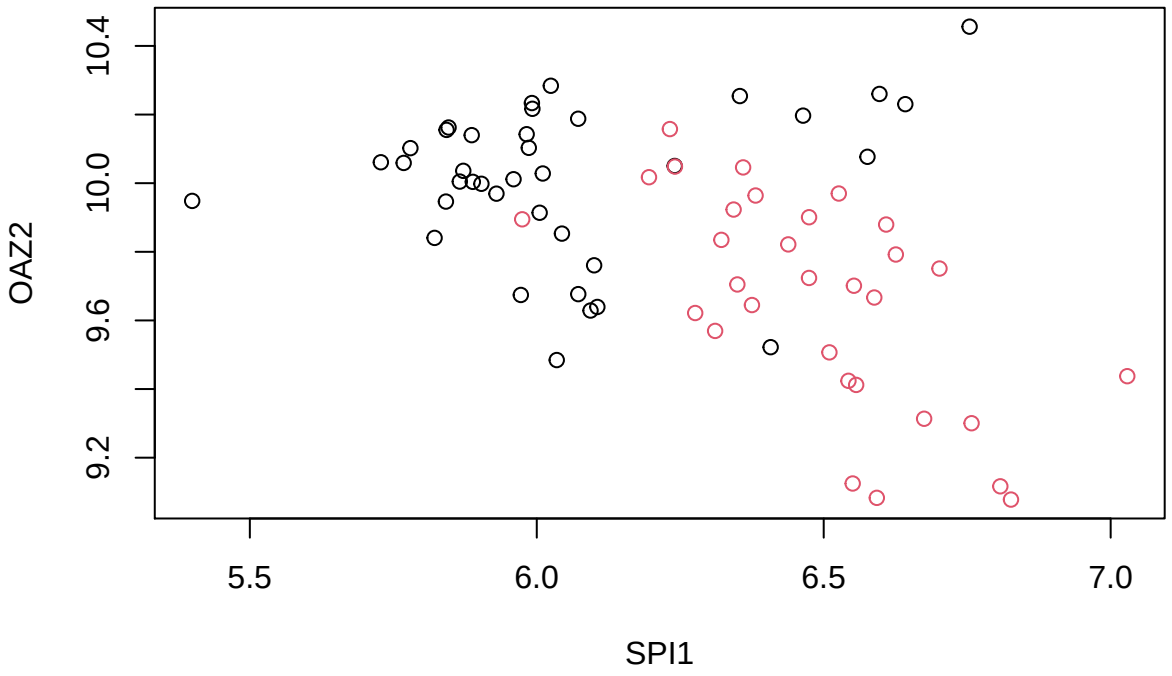


☐ A. C21orf62
☐ B. PLCB1
☐ C. RAB1B
☐ D. MSH4
☒ E. OAZ2

☒ F. SPI1
☐ G. SAPCD1
☐ H. IL18R1

You can see that it is different genes driving the algorithm now. This is because the predictor means change. In the previous exercises we saw that both LDA and QDA approaches worked well. For further exploration of the data, you can plot the predictor values for the two genes with the largest differences between the two groups in a scatter plot to see how they appear to follow a bivariate distribution as assumed by the LDA and QDA approaches, coloring the points by the outcome, using the following code:

```
d <- apply(fit_lda$finalModel$means, 2, diff)
ind <- order(abs(d), decreasing = TRUE)[1:2]
plot(x[, ind], col = y)
```



6. Now we are going to increase the complexity of the challenge slightly. Repeat the LDA analysis from Q5 but using all tissue types. Use the following code to create your dataset:

```
data("tissue_gene_expression")

# set.seed(1993) # if using R 3.5 or earlier
set.seed(1993, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1993, sample.kind = "Rounding"): non-uniform 'Rounding'
## sampler used
```

```
y <- tissue_gene_expression$y
x <- tissue_gene_expression$x
x <- x[, sample(ncol(x), 10)]
```

What is the accuracy using LDA?

```r
fit_lda <- train(x, y, method = "lda", preProcess = c("center"))
fit_lda$results["Accuracy"]
```

```
##    Accuracy
## 1 0.8194837
```

Section 5 - Classification with More than Two Classes and the Caret Package

In the **Classification with More than Two Classes and the Caret Package** section, you will learn how to overcome the curse of dimensionality using methods that adapt to higher dimensions and how to use the caret package to implement many different machine learning algorithms.

After completing this section, you will be able to:

- Use **classification and regression trees**.
- Use **classification (decision) trees**.
- Apply **random forests** to address the shortcomings of decision trees.
- Use the **caret** package to implement a variety of machine learning algorithms.

This section has three parts: **classification with more than two classes, caret package**, and a **set of exercises** on the Titanic.

Trees Motivation

There is a link to the relevant section of the textbook: The curse of dimensionality

Key points

- LDA and QDA are not **meant to be used with many predictors** p because the number of parameters needed to be estimated becomes too large.
- **Curse of dimensionality:** For kernel methods such as kNN or local regression, when they have multiple predictors used, the span/neighborhood/window made to include a given percentage of the data become large. With larger neighborhoods, our methods lose flexibility. The dimension here refers to the fact that when we have p predictors, the distance between two observations is computed in p-dimensional space.

Classification and Regression Trees (CART)

There is a link to the relevant sections of the textbook: CART motivation and Regression trees

Key points

- A tree is basically a **flow chart of yes or no questions**. The general idea of the methods we are describing is to define an algorithm that uses data to create these trees with predictions at the ends, referred to as nodes.
- When the outcome is continuous, we call the decision tree method a **regression tree**.
- Regression and decision trees operate by predicting an outcome variable Y by **partitioning the predictors**.

- The general idea here is to **build a decision tree** and, at end of each node, obtain a predictor $\hat{y}$. Mathematically, we are **partitioning the predictor space** into J non-overlapping regions, R_1, R_2, ..., R_J and then for any predictor x that falls within region R_j, estimate $f(x)$ with the average of the training observations y_i for which the associated predictor x_i in also in R_j.
- To pick j and its value s, we find the pair that **minimizes the residual sum of squares (RSS)**:

$$\sum_{i:x_i R_1(j,s)}(y_i - \hat{y}_{R_1})^2 + \sum_{i:x_i R_2(j,s)}(y_i - \hat{y}_{R_2})^2$$

- To fit the regression tree model, we can use the `rpart()` function in the **rpart** package.
- Two common parameters used for partition decision are the **complexity parameter** (`cp`) and the **minimum number of observations required in a partition** before partitioning it further (`minsplit` in the **rpart** package).
- If we already have a tree and want to apply a higher `cp` value, we can use the `prune()` function. We call this pruning a tree because we are snipping off partitions that do not meet a cp criterion.

Code

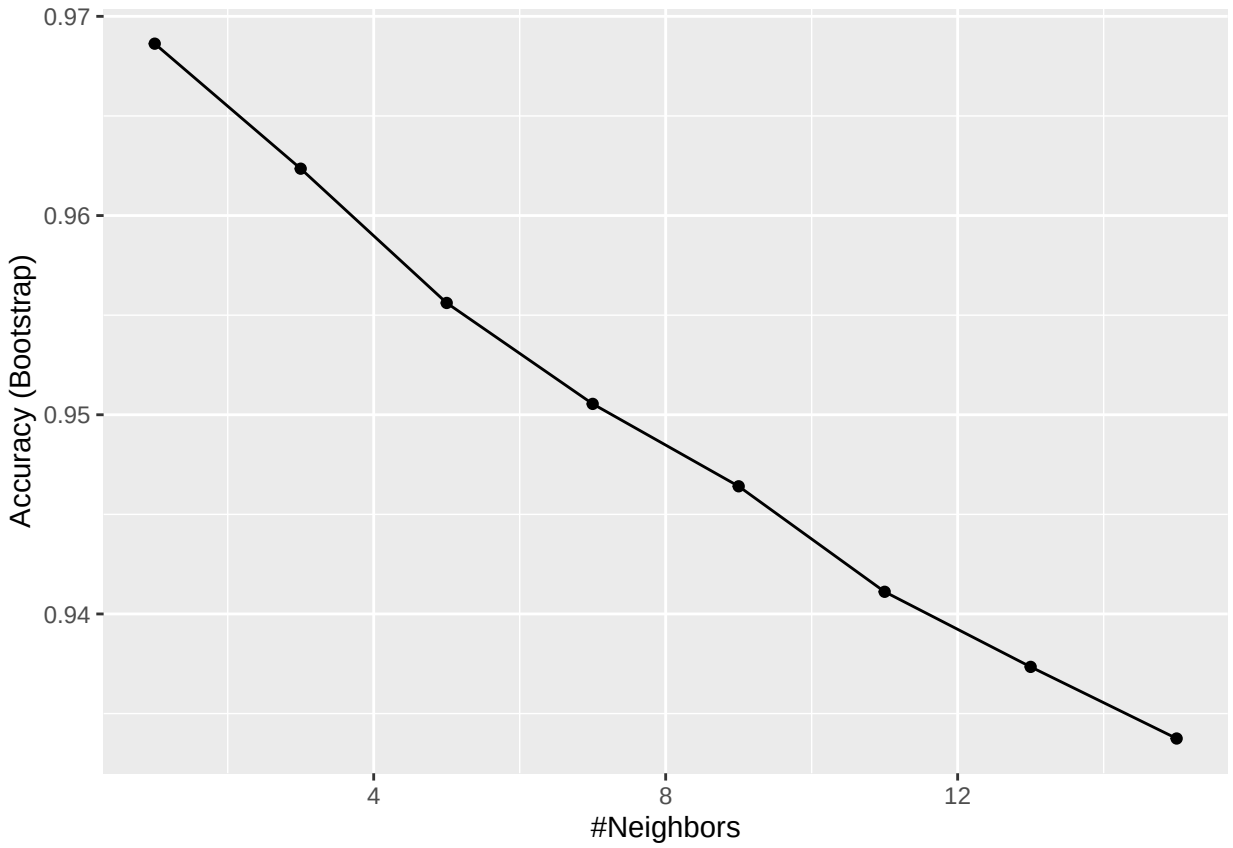
```
# Load data
data("olive")
olive %>% as_tibble()
```

```
## # A tibble: 572 x 10
##    region area  palmitic palmitoleic stearic oleic linoleic linolenic arachidic
##    <fct>  <fct>    <dbl>       <dbl>   <dbl> <dbl>    <dbl>     <dbl>     <dbl>
##  1 South~ Nort~    10.8        0.75     2.26  78.2     6.72      0.36      0.6
##  2 South~ Nort~    10.9        0.73     2.24  77.1     7.81      0.31      0.61
##  3 South~ Nort~     9.11       0.54     2.46  81.1     5.49      0.31      0.63
##  4 South~ Nort~     9.66       0.570    2.4   79.5     6.19      0.5       0.78
##  5 South~ Nort~    10.5        0.67     2.59  77.7     6.72      0.5       0.8
##  6 South~ Nort~     9.11       0.49     2.68  79.2     6.78      0.51      0.7
##  7 South~ Nort~     9.22       0.66     2.64  79.9     6.18      0.49      0.56
##  8 South~ Nort~    11          0.61     2.35  77.3     7.34      0.39      0.64
##  9 South~ Nort~    10.8        0.6      2.39  77.4     7.09      0.46      0.83
## 10 South~ Nort~    10.4        0.55     2.13  79.4     6.33      0.26      0.52
## # ... with 562 more rows, and 1 more variable: eicosenoic <dbl>
```

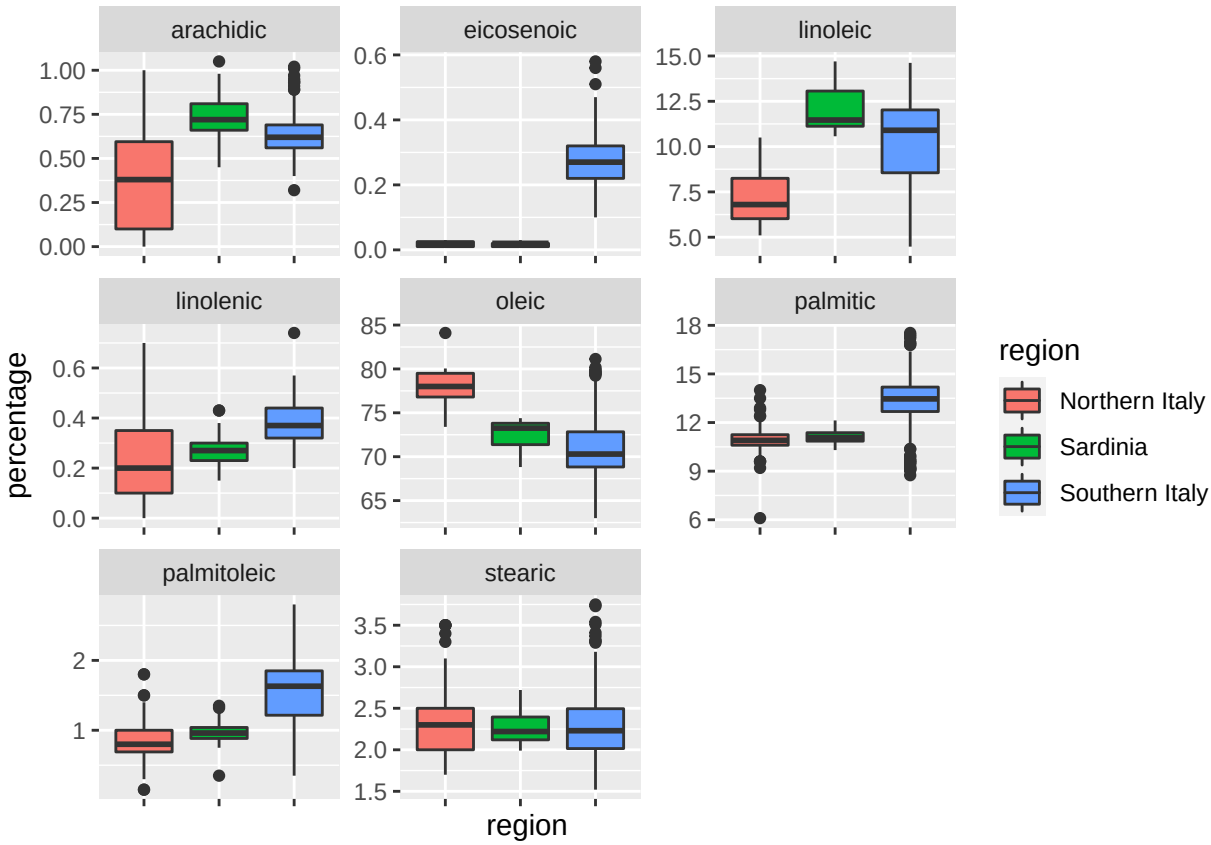
```
table(olive$region)
```

```
##
## Northern Italy       Sardinia Southern Italy
##            151              98            323
```

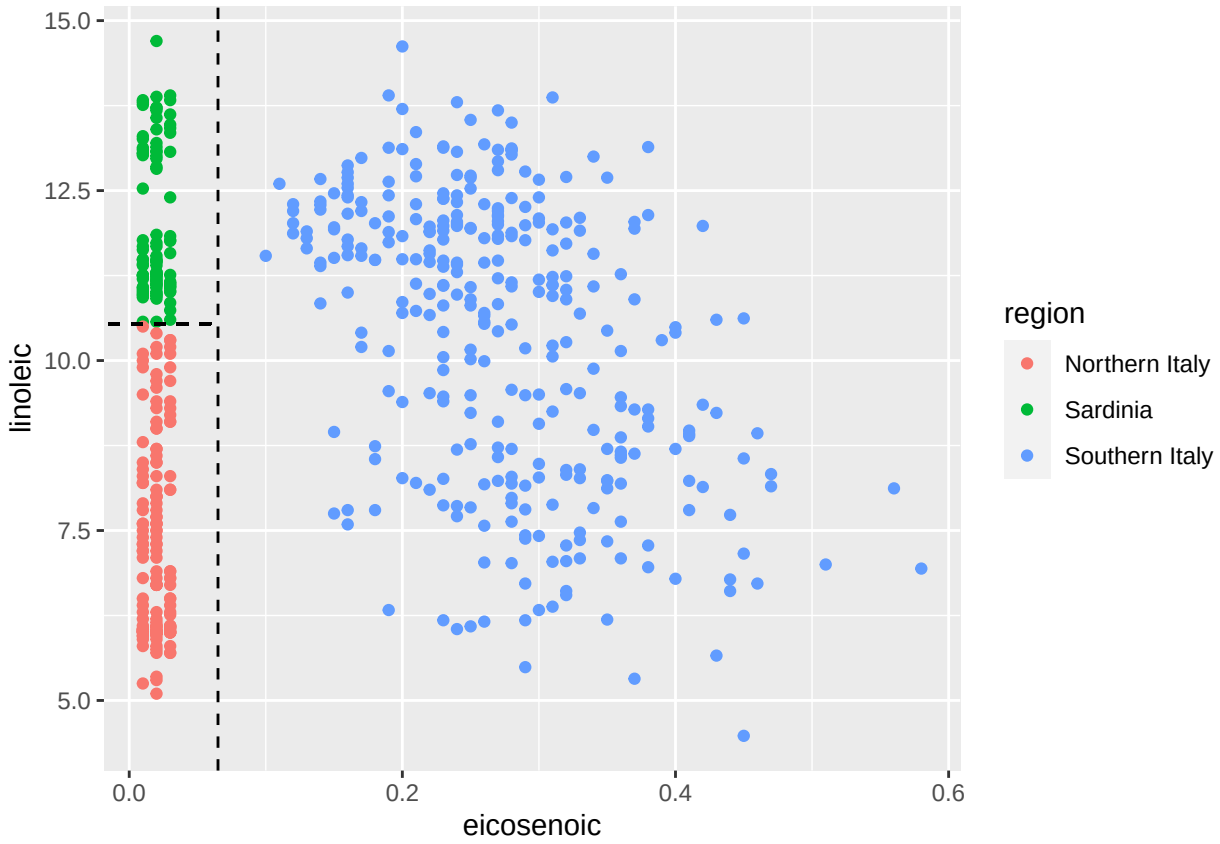
```
olive <- dplyr::select(olive, -area)

# Predict region using KNN
fit <- train(region ~ .,  method = "knn",
             tuneGrid = data.frame(k = seq(1, 15, 2)),
             data = olive)
ggplot(fit)
```



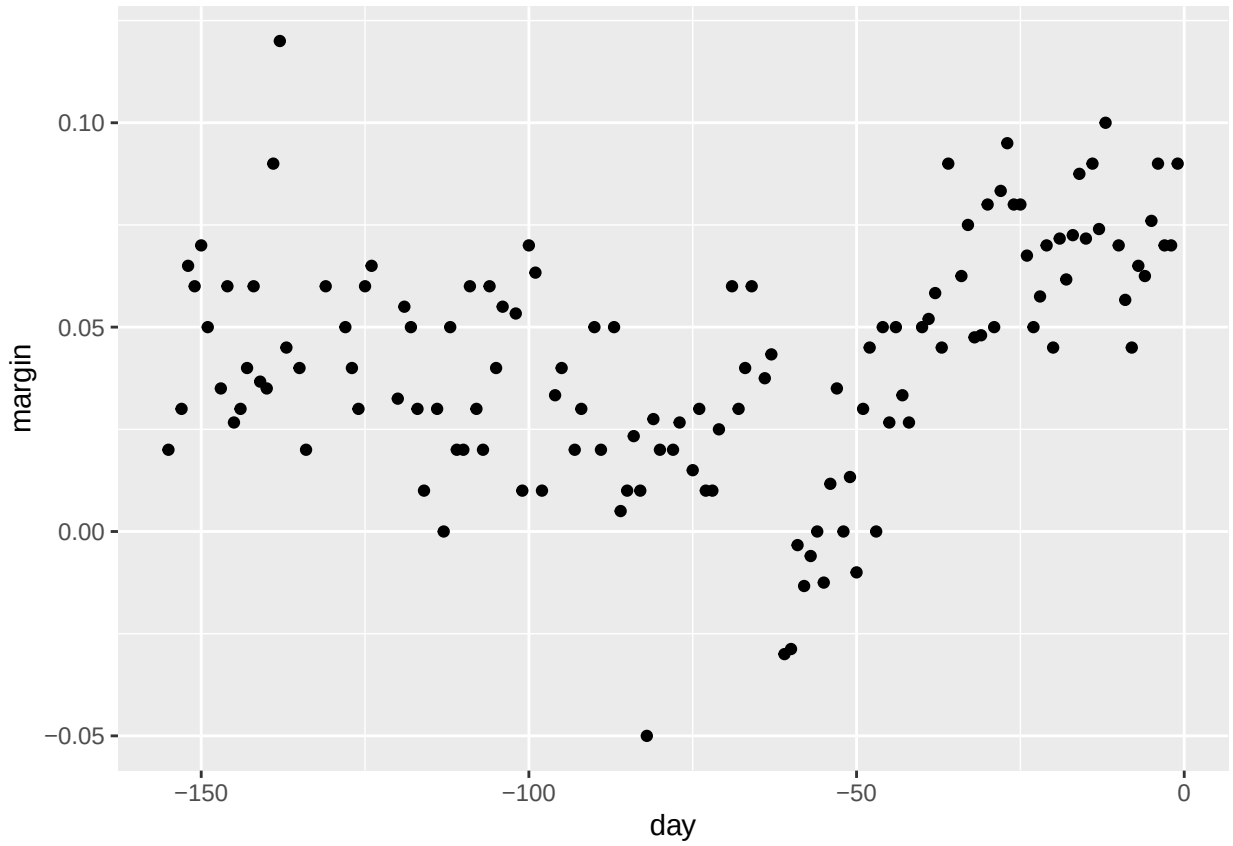

```
# Plot distribution of each predictor stratified by region
olive %>% gather(fatty_acid, percentage, -region) %>%
  ggplot(aes(region, percentage, fill = region)) +
  geom_boxplot() +
  facet_wrap(~fatty_acid, scales = "free") +
  theme(axis.text.x = element_blank())
```




```
# plot values for eicosenoic and linoleic
p <- olive %>%
  ggplot(aes(eicosenoic, linoleic, color = region)) +
  geom_point()
p + geom_vline(xintercept = 0.065, lty = 2) +
  geom_segment(x = -0.2, y = 10.54, xend = 0.065, yend = 10.54, color = "black", lty = 2)
```



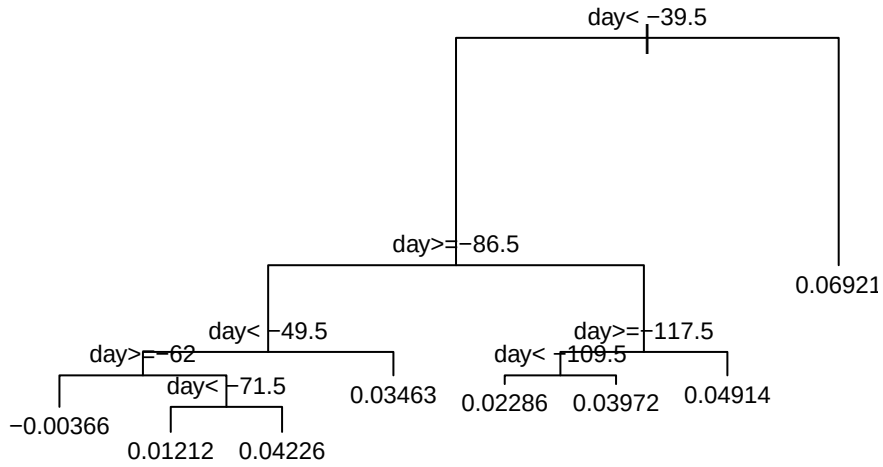

```
# load data for regression tree
data("polls_2008")
qplot(day, margin, data = polls_2008)
```



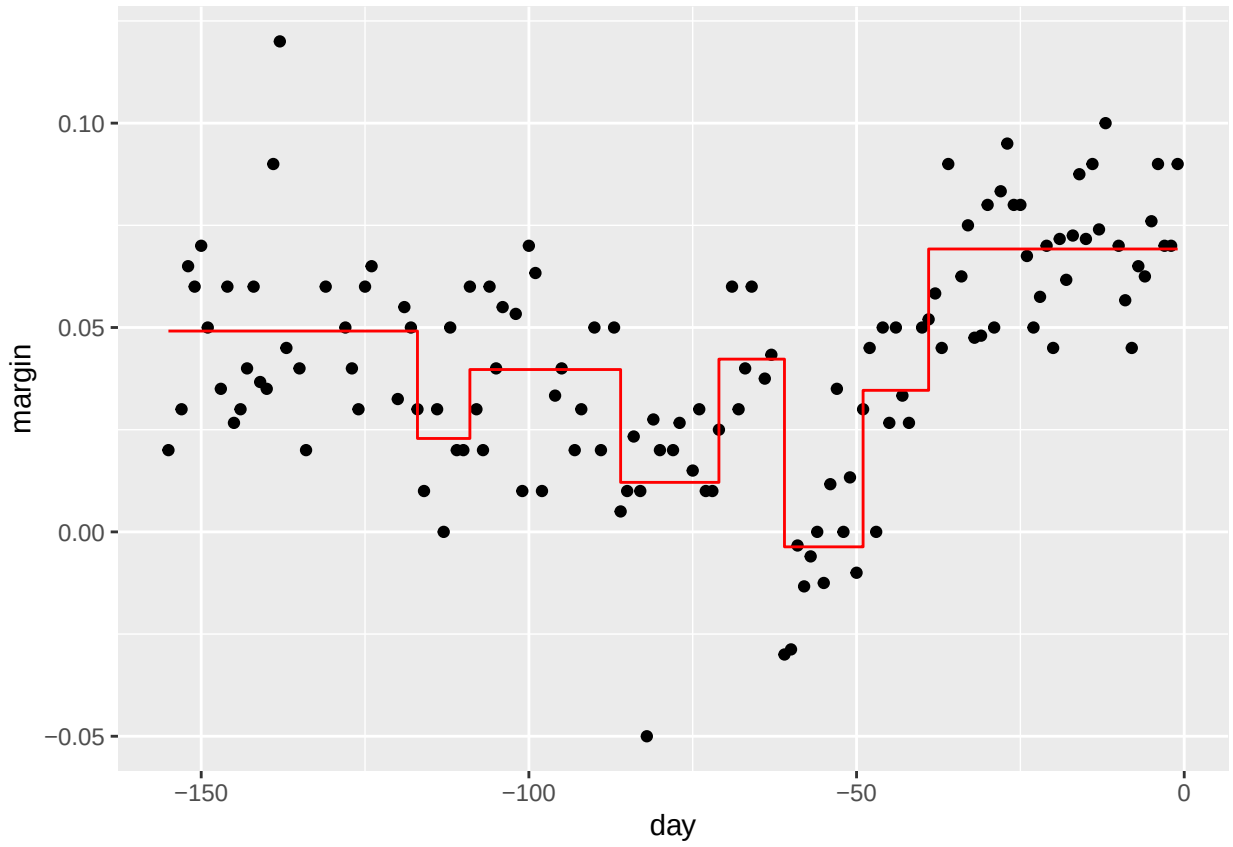

```
if(!require(rpart)) install.packages("rpart")
```

```
## Loading required package: rpart
```

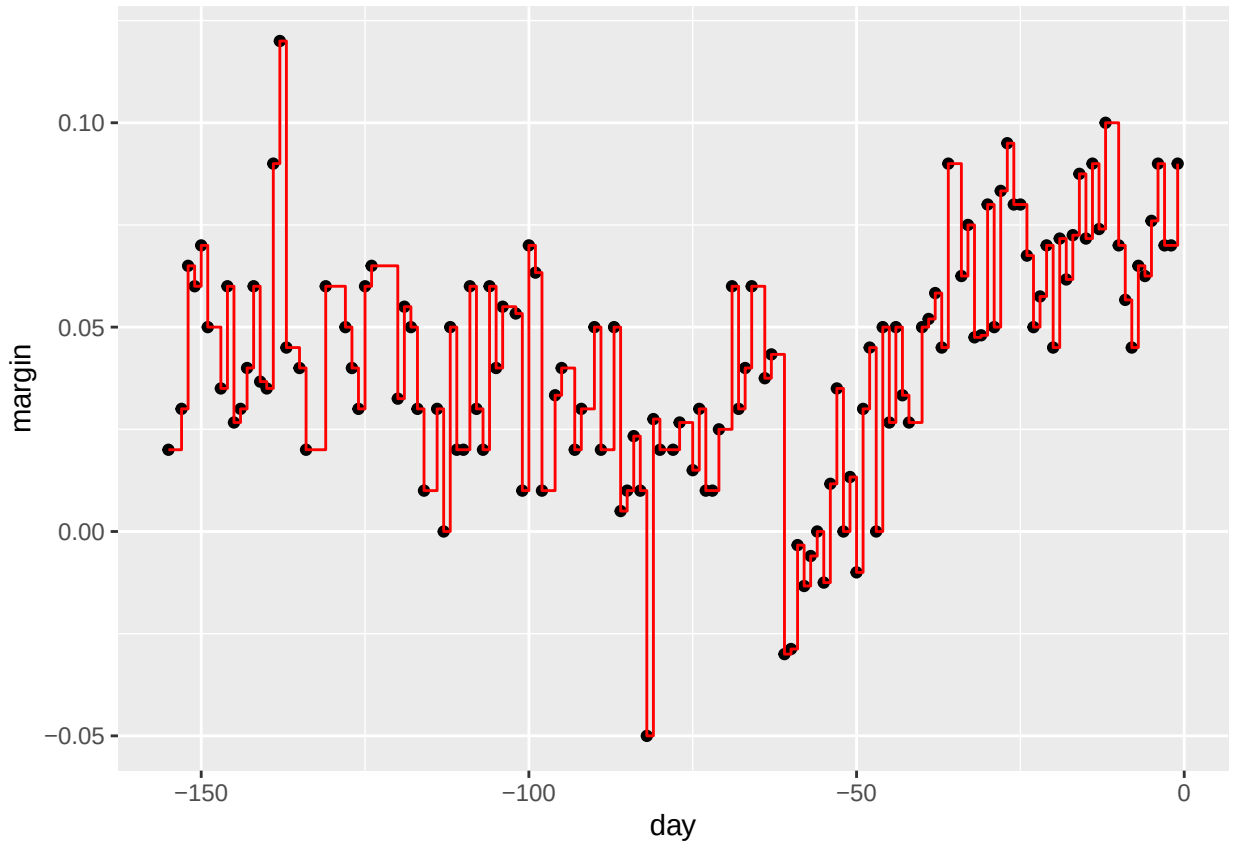
```
library(rpart)
fit <- rpart(margin ~ ., data = polls_2008)

# visualize the splits
plot(fit, margin = 0.1)
text(fit, cex = 0.75)
```



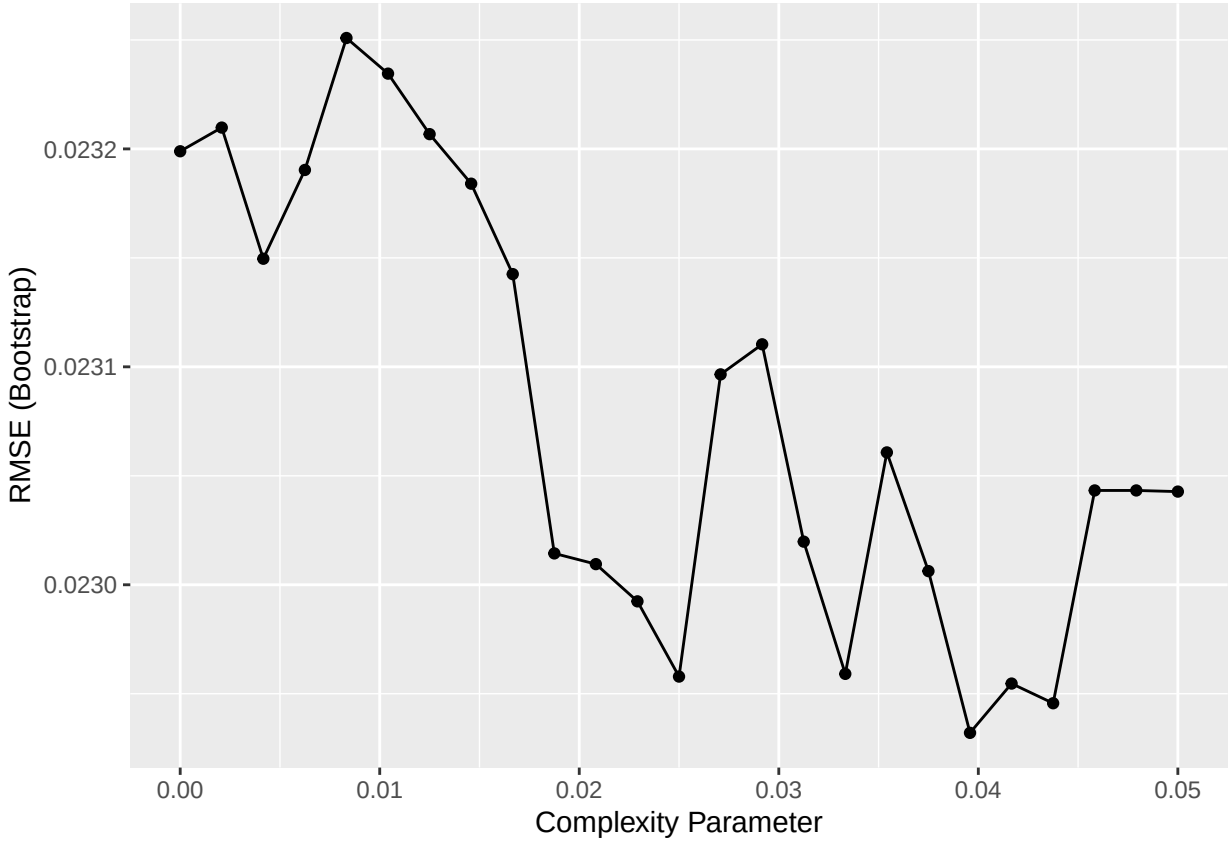
```
polls_2008 %>%
  mutate(y_hat = predict(fit)) %>%
  ggplot() +
  geom_point(aes(day, margin)) +
  geom_step(aes(day, y_hat), col="red")
```



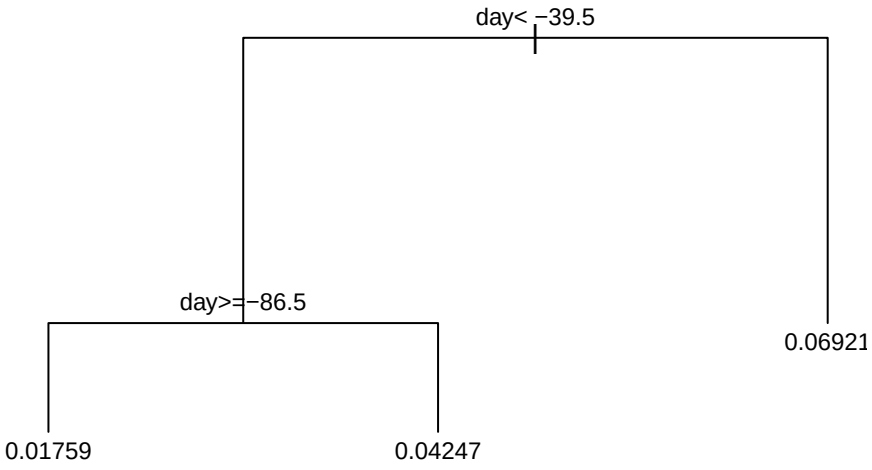

```
# change parameters
fit <- rpart(margin ~ ., data = polls_2008, control = rpart.control(cp = 0, minsplit = 2))
polls_2008 %>%
  mutate(y_hat = predict(fit)) %>%
  ggplot() +
  geom_point(aes(day, margin)) +
  geom_step(aes(day, y_hat), col="red")
```



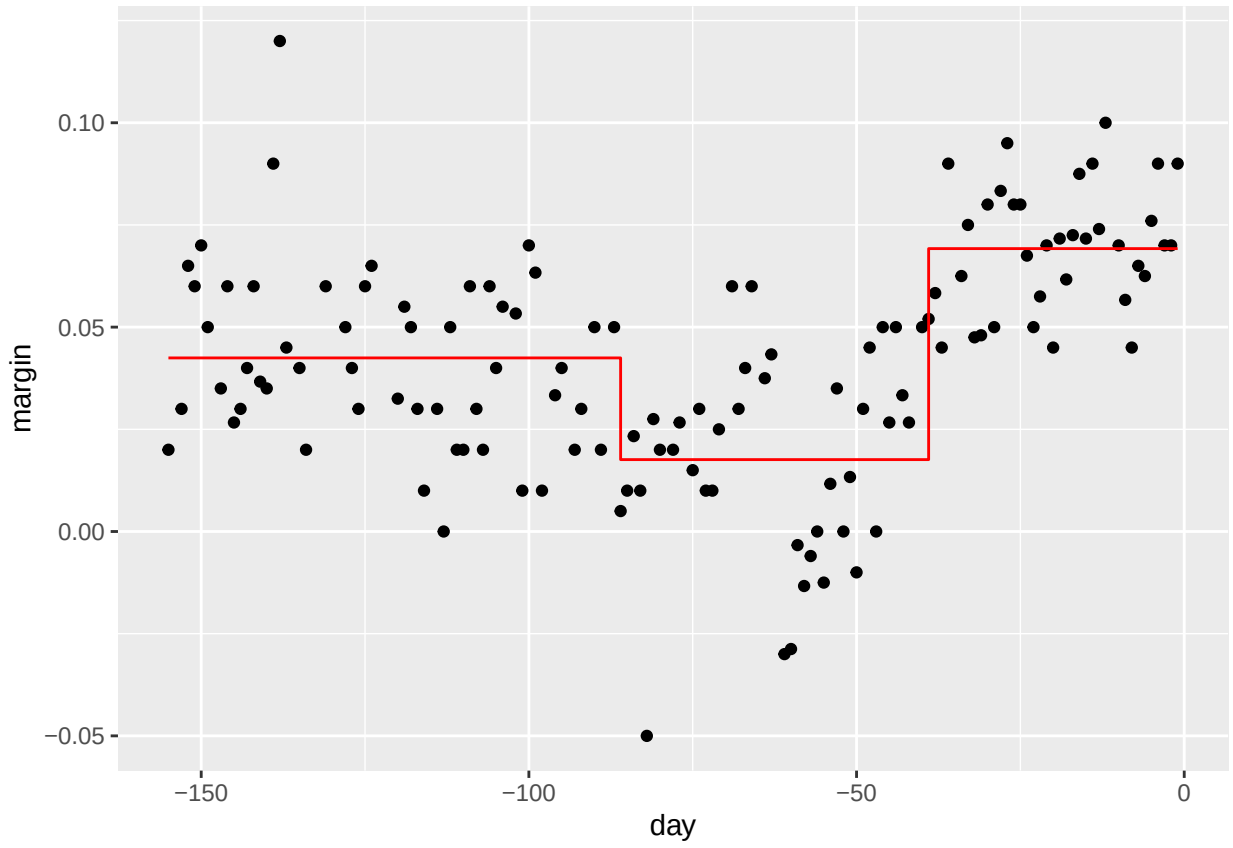

```
# use cross validation to choose cp
train_rpart <- train(margin ~ ., method = "rpart", tuneGrid = data.frame(cp = seq(0, 0.05, len = 25)), c
ggplot(train_rpart)
```




```
# access the final model and plot it
plot(train_rpart$finalModel, margin = 0.1)
text(train_rpart$finalModel, cex = 0.75)
```




```
polls_2008 %>%
  mutate(y_hat = predict(train_rpart)) %>%
  ggplot() +
  geom_point(aes(day, margin)) +
  geom_step(aes(day, y_hat), col="red")
```




```
# prune the tree
pruned_fit <- prune(fit, cp = 0.01)
```

Classification (Decision) Trees

There is a link to the relevant section of the textbook: Classification (decision) trees

Key points

- **Classification trees**, or decision trees, are used in prediction problems where the **outcome is categorical**.
- Decision trees form predictions by calculating **which class is the most common** among the training set observations within the partition, rather than taking the average in each partition.
- Two of the more popular metrics to choose the partitions are the **Gini index** and **entropy**.

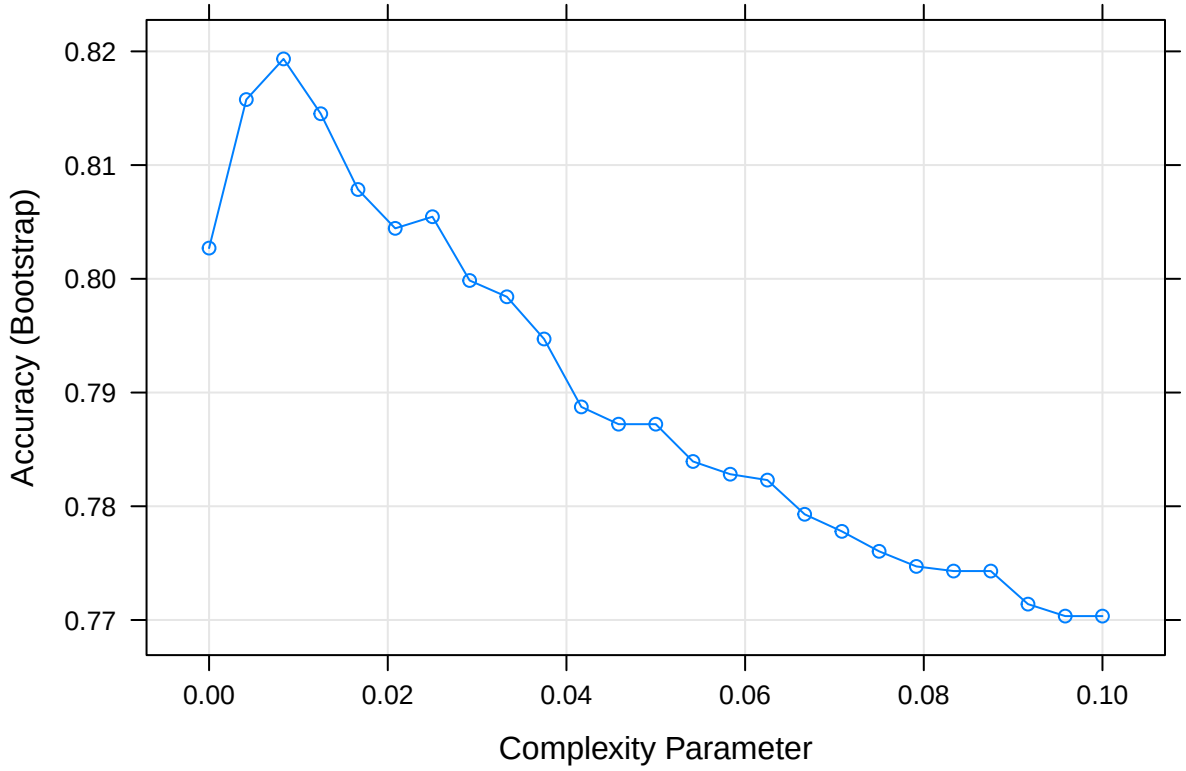
$\text{Gini}(j) = \sum_{k=1}^{K} \hat{p}_{j,k}(1 - \hat{p}_{j,k})$

$\text{entropy}(j) = -\sum_{k=1}^{K} \hat{p}_{j,k} log(\hat{p}_{j,k}), \text{with } 0 \times \log(0) \text{defined as } 0$

- Pros: Classification trees are highly interpretable and easy to visualize.They can model human decision processes and don't require use of dummy predictors for categorical variables.
- Cons: The approach via recursive partitioning can easily over-train and is therefore a bit harder to train than. Furthermore, in terms of accuracy, it is rarely the best performing method since it is not very flexible and is highly unstable to changes in training data.

Code

```
# fit a classification tree and plot it
train_rpart <- train(y ~ .,
                     method = "rpart",
                     tuneGrid = data.frame(cp = seq(0.0, 0.1, len = 25)),
                     data = mnist_27$train)
plot(train_rpart)
```




```
# compute accuracy
confusionMatrix(predict(train_rpart, mnist_27$test), mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##     0.82
```

Random Forests

There is a link to the relevant section of the textbook: Random forests

Key points

- **Random forests** are a very popular machine learning approach that addresses the shortcomings of decision trees. The goal is to improve prediction performance and reduce instability by **averaging multiple decision trees** (a forest of trees constructed with randomness).
- The general idea of random forests is to generate many predictors, each using regression or classification trees, and then **forming a final prediction based on the average prediction of all these trees**. To assure that the individual trees are not the same, we use the **bootstrap to induce randomness**.

- A **disadvantage** of random forests is that we **lose interpretability**.
- An approach that helps with interpretability is to examine **variable importance**. To define variable importance we **count how often a predictor is used in the individual trees**. The **caret** package includes the function `varImp` that extracts variable importance from any model in which the calculation is implemented.

Code

```
if(!require(randomForest)) install.packages("randomForest")
```

```
## Loading required package: randomForest
```

```
## randomForest 4.6-14
```

```
## Type rfNews() to see new features/changes/bug fixes.
```

```
##
## Attaching package: 'randomForest'
```

```
## The following object is masked from 'package:gridExtra':
##
##     combine
```

```
## The following object is masked from 'package:dplyr':
##
##     combine
```

```
## The following object is masked from 'package:ggplot2':
##
##     margin
```

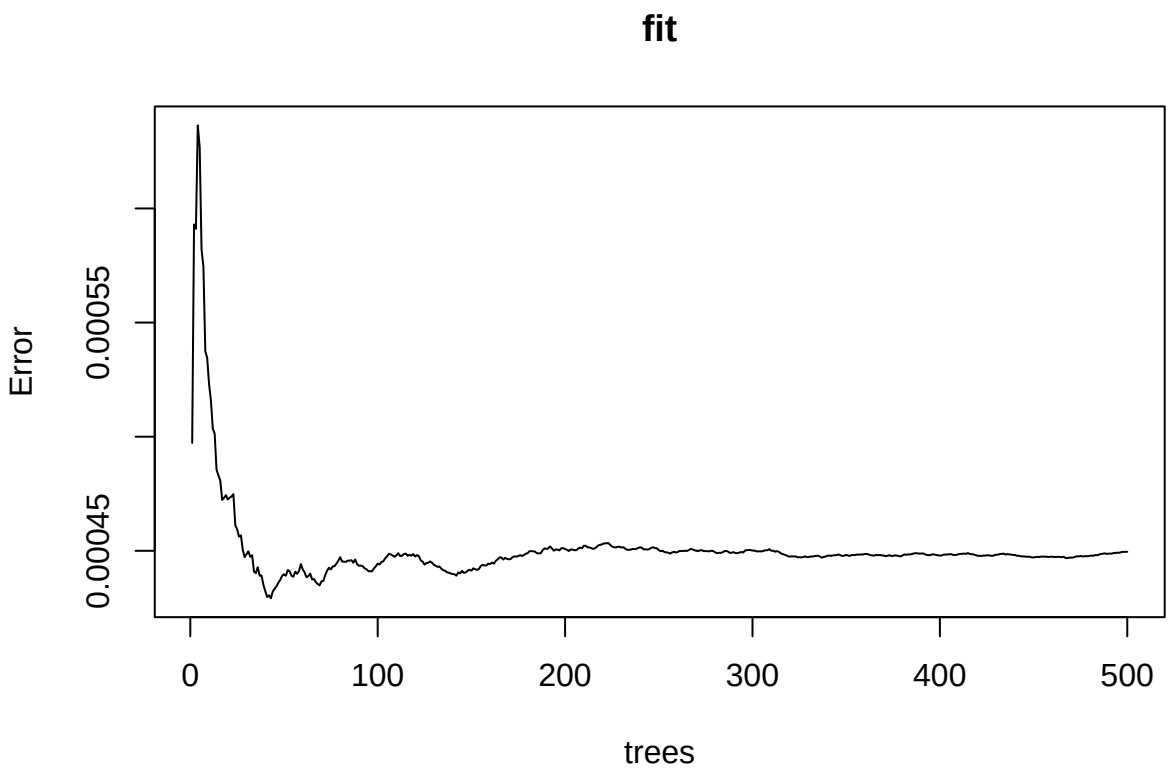
```
if(!require(Rborist)) install.packages("Rborist")
```

```
## Loading required package: Rborist
```

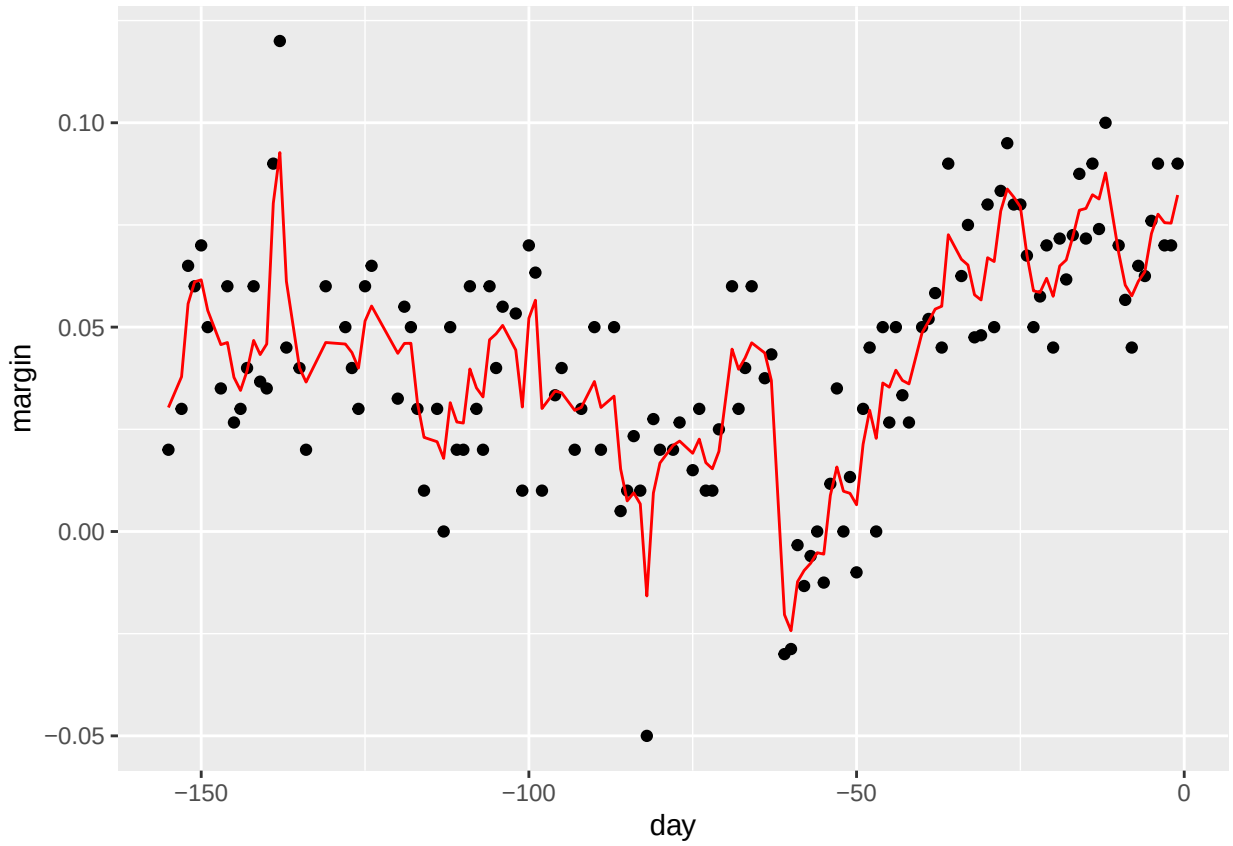
```
## Rborist 0.2-3
```

```
## Type RboristNews() to see new features/changes/bug fixes.
```

```
library(randomForest)
fit <- randomForest(margin~., data = polls_2008)
plot(fit)
```




```
polls_2008 %>%
  mutate(y_hat = predict(fit, newdata = polls_2008)) %>%
  ggplot() +
  geom_point(aes(day, margin)) +
  geom_line(aes(day, y_hat), col="red")
```




```
train_rf <- randomForest(y ~ ., data=mnist_27$train)
confusionMatrix(predict(train_rf, mnist_27$test), mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##    0.785
```

```
# use cross validation to choose parameter
train_rf_2 <- train(y ~ .,
      method = "Rborist",
      tuneGrid = data.frame(predFixed = 2, minNode = c(3, 50)),
      data = mnist_27$train)
confusionMatrix(predict(train_rf_2, mnist_27$test), mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##      0.8
```

Comprehension Check - Trees and Random Forests

1. Create a simple dataset where the outcome grows 0.75 units on average for every increase in a predictor, using this code:

```
n <- 1000
sigma <- 0.25
# set.seed(1) # if using R 3.5 or ealier
set.seed(1, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

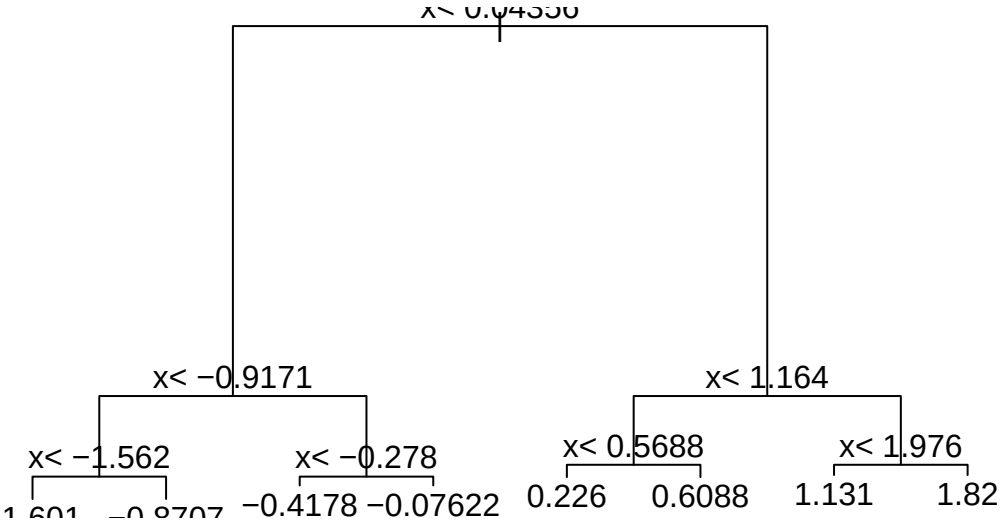
```
x <- rnorm(n, 0, 1)
y <- 0.75 * x + rnorm(n, 0, sigma)
dat <- data.frame(x = x, y = y)
```

Which code correctly uses rpart() to fit a regression tree and saves the result to fit?

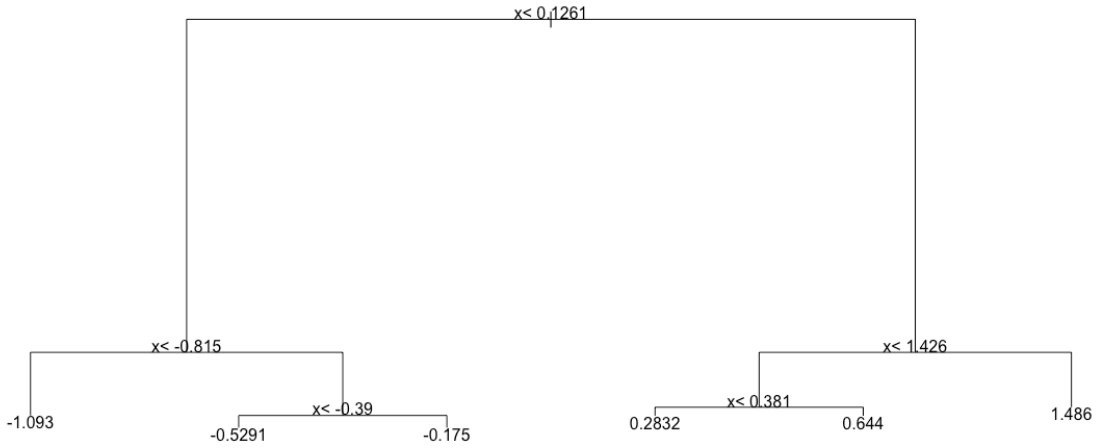
- ☐ A. `fit <- rpart(y ~ .)`
- ☐ B. `fit <- rpart(y, ., data = dat)`
- ☐ C. `fit <- rpart(x ~ ., data = dat)`
- ☒ D. `fit <- rpart(y ~ ., data = dat)`

2. Which of the following plots has the same tree shape obtained in Q1?

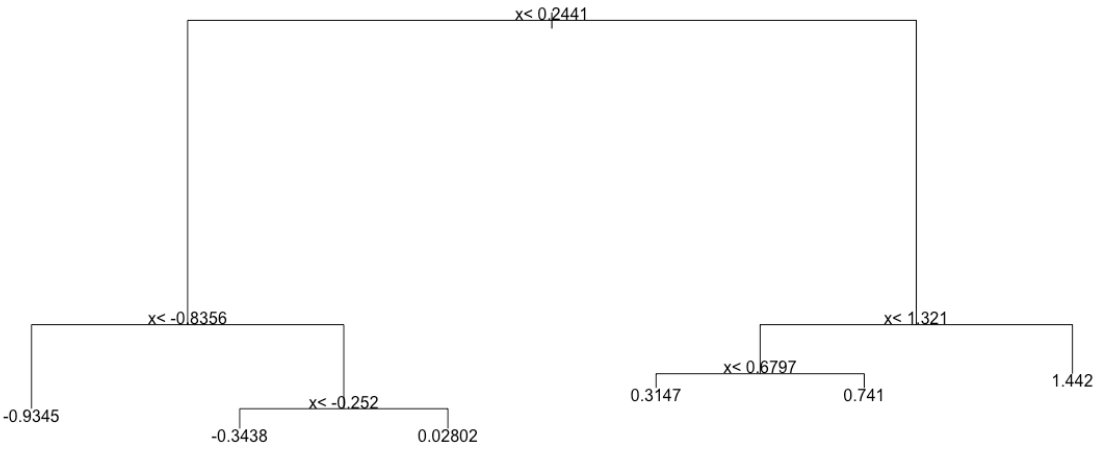
```
fit <- rpart(y ~ ., data = dat)
plot(fit)
text(fit)
```



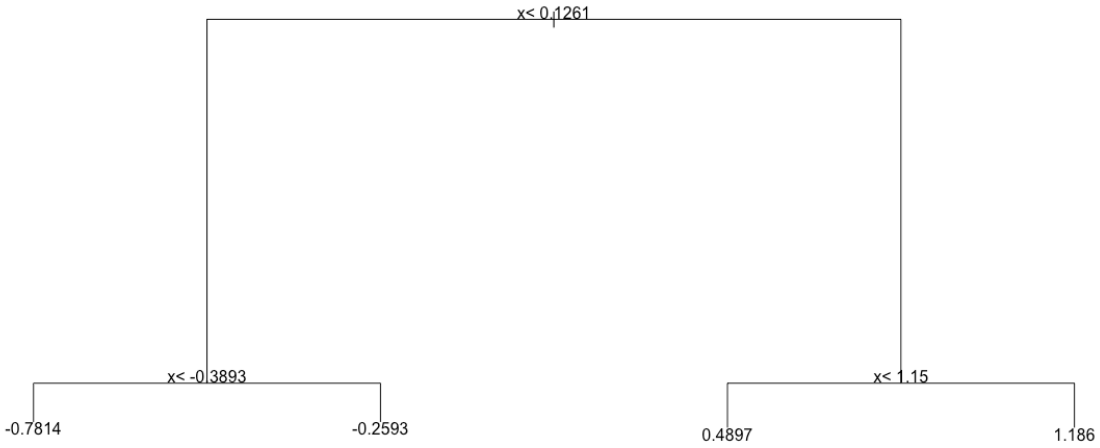
- ☐ A.


x< 0.1261
x< -0.815
x< 1.426
-1.093
x< -0.39
x< 0.381
1.486
-0.5291
-0.175
0.2832
0.644

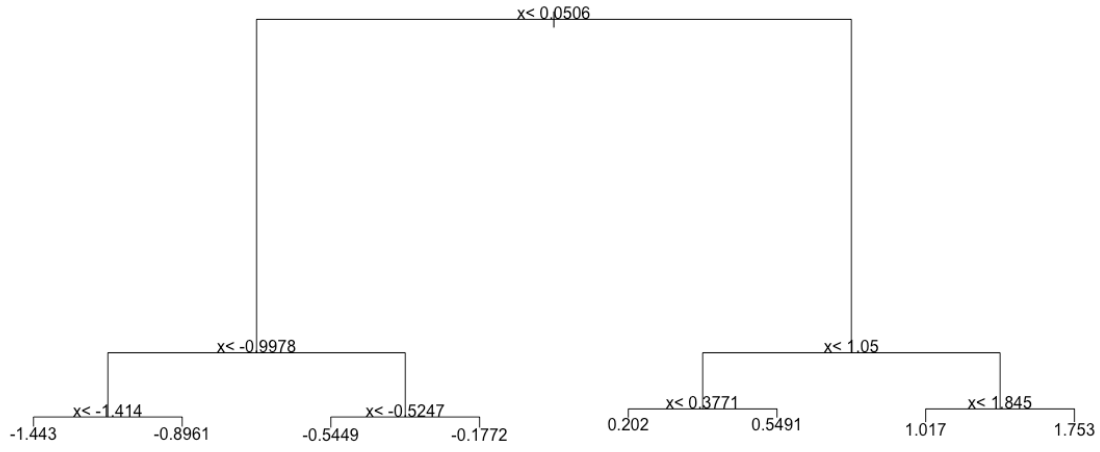
☐ B.


x< 0.2441
x< -0.8356
x< 1.321
-0.9345
x< -0.252
x< 0.6797
1.442
-0.3438
0.02802
0.3147
0.741

☐ C.



☒ D.

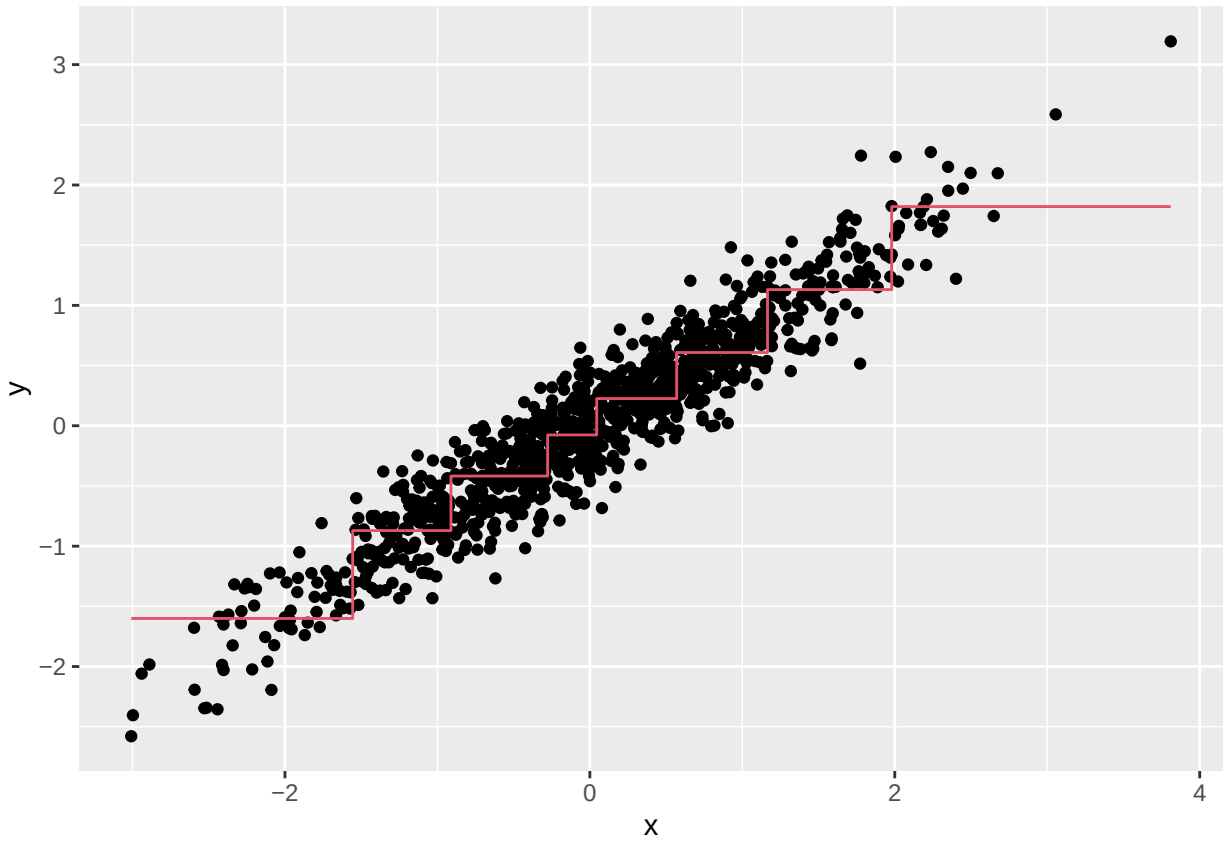


3. Below is most of the code to make a scatter plot of `y` versus `x` along with the predicted values based on the fit.

```
dat %>%
mutate(y_hat = predict(fit)) %>%
ggplot() +
geom_point(aes(x, y)) +
#BLANK
```

Which line of code should be used to replace #BLANK in the code above?

```
dat %>%
mutate(y_hat = predict(fit)) %>%
ggplot() +
geom_point(aes(x, y)) +
geom_step(aes(x, y_hat), col=2)
```



☒ A. `geom_step(aes(x, y_hat), col=2)`

☐ B. `geom_smooth(aes(y_hat, x), col=2)`

☐ C. `geom_quantile(aes(x, y_hat), col=2)`

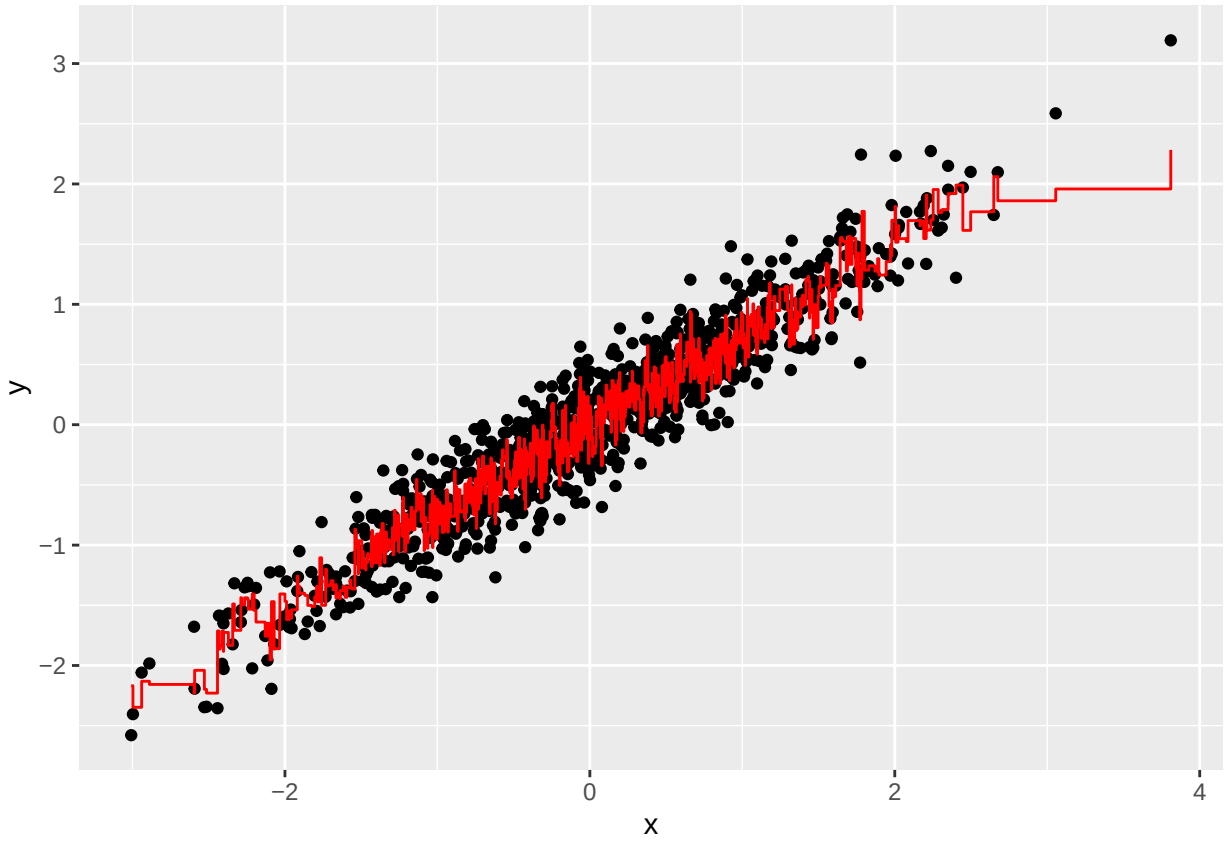
☐ D. `geom_step(aes(y_hat, x), col=2)`

4. Now run Random Forests instead of a regression tree using `randomForest()` from the **randomForest** package, and remake the scatterplot with the prediction line. Part of the code is provided for you below.

```
library(randomForest)
fit <- #BLANK
dat %>%
    mutate(y_hat = predict(fit)) %>%
    ggplot() +
    geom_point(aes(x, y)) +
    geom_step(aes(x, y_hat), col = "red")
```

What code should replace #BLANK in the provided code?

```
library(randomForest)
fit <- randomForest(y ~ x, data = dat)
dat %>%
    mutate(y_hat = predict(fit)) %>%
    ggplot() +
    geom_point(aes(x, y)) +
    geom_step(aes(x, y_hat), col = "red")
```



☒ A. `randomForest(y ~ x, data = dat)`

☐ B. `randomForest(x ~ y, data = dat)`

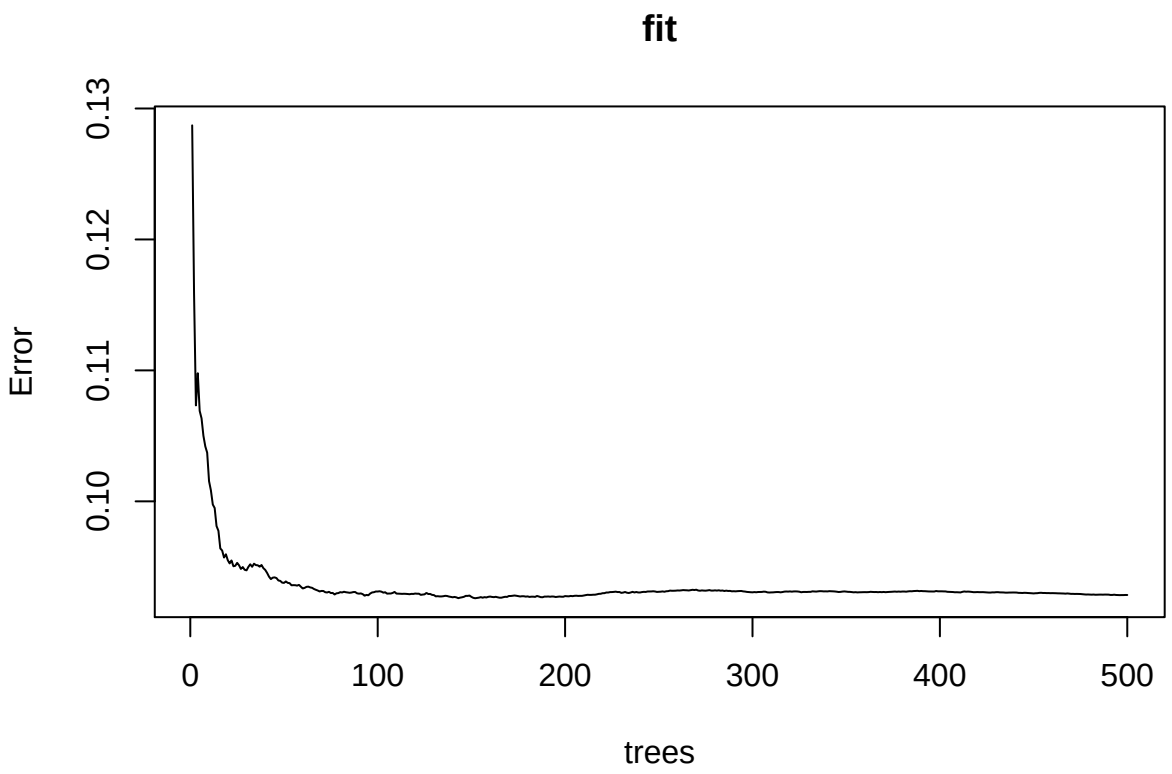
☐ C. `randomForest(y ~ x, data = data)`

☐ D. `randomForest(x ~ y)`

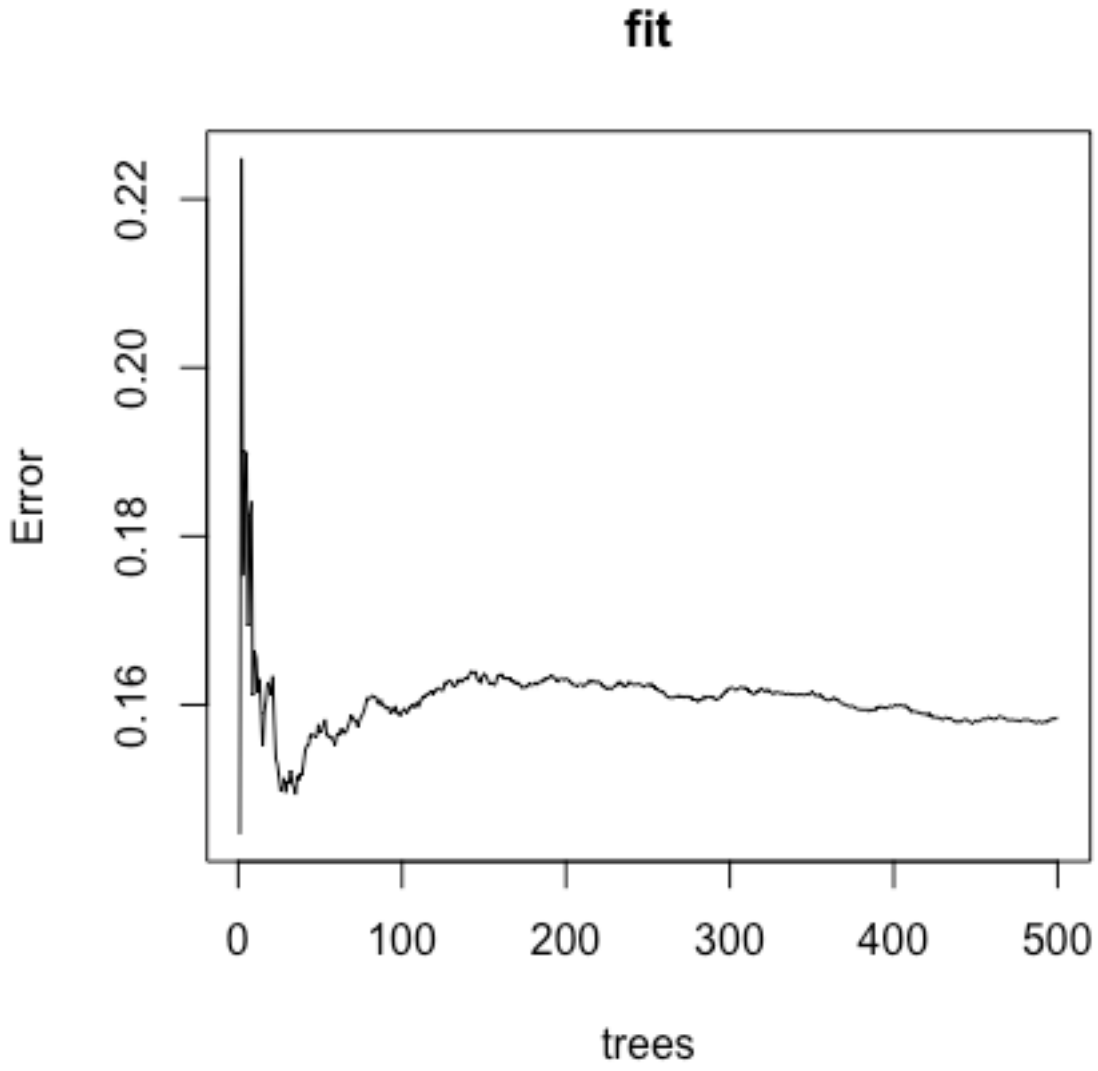
5. Use the `plot()` function to see if the Random Forest from Q4 has converged or if we need more trees.

Which of these graphs is most similar to the one produced by plotting the random forest? Note that there may be slight differences due to the seed not being set.

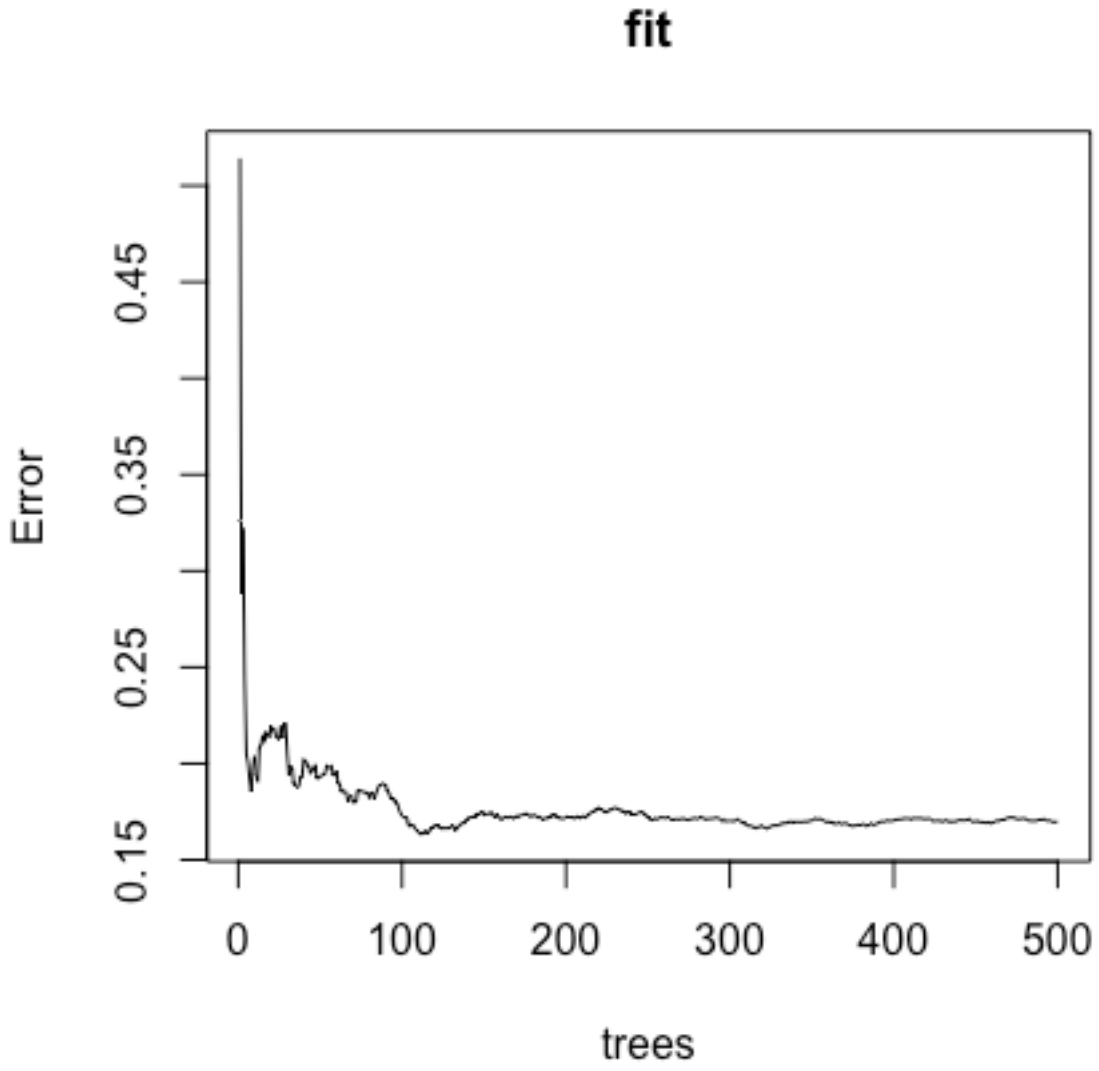
```
plot(fit)
```



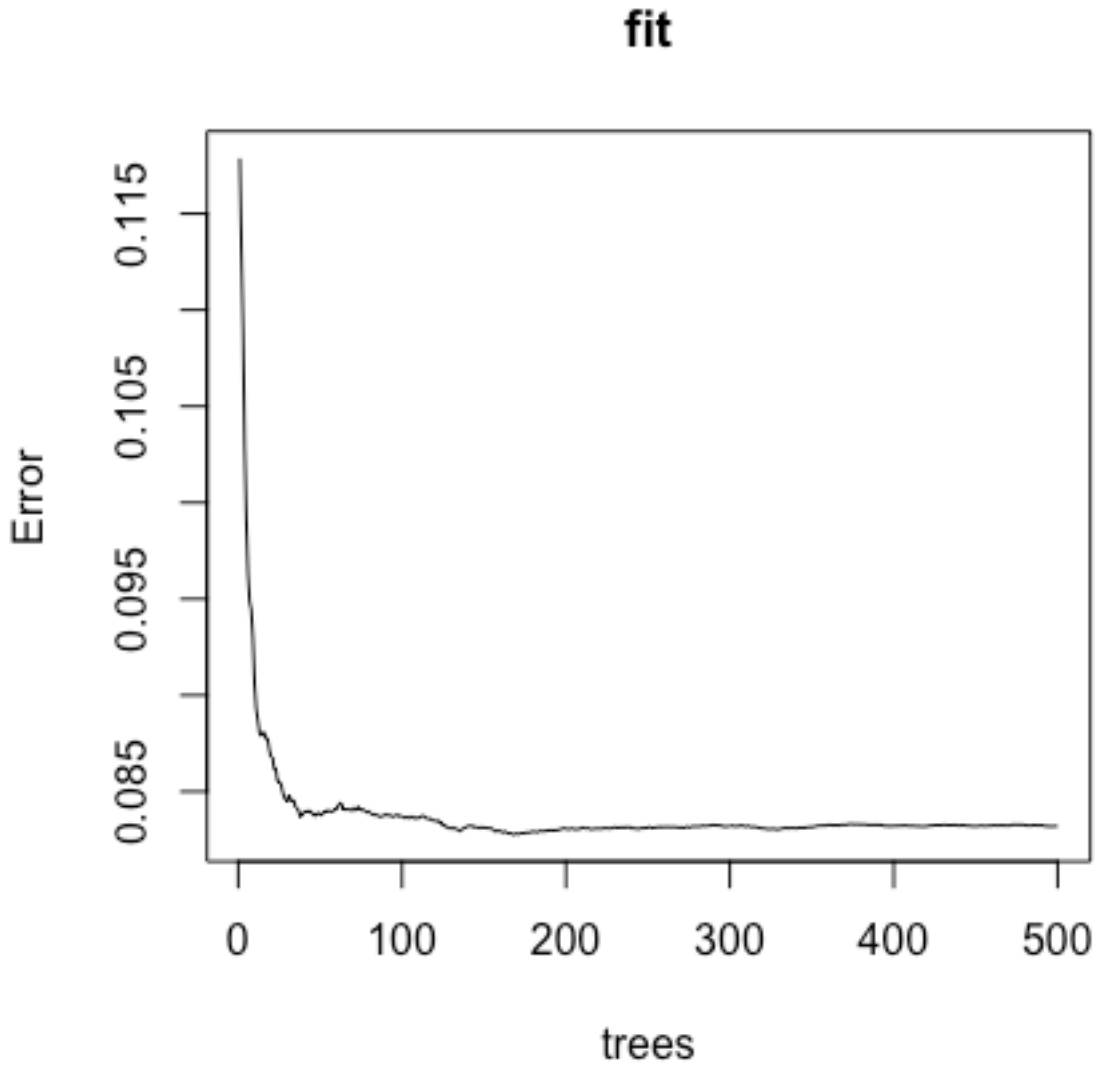
□ A.



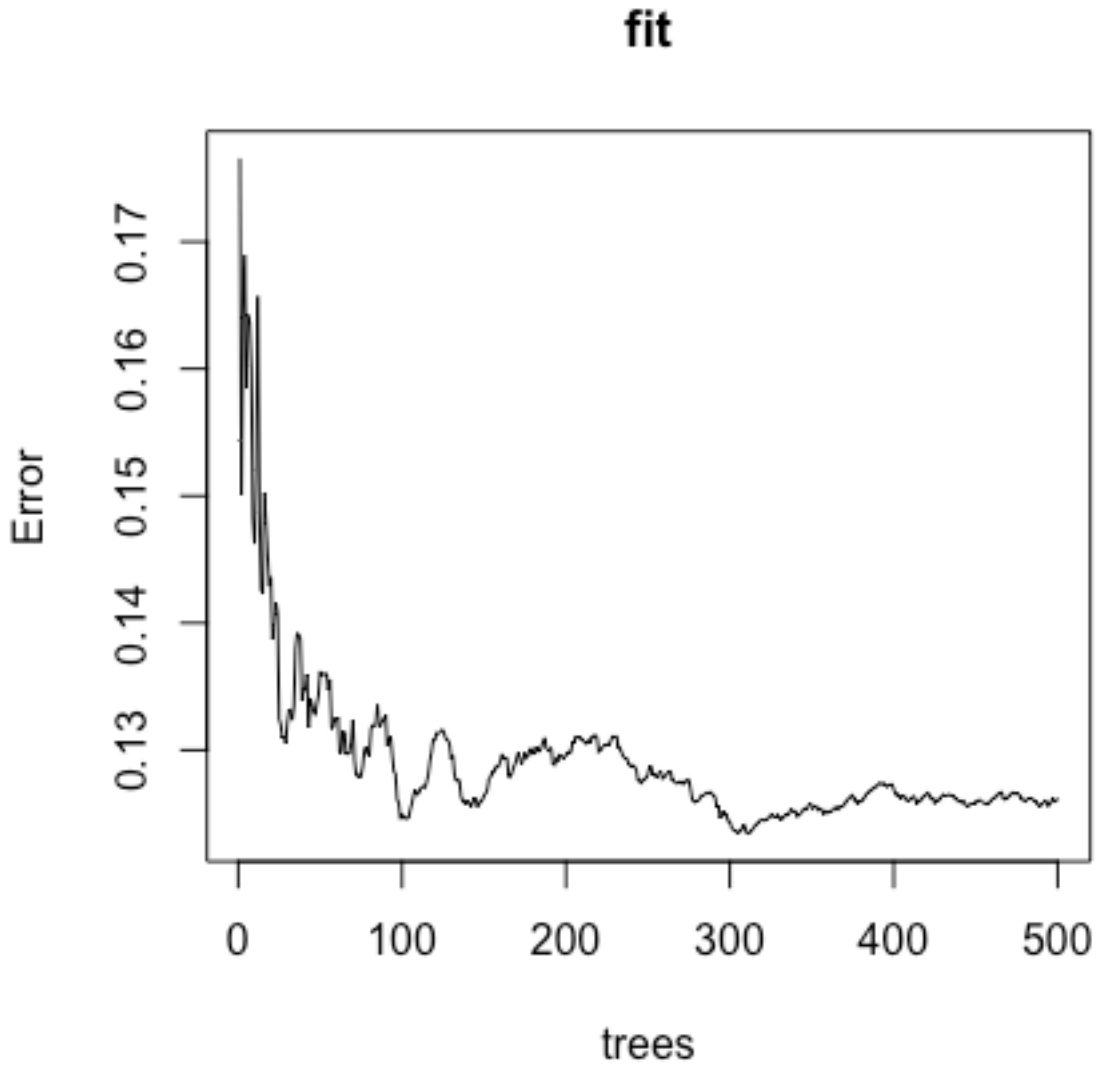
□ B.



☒ C.



□ D.



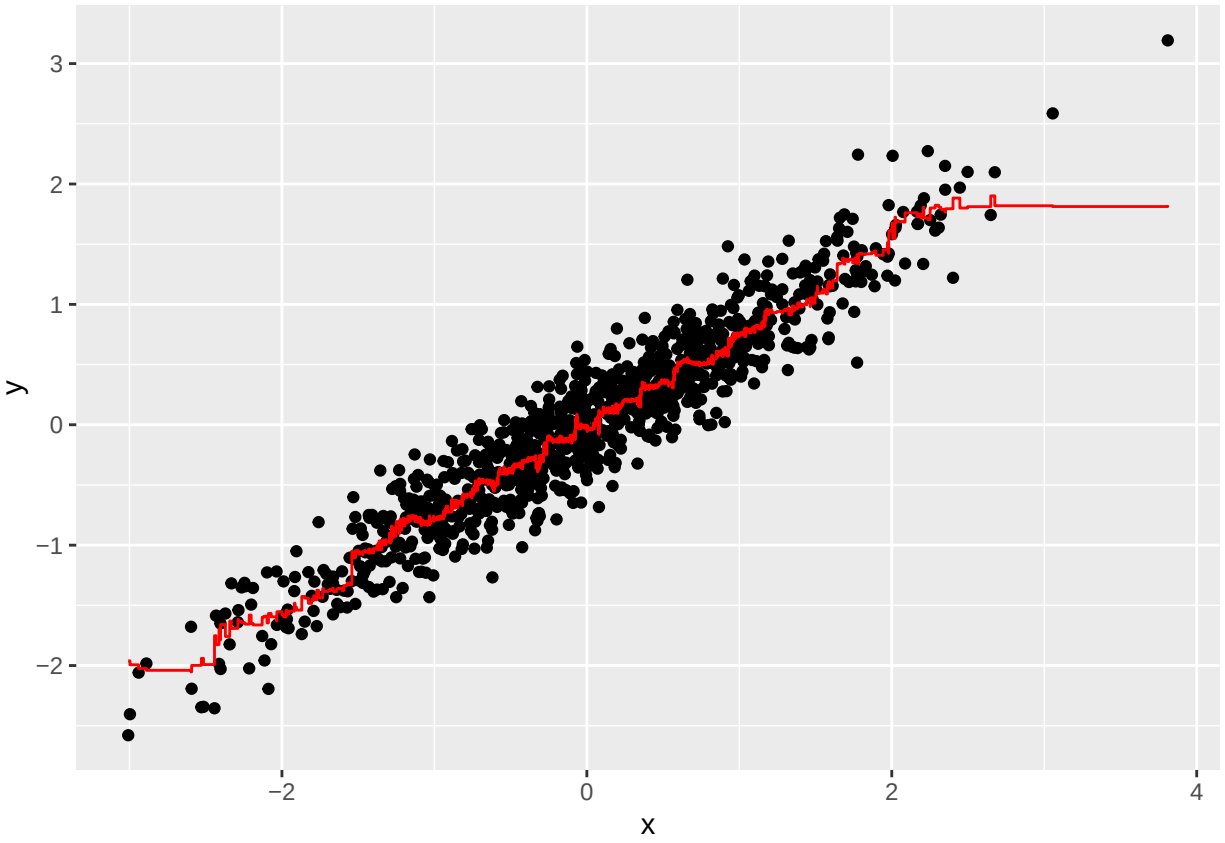
6. It seems that the default values for the Random Forest result in an estimate that is too flexible (unsmooth). Re-run the Random Forest but this time with a node size of 50 and a maximum of 25 nodes. Remake the plot.

Part of the code is provided for you below.

```
library(randomForest)
fit <- #BLANK
dat %>%
    mutate(y_hat = predict(fit)) %>%
    ggplot() +
    geom_point(aes(x, y)) +
    geom_step(aes(x, y_hat), col = "red")
```

What code should replace #BLANK in the provided code?

```
library(randomForest)
fit <- randomForest(y ~ x, data = dat, nodesize = 50, maxnodes = 25)
dat %>%
    mutate(y_hat = predict(fit)) %>%
    ggplot() +
    geom_point(aes(x, y)) +
    geom_step(aes(x, y_hat), col = "red")
```



☐ A. `randomForest(y ~ x, data = dat, nodesize = 25, maxnodes = 25)`

☐ B. `randomForest(y ~ x, data = dat, nodes = 50, max = 25)`

☐ C. `randomForest(x ~ y, data = dat, nodes = 50, max = 25)`

☒ D. `randomForest(y ~ x, data = dat, nodesize = 50, maxnodes = 25)`

☐ E. `randomForest(x ~ y, data = dat, nodesize = 50, maxnodes = 25)`

Caret Package

There is a link to the relevant section of the textbook: The caret package

Caret package links

http://topepo.github.io/caret/available-models.html

http://topepo.github.io/caret/train-models-by-tag.html

Key points

- The **caret** package helps provides a uniform interface and standardized syntax for the many different machine learning packages in R. Note that **caret** does not automatically install the packages needed.

Code

```
data("mnist_27")

train_glm <- train(y ~ ., method = "glm", data = mnist_27$train)
train_knn <- train(y ~ ., method = "knn", data = mnist_27$train)

y_hat_glm <- predict(train_glm, mnist_27$test, type = "raw")
y_hat_knn <- predict(train_knn, mnist_27$test, type = "raw")

confusionMatrix(y_hat_glm, mnist_27$test$y)$overall[["Accuracy"]]
```

```
## [1] 0.75
```

```
confusionMatrix(y_hat_knn, mnist_27$test$y)$overall[["Accuracy"]]
```

```
## [1] 0.84
```

Tuning Parameters with Caret

There is a link to the relevant section of the textbook: Cross validation

Key points

- The `train()` function automatically uses cross-validation to decide among a few default values of a tuning parameter.
- The `getModelInfo()` and `modelLookup()` functions can be used to learn more about a model and the parameters that can be optimized.
- We can use the `tunegrid()` parameter in the `train()` function to select a grid of values to be compared.
- The `trControl` parameter and `trainControl()` function can be used to change the way cross-validation is performed.
- Note that **not all parameters in machine learning algorithms are tuned**. We use the `train()` function to only optimize parameters that are tunable.

Code

```
getModelInfo("knn")
```

```
## $kknn
## $kknn$label
## [1] "k-Nearest Neighbors"
##
## $kknn$library
## [1] "kknn"
##
## $kknn$loop
## NULL
##
```

```
## $kknn$type
## [1] "Regression"     "Classification"
##
## $kknn$parameters
##   parameter     class           label
## 1      kmax   numeric Max. #Neighbors
## 2  distance   numeric        Distance
## 3    kernel character          Kernel
##
## $kknn$grid
## function(x, y, len = NULL, search = "grid") {
##                     if(search == "grid") {
##                       out <- data.frame(kmax = (5:((2 * len)+4))[(5:((2 * len)+4))%%2 > 0],
##                                         distance = 2,
##                                         kernel = "optimal")
##                     } else {
##                       by_val <- if(is.factor(y)) length(levels(y)) else 1
##                       kerns <- c("rectangular", "triangular", "epanechnikov", "biweight", "triweight
##                                  "cos", "inv", "gaussian")
##                       out <- data.frame(kmax = sample(seq(1, floor(nrow(x)/3), by = by_val), size = l
##                                         distance = runif(len, min = 0, max = 3),
##                                         kernel = sample(kerns, size = len, replace = TRUE))
##                     }
##                     out
##                   }
##
## $kknn$fit
## function(x, y, wts, param, lev, last, classProbs, ...) {
##                     dat <- if(is.data.frame(x)) x else as.data.frame(x, stringsAsFactors = TRUE)
##                     dat$.outcome <- y
##                     kknn::train.kknn(.outcome ~ ., data = dat,
##                               kmax = param$kmax,
##                               distance = param$distance,
##                               kernel = as.character(param$kernel), ...)
##                   }
##
## $kknn$predict
## function(modelFit, newdata, submodels = NULL) {
##                     if(!is.data.frame(newdata)) newdata <- as.data.frame(newdata, stringsAsFactors =
##                     predict(modelFit, newdata)
##                   }
##
## $kknn$levels
## function(x) x$obsLevels
##
## $kknn$tags
## [1] "Prototype Models"
##
## $kknn$prob
## function(modelFit, newdata, submodels = NULL) {
##                     if(!is.data.frame(newdata)) newdata <- as.data.frame(newdata, stringsAsFactors =
##                     predict(modelFit, newdata, type = "prob")
##                   }
##
```

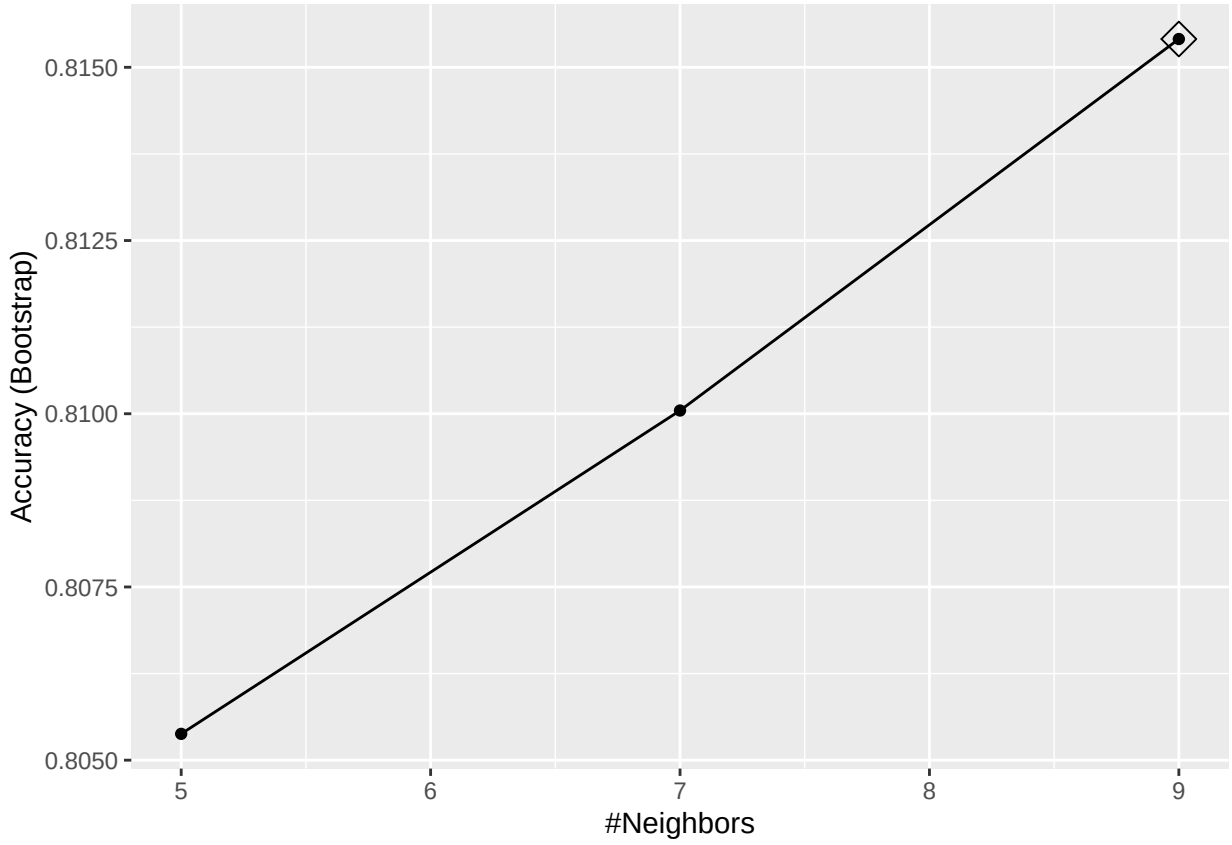
```
## $kknn$sort
## function(x) x[order(-x[,1]),]
##
##
## $knn
## $knn$label
## [1] "k-Nearest Neighbors"
##
## $knn$library
## NULL
##
## $knn$loop
## NULL
##
## $knn$type
## [1] "Classification" "Regression"
##
## $knn$parameters
##   parameter   class      label
## 1         k numeric #Neighbors
##
## $knn$grid
## function(x, y, len = NULL, search = "grid"){
##                      if(search == "grid") {
##                        out <- data.frame(k = (5:((2 * len)+4))[(5:((2 * len)+4))%%2 > 0])
##                      } else {
##                        by_val <- if(is.factor(y)) length(levels(y)) else 1
##                        out <- data.frame(k = sample(seq(1, floor(nrow(x)/3), by = by_val), size = len
##                      }
##                    }
##
## $knn$fit
## function(x, y, wts, param, lev, last, classProbs, ...) {
##                      if(is.factor(y))
##                      {
##                        knn3(as.matrix(x), y, k = param$k, ...)
##                      } else {
##                        knnreg(as.matrix(x), y, k = param$k, ...)
##                      }
##                    }
##
## $knn$predict
## function(modelFit, newdata, submodels = NULL) {
##                      if(modelFit$problemType == "Classification")
##                      {
##                        out <- predict(modelFit, newdata,  type = "class")
##                      } else {
##                        out <- predict(modelFit, newdata)
##                      }
##                      out
##                    }
##
## $knn$predictors
## function(x, ...) colnames(x$learn$X)
```

```
##
## $knn$tags
## [1] "Prototype Models"
##
## $knn$prob
## function(modelFit, newdata, submodels = NULL)
##                      predict(modelFit, newdata, type = "prob")
##
## $knn$levels
## function(x) levels(x$learn$y)
##
## $knn$sort
## function(x) x[order(-x[,1]),]
```

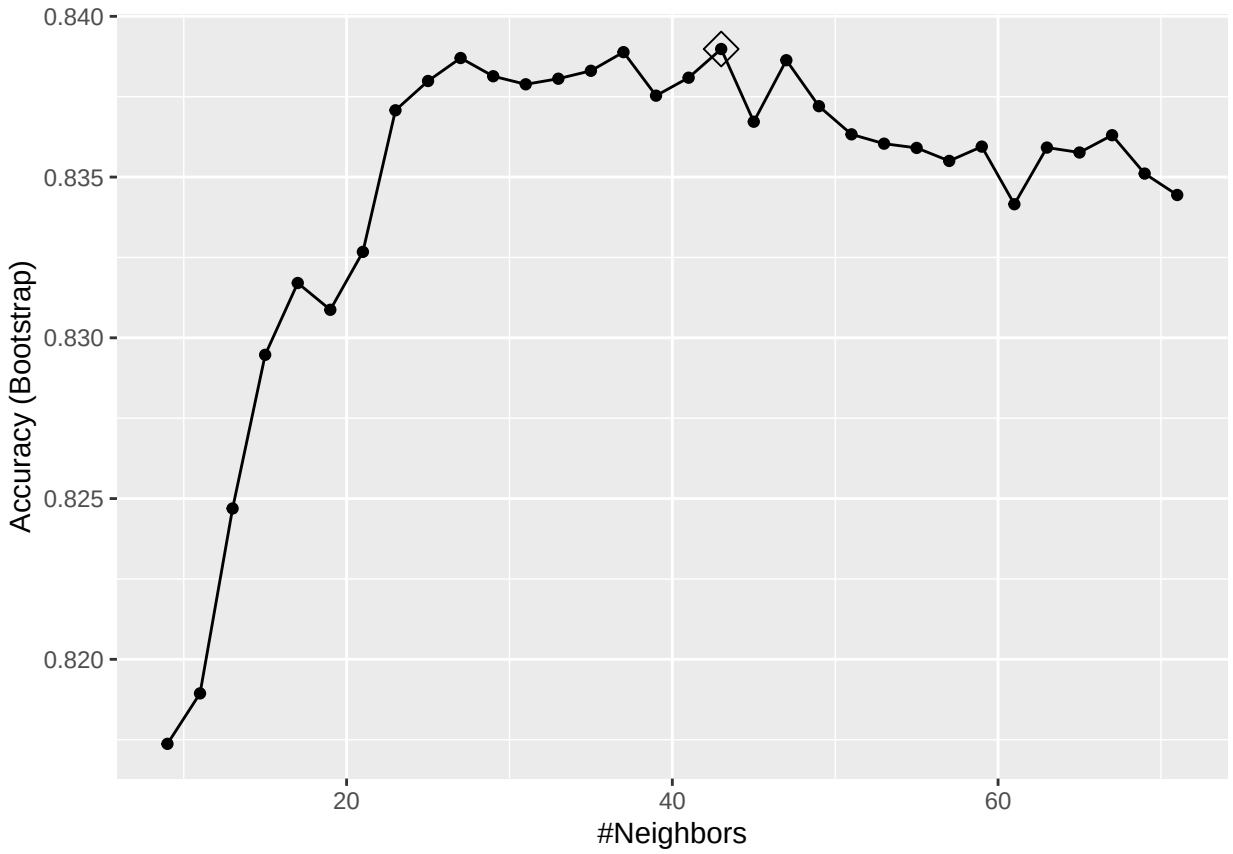
```
modelLookup("knn")
```

```
##   model parameter      label forReg forClass probModel
## 1   knn         k #Neighbors   TRUE     TRUE      TRUE
```

```
train_knn <- train(y ~ ., method = "knn", data = mnist_27$train)
ggplot(train_knn, highlight = TRUE)
```




```
train_knn <- train(y ~ ., method = "knn",
                   data = mnist_27$train,
                   tuneGrid = data.frame(k = seq(9, 71, 2)))
ggplot(train_knn, highlight = TRUE)
```




```
train_knn$bestTune
```

```
##     k
## 18 43
```

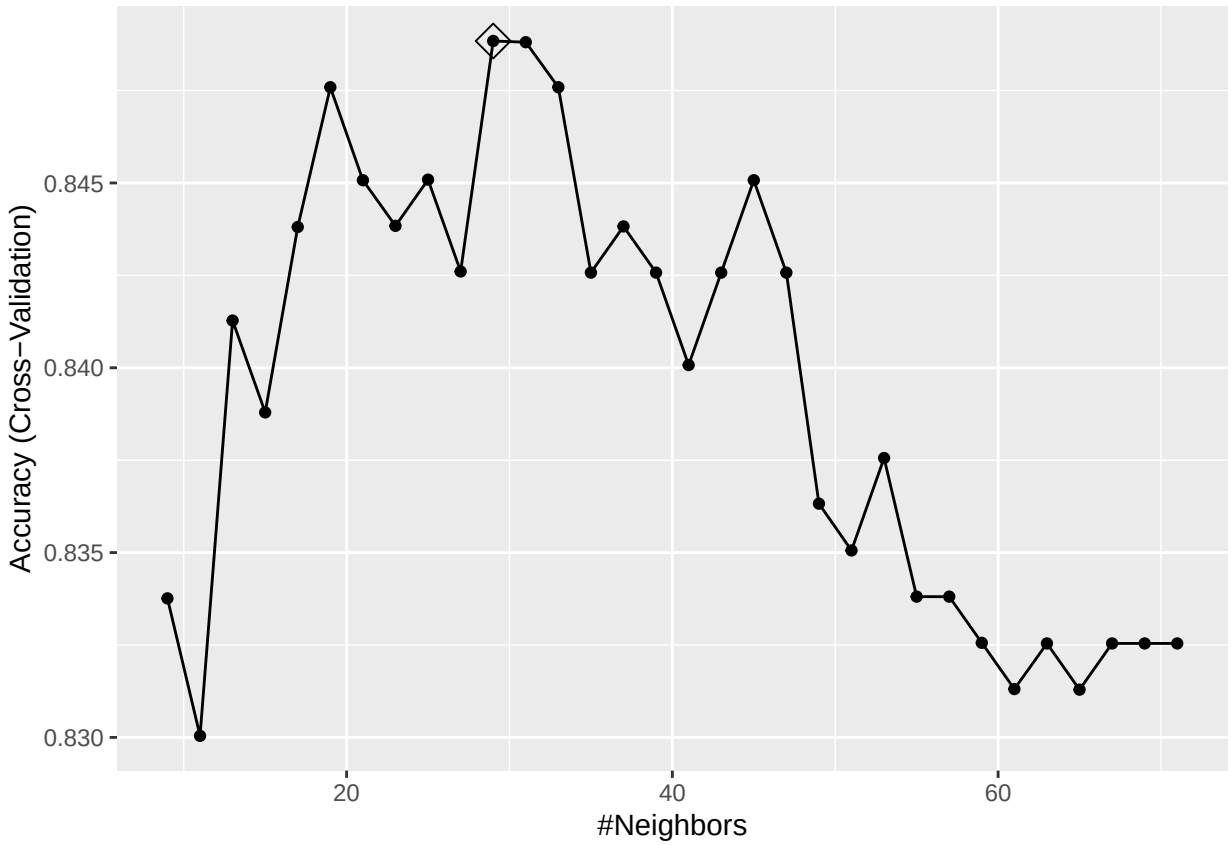
```
train_knn$finalModel
```

```
## 43-nearest neighbor model
## Training set outcome distribution:
##
##   2   7
## 379 421
```

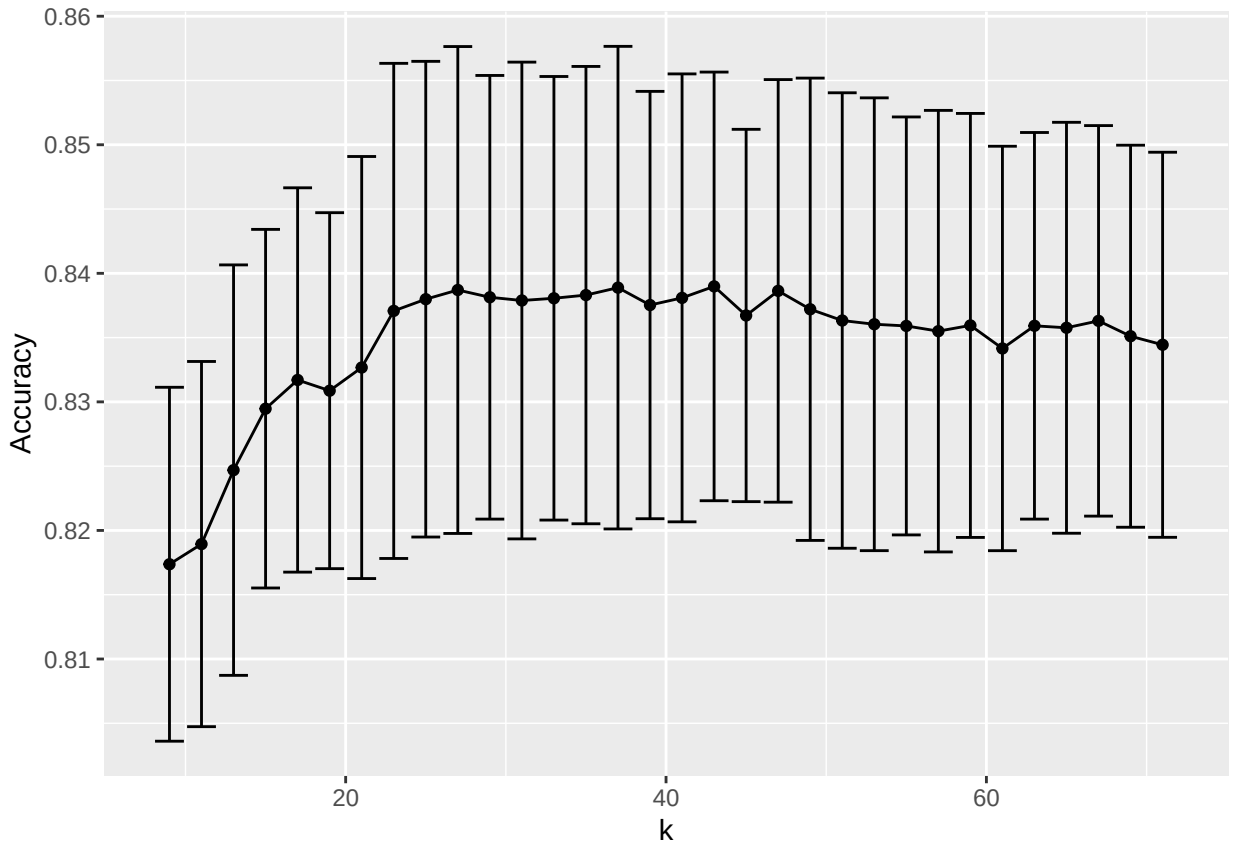
```
confusionMatrix(predict(train_knn, mnist_27$test, type = "raw"),
                mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##    0.855
```

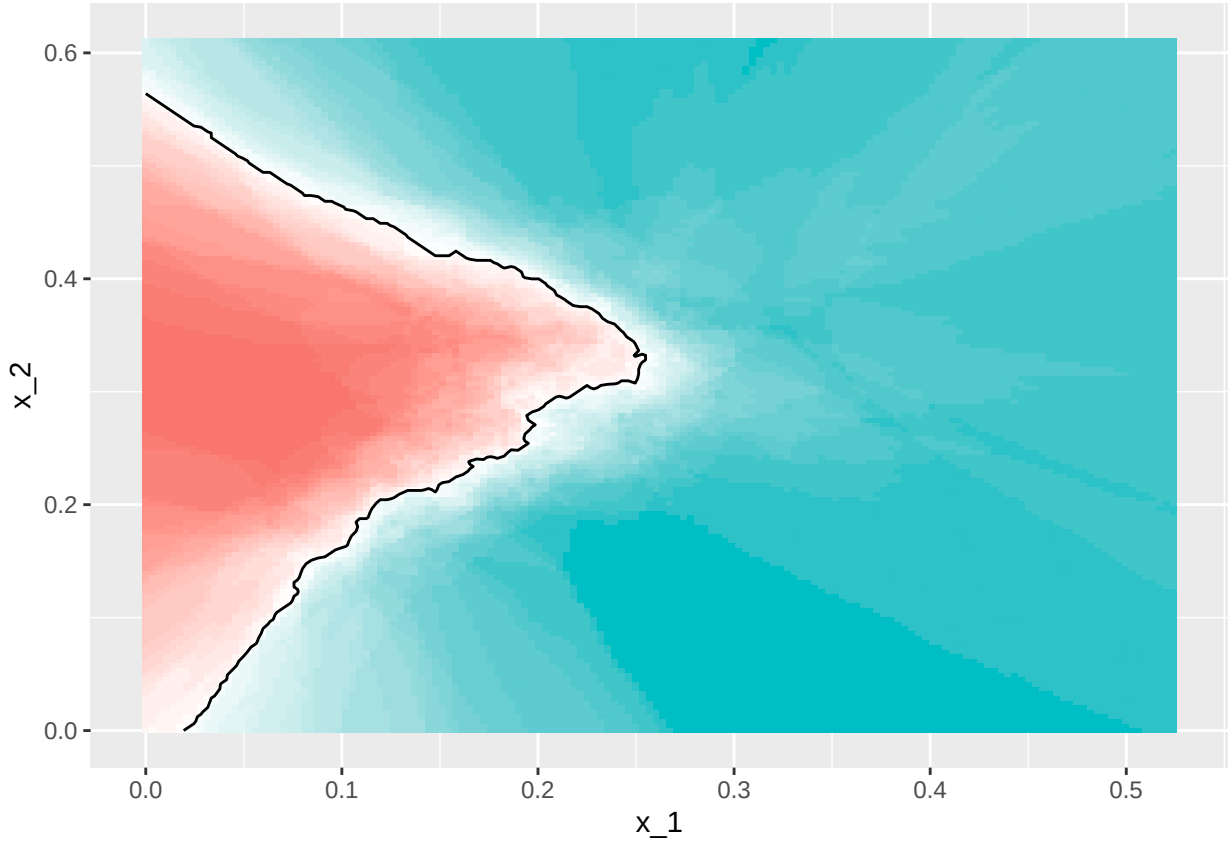
```
control <- trainControl(method = "cv", number = 10, p = .9)
train_knn_cv <- train(y ~ ., method = "knn",
                      data = mnist_27$train,
                      tuneGrid = data.frame(k = seq(9, 71, 2)),
                      trControl = control)
ggplot(train_knn_cv, highlight = TRUE)
```




```
train_knn$results %>%
     ggplot(aes(x = k, y = Accuracy)) +
     geom_line() +
     geom_point() +
     geom_errorbar(aes(x = k,
                       ymin = Accuracy - AccuracySD,
                       ymax = Accuracy + AccuracySD))
```




```
plot_cond_prob <- function(p_hat=NULL){
     tmp <- mnist_27$true_p
     if(!is.null(p_hat)){
          tmp <- mutate(tmp, p=p_hat)
     }
     tmp %>% ggplot(aes(x_1, x_2, z=p, fill=p)) +
     geom_raster(show.legend = FALSE) +
          scale_fill_gradientn(colors=c("#F8766D","white","#00BFC4")) +
          stat_contour(breaks=c(0.5),color="black")
}

plot_cond_prob(predict(train_knn, mnist_27$true_p, type = "prob")[,2])
```




```
if(!require(gam)) install.packages("gam")
```

```
## Loading required package: gam
```

```
## Loading required package: splines
```

```
## Loading required package: foreach
```

```
##
## Attaching package: 'foreach'
```

```
## The following objects are masked from 'package:purrr':
##
##     accumulate, when
```

```
## Loaded gam 1.20
```

```
modelLookup("gamLoess")
```

```
##      model parameter  label forReg forClass probModel
## 1 gamLoess      span   Span   TRUE     TRUE      TRUE
## 2 gamLoess    degree Degree   TRUE     TRUE      TRUE
```

```
grid <- expand.grid(span = seq(0.15, 0.65, len = 10), degree = 1)

train_loess <- train(y ~ .,
                method = "gamLoess",
                tuneGrid=grid,
                data = mnist_27$train)
ggplot(train_loess, highlight = TRUE)

confusionMatrix(data = predict(train_loess, mnist_27$test),
                 reference = mnist_27$test$y)$overall["Accuracy"]

p1 <- plot_cond_prob(predict(train_loess, mnist_27$true_p, type = "prob")[,2])
p1
```

Comprehension Check - Caret Package

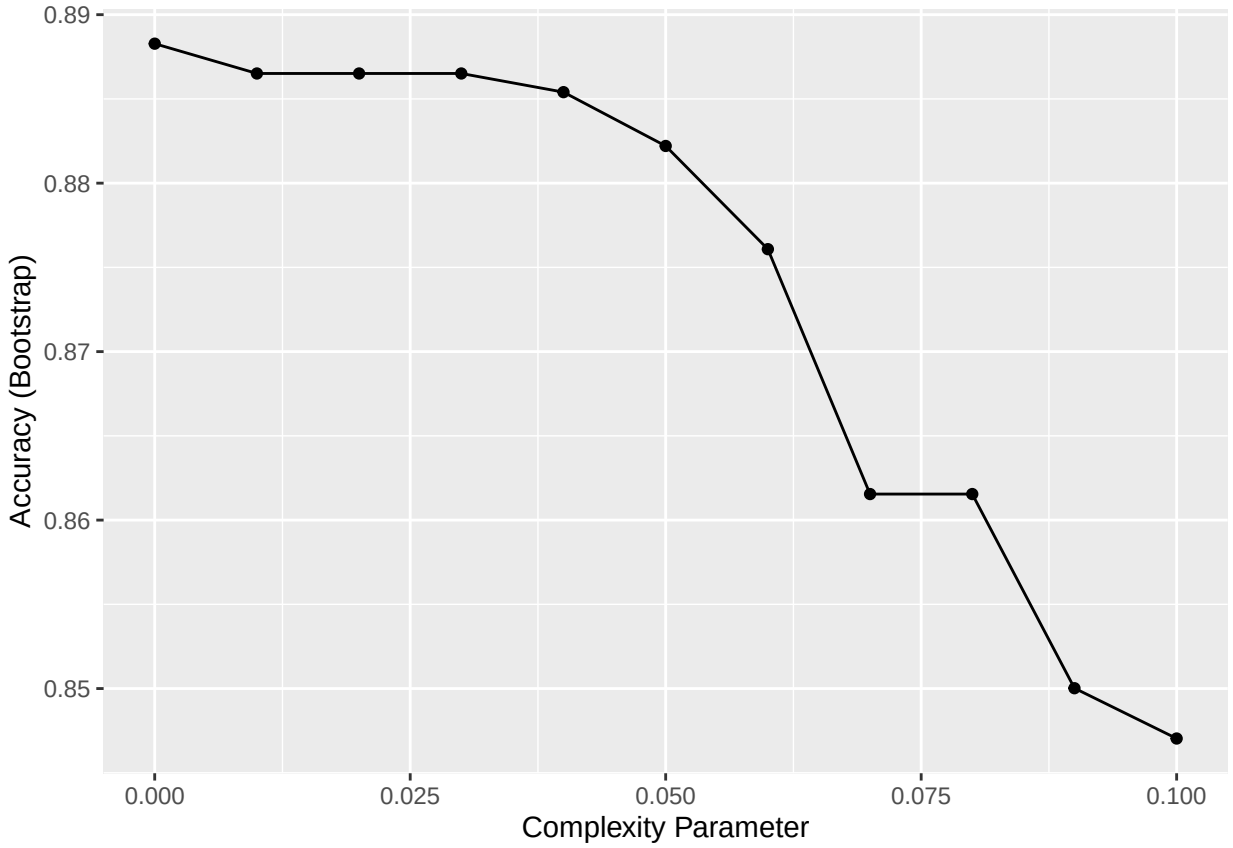
1. Load the **rpart** package and then use the `caret::train()` function with `method = "rpart"` to fit a classification tree to the `tissue_gene_expression` dataset. Try out `cp` values of `seq(0, 0.1, 0.01)`. Plot the accuracies to report the results of the best model. Set the seed to 1991.

Which value of cp gives the highest accuracy? `0`

```
set.seed(1991, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1991, sample.kind = "Rounding"): non-uniform 'Rounding'
## sampler used
```

```
data("tissue_gene_expression")

fit <- with(tissue_gene_expression,
                train(x, y, method = "rpart",
                      tuneGrid = data.frame(cp = seq(0, 0.1, 0.01))))

ggplot(fit)
```



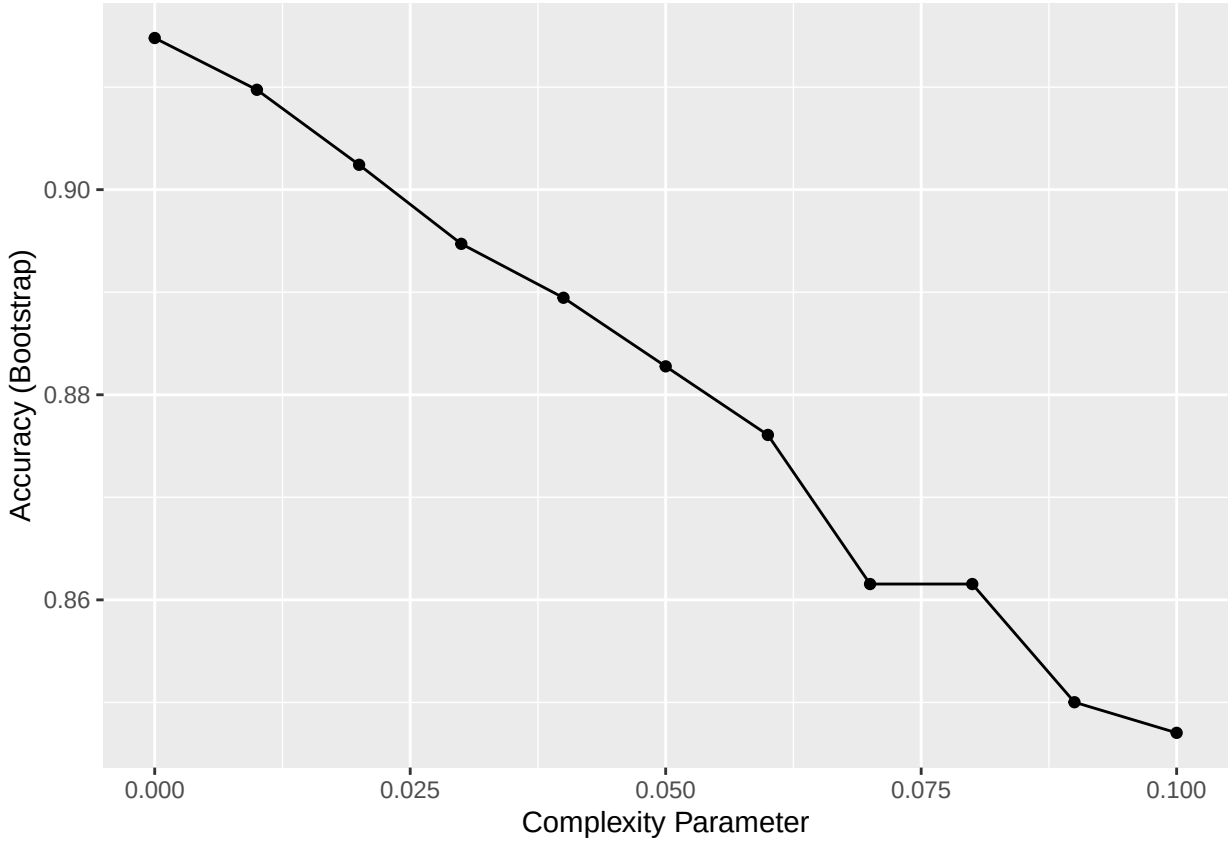
2. Note that there are only 6 placentas in the dataset. By default, `rpart` requires 20 observations before splitting a node. That means that it is difficult to have a node in which placentas are the majority. Rerun the analysis you did in Q1 with `caret::train()`, but this time with `method = "rpart"` and allow it to split any node by using the argument `control = rpart.control(minsplit = 0)`. Look at the confusion matrix again to determine whether the accuracy increases. Again, set the seed to 1991.

What is the accuracy now?

```
# set.seed(1991) # if using R 3.5 or earlier
set.seed(1991, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1991, sample.kind = "Rounding"): non-uniform 'Rounding'
## sampler used
```

```
fit_rpart <- with(tissue_gene_expression,
                  train(x, y, method = "rpart",
                        tuneGrid = data.frame(cp = seq(0, 0.10, 0.01)),
                        control = rpart.control(minsplit = 0)))
ggplot(fit_rpart)
```



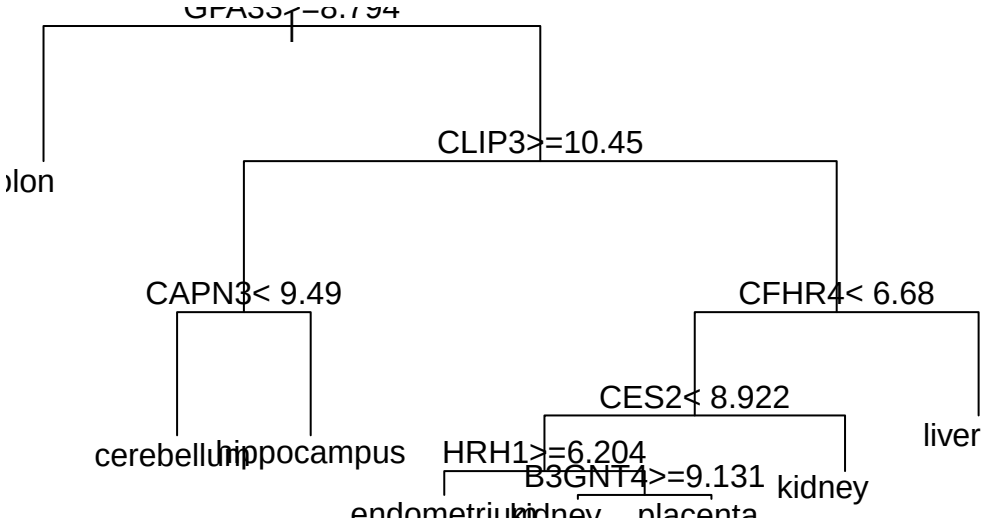

```
confusionMatrix(fit_rpart)
```

```
## Bootstrapped (25 reps) Confusion Matrix
##
## (entries are percentual average cell counts across resamples)
##
##              Reference
## Prediction    cerebellum colon endometrium hippocampus kidney liver placenta
##   cerebellum        19.5   0.0         0.2         0.9    0.4   0.0       0.1
##   colon              0.3  16.5         0.1         0.0    0.1   0.0       0.1
##   endometrium        0.1   0.2         6.4         0.1    0.9   0.1       0.5
##   hippocampus        0.2   0.0         0.0        15.6    0.1   0.0       0.0
##   kidney             0.3   0.3         0.9         0.1   19.1   0.5       0.3
##   liver              0.0   0.0         0.3         0.0    0.3  12.6       0.2
##   placenta           0.1   0.1         0.5         0.0    0.6   0.1       1.8
##
##  Accuracy (average) : 0.9141
```

3. Plot the tree from the best fitting model of the analysis you ran in Q2.

Which gene is at the first split?

```
plot(fit_rpart$finalModel)
text(fit_rpart$finalModel)
```



- ☐ A. B3GNT4
- ☐ B. CAPN3
- ☐ C. CES2
- ☐ D. CFHR4
- ☐ E. CLIP3
- ☒ F. GPA33
- ☐ G. HRH1

4. We can see that with just seven genes, we are able to predict the tissue type. Now let's see if we can predict the tissue type with even fewer genes using a Random Forest. Use the `train()` function and the `rf` method to train a Random Forest model and save it to an object called `fit`. Try out values of `mtry` ranging from `seq(50, 200, 25)` (you can also explore other values on your own). What `mtry` value maximizes accuracy? To permit small `nodesize` to grow as we did with the classification trees, use the following argument: `nodesize = 1`.

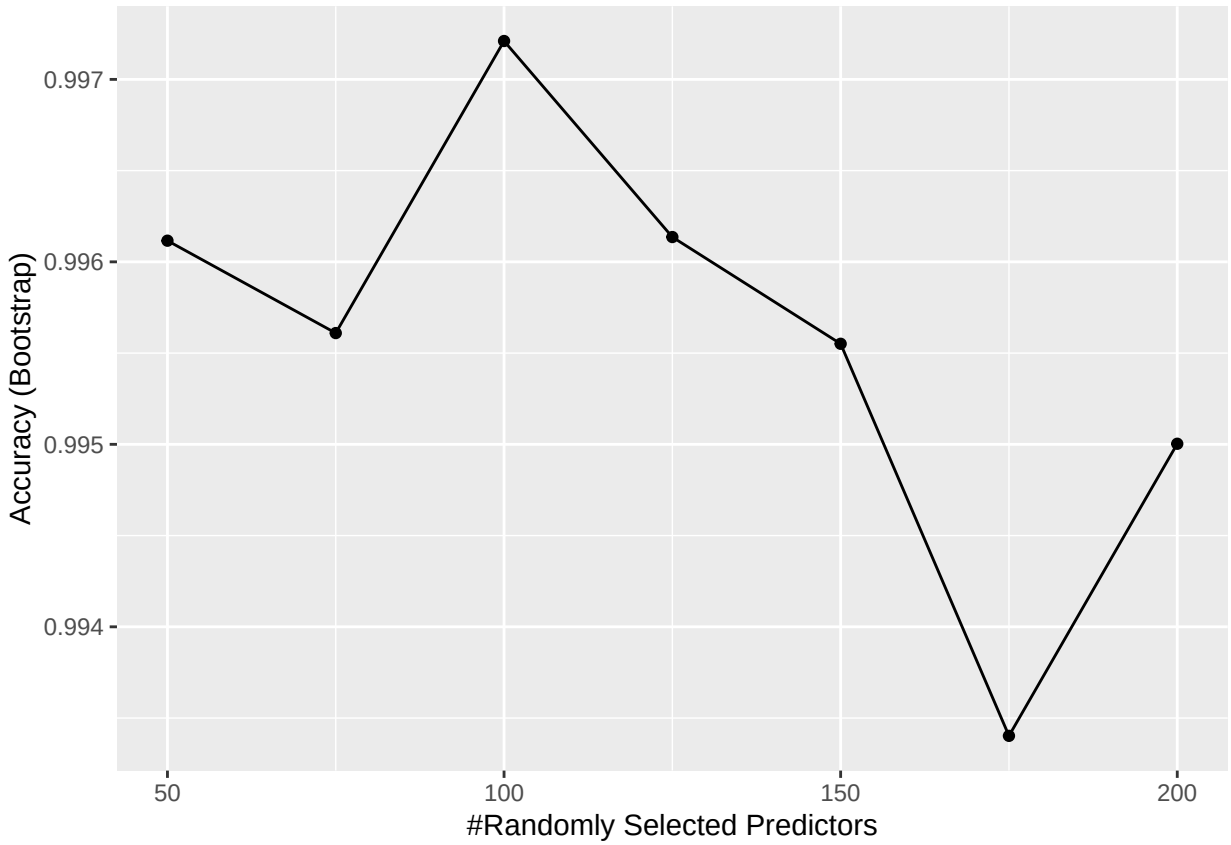
Note: This exercise will take some time to run. If you want to test out your code first, try using smaller values with `ntree`. Set the seed to 1991 again.

What value of mtry maximizes accuracy? `100`

```
# set.seed(1991) # if using R 3.5 or earlier
set.seed(1991, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1991, sample.kind = "Rounding"): non-uniform 'Rounding'
## sampler used
```

```
library(randomForest)
fit <- with(tissue_gene_expression,
                train(x, y, method = "rf",
                      nodesize = 1,
                      tuneGrid = data.frame(mtry = seq(50, 200, 25))))

ggplot(fit)
```



5. Use the function `varImp()` on the output of `train()` and save it to an object called `imp`:

```
imp <- #BLANK
imp
```

What should replace #BLANK in the code above?

```
imp <- varImp(fit)
imp
```

```
## rf variable importance
##
##   only 20 most important variables shown (out of 500)
##
##          Overall
## GPA33     100.00
## BIN1       64.65
## GPM6B      62.35
## KIF2C      62.15
## CLIP3      52.09
## COLGALT2   46.48
## CFHR4      35.03
## SHANK2     34.90
## TFR2       33.61
## GALNT11    30.70
```

```
## CEP55      30.49
## TCN2       27.96
## CAPN3      27.52
## CYP4F11    25.74
## GTF2IRD1   24.89
## KCTD2      24.34
## FCN3       22.68
## SUSD6      22.24
## DOCK4      22.02
## RARRES2    21.53
```

6. The `rpart()` model we ran above in Q2 produced a tree that used just seven predictors. Extracting the predictor names is not straightforward, but can be done. If the output of the call to train was `fit_rpart`, we can extract the names like this: 1/1 point (graded)

```
tree_terms <- as.character(unique(fit_rpart$finalModel$frame$var[!(fit_rpart$finalModel$frame$var == "<
tree_terms
```

```
## [1] "GPA33"  "CLIP3"  "CAPN3"  "CFHR4"  "CES2"   "HRH1"   "B3GNT4"
```

Calculate the variable importance in the Random Forest call from Q4 for these seven predictors and examine where they rank.

What is the importance of the CFHR4 gene in the Random Forest call? `35.0`

What is the rank of the CFHR4 gene in the Random Forest call? `7`

```
data_frame(term = rownames(imp$importance),
       importance = imp$importance$Overall) %>%
mutate(rank = rank(-importance)) %>% arrange(desc(importance)) %>%
filter(term %in% tree_terms)
```

```
## # A tibble: 7 x 3
##   term   importance  rank
##   <chr>       <dbl> <dbl>
## 1 GPA33     100         1
## 2 CLIP3      52.1       5
## 3 CFHR4      35.0       7
## 4 CAPN3      27.5      13
## 5 CES2       20.0      22
## 6 HRH1        2.35     97
## 7 B3GNT4      0.136   343
```

Titanic Exercises - Part 1

These exercises cover everything you have learned in this course so far. You will use the background information to provided to train a number of different types of models on this dataset.

Background

The Titanic was a British ocean liner that struck an iceberg and sunk on its maiden voyage in 1912 from the United Kingdom to New York. More than 1,500 of the estimated 2,224 passengers and crew died in the accident, making this one of the largest maritime disasters ever outside of war. The ship carried a wide

range of passengers of all ages and both genders, from luxury travelers in first-class to immigrants in the lower classes. However, not all passengers were equally likely to survive the accident. You will use real data about a selection of 891 passengers to predict which passengers survived.

```
if(!require(titanic)) install.packages("titanic")
```

```
## Loading required package: titanic
```

```
library(titanic)    # loads titanic_train data frame

# 3 significant digits
options(digits = 3)

# clean the data - `titanic_train` is loaded with the titanic package
titanic_clean <- titanic_train %>%
    mutate(Survived = factor(Survived),
           Embarked = factor(Embarked),
           Age = ifelse(is.na(Age), median(Age, na.rm = TRUE), Age), # NA age to median age
           FamilySize = SibSp + Parch + 1) %>%    # count family members
    dplyr::select(Survived,  Sex, Pclass, Age, Fare, SibSp, Parch, FamilySize, Embarked)
```

1. Training and test sets

Split `titanic_clean` into test and training sets - after running the setup code, it should have 891 rows and 9 variables.

Set the seed to 42, then use the **caret** package to create a 20% data partition based on the `Survived` column. Assign the 20% partition to `test_set` and the remaining 80% partition to `train_set`.

How many observations are in the training set?

```
#set.seed(42) # if using R 3.5 or earlier
set.seed(42, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(42, sample.kind = "Rounding"): non-uniform 'Rounding'
## sampler used
```

```
test_index <- createDataPartition(titanic_clean$Survived, times = 1, p = 0.2, list = FALSE) # create a
test_set <- titanic_clean[test_index,]
train_set <- titanic_clean[-test_index,]

nrow(train_set)
```

```
## [1] 712
```

How many observations are in the test set?

```
nrow(test_set)
```

```
## [1] 179
```

What proportion of individuals in the training set survived?

```r
mean(train_set$Survived == 1)
```

```
## [1] 0.383
```

2. Baseline prediction by guessing the outcome

The simplest prediction method is randomly guessing the outcome without using additional predictors. These methods will help us determine whether our machine learning algorithm performs better than chance. How accurate are two methods of guessing Titanic passenger survival?

Set the seed to 3. For each individual in the test set, randomly guess whether that person survived or not by sampling from the vector `c(0,1)` (Note: use the default argument setting of prob from the `sample` function).

What is the accuracy of this guessing method?

```r
#set.seed(3)
set.seed(3, sample.kind = "Rounding")
```

```
## Warning in set.seed(3, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```r
# guess with equal probability of survival
guess <- sample(c(0,1), nrow(test_set), replace = TRUE)
mean(guess == test_set$Survived)
```

```
## [1] 0.475
```

3a. Predicting survival by sex

Use the training set to determine whether members of a given sex were more likely to survive or die. Apply this insight to generate survival predictions on the test set.

What proportion of training set females survived?

```r
train_set %>%
    group_by(Sex) %>%
    summarize(Survived = mean(Survived == 1)) %>%
    filter(Sex == "female") %>%
    pull(Survived)
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
## [1] 0.731
```

What proportion of training set males survived?

```r
train_set %>%
    group_by(Sex) %>%
    summarize(Survived = mean(Survived == 1)) %>%
    filter(Sex == "male") %>%
    pull(Survived)
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
## [1] 0.197
```

3b. Predicting survival by sex

Predict survival using sex on the test set: if the survival rate for a sex is over 0.5, predict survival for all individuals of that sex, and predict death if the survival rate for a sex is under 0.5.

What is the accuracy of this sex-based prediction method on the test set?

```
sex_model <- ifelse(test_set$Sex == "female", 1, 0)    # predict Survived=1 if female, 0 if male
mean(sex_model == test_set$Survived)    # calculate accuracy
```

```
## [1] 0.821
```

4a. Predicting survival by passenger class

In the training set, which class(es) (Pclass) were passengers more likely to survive than die?

```
train_set %>%
    group_by(Pclass) %>%
    summarize(Survived = mean(Survived == 1))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
## # A tibble: 3 x 2
##   Pclass Survived
##    <int>    <dbl>
## 1      1    0.619
## 2      2    0.5
## 3      3    0.242
```

Select ALL that apply.

- ☒ A. 1
- ☐ B. 2
- ☐ C. 3

4b. Predicting survival by passenger class

Predict survival using passenger class on the test set: predict survival if the survival rate for a class is over 0.5, otherwise predict death.

What is the accuracy of this class-based prediction method on the test set?

```
class_model <- ifelse(test_set$Pclass == 1, 1, 0)    # predict survival only if first class
mean(class_model == test_set$Survived)    # calculate accuracy
```

```
## [1] 0.704
```

4c. Predicting survival by passenger class

Use the training set to group passengers by both sex and passenger class.

Which sex and class combinations were more likely to survive than die?

```r
train_set %>%
    group_by(Sex, Pclass) %>%
    summarize(Survived = mean(Survived == 1)) %>%
    filter(Survived > 0.5)
```

```
## `summarise()` regrouping output by 'Sex' (override with `.groups` argument)
```

```
## # A tibble: 2 x 3
## # Groups:   Sex [1]
##   Sex    Pclass Survived
##   <chr>   <int>    <dbl>
## 1 female      1    0.957
## 2 female      2    0.919
```

Select ALL that apply.

- ☒ A. female 1st class
- ☒ B. female 2nd class
- ☐ C. female 3rd class
- ☐ D. male 1st class
- ☐ E. male 2nd class
- ☐ F. male 3rd class

4d. Predicting survival by passenger class

Predict survival using both sex and passenger class on the test set. Predict survival if the survival rate for a sex/class combination is over 0.5, otherwise predict death.

What is the accuracy of this sex- and class-based prediction method on the test set?

```r
sex_class_model <- ifelse(test_set$Sex == "female" & test_set$Pclass != 3, 1, 0)
mean(sex_class_model == test_set$Survived)
```

```
## [1] 0.821
```

5a. Confusion matrix

Use the `confusionMatrix()` function to create confusion matrices for the sex model, class model, and combined sex and class model. You will need to convert predictions and survival status to factors to use this function.

```r
confusionMatrix(data = factor(sex_model), reference = factor(test_set$Survived))
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  0  1
##          0 96 18
##          1 14 51
##
##                Accuracy : 0.821
##                  95% CI : (0.757, 0.874)
```

```
##     No Information Rate : 0.615
##     P-Value [Acc > NIR] : 1.72e-09
##
##                   Kappa : 0.619
##
##  Mcnemar's Test P-Value : 0.596
##
##             Sensitivity : 0.873
##             Specificity : 0.739
##          Pos Pred Value : 0.842
##          Neg Pred Value : 0.785
##              Prevalence : 0.615
##          Detection Rate : 0.536
##    Detection Prevalence : 0.637
##       Balanced Accuracy : 0.806
##
##        'Positive' Class : 0
##
```

```
confusionMatrix(data = factor(class_model), reference = factor(test_set$Survived))
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  0  1
##          0 94 37
##          1 16 32
##
##                Accuracy : 0.704
##                  95% CI : (0.631, 0.77)
##     No Information Rate : 0.615
##     P-Value [Acc > NIR] : 0.00788
##
##                   Kappa : 0.337
##
##  Mcnemar's Test P-Value : 0.00601
##
##             Sensitivity : 0.855
##             Specificity : 0.464
##          Pos Pred Value : 0.718
##          Neg Pred Value : 0.667
##              Prevalence : 0.615
##          Detection Rate : 0.525
##    Detection Prevalence : 0.732
##       Balanced Accuracy : 0.659
##
##        'Positive' Class : 0
##
```

```
confusionMatrix(data = factor(sex_class_model), reference = factor(test_set$Survived))
```

```
## Confusion Matrix and Statistics
##
```

```
##           Reference
## Prediction   0   1
##          0 109  31
##          1   1  38
##
##                Accuracy : 0.821
##                  95% CI : (0.757, 0.874)
##     No Information Rate : 0.615
##     P-Value [Acc > NIR] : 1.72e-09
##
##                   Kappa : 0.589
##
##  Mcnemar's Test P-Value : 2.95e-07
##
##             Sensitivity : 0.991
##             Specificity : 0.551
##          Pos Pred Value : 0.779
##          Neg Pred Value : 0.974
##              Prevalence : 0.615
##          Detection Rate : 0.609
##    Detection Prevalence : 0.782
##       Balanced Accuracy : 0.771
##
##        'Positive' Class : 0
##
```

What is the "positive" class used to calculate confusion matrix metrics?

- ☒ A. 0
- ☐ B. 1

Which model has the highest sensitivity?

- ☐ A. sex only
- ☐ B. class only
- ☒ C. sex and class combined

Which model has the highest specificity?

- ☒ A. sex only
- ☐ B. class only
- ☐ C. sex and class combined

Which model has the highest balanced accuracy?

- ☒ A. sex only
- ☐ B. class only
- ☐ C. sex and class combined

5b. Confusion matrix

What is the maximum value of balanced accuracy? `0.806`

6. F1 scores

Use the `F_meas()` function to calculate F_1 scores for the sex model, class model, and combined sex and class model. You will need to convert predictions to factors to use this function.

Which model has the highest F_1 score?

```
F_meas(data = factor(sex_model), reference = test_set$Survived)
```

```
## [1] 0.857
```

```
F_meas(data = factor(class_model), reference = test_set$Survived)
```

```
## [1] 0.78
```

```
F_meas(data = factor(sex_class_model), reference = test_set$Survived)
```

```
## [1] 0.872
```

- ☐ A. sex only
- ☐ B. class only
- ☒ C. sex and class combined

What is the maximum value of the F_1 score? `0.872`

Titanic Exercises - Part 2

7. Survival by fare - LDA and QDA

Set the seed to 1. Train a model using linear discriminant analysis (LDA) with the **caret** `lda` method using fare as the only predictor.

What is the accuracy on the test set for the LDA model?

```
#set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
train_lda <- train(Survived ~ Fare, method = "lda", data = train_set)
lda_preds <- predict(train_lda, test_set)
mean(lda_preds == test_set$Survived)
```

```
## [1] 0.693
```

Set the seed to 1. Train a model using quadratic discriminant analysis (QDA) with the **caret** `qda` method using fare as the only predictor.

What is the accuracy on the test set for the QDA model?

```
#set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
train_qda <- train(Survived ~ Fare, method = "qda", data = train_set)
qda_preds <- predict(train_qda, test_set)
mean(qda_preds == test_set$Survived)
```

```
## [1] 0.693
```

Note: when training models for Titanic Exercises Part 2, please use the S3 method for class formula rather than the default S3 method of **caret** `train()` (see `?caret::train` for details).

8. Logistic regression models

Set the seed to 1. Train a logistic regression model with the **caret** `glm` method using age as the only predictor.

What is the accuracy of your model (using age as the only predictor) on the test set ?

```
#set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
train_glm_age <- train(Survived ~ Age, method = "glm", data = train_set)
glm_preds_age <- predict(train_glm_age, test_set)
mean(glm_preds_age == test_set$Survived)
```

```
## [1] 0.615
```

Set the seed to 1. Train a logistic regression model with the **caret** `glm` method using four predictors: sex, class, fare, and age.

What is the accuracy of your model (using these four predictors) on the test set?

```
#set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
train_glm <- train(Survived ~ Sex + Pclass + Fare + Age, method = "glm", data = train_set)
glm_preds <- predict(train_glm, test_set)
mean(glm_preds == test_set$Survived)
```

```
## [1] 0.849
```

Set the seed to 1. Train a logistic regression model with the **caret** `glm` method using all predictors. Ignore warnings about rank-deficient fit.

What is the accuracy of your model (using all predictors) on the test set?

```
#set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
train_glm_all <- train(Survived ~ ., method = "glm", data = train_set)
```

```
## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
```

```
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading

## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading
```

```
glm_all_preds <- predict(train_glm_all, test_set)
```

```
## Warning in predict.lm(object, newdata, se.fit, scale = 1, type = if (type == :
## prediction from a rank-deficient fit may be misleading
```

```
mean(glm_all_preds == test_set$Survived)
```

```
## [1] 0.849
```

9a. kNN model

Set the seed to 6. Train a kNN model on the training set using the **caret** `train` function. Try tuning with `k = seq(3, 51, 2)`.

What is the optimal value of the number of neighbors `k`?

```
#set.seed(6)
set.seed(6, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(6, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
train_knn <- train(Survived ~ .,
                   method = "knn",
                   data = train_set,
                   tuneGrid = data.frame(k = seq(3, 51, 2)))
train_knn$bestTune
```

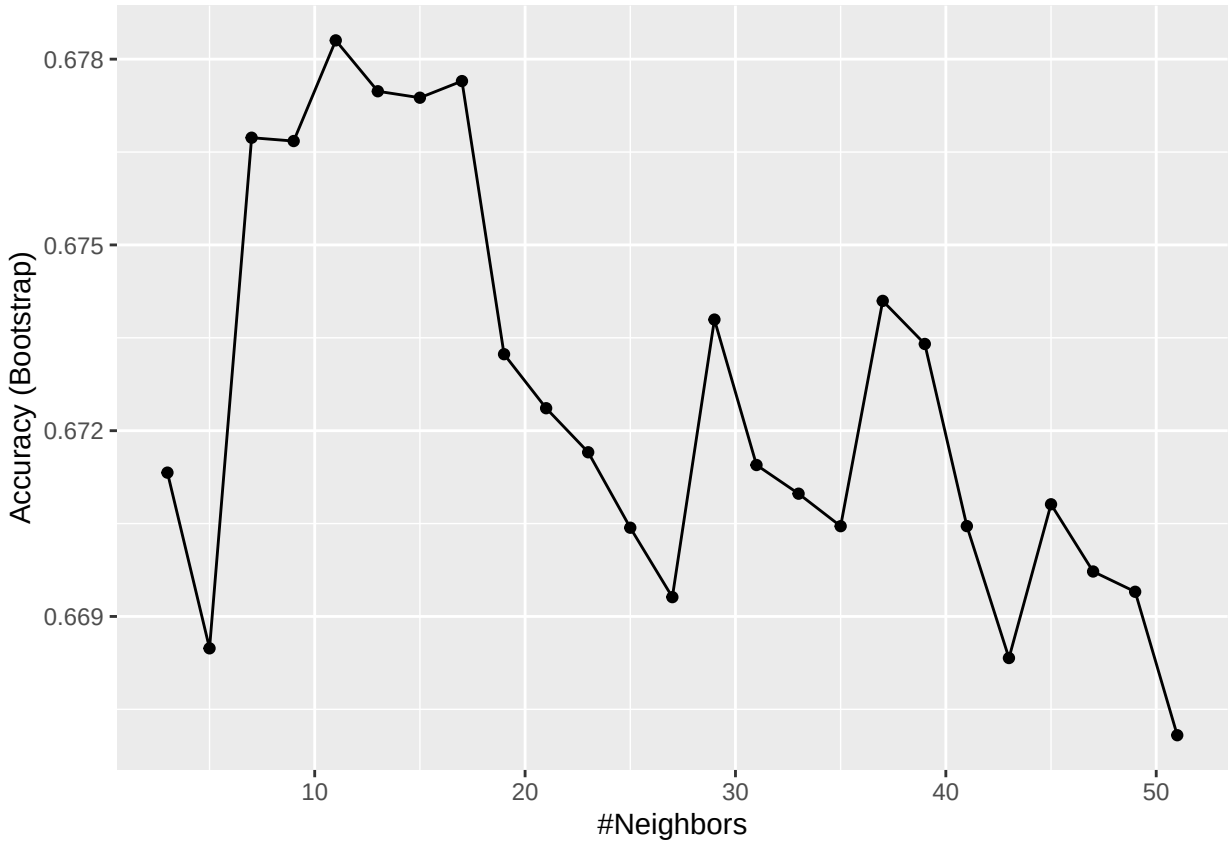
```
##    k
## 5 11
```

9b. kNN model

Plot the kNN model to investigate the relationship between the number of neighbors and accuracy on the training set.

Of these values of k, which yields the highest accuracy?

```
ggplot(train_knn)
```



☐ A. 7

☒ B. 11
☐ C. 17
☐ D. 21

9c. kNN model

What is the accuracy of the kNN model on the test set?

```
knn_preds <- predict(train_knn, test_set)
mean(knn_preds == test_set$Survived)
```

```
## [1] 0.709
```

10. Cross-validation

Set the seed to 8 and train a new kNN model. Instead of the default training control, use 10-fold cross-validation where each partition consists of 10% of the total. Try tuning with `k = seq(3, 51, 2)`.

What is the optimal value of `k` using cross-validation?

```
#set.seed(8)
set.seed(8, sample.kind = "Rounding")    # simulate R 3.5
```

```
## Warning in set.seed(8, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
train_knn_cv <- train(Survived ~ .,
                      method = "knn",
                      data = train_set,
                      tuneGrid = data.frame(k = seq(3, 51, 2)),
                      trControl = trainControl(method = "cv", number = 10, p = 0.9))
train_knn_cv$bestTune
```

```
##   k
## 2 5
```

What is the accuracy on the test set using the cross-validated kNN model?

```
knn_cv_preds <- predict(train_knn_cv, test_set)
mean(knn_cv_preds == test_set$Survived)
```

```
## [1] 0.648
```

11a. Classification tree model

Set the seed to 10. Use **caret** to train a decision tree with the `rpart` method. Tune the complexity parameter with `cp = seq(0, 0.05, 0.002)`.

What is the optimal value of the complexity parameter (`cp`)?

```
#set.seed(10)
set.seed(10, sample.kind = "Rounding")    # simulate R 3.5
```

```
## Warning in set.seed(10, sample.kind = "Rounding"): non-uniform 'Rounding'
## sampler used
```

```
train_rpart <- train(Survived ~ .,
                     method = "rpart",
                     tuneGrid = data.frame(cp = seq(0, 0.05, 0.002)),
                     data = train_set)
train_rpart$bestTune
```

```
##      cp
## 9 0.016
```

What is the accuracy of the decision tree model on the test set?

```
rpart_preds <- predict(train_rpart, test_set)
mean(rpart_preds == test_set$Survived)
```

```
## [1] 0.838
```

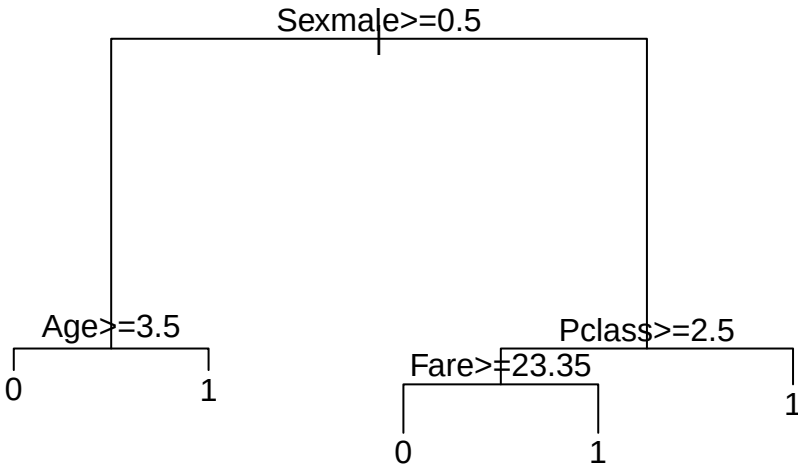
11b. Classification tree model

Inspect the final model and plot the decision tree.

```
train_rpart$finalModel # inspect final model
```

```
## n= 712
##
## node), split, n, loss, yval, (yprob)
##       * denotes terminal node
##
##  1) root 712 273 0 (0.6166 0.3834)
##    2) Sexmale>=0.5 463  91 0 (0.8035 0.1965)
##      4) Age>=3.5 449  80 0 (0.8218 0.1782) *
##      5) Age< 3.5 14   3 1 (0.2143 0.7857) *
##    3) Sexmale< 0.5 249  67 1 (0.2691 0.7309)
##      6) Pclass>=2.5 118  59 0 (0.5000 0.5000)
##       12) Fare>=23.4 24   3 0 (0.8750 0.1250) *
##       13) Fare< 23.4 94  38 1 (0.4043 0.5957) *
##      7) Pclass< 2.5 131   8 1 (0.0611 0.9389) *
```

```
# make plot of decision tree
plot(train_rpart$finalModel, margin = 0.1)
text(train_rpart$finalModel)
```



Which variables are used in the decision tree?

Select ALL that apply.

- ☐ A. Survived
- ☒ B. Sex
- ☒ C. Pclass
- ☒ D. Age
- ☒ E. Fare
- ☐ F. Parch
- ☐ G. Embarked

11c. Classification tree model

Using the decision rules generated by the final model, predict whether the following individuals would survive.

- A 28-year-old male `would NOT survive`
- A female in the second passenger class `would survive`
- A third-class female who paid a fare of $8 `would survive`
- A 5-year-old male with 4 siblings `would NOT survive`
- A third-class female who paid a fare of $25 `would NOT survive`
- A first-class 17-year-old female with 2 siblings `would survive`
- A first-class 17-year-old male with 2 siblings `would NOT survive`

12. Random forest model

Set the seed to 14. Use the **caret** `train()` function with the `rf` method to train a random forest. Test values of `mtry = seq(1:7)`. Set `ntree` to 100.

What `mtry` value maximizes accuracy?

```
#set.seed(14)
set.seed(14, sample.kind = "Rounding")    # simulate R 3.5
```

```
## Warning in set.seed(14, sample.kind = "Rounding"): non-uniform 'Rounding'
## sampler used
```

```
train_rf <- train(Survived ~ .,
                  data = train_set,
                  method = "rf",
                  ntree = 100,
                  tuneGrid = data.frame(mtry = seq(1:7)))
train_rf$bestTune
```

```
##   mtry
## 2    2
```

What is the accuracy of the random forest model on the test set?

```
rf_preds <- predict(train_rf, test_set)
mean(rf_preds == test_set$Survived)
```

```
## [1] 0.844
```

Use `varImp()` on the random forest model object to determine the importance of various predictors to the random forest model.

What is the most important variable?

```
varImp(train_rf)    # first row
```

```
## rf variable importance
##
##             Overall
## Sexmale    100.000
## Fare        65.091
## Age         45.533
## Pclass      32.529
## FamilySize  18.275
## SibSp        7.881
## Parch        7.150
## EmbarkedS    2.839
## EmbarkedQ    0.122
## EmbarkedC    0.000
```

Section 6 - Model Fitting and Recommendation Systems Overview

In the **Model Fitting and Recommendation Systems** section, you will learn how to apply the machine learning algorithms you have learned.

After completing this section, you will be able to:

- Apply the methods we have learned to an example, the **MNIST digits**.
- Build a **movie recommendation system** using machine learning.
- Penalize large estimates that come from small sample sizes using **regularization**.

This section has three parts: **case study: MNIST, recommendation systems**, and **regularization**.

Case Study: MNIST

There is a link to the relevant section of the textbook: Machine learning in practice

Key points

- We will apply what we have learned in the course on the Modified National Institute of Standards and Technology database (MNIST) digits, a popular dataset used in machine learning competitions.

Code

```
mnist <- read_mnist()

names(mnist)
```

```
## [1] "train" "test"
```

```
dim(mnist$train$images)
```

```
## [1] 60000   784
```

```
class(mnist$train$labels)
```

```
## [1] "integer"
```

```
table(mnist$train$labels)
```

```
##
##    0    1    2    3    4    5    6    7    8    9
## 5923 6742 5958 6131 5842 5421 5918 6265 5851 5949
```

```
# sample 10k rows from training set, 1k rows from test set
set.seed(123)
index <- sample(nrow(mnist$train$images), 10000)
x <- mnist$train$images[index,]
y <- factor(mnist$train$labels[index])

index <- sample(nrow(mnist$test$images), 1000)
#note that the line above is the corrected code - code in video at 0:52 is incorrect
x_test <- mnist$test$images[index,]
y_test <- factor(mnist$test$labels[index])
```

Preprocessing MNIST Data

There is a link to the relevant section of the textbook: Preprocessing

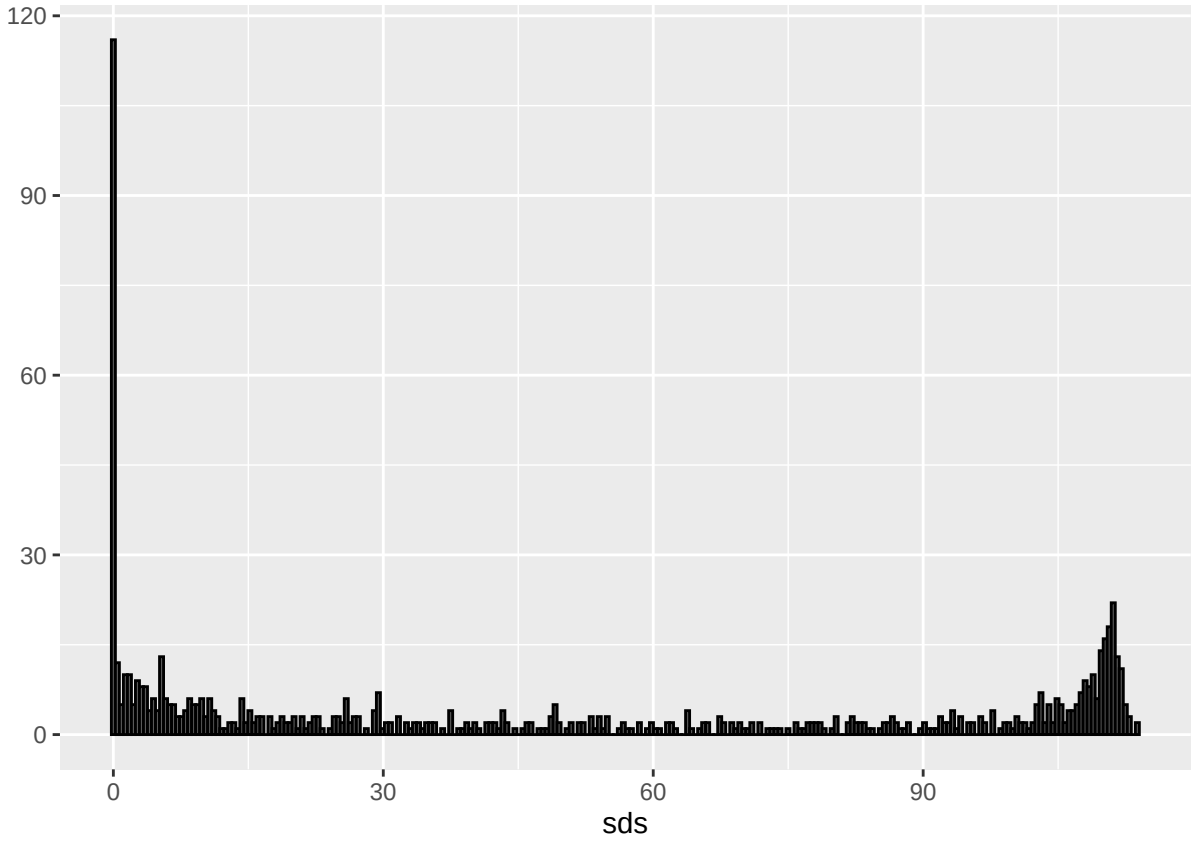
Key points

- Common **preprocessing steps include:

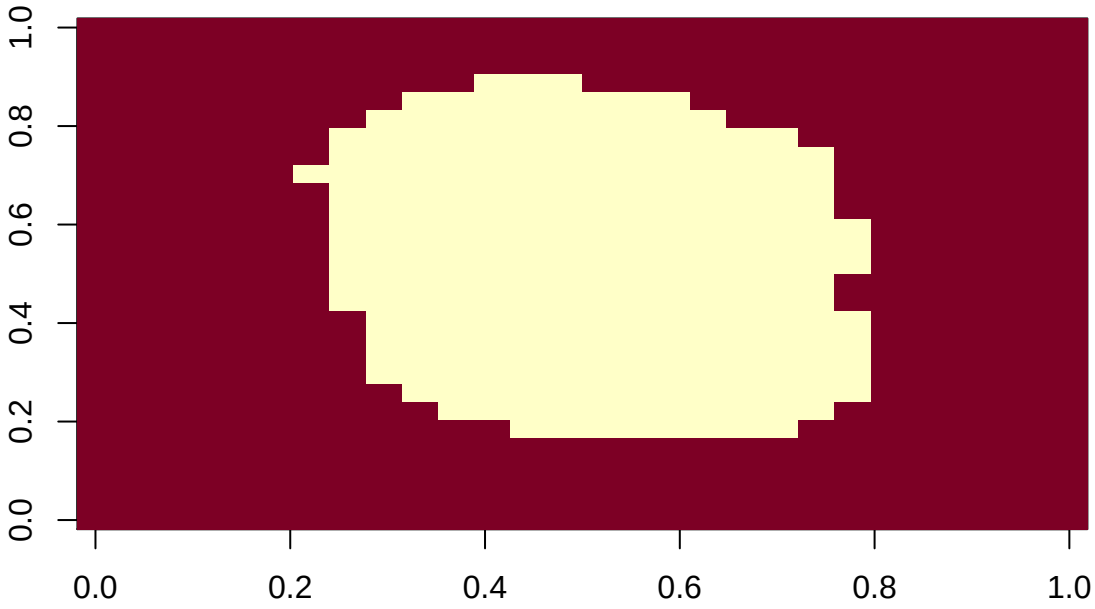
1. standardizing or transforming predictors and
2. removing predictors that are not useful, are highly correlated with others, have very few non-unique values, or have close to zero variation.

Code

```
sds <- colSds(x)
qplot(sds, bins = 256, color = I("black"))
```




```
nzv <- nearZeroVar(x)
image(matrix(1:784 %in% nzv, 28, 28))
```




```
col_index <- setdiff(1:ncol(x), nzv)
length(col_index)
```

```
## [1] 252
```

Model Fitting for MNIST Data

There is a link to the relevant section of the textbook: k-nearest neighbor and random forest

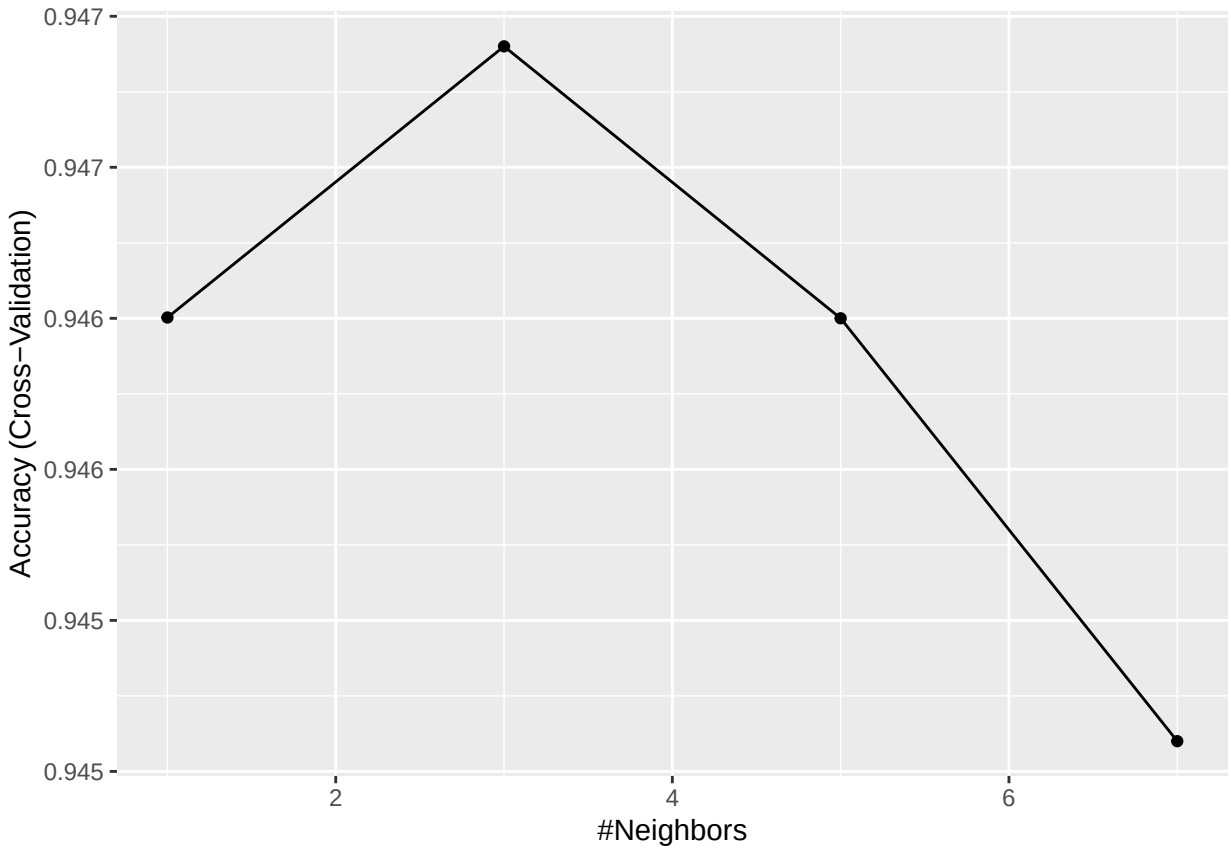
Key points

- The **caret** package requires that we **add column names** to the feature matrices.
- In general, it is a good idea to **test out a small subset of the data** first to get an idea of how long your code will take to run.

Code

```
colnames(x) <- 1:ncol(mnist$train$images)
colnames(x_test) <- colnames(x)

control <- trainControl(method = "cv", number = 10, p = .9)
train_knn <- train(x[,col_index], y,
                                method = "knn",
                                tuneGrid = data.frame(k = c(1,3,5,7)),
                                trControl = control)
ggplot(train_knn)
```




```
n <- 1000
b <- 2
index <- sample(nrow(x), n)
control <- trainControl(method = "cv", number = b, p = .9)
train_knn <- train(x[index ,col_index], y[index],
                   method = "knn",
                   tuneGrid = data.frame(k = c(3,5,7)),
                   trControl = control)
fit_knn <- knn3(x[ ,col_index], y,  k = 3)

y_hat_knn <- predict(fit_knn,
                     x_test[, col_index],
                     type="class")
cm <- confusionMatrix(y_hat_knn, factor(y_test))
cm$overall["Accuracy"]
```

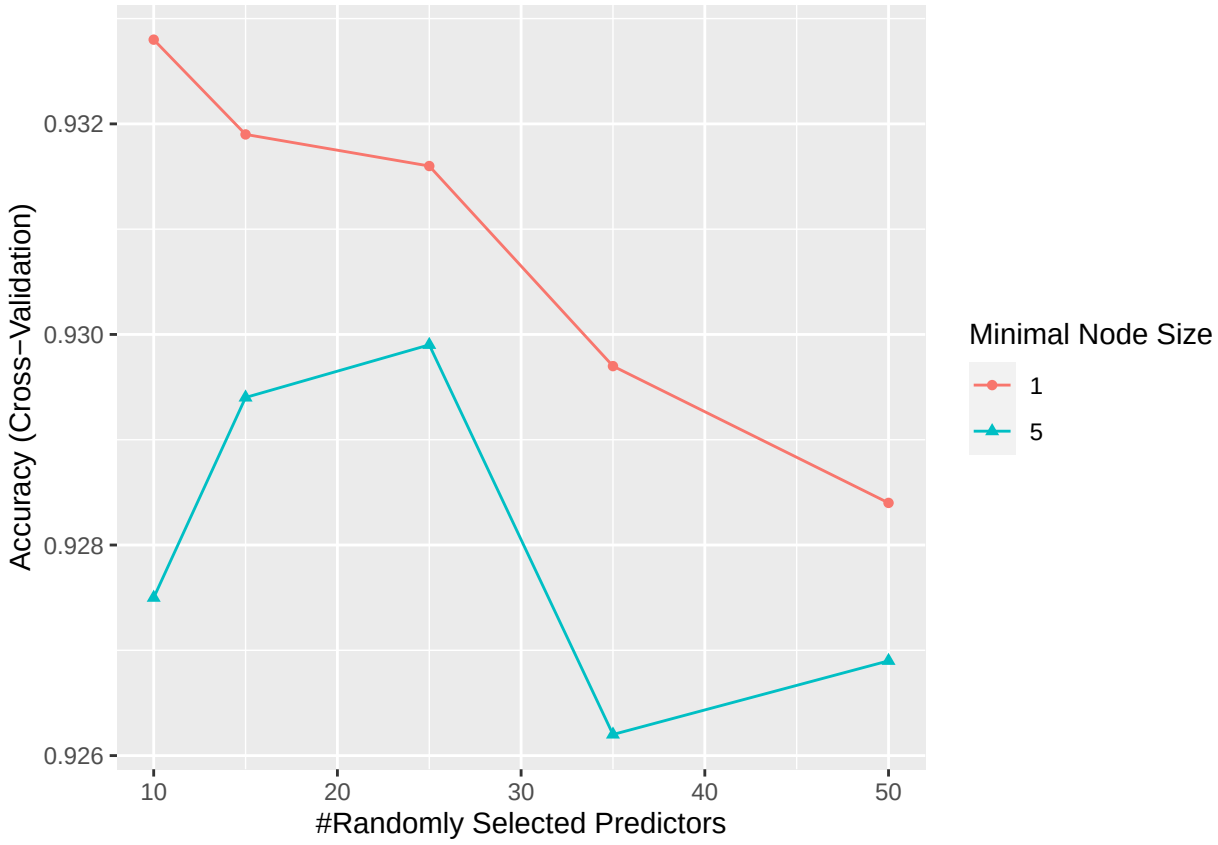
```
## Accuracy
##    0.955
```

```
cm$byClass[,1:2]
```

```
##          Sensitivity Specificity
## Class: 0       1.000       0.998
## Class: 1       1.000       0.992
## Class: 2       0.953       0.999
```

```
## Class: 3       0.917       0.993
## Class: 4       0.936       0.996
## Class: 5       0.971       0.991
## Class: 6       0.990       0.998
## Class: 7       0.945       0.994
## Class: 8       0.846       0.998
## Class: 9       0.971       0.991
```

```
control <- trainControl(method="cv", number = 5, p = 0.8)
grid <- expand.grid(minNode = c(1,5) , predFixed = c(10, 15, 25, 35, 50))
train_rf <-  train(x[, col_index], y,
                   method = "Rborist",
                   nTree = 50,
                   trControl = control,
                   tuneGrid = grid,
                   nSamp = 5000)
ggplot(train_rf)
```




```
train_rf$bestTune
```

```
##   predFixed minNode
## 1        10       1
```

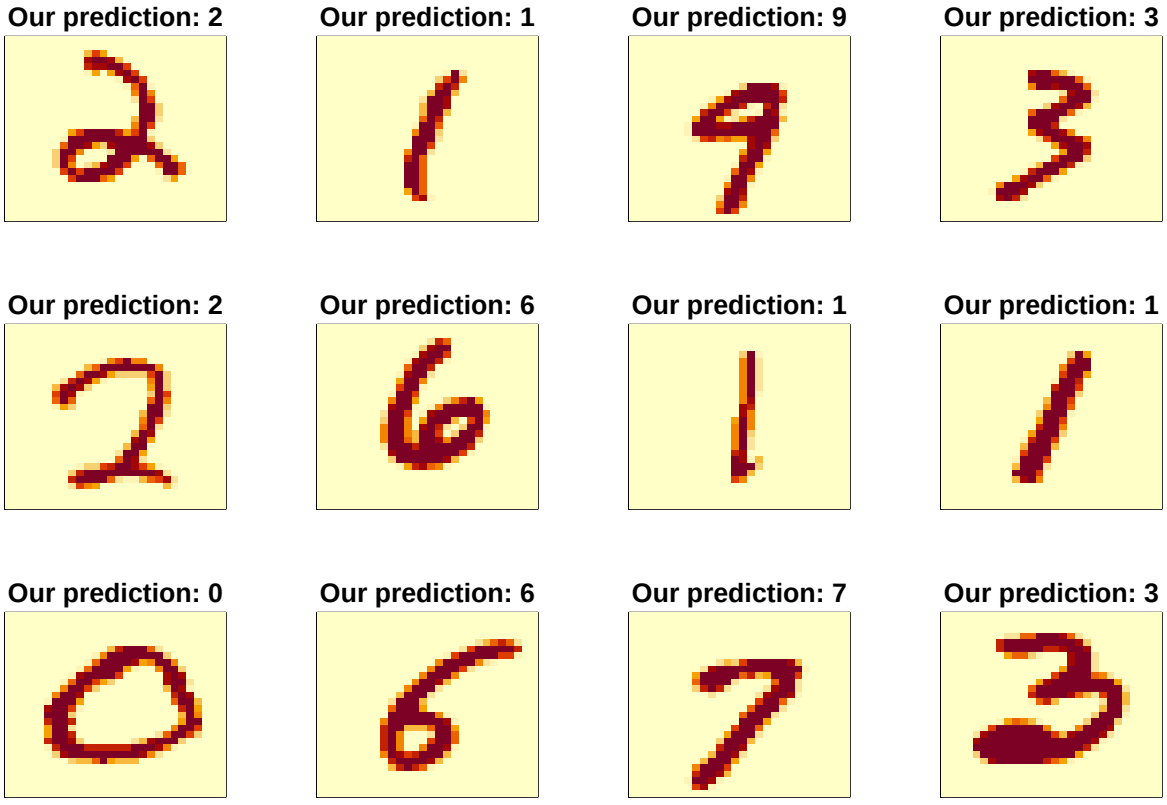
```
fit_rf <- Rborist(x[, col_index], y,
                  nTree = 1000,
```

```
                  minNode = train_rf$bestTune$minNode,
                  predFixed = train_rf$bestTune$predFixed)

y_hat_rf <- factor(levels(y)[predict(fit_rf, x_test[ ,col_index])$yPred])
cm <- confusionMatrix(y_hat_rf, y_test)
cm$overall["Accuracy"]
```

```
## Accuracy
##    0.959
```

```
rafalib::mypar(3,4)
for(i in 1:12){
     image(matrix(x_test[i,], 28, 28)[, 28:1],
           main = paste("Our prediction:", y_hat_rf[i]),
           xaxt="n", yaxt="n")
}
```



Variable Importance

There is a link to the relevant sections of the textbook: Variable importance and Visual assessments

Key points

- The **Rborist** package does not currently support variable importance calculations, but the **randomForest** package does.
- An important part of data science is visualizing results to determine why we are failing.

Code

```
x <- mnist$train$images[index,]
y <- factor(mnist$train$labels[index])
rf <- randomForest(x, y,  ntree = 50)
imp <- importance(rf)
imp
```

```
##     MeanDecreaseGini
## 1             0.0000
## 2             0.0000
## 3             0.0000
## 4             0.0000
## 5             0.0000
## 6             0.0000
## 7             0.0000
## 8             0.0000
## 9             0.0000
## 10            0.0000
## 11            0.0000
## 12            0.0000
## 13            0.0000
## 14            0.0000
## 15            0.0000
## 16            0.0000
## 17            0.0000
## 18            0.0000
## 19            0.0000
## 20            0.0000
## 21            0.0000
## 22            0.0000
## 23            0.0000
## 24            0.0000
## 25            0.0000
## 26            0.0000
## 27            0.0000
## 28            0.0000
## 29            0.0000
## 30            0.0000
## 31            0.0000
## 32            0.0000
## 33            0.0000
## 34            0.0000
## 35            0.0000
## 36            0.0000
## 37            0.0000
## 38            0.0000
## 39            0.0000
## 40            0.0000
## 41            0.0000
## 42            0.0000
## 43            0.0000
## 44            0.0000
## 45            0.0000
```

```
## 46          0.0000
## 47          0.0000
## 48          0.0000
## 49          0.0000
## 50          0.0000
## 51          0.0000
## 52          0.0000
## 53          0.0000
## 54          0.0000
## 55          0.0000
## 56          0.0000
## 57          0.0000
## 58          0.0000
## 59          0.0000
## 60          0.0000
## 61          0.0000
## 62          0.0000
## 63          0.0000
## 64          0.0000
## 65          0.0000
## 66          0.0000
## 67          0.0000
## 68          0.0000
## 69          0.0000
## 70          0.0200
## 71          0.0386
## 72          0.3364
## 73          0.4292
## 74          0.1083
## 75          0.1228
## 76          0.0000
## 77          0.0000
## 78          0.0359
## 79          0.0000
## 80          0.0000
## 81          0.0000
## 82          0.0000
## 83          0.0000
## 84          0.0000
## 85          0.0000
## 86          0.0000
## 87          0.0000
## 88          0.0000
## 89          0.0000
## 90          0.0000
## 91          0.0000
## 92          0.0000
## 93          0.0267
## 94          0.0702
## 95          0.0267
## 96          0.1533
## 97          0.5302
## 98          0.1691
## 99          0.1951
```

```
## 100          4.3825
## 101          3.7575
## 102          4.0716
## 103          1.4450
## 104          0.5788
## 105          0.0756
## 106          0.0300
## 107          0.0916
## 108          0.0000
## 109          0.0000
## 110          0.0000
## 111          0.0000
## 112          0.0000
## 113          0.0000
## 114          0.0000
## 115          0.0000
## 116          0.0000
## 117          0.0000
## 118          0.0000
## 119          0.0368
## 120          0.0958
## 121          0.0368
## 122          0.4054
## 123          0.1888
## 124          1.6623
## 125          1.0255
## 126          0.9706
## 127          0.9350
## 128          1.8896
## 129          2.3448
## 130          0.9726
## 131          0.7841
## 132          0.3058
## 133          0.2913
## 134          0.0611
## 135          0.4770
## 136          0.0000
## 137          0.0000
## 138          0.0000
## 139          0.0000
## 140          0.0000
## 141          0.0000
## 142          0.0000
## 143          0.0000
## 144          0.0000
## 145          0.0450
## 146          0.4217
## 147          0.1030
## 148          0.4381
## 149          0.2826
## 150          0.6646
## 151          1.4041
## 152          2.1603
## 153          3.1023
```

```
## 154          1.7377
## 155          2.9828
## 156          4.4697
## 157          4.6632
## 158          1.9789
## 159          1.1770
## 160          1.2593
## 161          1.1914
## 162          0.4314
## 163          0.9320
## 164          0.5088
## 165          0.0583
## 166          0.0000
## 167          0.0000
## 168          0.0000
## 169          0.0000
## 170          0.0000
## 171          0.0000
## 172          0.0337
## 173          0.0000
## 174          0.0467
## 175          0.0971
## 176          0.2638
## 177          0.8443
## 178          1.3889
## 179          2.3951
## 180          1.8932
## 181          3.7141
## 182          3.1491
## 183          2.5722
## 184          3.5550
## 185          3.7543
## 186          4.1136
## 187          1.2190
## 188          2.7119
## 189          1.3368
## 190          0.7848
## 191          0.5944
## 192          0.6998
## 193          0.0367
## 194          0.0000
## 195          0.0560
## 196          0.0000
## 197          0.0000
## 198          0.0000
## 199          0.0000
## 200          0.0000
## 201          0.0653
## 202          0.1618
## 203          0.2514
## 204          0.1467
## 205          0.7132
## 206          1.0696
## 207          1.8813
```

```
## 208          1.5488
## 209          1.6265
## 210          2.3821
## 211          4.1416
## 212          6.0898
## 213          2.8040
## 214          1.9544
## 215          2.9735
## 216          1.1595
## 217          1.2301
## 218          0.7179
## 219          0.8997
## 220          1.4020
## 221          0.8376
## 222          0.0376
## 223          0.0000
## 224          0.0000
## 225          0.0000
## 226          0.0000
## 227          0.0000
## 228          0.0000
## 229          0.1500
## 230          0.1951
## 231          0.6163
## 232          1.3442
## 233          0.8332
## 234          1.1122
## 235          3.0582
## 236          4.9129
## 237          3.2573
## 238          2.7814
## 239          2.9401
## 240          5.4603
## 241          3.9843
## 242          3.9568
## 243          1.1594
## 244          1.9290
## 245          1.5714
## 246          1.1573
## 247          0.9894
## 248          0.7398
## 249          0.2346
## 250          0.5157
## 251          0.0000
## 252          0.0000
## 253          0.0000
## 254          0.0000
## 255          0.0000
## 256          0.0000
## 257          0.0000
## 258          0.0722
## 259          0.6696
## 260          0.3971
## 261          1.1764
```

```
## 262          2.2870
## 263          2.6467
## 264          3.0094
## 265          5.8341
## 266          2.1984
## 267          3.1962
## 268          3.5770
## 269          2.7636
## 270          5.0814
## 271          4.8756
## 272          2.4102
## 273          2.2899
## 274          1.2372
## 275          0.3960
## 276          0.7806
## 277          0.2840
## 278          0.0000
## 279          0.0000
## 280          0.0000
## 281          0.0000
## 282          0.0000
## 283          0.0000
## 284          0.0000
## 285          0.1978
## 286          0.0691
## 287          0.8360
## 288          0.8459
## 289          0.9408
## 290          2.0882
## 291          4.3131
## 292          3.5580
## 293          3.2671
## 294          1.9374
## 295          1.9242
## 296          2.6329
## 297          3.0550
## 298          2.8851
## 299          3.3400
## 300          2.2500
## 301          2.8778
## 302          1.3096
## 303          0.5058
## 304          0.1055
## 305          0.1202
## 306          0.0000
## 307          0.0000
## 308          0.0000
## 309          0.0000
## 310          0.0000
## 311          0.0000
## 312          0.0000
## 313          0.0267
## 314          0.1652
## 315          1.0535
```

```
## 316          0.9770
## 317          1.1757
## 318          3.9662
## 319          7.4847
## 320          5.0866
## 321          3.2152
## 322          2.9141
## 323          3.5169
## 324          4.8595
## 325          3.6001
## 326          3.6972
## 327          2.4491
## 328          3.2116
## 329          1.3368
## 330          2.0959
## 331          0.6248
## 332          0.1734
## 333          0.1204
## 334          0.0000
## 335          0.0000
## 336          0.0000
## 337          0.0000
## 338          0.0000
## 339          0.0000
## 340          0.0669
## 341          0.0589
## 342          0.0710
## 343          0.7515
## 344          1.5224
## 345          2.9044
## 346          3.4698
## 347          2.9629
## 348          6.6917
## 349          2.8665
## 350          2.5272
## 351          5.2107
## 352          5.2579
## 353          2.5862
## 354          4.0516
## 355          3.9797
## 356          1.2102
## 357          1.9677
## 358          2.8926
## 359          2.4807
## 360          0.2659
## 361          0.0710
## 362          0.0000
## 363          0.0000
## 364          0.0000
## 365          0.0000
## 366          0.0000
## 367          0.0000
## 368          0.0000
## 369          0.0267
```

```
## 370          0.1961
## 371          0.6116
## 372          0.9917
## 373          2.6019
## 374          4.5573
## 375          5.0599
## 376          6.0905
## 377          5.3284
## 378          5.1077
## 379          9.6768
## 380          3.0461
## 381          4.7315
## 382          4.3859
## 383          4.5496
## 384          1.2225
## 385          2.1867
## 386          1.7976
## 387          1.3636
## 388          0.2294
## 389          0.0000
## 390          0.0000
## 391          0.0000
## 392          0.0000
## 393          0.0000
## 394          0.0000
## 395          0.0000
## 396          0.0000
## 397          0.2786
## 398          0.3010
## 399          1.2454
## 400          3.1789
## 401          4.4449
## 402          5.5182
## 403          4.3270
## 404          4.0243
## 405          4.0694
## 406          5.5033
## 407          6.6132
## 408          3.8076
## 409          5.1868
## 410          5.2291
## 411          4.3761
## 412          1.2487
## 413          1.6620
## 414          1.7047
## 415          3.3018
## 416          0.3135
## 417          0.0667
## 418          0.0000
## 419          0.0000
## 420          0.0000
## 421          0.0000
## 422          0.0000
## 423          0.0000
```

```
## 424          0.0200
## 425          0.1010
## 426          0.3706
## 427          0.8750
## 428          5.2063
## 429          3.6503
## 430          5.5588
## 431          6.5687
## 432          6.3710
## 433          3.7244
## 434          6.4584
## 435          3.8925
## 436          3.1450
## 437          4.6127
## 438          5.8932
## 439          3.6514
## 440          1.8678
## 441          0.7452
## 442          2.3169
## 443          1.7684
## 444          0.3237
## 445          0.0000
## 446          0.0000
## 447          0.0000
## 448          0.0000
## 449          0.0000
## 450          0.0000
## 451          0.0000
## 452          0.0384
## 453          0.0814
## 454          0.5199
## 455          0.5373
## 456          5.9110
## 457          2.8719
## 458          4.4087
## 459          2.8772
## 460          2.8043
## 461          4.5564
## 462          9.2761
## 463          3.5203
## 464          3.9495
## 465          3.0245
## 466          3.5809
## 467          2.6407
## 468          2.9175
## 469          1.9749
## 470          2.2785
## 471          0.5547
## 472          0.2392
## 473          0.1860
## 474          0.0200
## 475          0.0000
## 476          0.0000
## 477          0.0000
```

```
## 478          0.0000
## 479          0.0000
## 480          0.0383
## 481          0.0387
## 482          0.4292
## 483          1.6728
## 484          2.5022
## 485          0.4138
## 486          2.9169
## 487          3.0419
## 488          4.1365
## 489          7.1352
## 490          4.9019
## 491          2.8327
## 492          2.5211
## 493          1.7125
## 494          2.7378
## 495          2.8248
## 496          2.0614
## 497          2.3113
## 498          0.9727
## 499          1.6279
## 500          0.5343
## 501          0.3333
## 502          0.0000
## 503          0.0000
## 504          0.0000
## 505          0.0000
## 506          0.0000
## 507          0.0000
## 508          0.0676
## 509          0.2275
## 510          0.2708
## 511          2.4200
## 512          2.5823
## 513          3.0054
## 514          3.4622
## 515          4.5320
## 516          6.1263
## 517          2.3824
## 518          3.3455
## 519          1.9886
## 520          2.9348
## 521          1.1133
## 522          1.4845
## 523          3.0486
## 524          1.7594
## 525          2.0075
## 526          1.0956
## 527          0.7642
## 528          0.5527
## 529          0.0702
## 530          0.0000
## 531          0.0000
```

```
## 532          0.0000
## 533          0.0000
## 534          0.0000
## 535          0.0000
## 536          0.0000
## 537          0.1836
## 538          0.8058
## 539          3.7220
## 540          5.5971
## 541          1.8936
## 542          2.1503
## 543          5.3189
## 544          3.1706
## 545          2.5217
## 546          2.2154
## 547          1.6559
## 548          2.3495
## 549          0.9677
## 550          2.5048
## 551          2.7026
## 552          1.4848
## 553          1.0656
## 554          0.5196
## 555          0.4745
## 556          0.5605
## 557          0.1946
## 558          0.0000
## 559          0.0000
## 560          0.0000
## 561          0.0000
## 562          0.0000
## 563          0.0000
## 564          0.0000
## 565          0.0360
## 566          0.7484
## 567          2.0237
## 568          4.3082
## 569          3.1404
## 570          4.0156
## 571          3.2594
## 572          3.2163
## 573          3.2371
## 574          2.6207
## 575          1.3211
## 576          1.4396
## 577          1.4215
## 578          2.6131
## 579          2.1551
## 580          1.6976
## 581          0.4295
## 582          0.7656
## 583          0.1415
## 584          0.1012
## 585          0.0653
```

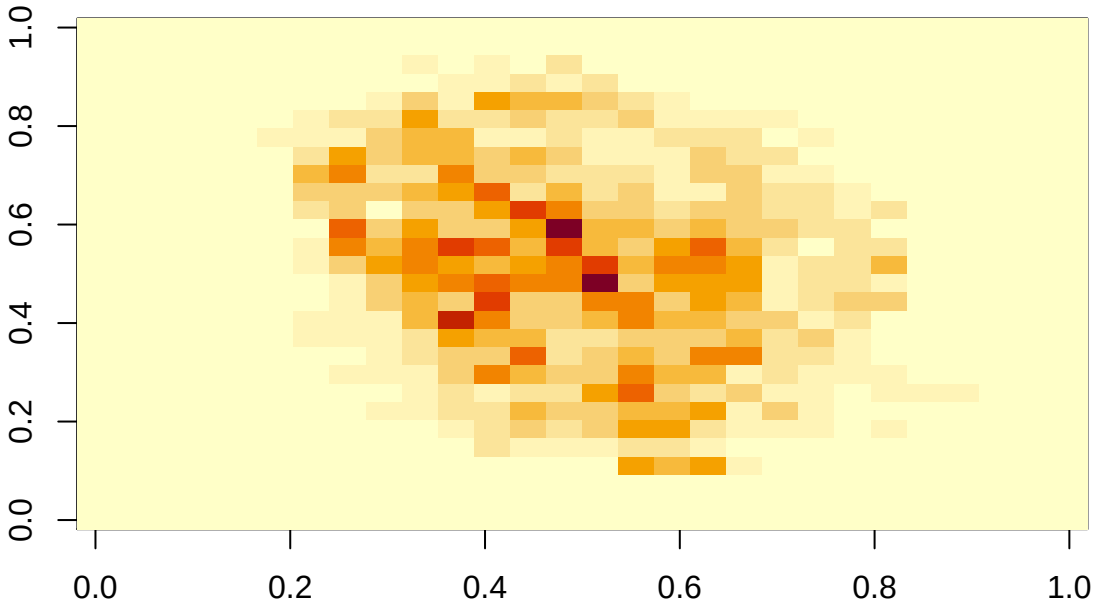
```
## 586          0.1405
## 587          0.0000
## 588          0.0000
## 589          0.0000
## 590          0.0000
## 591          0.0000
## 592          0.0000
## 593          0.3101
## 594          0.8712
## 595          1.2101
## 596          1.5286
## 597          3.0302
## 598          3.8308
## 599          3.8574
## 600          1.4988
## 601          1.4851
## 602          2.2346
## 603          1.6009
## 604          1.5888
## 605          1.7945
## 606          1.9097
## 607          1.8448
## 608          0.7688
## 609          1.4031
## 610          0.4461
## 611          0.1067
## 612          0.2739
## 613          0.0000
## 614          0.0000
## 615          0.0000
## 616          0.0000
## 617          0.0000
## 618          0.0000
## 619          0.0000
## 620          0.0390
## 621          0.1751
## 622          0.1036
## 623          1.4516
## 624          2.0503
## 625          1.8557
## 626          4.5113
## 627          2.0373
## 628          1.6867
## 629          2.8683
## 630          2.0734
## 631          1.8517
## 632          2.4817
## 633          1.4786
## 634          1.3862
## 635          1.1019
## 636          1.0241
## 637          0.4047
## 638          0.3250
## 639          0.0655
```

```
## 640          0.0000
## 641          0.0400
## 642          0.0000
## 643          0.0000
## 644          0.0000
## 645          0.0000
## 646          0.0000
## 647          0.0000
## 648          0.0000
## 649          0.0000
## 650          0.0360
## 651          0.5241
## 652          0.7703
## 653          1.3069
## 654          2.9215
## 655          1.3210
## 656          4.7766
## 657          3.5148
## 658          3.5579
## 659          2.7827
## 660          2.0031
## 661          1.1806
## 662          0.6780
## 663          0.4173
## 664          0.5286
## 665          0.0000
## 666          0.0840
## 667          0.1122
## 668          0.1322
## 669          0.0644
## 670          0.0000
## 671          0.0000
## 672          0.0000
## 673          0.0000
## 674          0.0000
## 675          0.0000
## 676          0.0000
## 677          0.0923
## 678          0.1728
## 679          0.2596
## 680          0.2985
## 681          0.2241
## 682          0.5979
## 683          1.1140
## 684          1.2162
## 685          1.9263
## 686          0.9836
## 687          1.6218
## 688          0.6831
## 689          0.4048
## 690          0.4089
## 691          0.4024
## 692          0.0845
## 693          0.1489
```

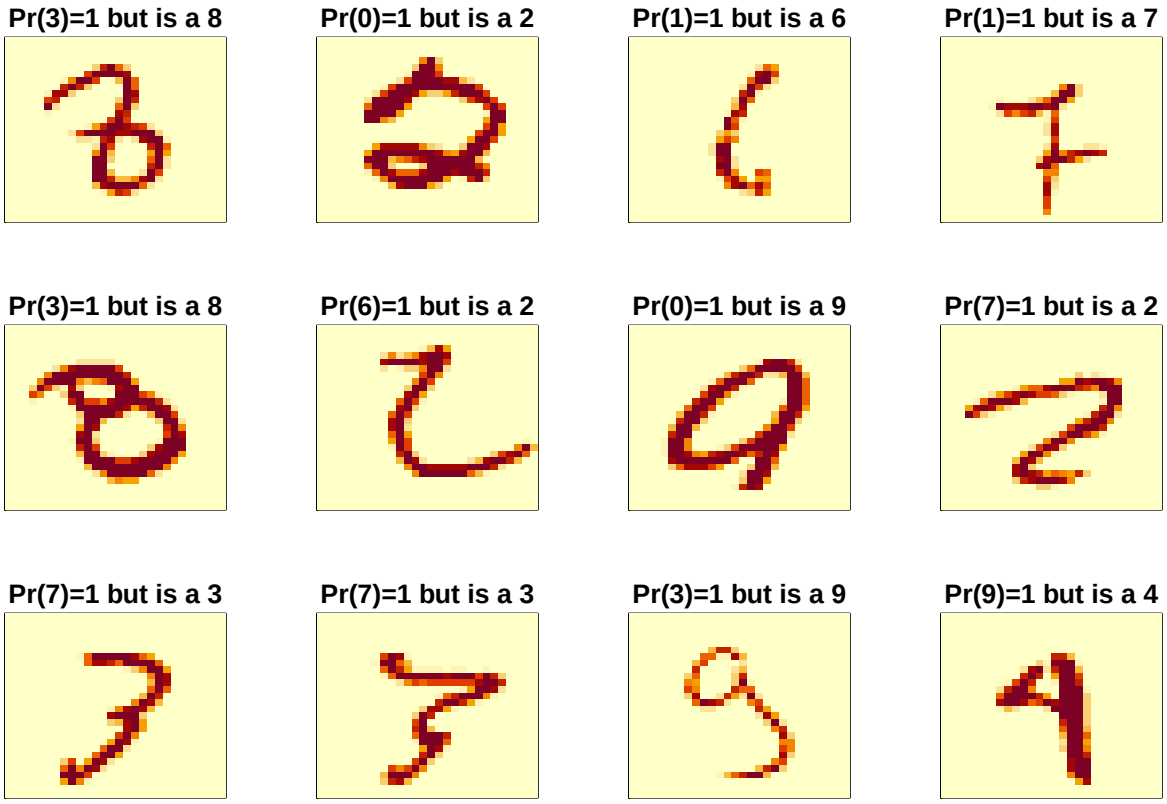
```
## 694          0.0533
## 695          0.0000
## 696          0.0394
## 697          0.0000
## 698          0.0000
## 699          0.0000
## 700          0.0000
## 701          0.0000
## 702          0.0000
## 703          0.0000
## 704          0.0000
## 705          0.0000
## 706          0.0378
## 707          0.0745
## 708          0.0460
## 709          0.0400
## 710          0.8688
## 711          0.5995
## 712          1.3124
## 713          0.3276
## 714          2.1420
## 715          0.5888
## 716          0.1989
## 717          0.6024
## 718          0.1311
## 719          0.1512
## 720          0.0356
## 721          0.0000
## 722          0.0000
## 723          0.1434
## 724          0.0000
## 725          0.0000
## 726          0.0000
## 727          0.0000
## 728          0.0000
## 729          0.0000
## 730          0.0000
## 731          0.0000
## 732          0.0000
## 733          0.0000
## 734          0.0000
## 735          0.0000
## 736          0.0367
## 737          0.0000
## 738          0.2851
## 739          0.5083
## 740          0.2420
## 741          0.0676
## 742          0.0320
## 743          0.0709
## 744          0.2129
## 745          0.0382
## 746          0.0350
## 747          0.0326
```

```
## 748           0.0000
## 749           0.0000
## 750           0.0393
## 751           0.0000
## 752           0.0000
## 753           0.0000
## 754           0.0000
## 755           0.0000
## 756           0.0000
## 757           0.0000
## 758           0.0000
## 759           0.0000
## 760           0.0000
## 761           0.0000
## 762           0.0000
## 763           0.0000
## 764           0.0000
## 765           0.0000
## 766           0.0000
## 767           0.0000
## 768           0.0000
## 769           0.0000
## 770           0.0000
## 771           0.0371
## 772           0.0000
## 773           0.0000
## 774           0.0000
## 775           0.0000
## 776           0.0000
## 777           0.0000
## 778           0.0000
## 779           0.0000
## 780           0.0000
## 781           0.0000
## 782           0.0000
## 783           0.0000
## 784           0.0000
```

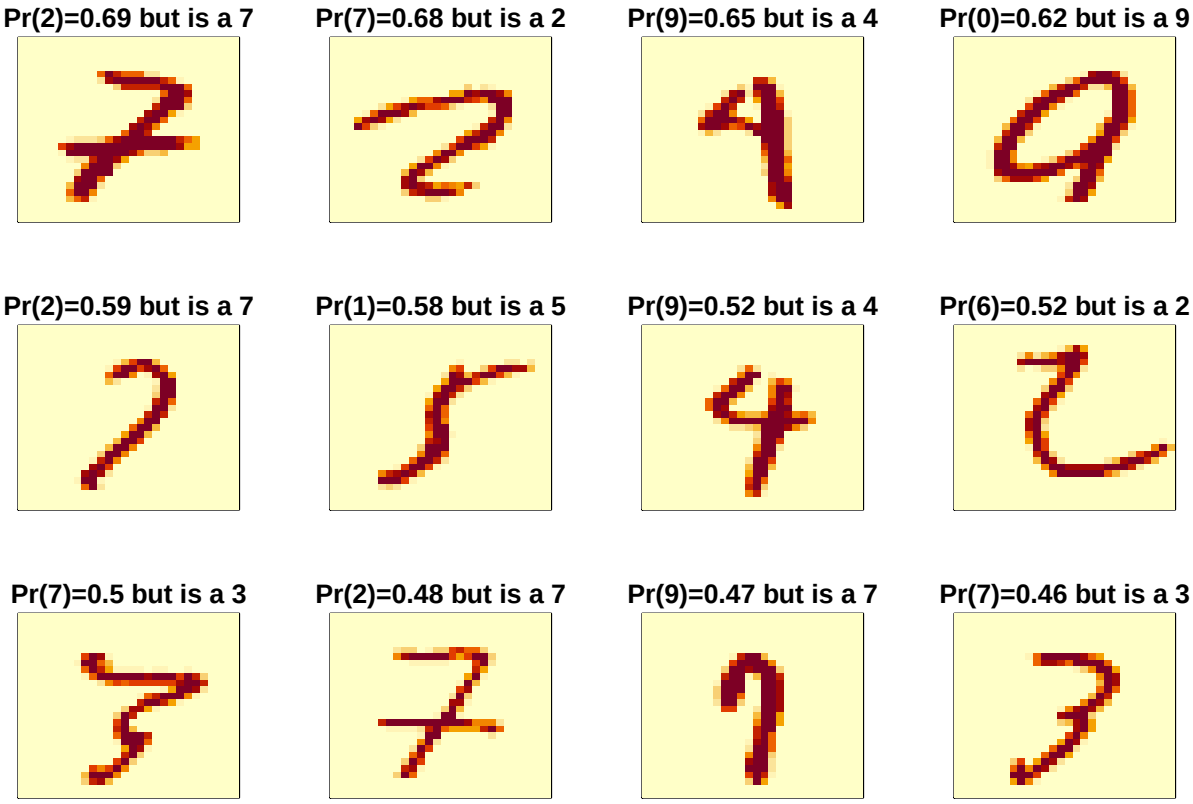
```
image(matrix(imp, 28, 28))
```




```
p_max <- predict(fit_knn, x_test[,col_index])
p_max <- apply(p_max, 1, max)
ind  <- which(y_hat_knn != y_test)
ind <- ind[order(p_max[ind], decreasing = TRUE)]
rafalib::mypar(3,4)
for(i in ind[1:12]){
    image(matrix(x_test[i,], 28, 28)[, 28:1],
                main = paste0("Pr(",y_hat_knn[i],")=",round(p_max[i], 2),
                                                                    " but is a ",y_test[i]),
                xaxt="n", yaxt="n")
}
```




```
p_max <- predict(fit_rf, x_test[,col_index])$census
p_max <- p_max / rowSums(p_max)
p_max <- apply(p_max, 1, max)
ind  <- which(y_hat_rf != y_test)
ind <- ind[order(p_max[ind], decreasing = TRUE)]
rafalib::mypar(3,4)
for(i in ind[1:12]){
    image(matrix(x_test[i,], 28, 28)[, 28:1],
                main = paste0("Pr(",y_hat_rf[i],")=",round(p_max[i], 2),
                              " but is a ",y_test[i]),
                xaxt="n", yaxt="n")
}
```



Ensembles

There is a link to the relevant sections of the textbook: Ensembles

Key points

- **Ensembles** combine multiple machine learning algorithms into one model to improve predictions.

Code

```
p_rf <- predict(fit_rf, x_test[,col_index])$census
p_rf <- p_rf / rowSums(p_rf)
p_knn <- predict(fit_knn, x_test[,col_index])
p <- (p_rf + p_knn)/2
y_pred <- factor(apply(p, 1, which.max)-1)
confusionMatrix(y_pred, y_test)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1   2   3   4   5   6   7   8   9
##          0 102   0   1   0   0   0   0   0   0   1
##          1   0 121   1   0   1   1   1   2   0   0
##          2   0   0 102   1   0   0   0   3   0   0
##          3   0   0   0  78   0   1   0   0   3   2
##          4   0   0   0   0 102   0   0   1   1   0
##          5   0   0   0   2   0  68   0   0   5   0
```

```
##          6   0   0   1   0   1   0 101   0   0   0
##          7   0   0   1   2   0   0   0 102   0   0
##          8   0   0   0   1   0   0   0   0  81   0
##          9   0   0   0   0   5   0   0   2   1 102
##
## Overall Statistics
##
##                Accuracy : 0.959
##                  95% CI : (0.945, 0.97)
##     No Information Rate : 0.121
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.954
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 0 Class: 1 Class: 2 Class: 3 Class: 4 Class: 5
## Sensitivity             1.000    1.000    0.962    0.929    0.936    0.971
## Specificity             0.998    0.993    0.996    0.993    0.998    0.992
## Pos Pred Value          0.981    0.953    0.962    0.929    0.981    0.907
## Neg Pred Value          1.000    1.000    0.996    0.993    0.992    0.998
## Prevalence              0.102    0.121    0.106    0.084    0.109    0.070
## Detection Rate          0.102    0.121    0.102    0.078    0.102    0.068
## Detection Prevalence    0.104    0.127    0.106    0.084    0.104    0.075
## Balanced Accuracy       0.999    0.997    0.979    0.961    0.967    0.982
##                      Class: 6 Class: 7 Class: 8 Class: 9
## Sensitivity             0.990    0.927    0.890    0.971
## Specificity             0.998    0.997    0.999    0.991
## Pos Pred Value          0.981    0.971    0.988    0.927
## Neg Pred Value          0.999    0.991    0.989    0.997
## Prevalence              0.102    0.110    0.091    0.105
## Detection Rate          0.101    0.102    0.081    0.102
## Detection Prevalence    0.103    0.105    0.082    0.110
## Balanced Accuracy       0.994    0.962    0.945    0.981
```

Comprehension Check - Ensembles

1. Use the training set to build a model with several of the models available from the caret package. We will test out 10 of the most common machine learning models in this exercise:

```
models <- c("glm", "lda", "naive_bayes", "svmLinear", "knn", "gamLoess", "multinom", "qda", "rf", "adabo
```

Apply all of these models using `train()` with all the default parameters. You may need to install some packages. Keep in mind that you will probably get some warnings. Also, it will probably take a while to train all of the models - be patient!

Run the following code to train the various models:

```
# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind = "Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
data("mnist_27")

fits <- lapply(models, function(model){
    print(model)
    train(y ~ ., method = model, data = mnist_27$train)
})
```

```
## [1] "glm"
## [1] "lda"
## [1] "naive_bayes"
## [1] "svmLinear"
## [1] "knn"
## [1] "gamLoess"

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.46667

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.41586

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.4375

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.41586

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.089286

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.10703

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.094737

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.10703
```

```
## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.089286

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.092518

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.57895

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.54068

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.46667

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.43969

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.46667

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.43969

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.089286

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.092518

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.57895
```

```
## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.54068

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.46667

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.43969

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.089286

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.092316

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.089286

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.092316

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.53846

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.53555

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.57895

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.53555

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending
```

```
## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.46667

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.43969

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.089286

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.10703

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.094737

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.10703

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.57895

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.54071

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.46667

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.43969

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.089286

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.092316
```

```
## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.46667

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.40628

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.41379

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.40628

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.4375

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.40628

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.089286

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.092518

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.57895

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.54068

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.089286
```

```
## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.10703

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.094737

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.10703

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.46667

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.43969

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.46667

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.402

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.40323

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.402

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.41379

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.402

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending
```

```
## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.40426

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.402

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.4375

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.402

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.46667

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.41586

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.4375

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.41586

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.46667

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.43969

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.57895

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.54071
```

```
## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.46667

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.41586

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.4375

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.41586

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.089286

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.092316

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.089286

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.092518

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.57895

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.54068

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.089286
```

```
## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.10877

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.094737

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.10877

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.089286

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## lowerlimit 0.092316

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.46667

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.43969

## Warning in gam.lo(data[["lo(x_1, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.53846

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.50797

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.51111

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.50797

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending
```

```
## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.57895

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.50797

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## eval 0.53333

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## upperlimit 0.50797

## Warning in gam.lo(data[["lo(x_2, span = 0.5, degree = 1)"]], z, w, span = 0.5, :
## extrapolation not allowed with blending

## [1] "multinom"
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 384.794809
## final  value 384.794775
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 421.251454
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 384.848555
## final  value 384.848522
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 358.466023
## final  value 358.466014
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 400.257332
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 358.528966
## final  value 358.528958
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 345.361326
## final  value 345.361319
## converged
```

```
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 389.162400
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 345.427631
## final  value 345.427624
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 370.819967
## iter  10 value 370.819967
## iter  10 value 370.819967
## final  value 370.819967
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 411.520894
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 370.881269
## iter  10 value 370.881269
## iter  10 value 370.881269
## final  value 370.881269
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 338.339240
## final  value 337.642174
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 389.552735
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 337.725860
## final  value 337.725851
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 362.651997
## iter  10 value 362.651996
## iter  10 value 362.651996
## final  value 362.651996
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 404.947235
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
```

```
## iter  10 value 362.716896
## iter  10 value 362.716895
## iter  10 value 362.716894
## final  value 362.716894
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 353.360649
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 396.615883
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 353.427369
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 331.505876
## final  value 331.505837
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 382.233327
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 331.587049
## final  value 331.587010
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 364.158073
## iter  10 value 364.158073
## iter  10 value 364.158073
## final  value 364.158073
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 400.438283
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 364.210111
## iter  10 value 364.210111
## iter  10 value 364.210111
## final  value 364.210111
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 343.760429
## final  value 343.760410
## converged
```

```
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 387.083157
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 343.826126
## final  value 343.826108
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 377.277862
## iter  10 value 377.277862
## iter  10 value 377.277861
## final  value 377.277861
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 413.479657
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 377.330740
## iter  10 value 377.330739
## iter  10 value 377.330738
## final  value 377.330738
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 363.527477
## final  value 363.527449
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 405.904614
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 363.591426
## final  value 363.591399
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 346.706756
## iter  10 value 346.706754
## iter  10 value 346.706754
## final  value 346.706754
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 393.064300
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
```

```
## iter  10 value 346.778579
## iter  10 value 346.778577
## iter  10 value 346.778577
## final  value 346.778577
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 350.308158
## final  value 350.308124
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 394.686750
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 350.376208
## final  value 350.376174
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 365.423988
## final  value 365.423967
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 407.046095
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 365.486830
## final  value 365.486809
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 375.942875
## final  value 375.942868
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 412.738783
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 375.996860
## final  value 375.996853
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 369.004020
## final  value 369.003531
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
```

```
## final  value 407.374841
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 369.060934
## final  value 369.060455
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 360.551961
## iter  10 value 360.551959
## iter  10 value 360.551959
## final  value 360.551959
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 400.866217
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 360.611945
## iter  10 value 360.611943
## iter  10 value 360.611943
## final  value 360.611943
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 370.467778
## final  value 370.414135
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 406.680836
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 370.519928
## final  value 370.466715
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 355.236387
## final  value 355.236347
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 401.370189
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 355.308279
## final  value 355.308240
## converged
## # weights:  4 (3 variable)
```

```
## initial  value 554.517744
## iter  10 value 364.714111
## final  value 364.714051
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 407.312950
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 364.779508
## final  value 364.779448
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 347.812292
## final  value 347.812150
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 389.764148
## iter  10 value 389.764145
## iter  10 value 389.764145
## final  value 389.764145
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 347.875247
## final  value 347.875105
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 319.870357
## final  value 319.870338
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 372.994080
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 319.955663
## final  value 319.955644
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 312.576095
## final  value 312.576064
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 367.284329
## iter  10 value 367.284329
## iter  10 value 367.284329
```

```
## final  value 367.284329
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 312.666550
## final  value 312.666520
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 363.313712
## iter  10 value 363.313712
## iter  10 value 363.313712
## final  value 363.313712
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## final  value 403.175943
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 363.373575
## iter  10 value 363.373575
## iter  10 value 363.373575
## final  value 363.373575
## converged
## # weights:  4 (3 variable)
## initial  value 554.517744
## iter  10 value 358.900453
## iter  10 value 358.900452
## iter  10 value 358.900452
## final  value 358.900452
## converged
## [1] "qda"
## [1] "rf"
## note: only 1 unique complexity parameters in default grid. Truncating the grid to 1 .
##
## [1] "adaboost"
```

```
names(fits) <- models
```

Did you train all of the models?

- ☒ A. Yes
- ☐ B. No

2. Now that you have all the trained models in a list, use `sapply()` or `map()` to create a matrix of predictions for the test set. You should end up with a matrix with `length(mnist_27$test$y)` rows and `length(models)` columns.

What are the dimensions of the matrix of predictions?

```
pred <- sapply(fits, function(object)
    predict(object, newdata = mnist_27$test))
dim(pred)
```

```
## [1] 200  10
```

3. Now compute accuracy for each model on the test set.

Report the mean accuracy across all models.

```
acc <- colMeans(pred == mnist_27$test$y)
acc
```

```
##         glm         lda naive_bayes   svmLinear         knn    gamLoess
##       0.750       0.750       0.795       0.755       0.840       0.845
##    multinom         qda          rf    adaboost
##       0.750       0.820       0.780       0.805
```

```
mean(acc)
```

```
## [1] 0.789
```

4. Next, build an ensemble prediction by majority vote and compute the accuracy of the ensemble. Vote 7 if more than 50% of the models are predicting a 7, and 2 otherwise.

What is the accuracy of the ensemble?

```
votes <- rowMeans(pred == "7")
y_hat <- ifelse(votes > 0.5, "7", "2")
mean(y_hat == mnist_27$test$y)
```

```
## [1] 0.815
```

5. In Q3, we computed the accuracy of each method on the test set and noticed that the individual accuracies varied.

How many of the individual methods do better than the ensemble?

Which individual methods perform better than the ensemble?

```
ind <- acc > mean(y_hat == mnist_27$test$y)
sum(ind)
```

```
## [1] 3
```

```
models[ind]
```

```
## [1] "knn"      "gamLoess" "qda"
```

☐ A. glm
☐ B. lda
☐ C. naive_bayes
☐ D. svmLinear
☒ E. knn
☒ F. gamLoess
☐ G. multinom
☒ H. qda
☐ I. rf
☐ J. adaboost

6. It is tempting to remove the methods that do not perform well and re-do the ensemble. The problem with this approach is that we are using the test data to make a decision. However, we could use the minimum accuracy estimates obtained from cross validation with the training data for each model from `fit$results$Accuracy`. Obtain these estimates and save them in an object. Report the mean of these training set accuracy estimates.

What is the mean of these training set accuracy estimates?

```
acc_hat <- sapply(fits, function(fit) min(fit$results$Accuracy))
mean(acc_hat)
```

```
## [1] 0.809
```

7. Now let's only consider the methods with an estimated accuracy of greater than or equal to 0.8 when constructing the ensemble. Vote 7 if 50% or more of the models are predicting a 7, and 2 otherwise.

What is the accuracy of the ensemble now?

```
ind <- acc_hat >= 0.8
votes <- rowMeans(pred[,ind] == "7")
y_hat <- ifelse(votes>=0.5, 7, 2)
mean(y_hat == mnist_27$test$y)
```

```
## [1] 0.825
```

Recommendation Systems

There is a link to the relevant section of the textbook: Recommendation systems

Netflix Challenge links

For more information about the "Netflix Challenge," you can check out these sites:

- https://bits.blogs.nytimes.com/2009/09/21/netflix-awards-1-million-prize-and-starts-a-new-contest/
- http://blog.echen.me/2011/10/24/winning-the-netflix-prize-a-summary/
- https://www.netflixprize.com/assets/GrandPrize2009_BPC_BellKor.pdf

Key points

- **Recommendation systems** are more complicated machine learning challenges because each outcome has a different set of predictors. For example, different users rate a different number of movies and rate different movies.

- To compare different models or to see how well we're doing compared to a baseline, we will use **root mean squared error (RMSE) as our loss function**. We can interpret RMSE similar to standard deviation.
- If N is the number of user-movie combinations, $y_{u,i}$ is the rating for movie i by user u, and $\hat{y}_{u,i}$ is our prediction, then **RMSE is defined as follows**:

$$\sqrt{\frac{1}{N}\sum_{u,i}(\hat{y}_{u,i} - y_{u,i})^2}$$

Code

```
data("movielens")

head(movielens)
```

```
##   movieId                                    title year
## 1      31                     Dangerous Minds 1995
## 2    1029                                Dumbo 1941
## 3    1061                             Sleepers 1996
## 4    1129                 Escape from New York 1981
## 5    1172 Cinema Paradiso (Nuovo cinema Paradiso) 1989
## 6    1263                     Deer Hunter, The 1978
##                             genres userId rating  timestamp
## 1                            Drama      1    2.5 1260759144
## 2 Animation|Children|Drama|Musical      1    3.0 1260759179
## 3                         Thriller      1    3.0 1260759182
## 4 Action|Adventure|Sci-Fi|Thriller      1    2.0 1260759185
## 5                            Drama      1    4.0 1260759205
## 6                      Drama|War      1    2.0 1260759151
```

```
movielens %>%
     summarize(n_users = n_distinct(userId),
               n_movies = n_distinct(movieId))
```

```
##   n_users n_movies
## 1     671     9066
```

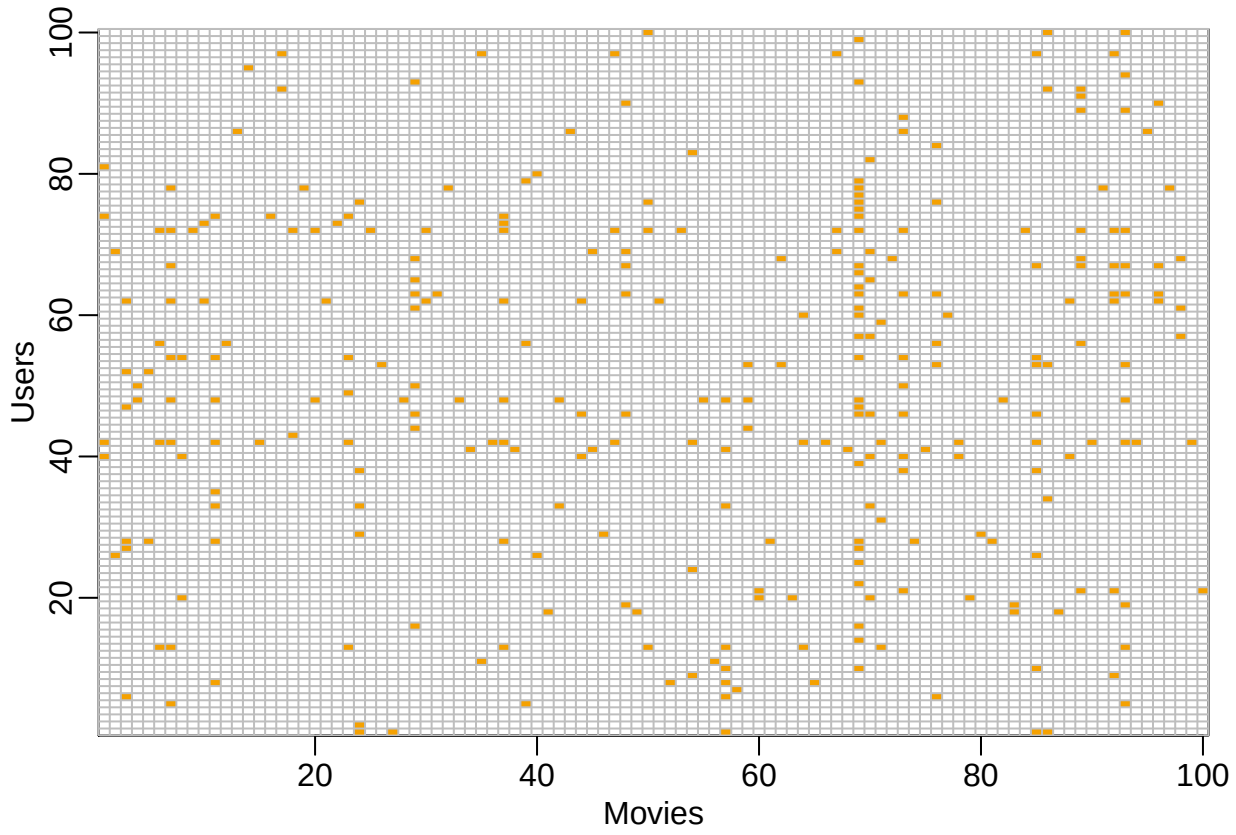
```
keep <- movielens %>%
     dplyr::count(movieId) %>%
     top_n(5) %>%
     pull(movieId)
```

```
## Selecting by n
```

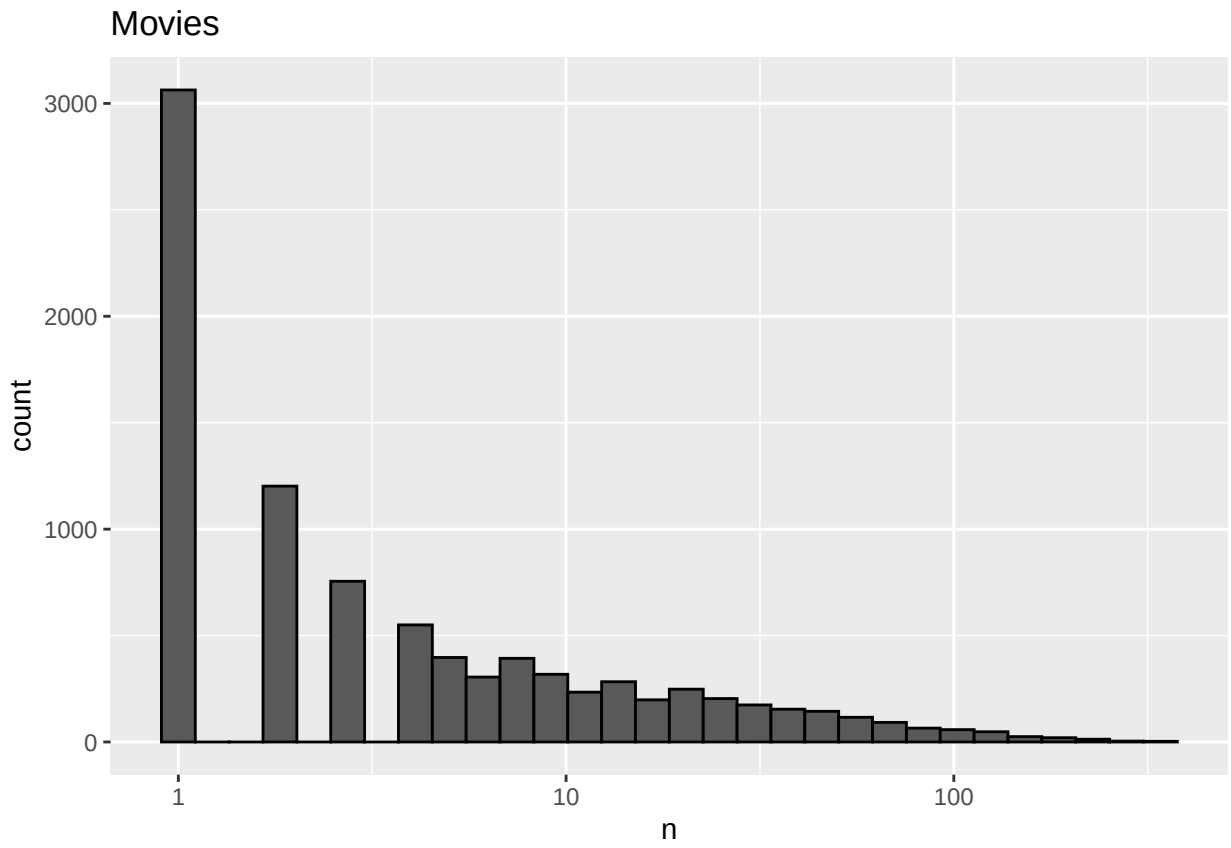
```
tab <- movielens %>%
     filter(userId %in% c(13:20)) %>%
     filter(movieId %in% keep) %>%
     dplyr::select(userId, title, rating) %>%
     spread(title, rating)
tab %>% knitr::kable()
```

userId	Forrest Gump	Pulp Fiction	Shawshank Redemption, The	Silence of the Lambs, The	Star Wars: Episode IV - A New Hope
13	5.0	3.5	4.5	NA	NA
15	1.0	5.0	2.0	5.0	5.0
16	NA	NA	4.0	NA	NA
17	2.5	5.0	5.0	4.5	3.5
18	NA	NA	NA	NA	3.0
19	5.0	5.0	4.0	3.0	4.0
20	2.0	0.5	4.5	0.5	1.5

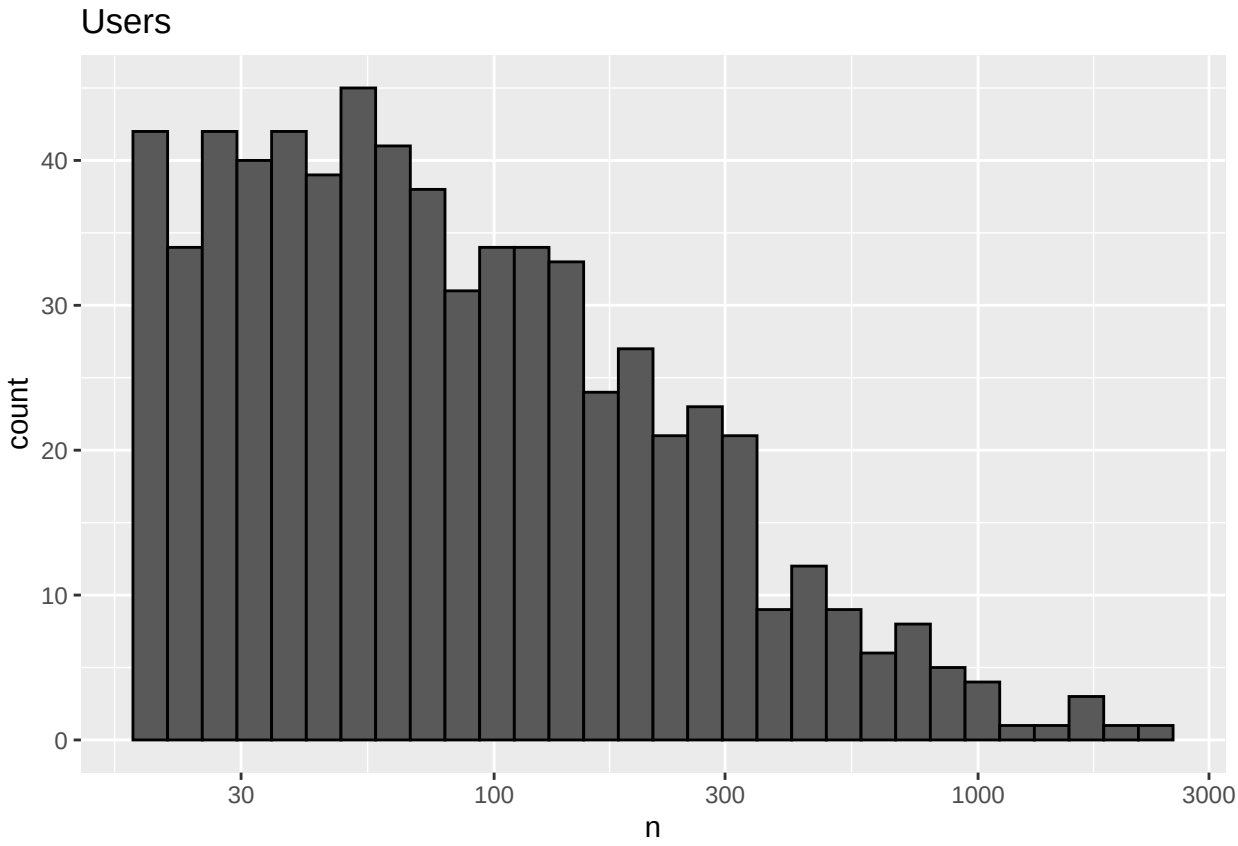
```
users <- sample(unique(movielens$userId), 100)
rafalib::mypar()
movielens %>% filter(userId %in% users) %>%
     dplyr::select(userId, movieId, rating) %>%
     mutate(rating = 1) %>%
     spread(movieId, rating) %>% dplyr::select(sample(ncol(.), 100)) %>%
     as.matrix() %>% t(.) %>%
     image(1:100, 1:100,. , xlab="Movies", ylab="Users")
abline(h=0:100+0.5, v=0:100+0.5, col = "grey")
```




```
movielens %>%
     dplyr::count(movieId) %>%
     ggplot(aes(n)) +
     geom_histogram(bins = 30, color = "black") +
     scale_x_log10() +
     ggtitle("Movies")
```




```
movielens %>%
     dplyr::count(userId) %>%
     ggplot(aes(n)) +
     geom_histogram(bins = 30, color = "black") +
     scale_x_log10() +
     ggtitle("Users")
```




```
library(caret)
set.seed(755)
test_index <- createDataPartition(y = movielens$rating, times = 1,
                                  p = 0.2, list = FALSE)
train_set <- movielens[-test_index,]
test_set <- movielens[test_index,]

test_set <- test_set %>%
     semi_join(train_set, by = "movieId") %>%
     semi_join(train_set, by = "userId")

RMSE <- function(true_ratings, predicted_ratings){
     sqrt(mean((true_ratings - predicted_ratings)^2))
}
```

Building the Recommendation System

There is a link to the relevant sections of the textbook: A first model,Modeling movie effects and User effects

Key points

- We start with a model that **assumes the same rating for all movies and all users**, with all the differences explained by random variation: If μ represents the true rating for all movies and users and ϵ represents independent errors sampled from the same distribution centered at zero, then:

$Y_{u,i} = \mu + \epsilon_{u,i}$

- In this case, the **least squares estimate of** μ — the estimate that minimizes the root mean squared error — is the average rating of all movies across all users.
- We can improve our model by adding a term, b_i, that represents the **average rating for movie** i:

$Y_{u,i} = \mu + b_i + \epsilon_{u,i}$

b_i is the average of $Y_{u,i}$ minus the overall mean for each movie i.

We can further improve our model by adding b_u, the **user-specific effect**:

$Y_{u,i} = \mu + b_i + b_u + \epsilon_{u,i}$

- Note that because there are thousands of b's, the `lm()` function will be very slow or cause R to crash, so **we don't recommend using linear regression to calculate these effects**.

Code

```
mu_hat <- mean(train_set$rating)
mu_hat
```

```
## [1] 3.54
```

```
naive_rmse <- RMSE(test_set$rating, mu_hat)
naive_rmse
```

```
## [1] 1.05
```

```
predictions <- rep(2.5, nrow(test_set))
RMSE(test_set$rating, predictions)
```

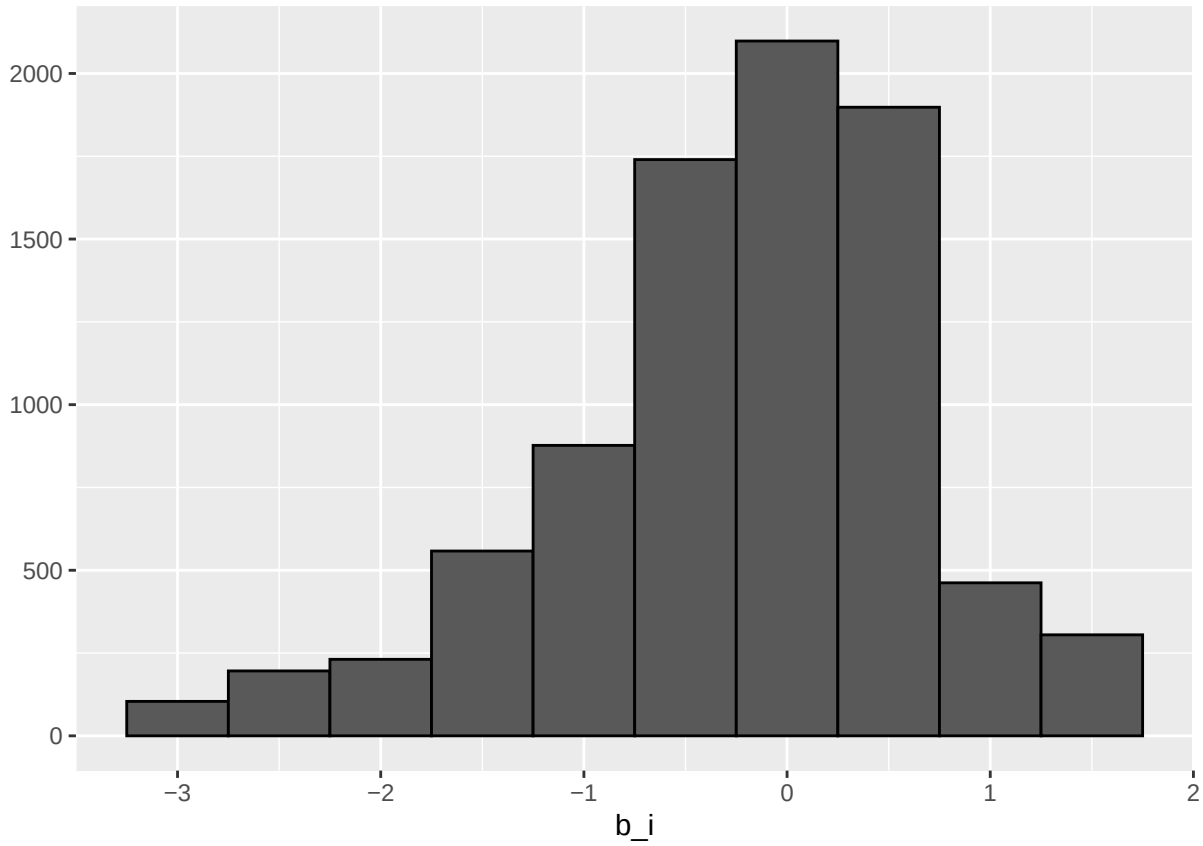
```
## [1] 1.49
```

```
rmse_results <- data_frame(method = "Just the average", RMSE = naive_rmse)

# fit <- lm(rating ~ as.factor(userId), data = movielens)
mu <- mean(train_set$rating)
movie_avgs <- train_set %>%
     group_by(movieId) %>%
     summarize(b_i = mean(rating - mu))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
movie_avgs %>% qplot(b_i, geom ="histogram", bins = 10, data = ., color = I("black"))
```




```
predicted_ratings <- mu + test_set %>%
     left_join(movie_avgs, by='movieId') %>%
     .$b_i

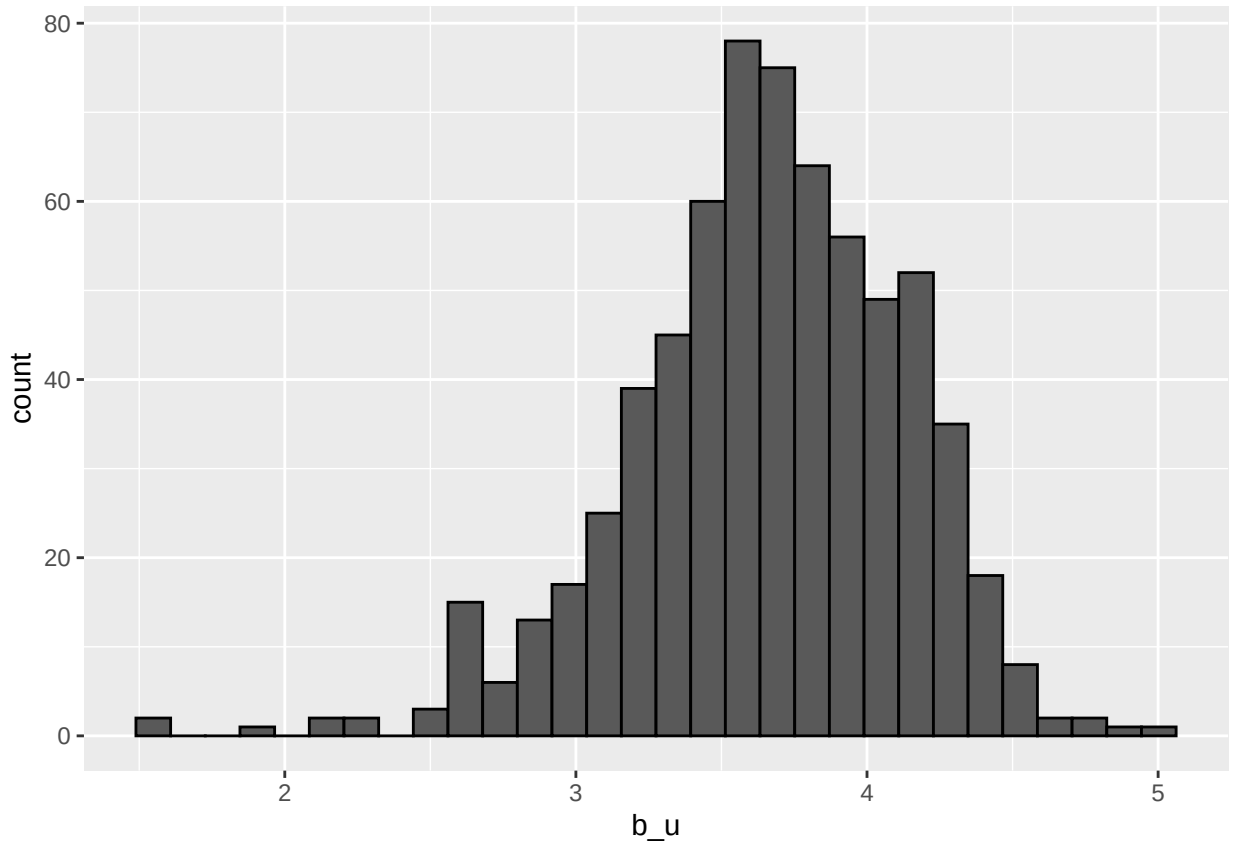
model_1_rmse <- RMSE(predicted_ratings, test_set$rating)
rmse_results <- bind_rows(rmse_results,
                          data_frame(method="Movie Effect Model",
                                     RMSE = model_1_rmse ))

rmse_results %>% knitr::kable()
```

method	RMSE
Just the average	1.048
Movie Effect Model	0.986

```
train_set %>%
     group_by(userId) %>%
     summarize(b_u = mean(rating)) %>%
     filter(n()>=100) %>%
     ggplot(aes(b_u)) +
     geom_histogram(bins = 30, color = "black")
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```




```
# lm(rating ~ as.factor(movieId) + as.factor(userId))
user_avgs <- test_set %>%
     left_join(movie_avgs, by='movieId') %>%
     group_by(userId) %>%
     summarize(b_u = mean(rating - mu - b_i))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
predicted_ratings <- test_set %>%
     left_join(movie_avgs, by='movieId') %>%
     left_join(user_avgs, by='userId') %>%
     mutate(pred = mu + b_i + b_u) %>%
     .$pred

model_2_rmse <- RMSE(predicted_ratings, test_set$rating)
rmse_results <- bind_rows(rmse_results,
                          data_frame(method="Movie + User Effects Model",
                                     RMSE = model_2_rmse ))
rmse_results %>% knitr::kable()
```

method	RMSE
Just the average	1.048
Movie Effect Model	0.986
Movie + User Effects Model	0.885

Comprehension Check - Recommendation Systems

The following exercises all work with the movielens data, which can be loaded using the following code:

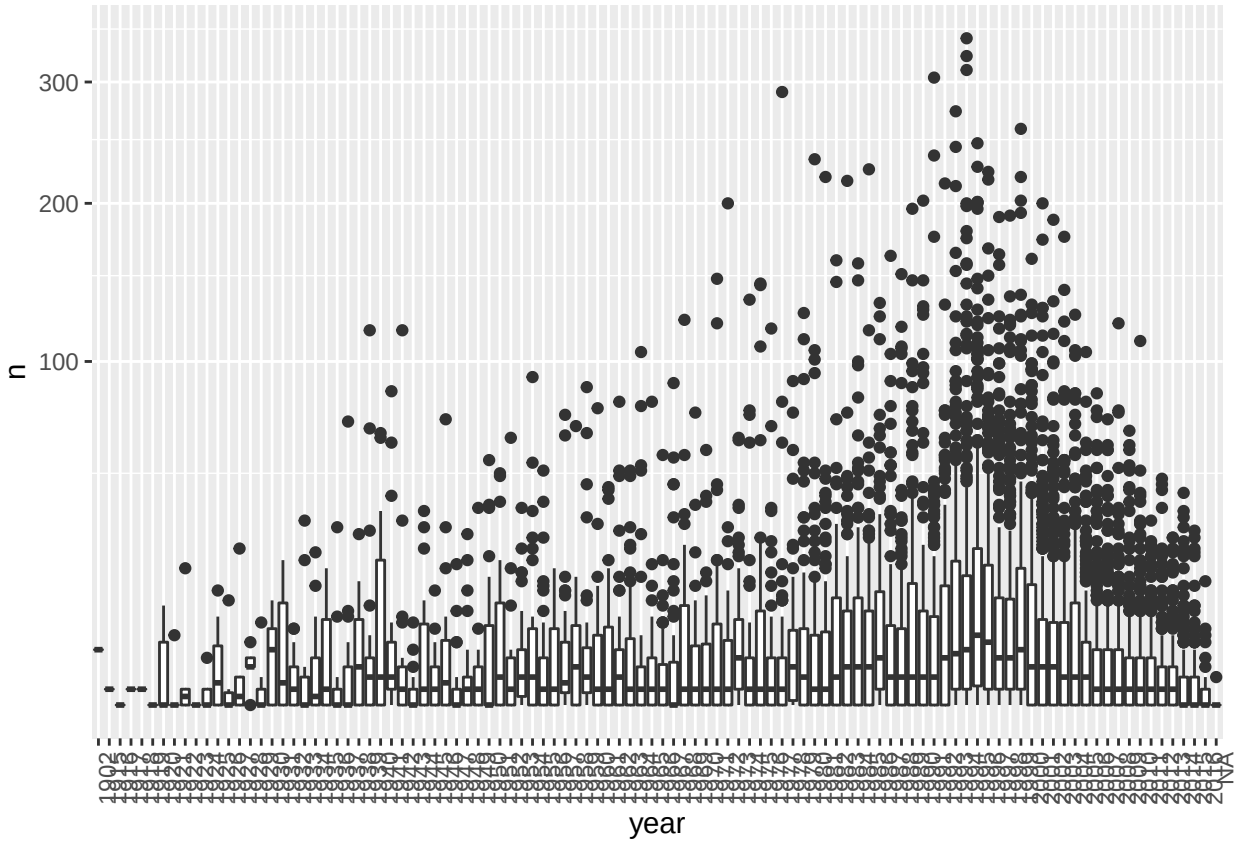
```
data("movielens")
```

1. Compute the number of ratings for each movie and then plot it against the year the movie came out using a boxplot for each year. Use the square root transformation on the y-axis (number of ratings) when creating your plot.

What year has the highest median number of ratings? 1995

```
movielens %>% group_by(movieId) %>%
    summarize(n = n(), year = as.character(first(year))) %>%
    qplot(year, n, data = ., geom = "boxplot") +
    coord_trans(y = "sqrt") +
    theme(axis.text.x = element_text(angle = 90, hjust = 1))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```



2. We see that, on average, movies that came out after 1993 get more ratings. We also see that with newer movies, starting in 1993, the number of ratings decreases with year: the more recent a movie is, the less time users have had to rate it.

Among movies that came out in 1993 or later, select the top 25 movies with the highest average number of ratings per year (n/year), and caculate the average rating of each of them. To calculate number of ratings per year, use 2018 as the end year.

What is the average rating for the movie The Shawshank Redemption?

What is the average number of ratings per year for the movie Forrest Gump?

```
movielens %>%
    filter(year >= 1993) %>%
    group_by(movieId) %>%
    summarize(n = n(), years = 2018 - first(year),
                title = title[1],
                rating = mean(rating)) %>%
    mutate(rate = n/years) %>%
    top_n(25, rate) %>%
    arrange(desc(rate))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
## # A tibble: 25 x 6
##    movieId     n years title                                        rating  rate
##      <int> <int> <dbl> <chr>                                         <dbl> <dbl>
##  1     356   341    24 Forrest Gump                                   4.05  14.2
##  2   79132   111     8 Inception                                      4.05  13.9
##  3    2571   259    19 Matrix, The                                    4.18  13.6
##  4     296   324    24 Pulp Fiction                                   4.26  13.5
##  5     318   311    24 Shawshank Redemption, The                      4.49  13.0
##  6   58559   121    10 Dark Knight, The                               4.24  12.1
##  7    4993   200    17 Lord of the Rings: The Fellowship of the Ri~   4.18  11.8
##  8    5952   188    16 Lord of the Rings: The Two Towers, The         4.06  11.8
##  9    7153   176    15 Lord of the Rings: The Return of the King, ~   4.13  11.7
## 10    2858   220    19 American Beauty                                4.24  11.6
## # ... with 15 more rows
```

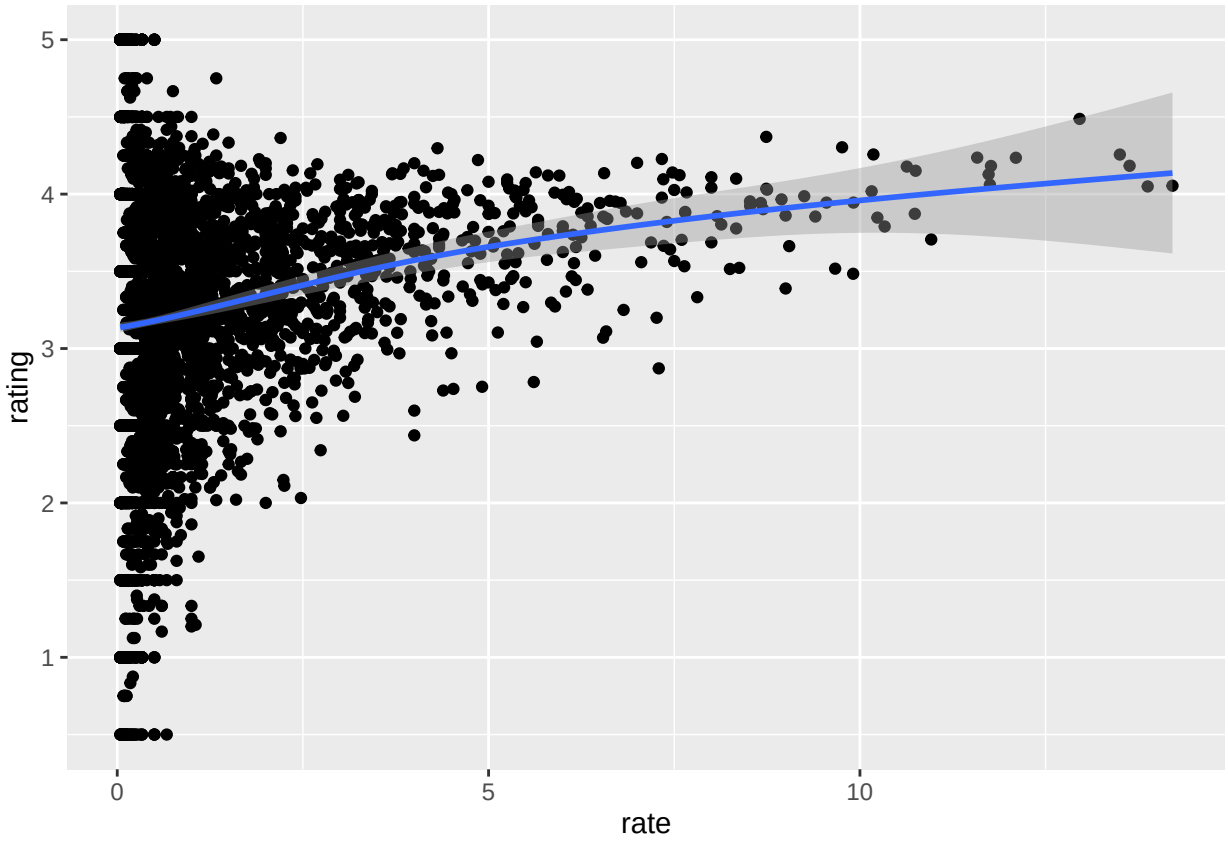
3. From the table constructed in Q2, we can see that the most frequently rated movies tend to have above average ratings. This is not surprising: more people watch popular movies. To confirm this, stratify the post-1993 movies by ratings per year and compute their average ratings. To calculate number of ratings per year, use 2018 as the end year. Make a plot of average rating versus ratings per year and show an estimate of the trend.

What type of trend do you observe?

```
movielens %>%
    filter(year >= 1993) %>%
    group_by(movieId) %>%
    summarize(n = n(), years = 2018 - first(year),
                title = title[1],
                rating = mean(rating)) %>%
    mutate(rate = n/years) %>%
    ggplot(aes(rate, rating)) +
    geom_point() +
    geom_smooth()
```

```
## `summarise()` ungrouping output (override with `.groups` argument)

## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
```



☐ A. There is no relationship between how often a movie is rated and its average rating.
☐ B. Movies with very few and very many ratings have the highest average ratings.
☒ C. The more often a movie is rated, the higher its average rating.
☐ D. The more often a movie is rated, the lower its average rating.

4. Suppose you are doing a predictive analysis in which you need to fill in the missing ratings with some value.

Given your observations in the exercise in Q3, which of the following strategies would be most appropriate?

☐ A. Fill in the missing values with the average rating across all movies.
☐ B. Fill in the missing values with 0.
☐ C. Fill in the missing values with a lower value than the average rating across all movies.
☒ D. Fill in the value with a higher value than the average rating across all movies.
☐ E. None of the above.

5. The `movielens` dataset also includes a time stamp. This variable represents the time and data in which the rating was provided. The units are seconds since January 1, 1970. Create a new column `date` with the date.

Which code correctly creates this new column?

```
movielens <- mutate(movielens, date = as_datetime(timestamp))
```

- ☐ A. `movielens <- mutate(movielens, date = as.date(timestamp))`
- ☒ B. `movielens <- mutate(movielens, date = as_datetime(timestamp))`
- ☐ C. `movielens <- mutate(movielens, date = as.data(timestamp))`
- ☐ D. `movielens <- mutate(movielens, date = timestamp)`

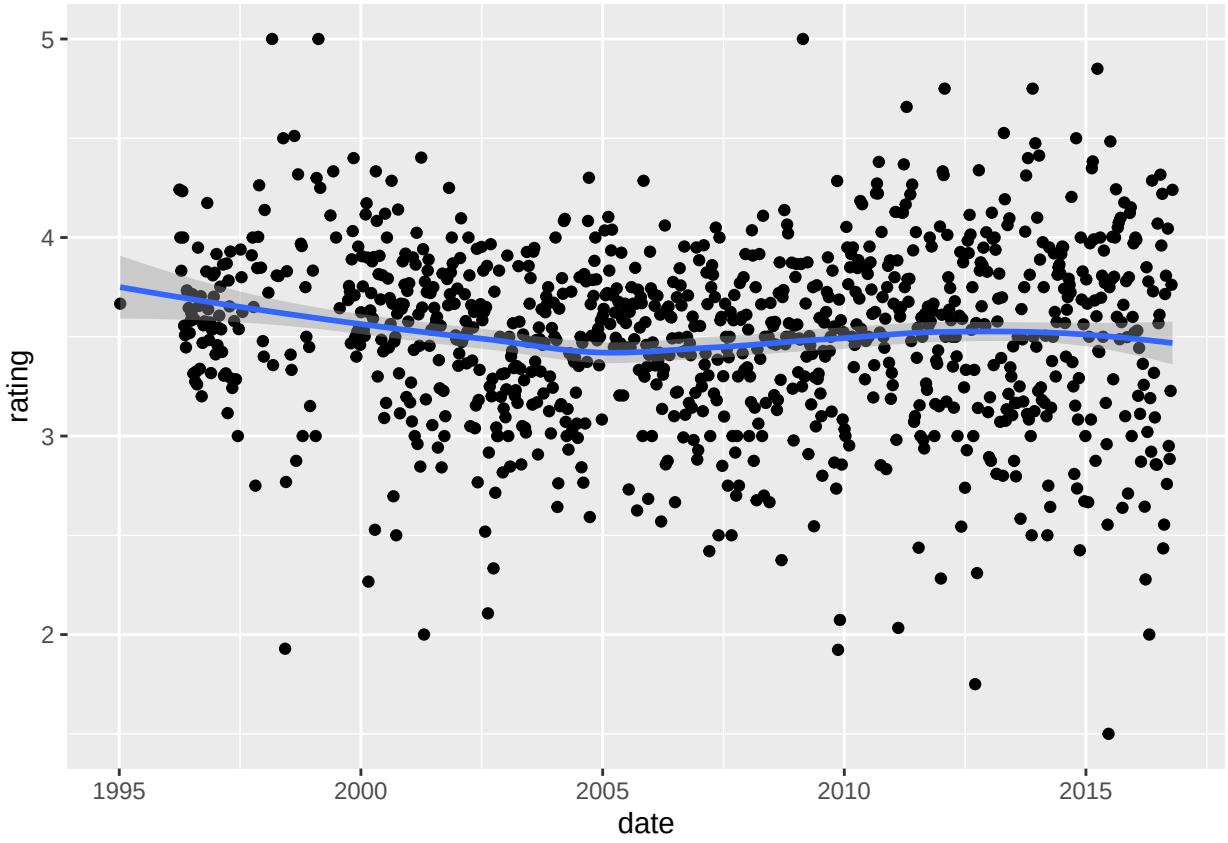
6. Compute the average rating for each week and plot this average against date. Hint: use the `round_date()` function before you `group_by()`.

What type of trend do you observe?

```
movielens %>% mutate(date = round_date(date, unit = "week")) %>%
    group_by(date) %>%
    summarize(rating = mean(rating)) %>%
    ggplot(aes(date, rating)) +
    geom_point() +
    geom_smooth()
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```



☐ A. There is very strong evidence of a time effect on average rating.
☒ B. There is some evidence of a time effect on average rating.
☐ C. There is no evidence of a time effect on average rating (straight horizontal line).

7. Consider again the plot you generated in Q6.

If we define $d_{u,i}$ as the day for user's u rating of movie i, which of the following models is most appropriate?

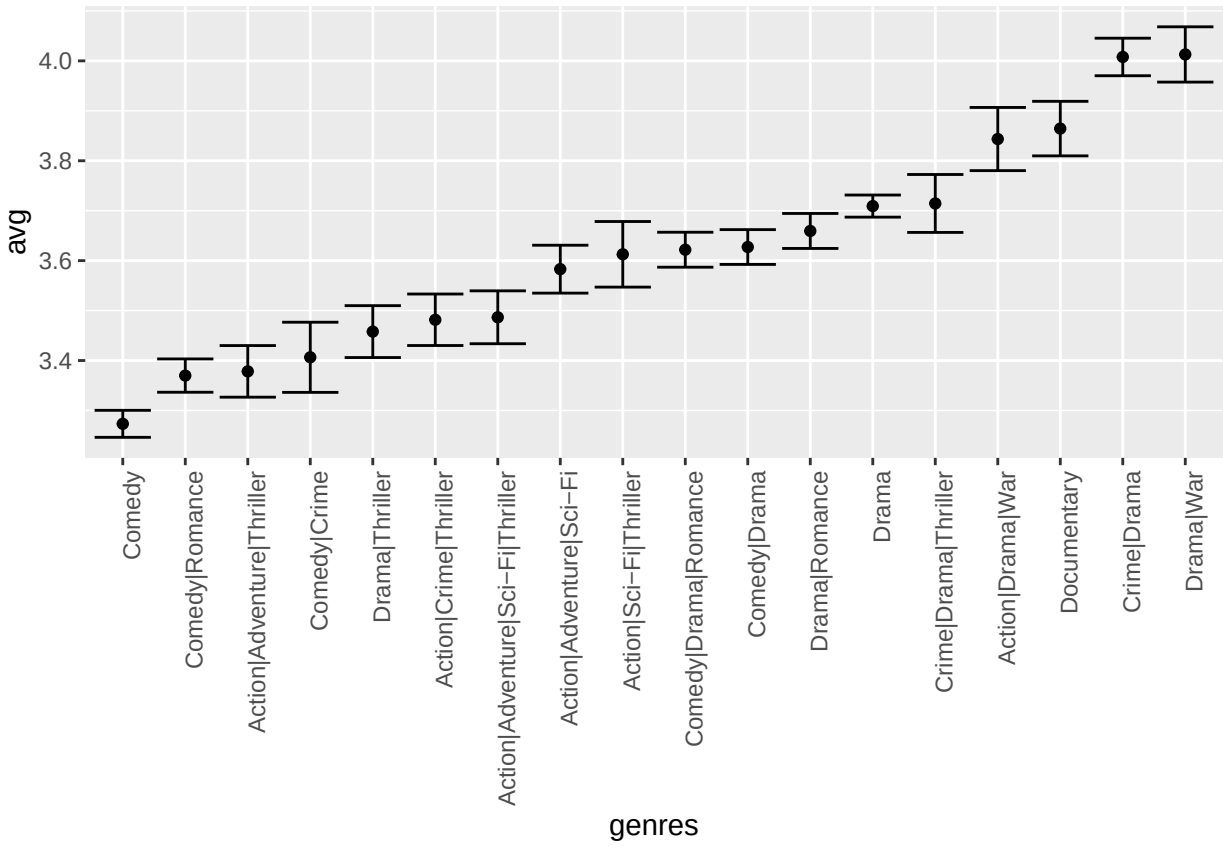
☐ A. $Y_{u,i} = \mu + b_i + b_u + d_{u,i} + \varepsilon_{u,i}$
☐ B. $Y_{u,i} = \mu + b_i + b_u + d_{u,i}\beta + \varepsilon_{u,i}$
☐ C. $Y_{u,i} = \mu + b_i + b_u + d_{u,i}\beta_i + \varepsilon_{u,i}$
☒ D. $Y_{u,i} = \mu + b_i + b_u + f(d_{u,i}) + \varepsilon_{u,i}$

8. The `movielens` data also has a `genres` column. This column includes every genre that applies to the movie. Some movies fall under several genres. Define a category as whatever combination appears in this column. Keep only categories with more than 1,000 ratings. Then compute the average and standard error for each category. Plot these as error bar plots.

Which genre has the lowest average rating?

```
movielens %>% group_by(genres) %>%
    summarize(n = n(), avg = mean(rating), se = sd(rating)/sqrt(n())) %>%
    filter(n >= 1000) %>%
    mutate(genres = reorder(genres, avg)) %>%
    ggplot(aes(x = genres, y = avg, ymin = avg - 2*se, ymax = avg + 2*se)) +
    geom_point() +
    geom_errorbar() +
    theme(axis.text.x = element_text(angle = 90, hjust = 1))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```



9. The plot you generated in Q8 shows strong evidence of a genre effect. Consider this plot as you answer the following question.

If we define $g_{u,i}$ as the genre for user u's rating of movie i, which of the following models is most appropriate?

☐ A. $Y_{u,i} = \mu + b_i + b_u + g_{u,i} + \varepsilon_{u,i}$
☐ B. $Y_{u,i} = \mu + b_i + b_u + g_{u,i}\beta + \varepsilon_{u,i}$
☒ C. $Y_{u,i} = \mu + b_i + b_u + \sum_{k=1}^{K} x_{u,i}^k \beta_k + \varepsilon_{u,i}$, with $x_{u,i}^k = 1$ if $g_{u,i}$ is genre k
☐ D. $Y_{u,i} = \mu + b_i + b_u + f(g_{u,i}) + \varepsilon_{u,i}$, with f a smooth function of $g_{u,i}$

Regularization

There is a link to the relevant section of the textbook: Regularization

Notes

- To improve our results, we will use **regularization**. Regularization constrains the total variability of the effect sizes by penalizing large estimates that come from small sample sizes.
- To estimate the b's, we will now **minimize this equation**, which contains a penalty term:

$\frac{1}{N}\sum_{u,i}(y_{u,i} - \mu - b_i)^2 + \lambda \sum_i b_i^2$

The first term is the mean squared error and the second is a penalty term that gets larger when many b's are large.

The values of b that minimize this equation are given by:

$\hat{b}_i(\lambda) = \frac{1}{\lambda + n_i} \sum_{u=1}^{n_i} (Y_{u,i} - \hat{\mu})$,

where n_i is a number of ratings b for movie i.

- The **larger λ is, the more we shrink**. λ is a tuning parameter, so we can use cross-validation to choose it. We should be using full cross-validation on just the training set, without using the test set until the final assessment.
- We can also use regularization to estimate the **user effect**. We will now minimize this equation:

$\frac{1}{N} \sum_{u,i} (y_{u,i} - \mu - b_i - b_u)^2 + \lambda(\sum_i b_i^2 + \sum_u b_u^2)$

Code

```
data("movielens")
set.seed(755)
test_index <- createDataPartition(y = movielens$rating, times = 1,
                                  p = 0.2, list = FALSE)
train_set <- movielens[-test_index,]
test_set <- movielens[test_index,]
test_set <- test_set %>%
     semi_join(train_set, by = "movieId") %>%
     semi_join(train_set, by = "userId")
RMSE <- function(true_ratings, predicted_ratings){
     sqrt(mean((true_ratings - predicted_ratings)^2))
}
mu_hat <- mean(train_set$rating)
naive_rmse <- RMSE(test_set$rating, mu_hat)
rmse_results <- data_frame(method = "Just the average", RMSE = naive_rmse)
mu <- mean(train_set$rating)
movie_avgs <- train_set %>%
     group_by(movieId) %>%
     summarize(b_i = mean(rating - mu))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
predicted_ratings <- mu + test_set %>%
     left_join(movie_avgs, by='movieId') %>%
     .$b_i
model_1_rmse <- RMSE(predicted_ratings, test_set$rating)
rmse_results <- bind_rows(rmse_results,
                          data_frame(method="Movie Effect Model",
                                     RMSE = model_1_rmse ))
user_avgs <- test_set %>%
     left_join(movie_avgs, by='movieId') %>%
     group_by(userId) %>%
     summarize(b_u = mean(rating - mu - b_i))
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
predicted_ratings <- test_set %>%
     left_join(movie_avgs, by='movieId') %>%
     left_join(user_avgs, by='userId') %>%
```

```
    mutate(pred = mu + b_i + b_u) %>%
    .$pred
model_2_rmse <- RMSE(predicted_ratings, test_set$rating)
rmse_results <- bind_rows(rmse_results,
                          data_frame(method="Movie + User Effects Model",
                                     RMSE = model_2_rmse ))

test_set %>%
    left_join(movie_avgs, by='movieId') %>%
    mutate(residual = rating - (mu + b_i)) %>%
    arrange(desc(abs(residual))) %>%
    dplyr::select(title,  residual) %>% slice(1:10) %>% knitr::kable()
```

title	residual
Day of the Beast, The (Día de la Bestia, El)	4.50
Horror Express	-4.00
No Holds Barred	4.00
Dear Zachary: A Letter to a Son About His Father	-4.00
Faust	-4.00
Hear My Song	-4.00
Confessions of a Shopaholic	-4.00
Twilight Saga: Breaking Dawn - Part 1, The	-4.00
Taxi Driver	-3.81
Taxi Driver	-3.81

```
movie_titles <- movielens %>%
    dplyr::select(movieId, title) %>%
    distinct()
movie_avgs %>% left_join(movie_titles, by="movieId") %>%
    arrange(desc(b_i)) %>%
    dplyr::select(title, b_i) %>%
    slice(1:10) %>%
    knitr::kable()
```

title	b_i
Lamerica	1.46
Love & Human Remains	1.46
Enfer, L'	1.46
Picture Bride (Bijo photo)	1.46
Red Firecracker, Green Firecracker (Pao Da Shuang Deng)	1.46
Faces	1.46
Maya Lin: A Strong Clear Vision	1.46
Heavy	1.46
Gate of Heavenly Peace, The	1.46
Death in the Garden (Mort en ce jardin, La)	1.46

```
movie_avgs %>% left_join(movie_titles, by="movieId") %>%
    arrange(b_i) %>%
    dplyr::select(title, b_i) %>%
```

```
     slice(1:10) %>%
     knitr::kable()
```

title	b_i
Santa with Muscles	-3.04
B*AP*S	-3.04
3 Ninjas: High Noon On Mega Mountain	-3.04
Barney's Great Adventure	-3.04
Merry War, A	-3.04
Day of the Beast, The (Día de la Bestia, El)	-3.04
Children of the Corn III	-3.04
Whiteboyz	-3.04
Catfish in Black Bean Sauce	-3.04
Watcher, The	-3.04

```
train_set %>% dplyr::count(movieId) %>%
     left_join(movie_avgs) %>%
     left_join(movie_titles, by="movieId") %>%
     arrange(desc(b_i)) %>%
     dplyr::select(title, b_i, n) %>%
     slice(1:10) %>%
     knitr::kable()
```

```
## Joining, by = "movieId"
```

title	b_i	n
Lamerica	1.46	1
Love & Human Remains	1.46	3
Enfer, L'	1.46	1
Picture Bride (Bijo photo)	1.46	1
Red Firecracker, Green Firecracker (Pao Da Shuang Deng)	1.46	3
Faces	1.46	1
Maya Lin: A Strong Clear Vision	1.46	2
Heavy	1.46	1
Gate of Heavenly Peace, The	1.46	1
Death in the Garden (Mort en ce jardin, La)	1.46	1

```
train_set %>% dplyr::count(movieId) %>%
     left_join(movie_avgs) %>%
     left_join(movie_titles, by="movieId") %>%
     arrange(b_i) %>%
     dplyr::select(title, b_i, n) %>%
     slice(1:10) %>%
     knitr::kable()
```

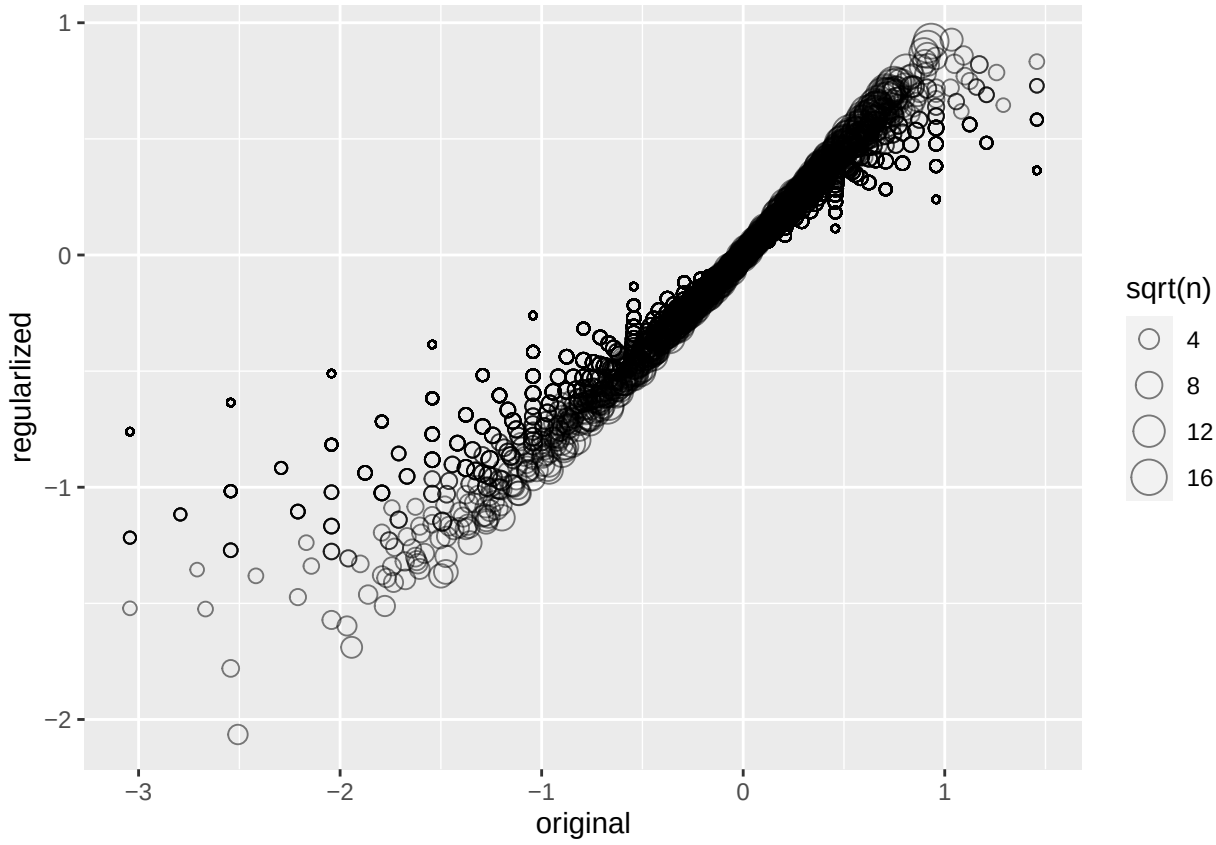
```
## Joining, by = "movieId"
```

title	b_i	n
Santa with Muscles	-3.04	1
B*A*P*S	-3.04	1
3 Ninjas: High Noon On Mega Mountain	-3.04	1
Barney's Great Adventure	-3.04	1
Merry War, A	-3.04	1
Day of the Beast, The (Día de la Bestia, El)	-3.04	1
Children of the Corn III	-3.04	1
Whiteboyz	-3.04	1
Catfish in Black Bean Sauce	-3.04	1
Watcher, The	-3.04	1

```
lambda <- 3
mu <- mean(train_set$rating)
movie_reg_avgs <- train_set %>%
     group_by(movieId) %>%
     summarize(b_i = sum(rating - mu)/(n()+lambda), n_i = n())
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
data_frame(original = movie_avgs$b_i,
           regularlized = movie_reg_avgs$b_i,
           n = movie_reg_avgs$n_i) %>%
     ggplot(aes(original, regularlized, size=sqrt(n))) +
     geom_point(shape=1, alpha=0.5)
```



```
train_set %>%
     dplyr::count(movieId) %>%
     left_join(movie_reg_avgs) %>%
     left_join(movie_titles, by="movieId") %>%
     arrange(desc(b_i)) %>%
     dplyr::select(title, b_i, n) %>%
     slice(1:10) %>%
     knitr::kable()
```

```
## Joining, by = "movieId"
```

title	b_i	n
All About Eve	0.927	26
Shawshank Redemption, The	0.921	240
Godfather, The	0.897	153
Godfather: Part II, The	0.871	100
Maltese Falcon, The	0.860	47
Best Years of Our Lives, The	0.859	11
On the Waterfront	0.847	23
Face in the Crowd, A	0.833	4
African Queen, The	0.832	36
All Quiet on the Western Front	0.824	11

```
train_set %>%
     dplyr::count(movieId) %>%
     left_join(movie_reg_avgs) %>%
     left_join(movie_titles, by="movieId") %>%
     arrange(b_i) %>%
     dplyr::select(title, b_i, n) %>%
     slice(1:10) %>%
     knitr::kable()
```

```
## Joining, by = "movieId"
```

title	b_i	n
Battlefield Earth	-2.06	14
Joe's Apartment	-1.78	7
Speed 2: Cruise Control	-1.69	20
Super Mario Bros.	-1.60	13
Police Academy 6: City Under Siege	-1.57	10
After Earth	-1.52	4
Disaster Movie	-1.52	3
Little Nicky	-1.51	17
Cats & Dogs	-1.47	6
Blade: Trinity	-1.46	11

```
predicted_ratings <- test_set %>%
     left_join(movie_reg_avgs, by='movieId') %>%
```

```
     mutate(pred = mu + b_i) %>%
     .$pred

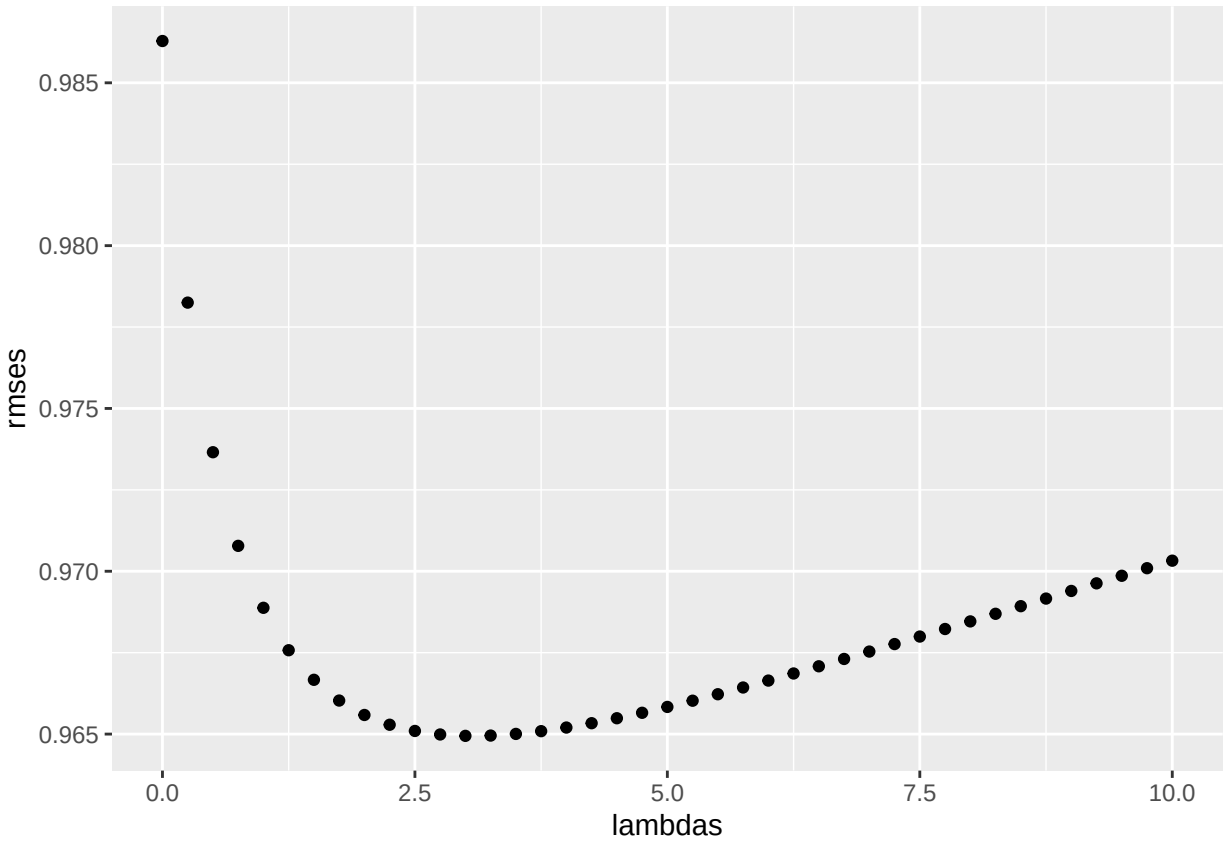
model_3_rmse <- RMSE(predicted_ratings, test_set$rating)
rmse_results <- bind_rows(rmse_results,
                          data_frame(method="Regularized Movie Effect Model",
                                     RMSE = model_3_rmse ))
rmse_results %>% knitr::kable()
```

method	RMSE
Just the average	1.048
Movie Effect Model	0.986
Movie + User Effects Model	0.885
Regularized Movie Effect Model	0.965

```
lambdas <- seq(0, 10, 0.25)
mu <- mean(train_set$rating)
just_the_sum <- train_set %>%
     group_by(movieId) %>%
     summarize(s = sum(rating - mu), n_i = n())
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```

```
rmses <- sapply(lambdas, function(l){
     predicted_ratings <- test_set %>%
          left_join(just_the_sum, by='movieId') %>%
          mutate(b_i = s/(n_i+l)) %>%
          mutate(pred = mu + b_i) %>%
          .$pred
     return(RMSE(predicted_ratings, test_set$rating))
})
qplot(lambdas, rmses)
```




```
lambdas[which.min(rmses)]
```

```
## [1] 3
```

```
lambdas <- seq(0, 10, 0.25)
rmses <- sapply(lambdas, function(l){
     mu <- mean(train_set$rating)
     b_i <- train_set %>%
          group_by(movieId) %>%
          summarize(b_i = sum(rating - mu)/(n()+l))
     b_u <- train_set %>%
          left_join(b_i, by="movieId") %>%
          group_by(userId) %>%
          summarize(b_u = sum(rating - b_i - mu)/(n()+l))
     predicted_ratings <-
          test_set %>%
          left_join(b_i, by = "movieId") %>%
          left_join(b_u, by = "userId") %>%
          mutate(pred = mu + b_i + b_u) %>%
          .$pred
     return(RMSE(predicted_ratings, test_set$rating))
})
```

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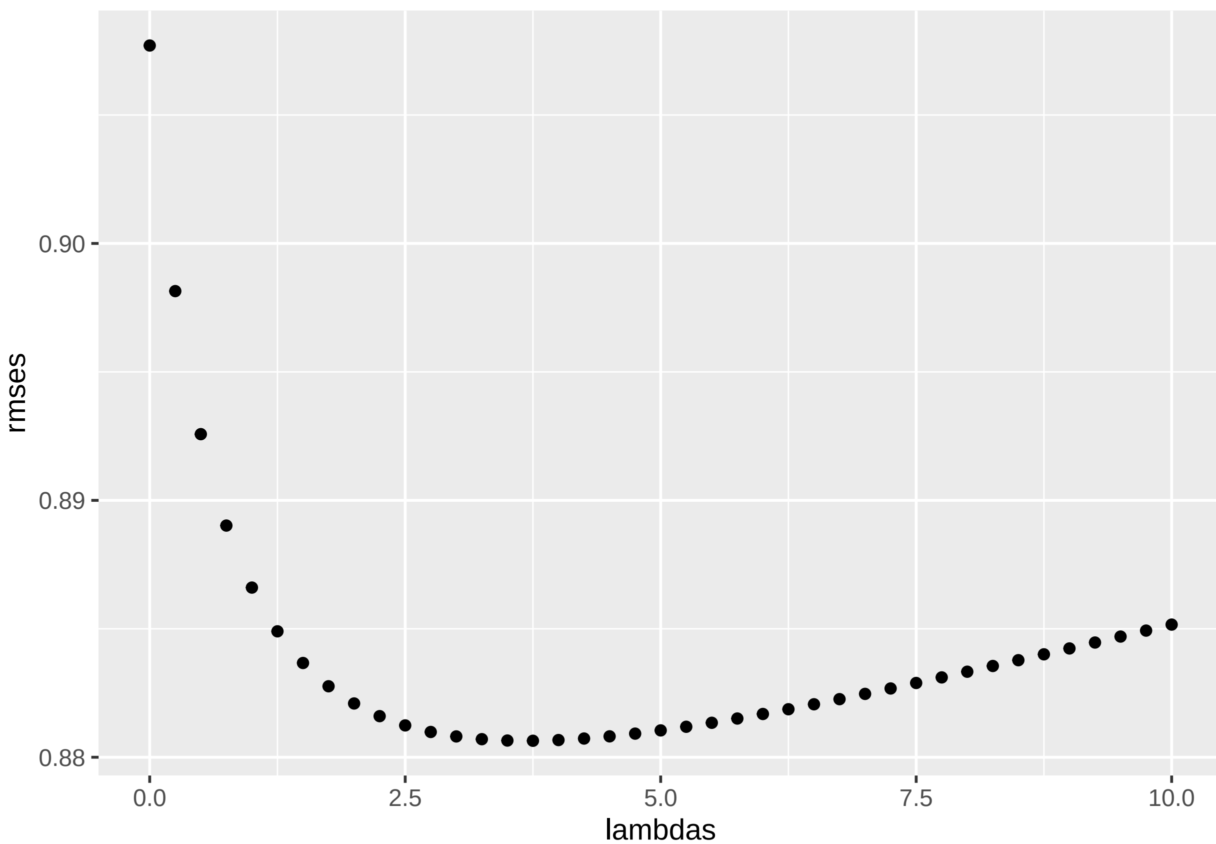
```

```
qplot(lambdas, rmses)
```



```
lambda <- lambdas[which.min(rmses)]
lambda
```

```
## [1] 3.75
```

```
rmse_results <- bind_rows(rmse_results,
                          data_frame(method="Regularized Movie + User Effect Model",
                                     RMSE = min(rmses)))
rmse_results %>% knitr::kable()
```

method	RMSE
Just the average	1.048
Movie Effect Model	0.986
Movie + User Effects Model	0.885
Regularized Movie Effect Model	0.965
Regularized Movie + User Effect Model	0.881

Comprehension Check - Regularization

The exercises in Q1-Q8 work with a simulated dataset for 1000 schools. This pre-exercise setup walks you through the code needed to simulate the dataset.

If you have not done so already since the Titanic Exercises, please restart R or reset the number of digits that are printed with `options(digits=7)`.

An education expert is advocating for smaller schools. The expert bases this recommendation on the fact that among the best performing schools, many are small schools. Let's simulate a dataset for 1000 schools. First, let's simulate the number of students in each school, using the following code:

```
# set.seed(1986) # if using R 3.5 or earlier
set.seed(1986, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1986, sample.kind = "Rounding"): non-uniform 'Rounding'
## sampler used
```

```
n <- round(2^rnorm(1000, 8, 1))
```

Now let's assign a **true** quality for each school that is completely independent from size. This is the parameter we want to estimate in our analysis. The true quality can be assigned using the following code:

```
# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
mu <- round(80 + 2*rt(1000, 5))
range(mu)
```

```
## [1] 67 94
```

```
schools <- data.frame(id = paste("PS",1:1000),
                      size = n,
                      quality = mu,
                      rank = rank(-mu))
```

We can see the top 10 schools using this code:

```
schools %>% top_n(10, quality) %>% arrange(desc(quality))
```

```
##         id size quality rank
## 1  PS 191 1036      94  1.0
## 2  PS 567  121      93  2.0
## 3   PS 95  235      91  3.0
## 4  PS 430   61      90  4.0
## 5  PS 343   78      89  5.0
## 6  PS 981  293      88  6.0
## 7  PS 558  196      87  7.0
## 8   PS 79  105      86 13.5
## 9  PS 113  653      86 13.5
## 10 PS 163  300      86 13.5
## 11 PS 266 2369      86 13.5
## 12 PS 400  550      86 13.5
## 13 PS 451  217      86 13.5
## 14 PS 477  341      86 13.5
## 15 PS 484  967      86 13.5
## 16 PS 561  723      86 13.5
## 17 PS 563  828      86 13.5
## 18 PS 865  586      86 13.5
## 19 PS 963  208      86 13.5
```

Now let's have the students in the school take a test. There is random variability in test taking, so we will simulate the test scores as normally distributed with the average determined by the school quality with a standard deviation of 30 percentage points. This code will simulate the test scores:

```
# set.seed(1) # if using R 3.5 or earlier
set.seed(1, sample.kind="Rounding") # if using R 3.6 or later
```

```
## Warning in set.seed(1, sample.kind = "Rounding"): non-uniform 'Rounding' sampler
## used
```

```
mu <- round(80 + 2*rt(1000, 5))

scores <- sapply(1:nrow(schools), function(i){
       scores <- rnorm(schools$size[i], schools$quality[i], 30)
       scores
})
schools <- schools %>% mutate(score = sapply(scores, mean))
```

1. What are the top schools based on the average score? Show just the ID, size, and the average score.

Report the ID of the top school and average score of the 10th school.

What is the ID of the top school?

What is the average score of the 10th school (after sorting from highest to lowest average score)?

```
schools %>% top_n(10, score) %>% arrange(desc(score)) %>% dplyr::select(id, size, score)
```

```
##        id size score
## 1  PS 567  121  95.8
## 2  PS 191 1036  93.5
## 3  PS 330  162  91.0
## 4  PS 701   83  90.5
## 5  PS 591  213  89.7
## 6  PS 205  172  89.3
## 7  PS 574  199  89.2
## 8  PS 963  208  89.0
## 9  PS 430   61  88.7
## 10 PS 756  245  88.0
```

2. Compare the median school size to the median school size of the top 10 schools based on the score.

What is the median school size overall?

What is the median school size of the of the top 10 schools based on the score?

```
median(schools$size)
```

```
## [1] 261
```

```
schools %>% top_n(10, score) %>% .$size %>% median()
```

```
## [1] 186
```

3. According to this analysis, it appears that small schools produce better test scores than large schools. Four out of the top 10 schools have 100 or fewer students. But how can this be? We constructed the simulation so that quality and size were independent. Repeat the exercise for the worst 10 schools.

What is the median school size of the bottom 10 schools based on the score?

```
median(schools$size)
```

```
## [1] 261
```

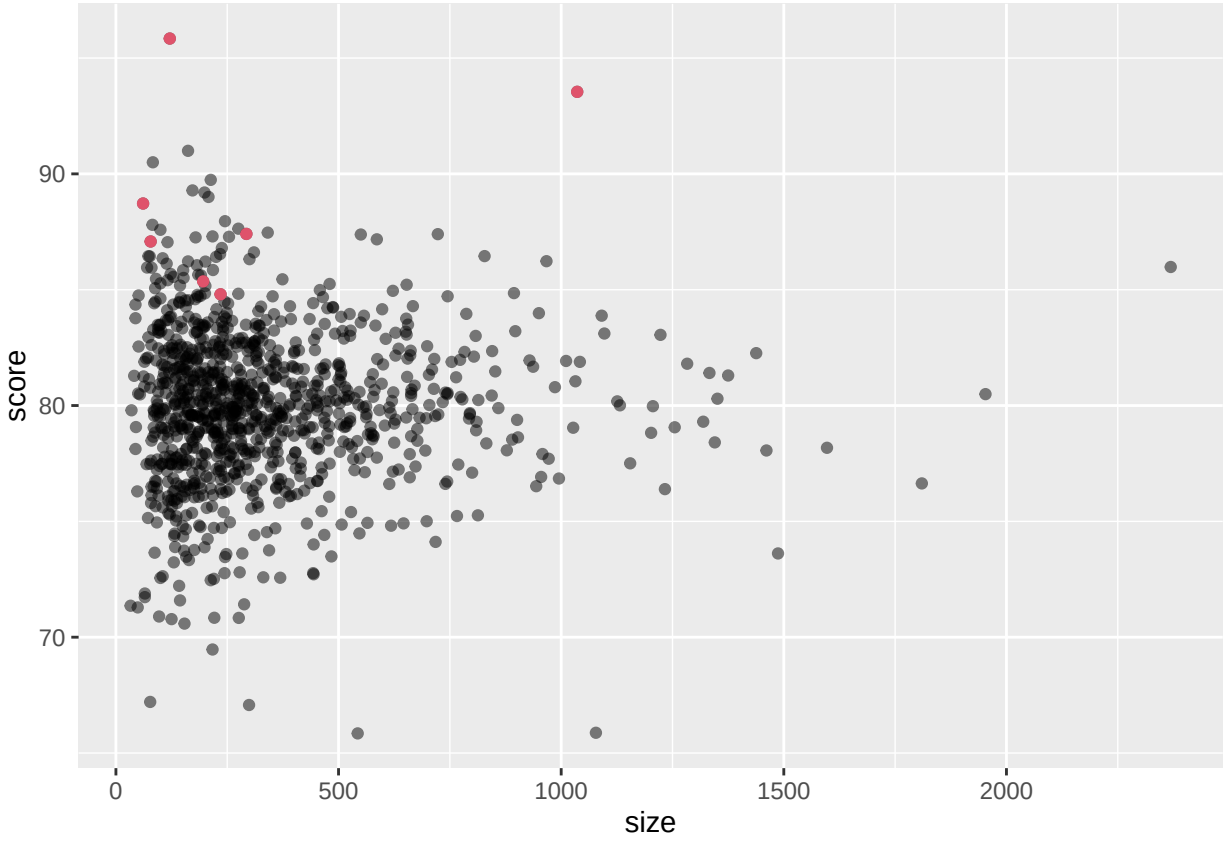
```
schools %>% top_n(-10, score) %>% .$size %>% median()
```

```
## [1] 219
```

4. From this analysis, we see that the worst schools are also small. Plot the average score versus school size to see what's going on. Highlight the top 10 schools based on the **true** quality.

What do you observe?

```
schools %>% ggplot(aes(size, score)) +
    geom_point(alpha = 0.5) +
    geom_point(data = filter(schools, rank<=10), col = 2)
```



- ☐ A. There is no difference in the standard error of the score based on school size; there must be an error in how we generated our data.
- ☒ B. The standard error of the score has larger variability when the school is smaller, which is why both the best and the worst schools are more likely to be small.
- ☐ C. The standard error of the score has smaller variability when the school is smaller, which is why both the best and the worst schools are more likely to be small.
- ☐ D. The standard error of the score has larger variability when the school is very small or very large, which is why both the best and the worst schools are more likely to be small.
- ☐ E. The standard error of the score has smaller variability when the school is very small or very large, which is why both the best and the worst schools are more likely to be small.

5. Let's use regularization to pick the best schools. Remember regularization **shrinks** deviations from the average towards 0. To apply regularization here, we first need to define the overall average for all schools, using the following code:

```
overall <- mean(sapply(scores, mean))
```

Then, we need to define, for each school, how it deviates from that average.

Write code that estimates the score above the average for each school but dividing by $n + \alpha$ instead of n, with n the school size and α a regularization parameter. Try $\alpha = 25$.

What is the ID of the top school with regularization?

What is the regularized score of the 10th school?

```
alpha <- 25
score_reg <- sapply(scores, function(x)  overall + sum(x-overall)/(length(x)+alpha))
schools %>% mutate(score_reg = score_reg) %>%
    top_n(10, score_reg) %>% arrange(desc(score_reg))
```

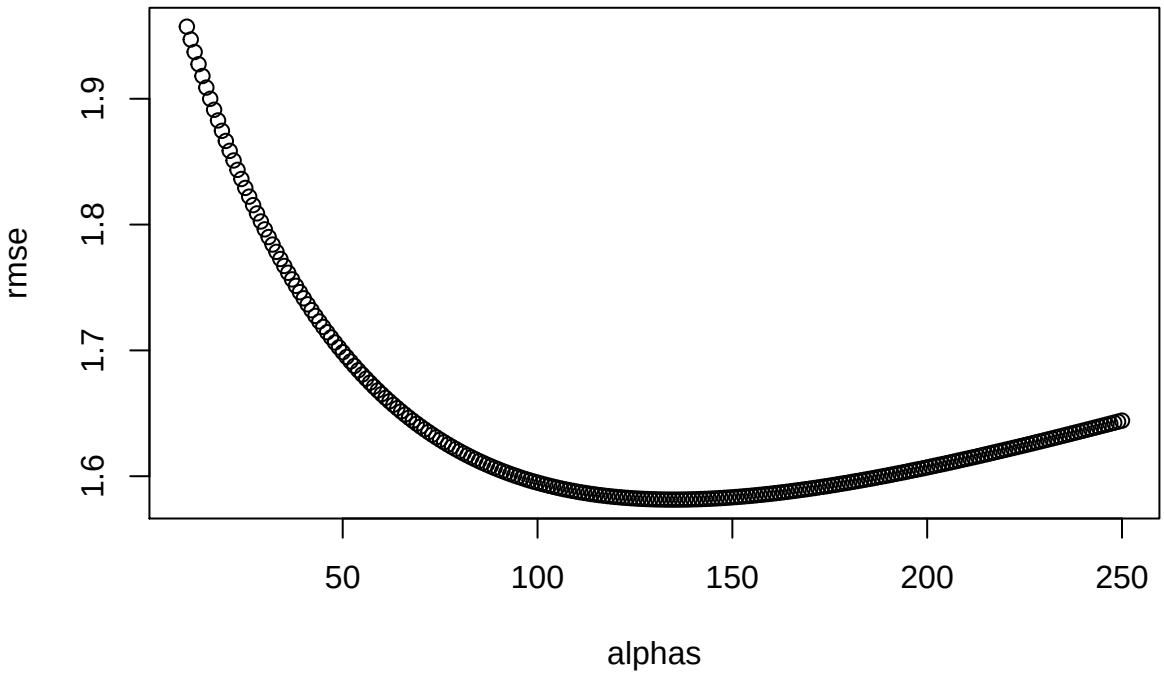
```
##         id size quality  rank score score_reg
## 1  PS 191 1036      94   1.0  93.5      93.2
## 2  PS 567  121      93   2.0  95.8      93.1
## 3  PS 330  162      84  53.5  91.0      89.5
## 4  PS 591  213      83 104.5  89.7      88.7
## 5  PS 574  199      84  53.5  89.2      88.2
## 6  PS 205  172      85  28.5  89.3      88.1
## 7  PS 701   83      83 104.5  90.5      88.1
## 8  PS 963  208      86  13.5  89.0      88.0
## 9  PS 756  245      83 104.5  88.0      87.2
## 10 PS 561  723      86  13.5  87.4      87.2
```

6. Notice that this improves things a bit. The number of small schools that are not highly ranked is now lower. Is there a better α? Using values of α from 10 to 250, find the α that minimizes the RMSE.

$\text{RMSE} = \sqrt{\frac{1}{1000}\sum_{i=1}^{1000}(\text{quality} - \text{estimate})^2}$

What value of α gives the minimum RMSE?

```
alphas <- seq(10,250)
rmse <- sapply(alphas, function(alpha){
    score_reg <- sapply(scores, function(x) overall+sum(x-overall)/(length(x)+alpha))
    sqrt(mean((score_reg - schools$quality)^2))
})
plot(alphas, rmse)
```




```
alphas[which.min(rmse)]
```

```
## [1] 135
```

7. Rank the schools based on the average obtained with the best α from Q6. Note that no small school is incorrectly included.

What is the ID of the top school now?

What is the regularized average score of the 10th school now?

```
alpha <- alphas[which.min(rmse)]
score_reg <- sapply(scores, function(x)
    overall+sum(x-overall)/(length(x)+alpha))
schools %>% mutate(score_reg = score_reg) %>%
    top_n(10, score_reg) %>% arrange(desc(score_reg))
```

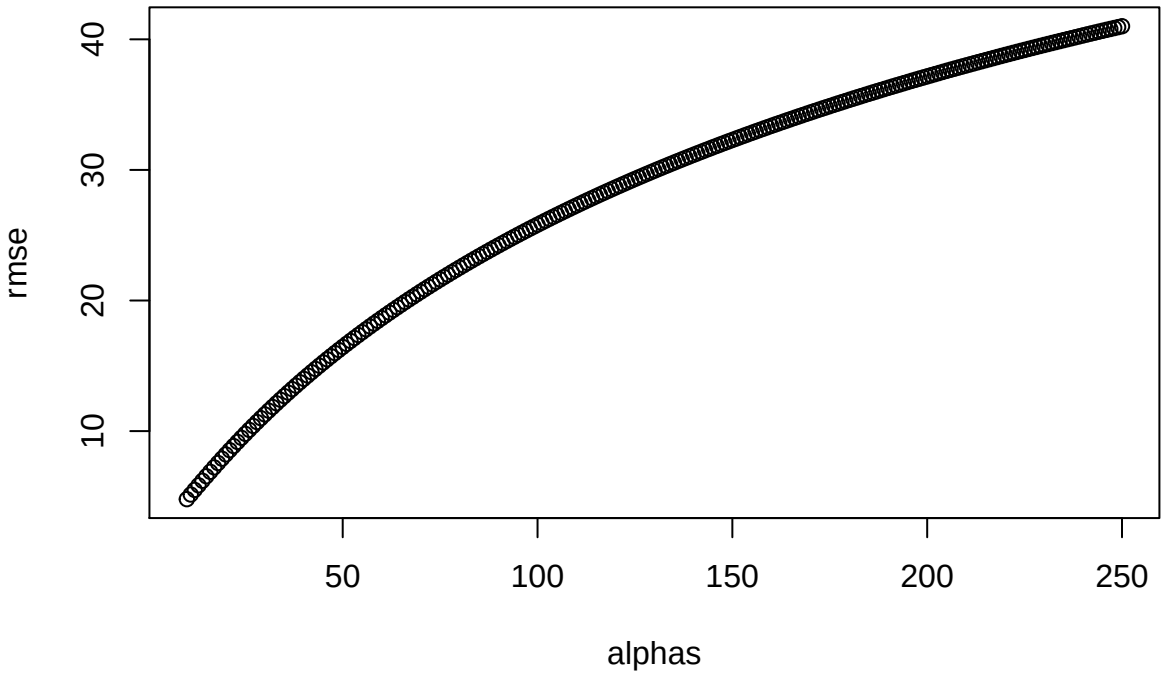
```
##        id size quality  rank score score_reg
## 1  PS 191 1036      94   1.0  93.5      92.0
## 2  PS 567  121      93   2.0  95.8      87.5
## 3  PS 561  723      86  13.5  87.4      86.2
## 4  PS 330  162      84  53.5  91.0      86.0
## 5  PS 591  213      83 104.5  89.7      86.0
## 6  PS 400  550      86  13.5  87.4      85.9
## 7  PS 865  586      86  13.5  87.2      85.8
## 8  PS 266 2369      86  13.5  86.0      85.7
## 9  PS 563  828      86  13.5  86.5      85.5
## 10 PS 574  199      84  53.5  89.2      85.5
```

8. A common mistake made when using regularization is shrinking values towards 0 that are not centered around 0. For example, if we don't subtract the overall average before shrinking, we actually obtain a

very similar result. Confirm this by re-running the code from the exercise in Q6 but without removing the overall mean.

What value of α gives the minimum RMSE here?

```
alphas <- seq(10,250)
rmse <- sapply(alphas, function(alpha){
    score_reg <- sapply(scores, function(x) sum(x)/(length(x)+alpha))
    sqrt(mean((score_reg - schools$quality)^2))
})
plot(alphas, rmse)
```




```
alphas[which.min(rmse)]
```

```
## [1] 10
```