

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, \dots, 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 $X_{i,1}, \dots, X_{i,784}$.
- 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 (\mathbf{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()
```

```

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

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

## Loading required package: dslabs

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

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

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

```

# 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

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

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)

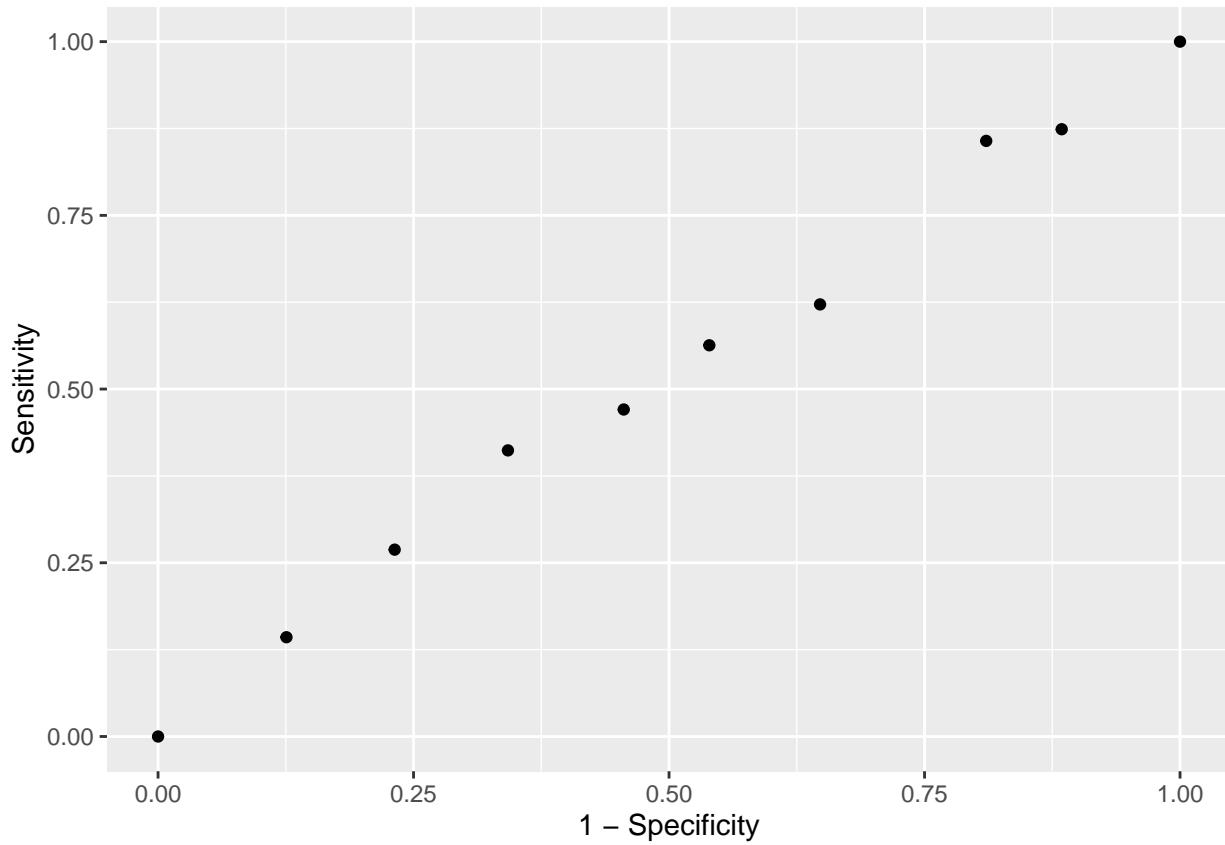
```

```

## [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:

$$p_k(x) = \Pr(Y = k|X = x), \text{ for } k = 1, \dots, K$$

- 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**:

$$p_k(x) = \Pr(Y = k|X = x), \text{ for } k = 1, \dots, K$$

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:

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

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): $P(\text{test}-|\text{healthy}) = 0.90$
- 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): $P(\text{test}-|\text{healthy}) = 0.90$
- 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 $0.1, 0.2, \dots, 0.9$ 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 distribution 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

- 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?

```

# 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] 0.6592608

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

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

```

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

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

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")
```

```

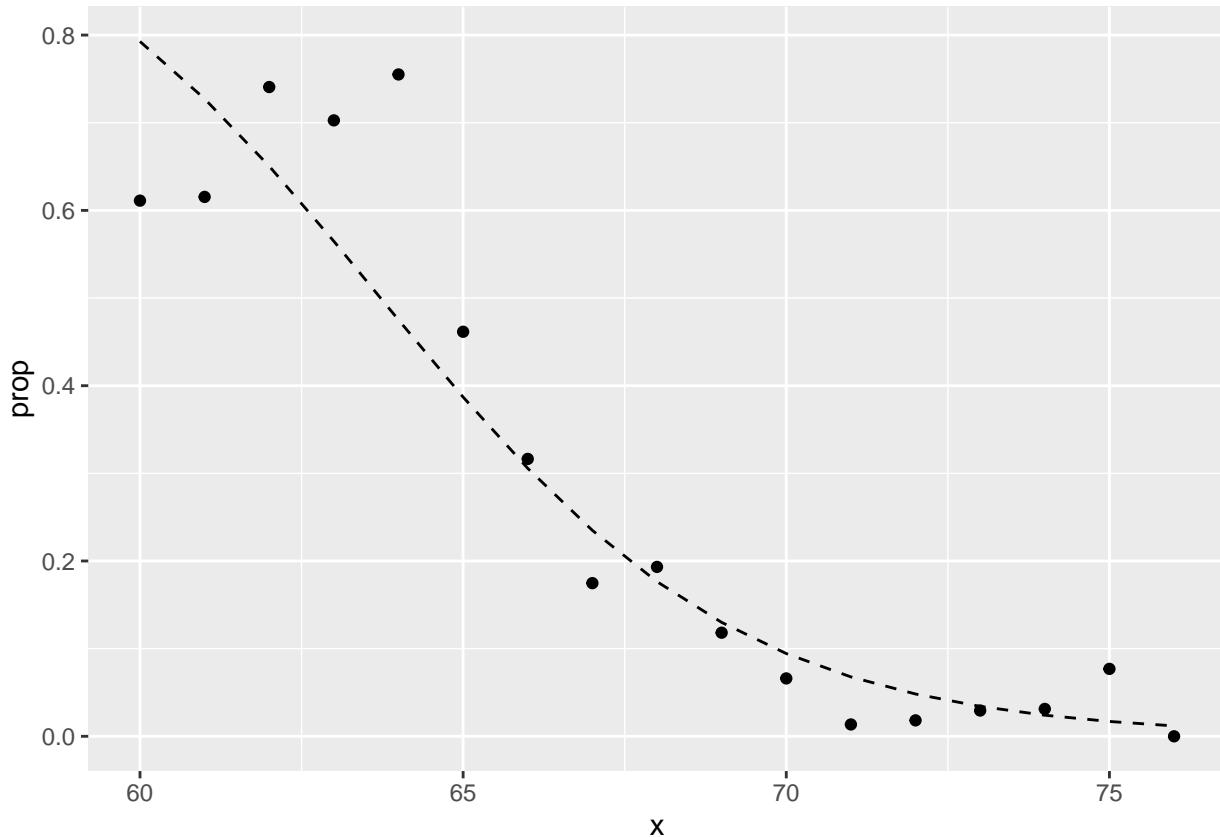
p_hat_logit <- predict(glm_fit, newdata = test_set, type = "response")

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

- 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?

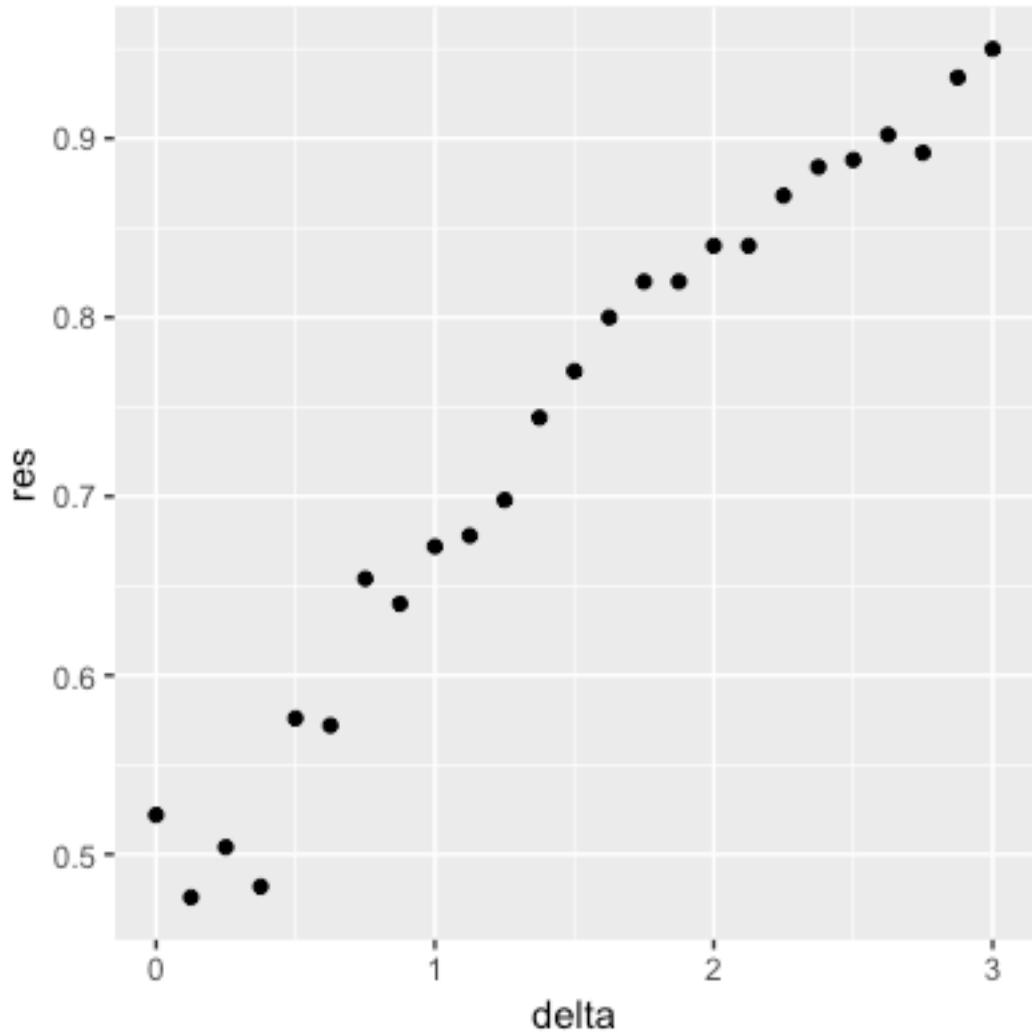
```
set.seed(1) #if you are using R 3.5 or earlier
set.seed(1, sample.kind="Rounding") #if you are using R 3.6 or later

## 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)
```



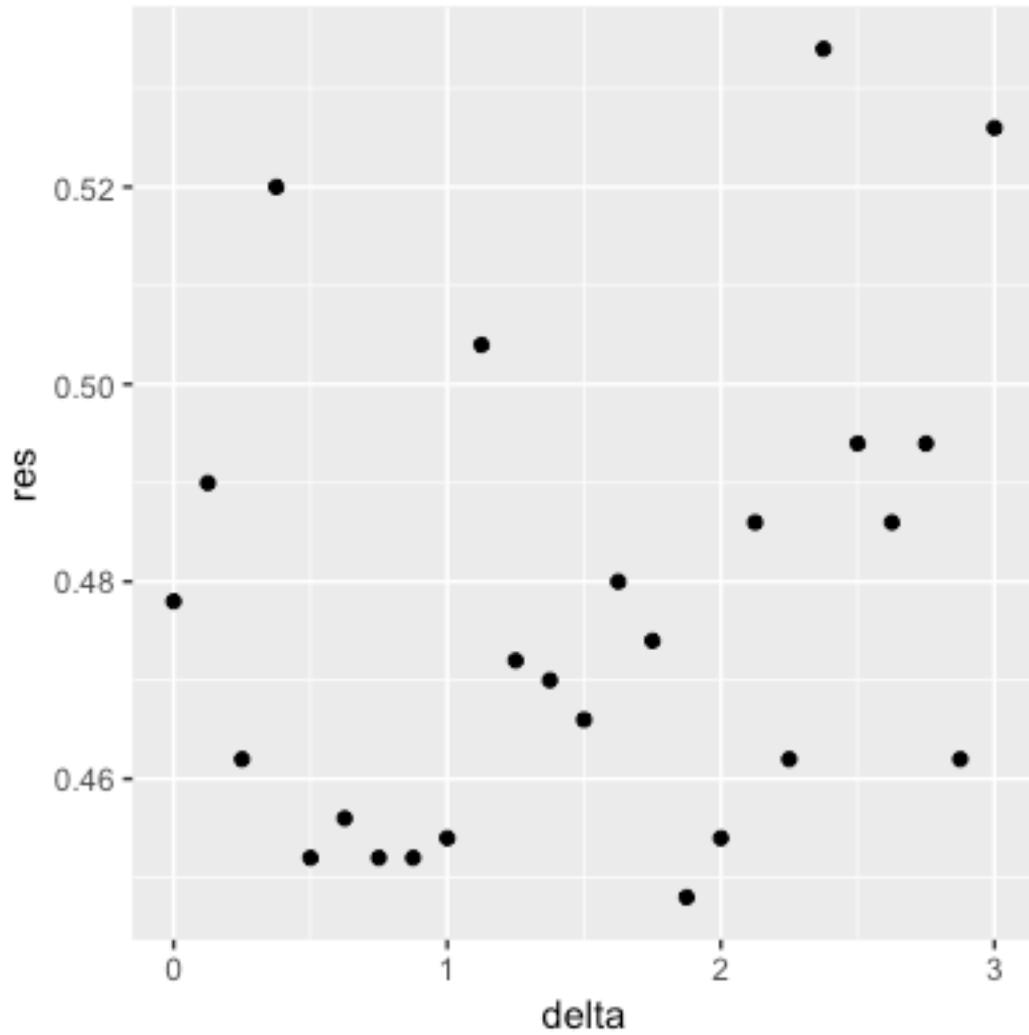
☒ A.



□ 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_2015-18180531.pdf", package="dslabs")
dat <- map_df(str_split(pdf_text(fn), "\n"), function(s){
  s <- str_trim(s)
  header_index <- strwhich(s, "2015")[1]
  tmp <- strsplit(s[header_index], "\\\s+", simplify = TRUE)
  month <- tmp[1]
  header <- tmp[-1]
})
  
```

```

tail_index <- strwhich(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)
```



1:28

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



1:28

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    0
## [2,]    0    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    0    0    0
## [2,]    0    0    0    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    0    0    0
## [2,]    0    0    0    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    0    0    0
## [2,]    0    0    0    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    0    0    0
## [2,]    0    0    0    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    0    0    0
## [2,]    0    0    0    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    0    0    0
## [2,]    0    0    0    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    0
## [2,]    0    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    0    0    0
## [2,]    0    0    0    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    0    0    0
## [2,]    0    0    0    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    0    0    0    51
## [2,]    0    0    0    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    0    0
## [2,]    0    0    0    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    0    0    0
## [2,]    0    0    0    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    0    0
## [,159] [,160] [,161] [,162] [,163] [,164] [,165] [,166] [,167] [,168]
## [1,] 252   237    0    0    0    0    0    0    0    0    0    0
## [2,]    0    0    67   232   39    0    0    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    0    0
## [2,]    0    0    0    0    62   81    0    0    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    0    0
## [,189] [,190] [,191] [,192] [,193] [,194] [,195] [,196] [,197] [,198]
## [1,] 57    6    0    0    0    0    0    0    0    0    0    0
## [2,] 120   180   39    0    0    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    0    0    10
## [2,]    0    0   126   163    0    0    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    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    0    0
## [2,] 40    0    0    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    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    0    0
## [2,]    0    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    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    0    7   135
## [2,]   98   56    0    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    0
## [2,]    0    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    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    0
## [2,]    0    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    0
## [2,]    0    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    0
## [2,]    0    0    0   169   254    57    0    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    0
## [2,]    0    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    0   114
## [2,]    0    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    0
## [2,]    0   169   254    57    0    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    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    0   169
## [,579] [,580] [,581] [,582] [,583] [,584] [,585] [,586] [,587] [,588]
## [1,]   56    0    0    0    0    0    0    0    0    0    0
## [2,]  255   94    0    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    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    0
## [2,]    0    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    0
## [,629] [,630] [,631] [,632] [,633] [,634] [,635] [,636] [,637] [,638]

```

```

## [1,] 252 233 145 0 0 0 0 0 0 0 0
## [2,] 0 0 0 0 0 169 254 153 0 0 0
## [,639] [,640] [,641] [,642] [,643] [,644] [,645] [,646] [,647] [,648]
## [1,] 0 0 0 0 0 0 0 0 0 0 0
## [2,] 0 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 0
## [,659] [,660] [,661] [,662] [,663] [,664] [,665] [,666] [,667] [,668]
## [1,] 0 0 0 0 0 0 0 0 0 0 0
## [2,] 0 0 0 169 255 153 0 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 0
## [2,] 0 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 0
## [2,] 0 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 0
## [2,] 0 96 254 153 0 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 0
## [2,] 0 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 0
## [2,] 0 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 0
## [2,] 0 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 0
## [2,] 0 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 0
## [2,] 0 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 0
## [2,] 0 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 0
## [2,] 0 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 0
## [2,] 0 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
```

```
#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:

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

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

```
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:

```
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

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

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

#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)`
- E. `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"

```

```
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
```

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



```
#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 ~ predictor1 + predictor2 + predictor3`. 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

- 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 $k = \text{seq}(1, 11, 2)$ 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//RtmpLmy1gi/downloaded_packages

## Old packages: 'tm'

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 redefining `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

```

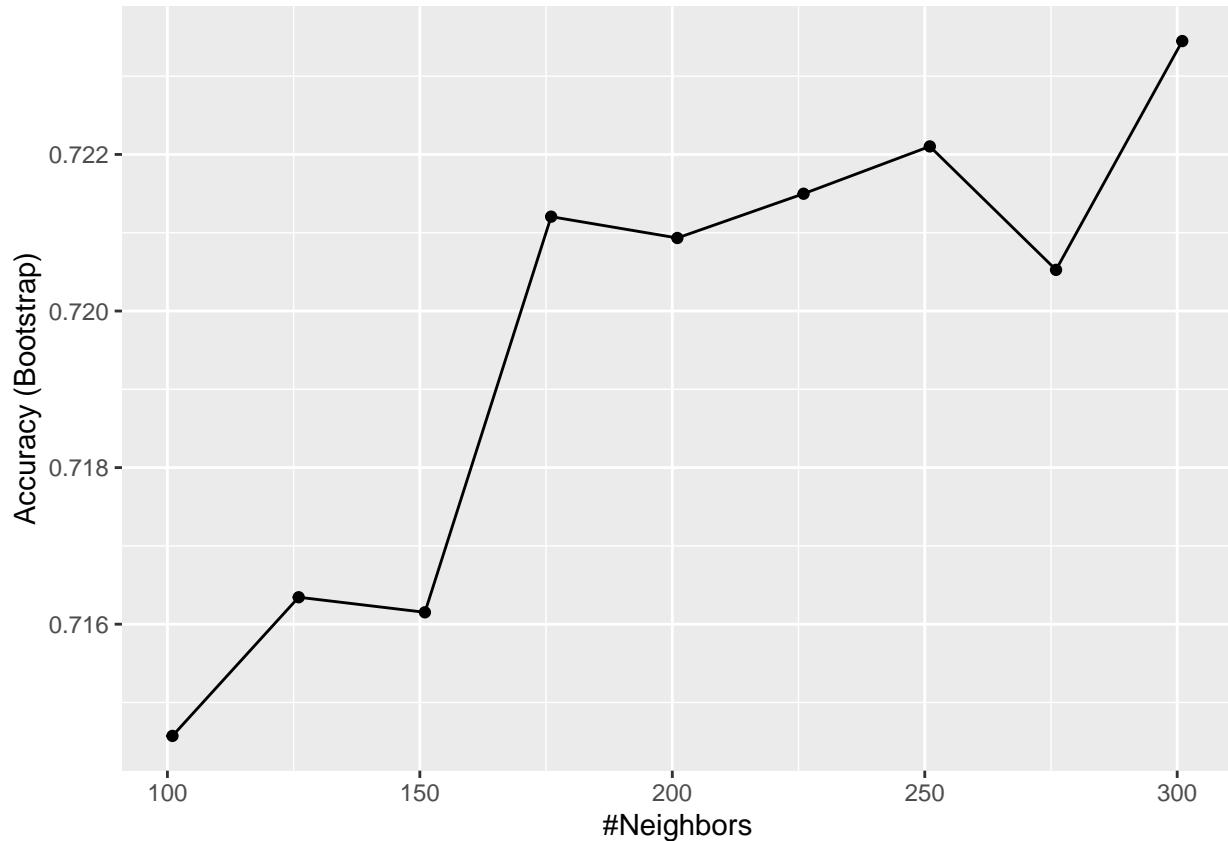
5. Re-run the cross-validation again, but this time using kNN. Try out the following grid `k = seq(101, 301, 25)` of tuning parameters. Make a plot of the resulting accuracies.

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.

```

# 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

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

mean(q_75)

## [1] 0.6656107

sd(q_75)

## [1] 0.1353809

```

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

```

# 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

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.

```

# 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

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 $\hat{p}(x)$ 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.legends=TRUE)

```



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. OA2Z
- 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()
```

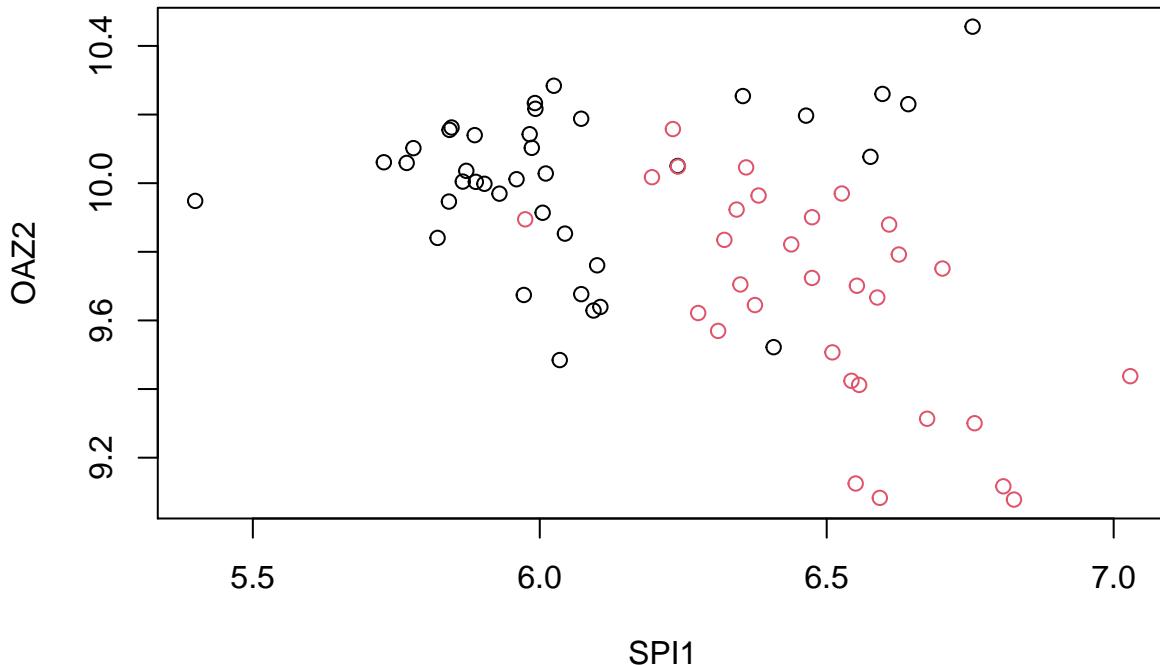


- A. C21orf62
- B. PLCB1
- C. RAB1B
- D. MSH4
- E. OAZ2

- 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)
```



- 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?

```
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, \dots, 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 is also in R_j .
- To pick j and its value s , we find the pair that **minimizes the residual sum of squares (RSS)**:

$$\sum_{i:x_i \in R_1(j,s)} (y_i - \hat{y}_{R_1})^2 + \sum_{i:x_i \in R_2(j,s)} (y_i - \hat{y}_{R_2})^2$$

- 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>  <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)
```



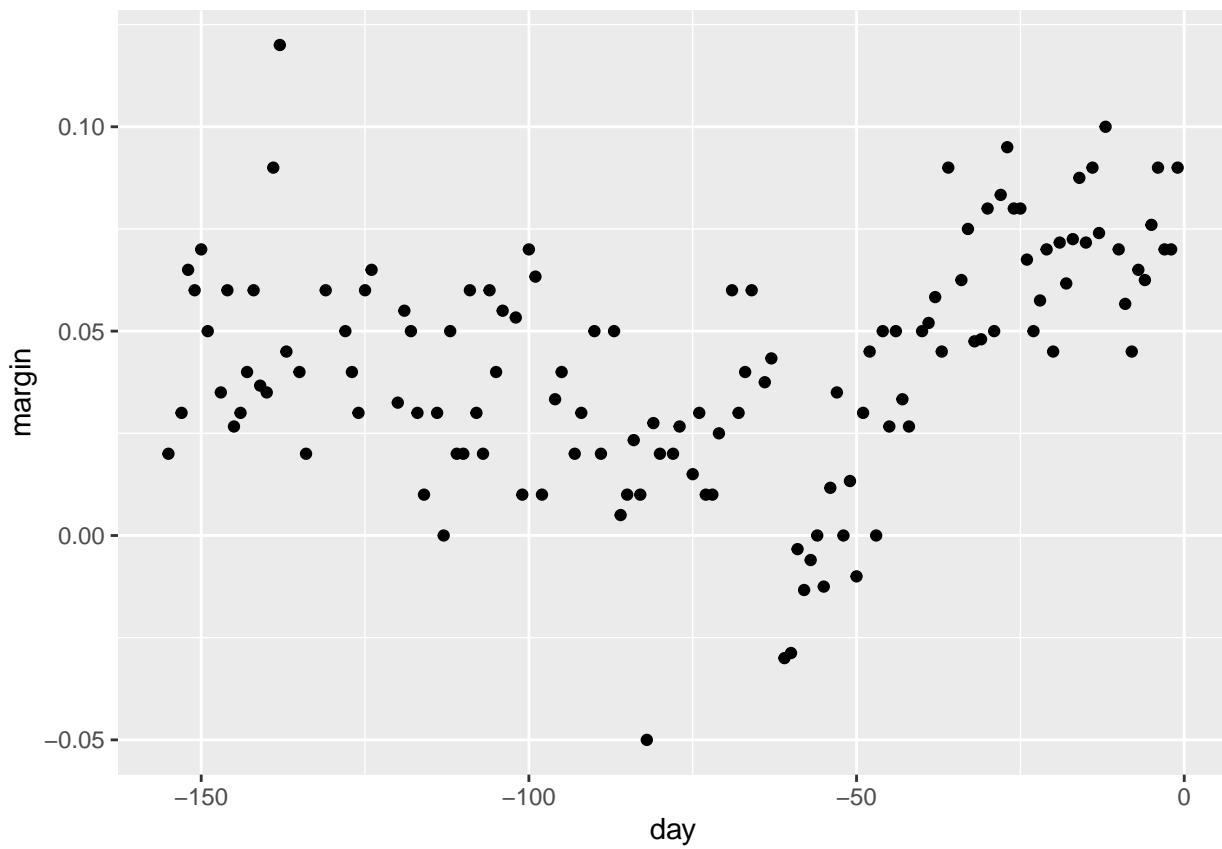
```
# Plot distribution of each predictor stratified by region
olive %>% gather(fatty_acid, percentage, -region) %>%
  ggplot(aes(region, percentage, fill = region)) +
  geom_boxplot() +
  facet_wrap(~fatty_acid, scales = "free") +
  theme(axis.text.x = element_blank())
```



```
# 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")

```



```

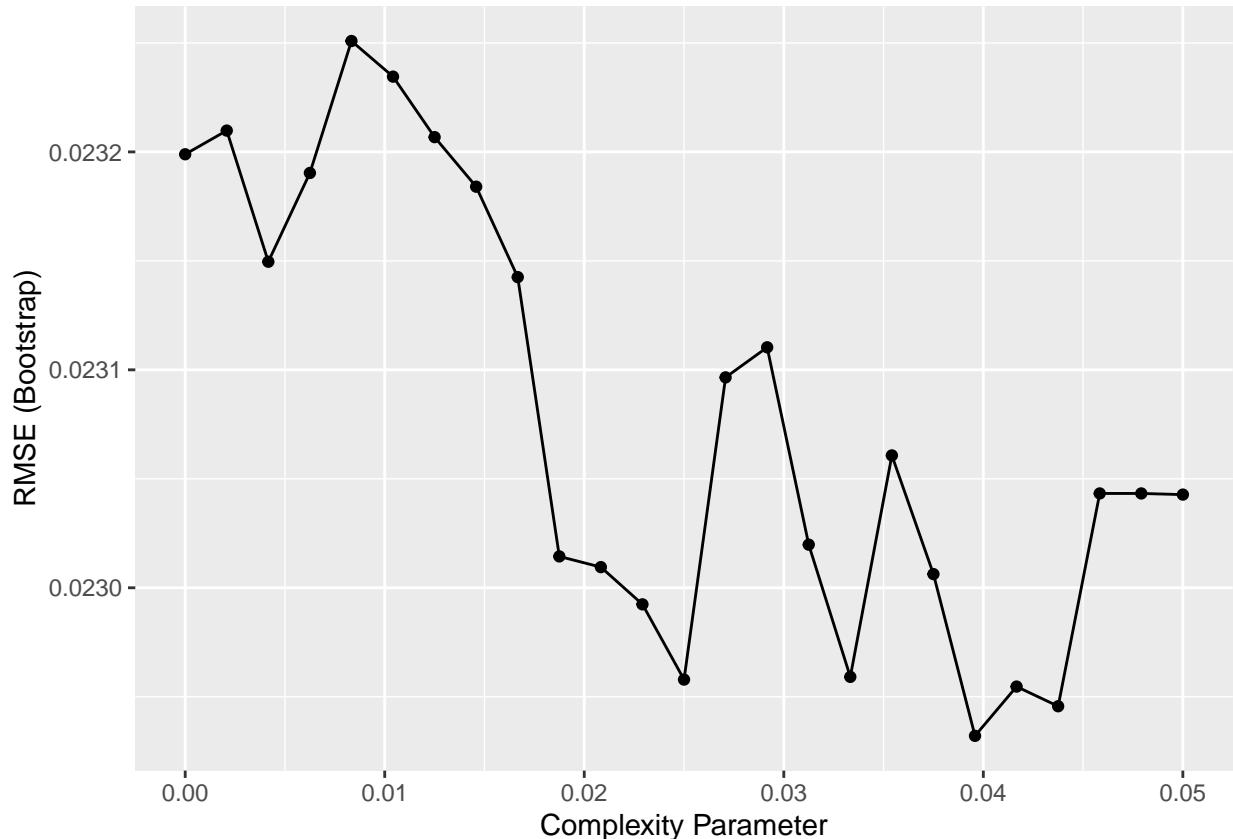
# change parameters
fit <- rpart(margin ~ ., data = polls_2008, control = rpart.control(cp = 0, minsplit = 2))
polls_2008 %>%
  mutate(y_hat = predict(fit)) %>%
  ggplot() +
  geom_point(aes(day, margin)) +
  geom_step(aes(day, y_hat), col="red")

```

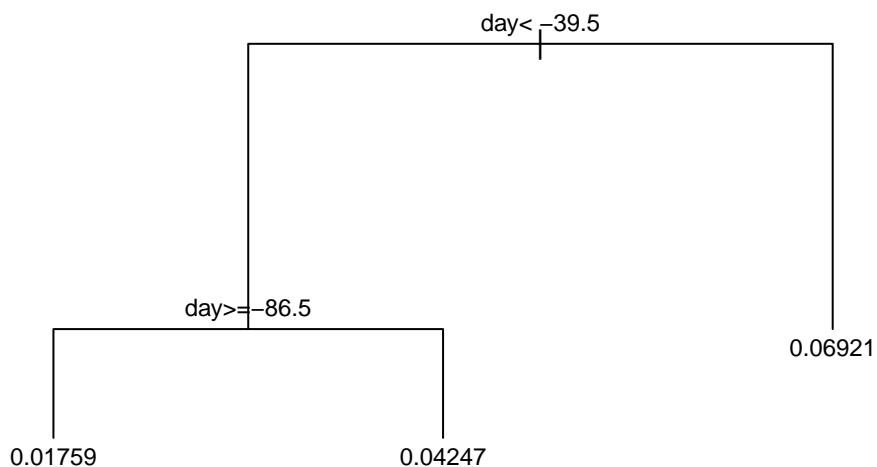


```
# use cross validation to choose cp
```

```
train_rpart <- train(margin ~ ., method = "rpart", tuneGrid = data.frame(cp = seq(0, 0.05, len = 25)),  
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**.

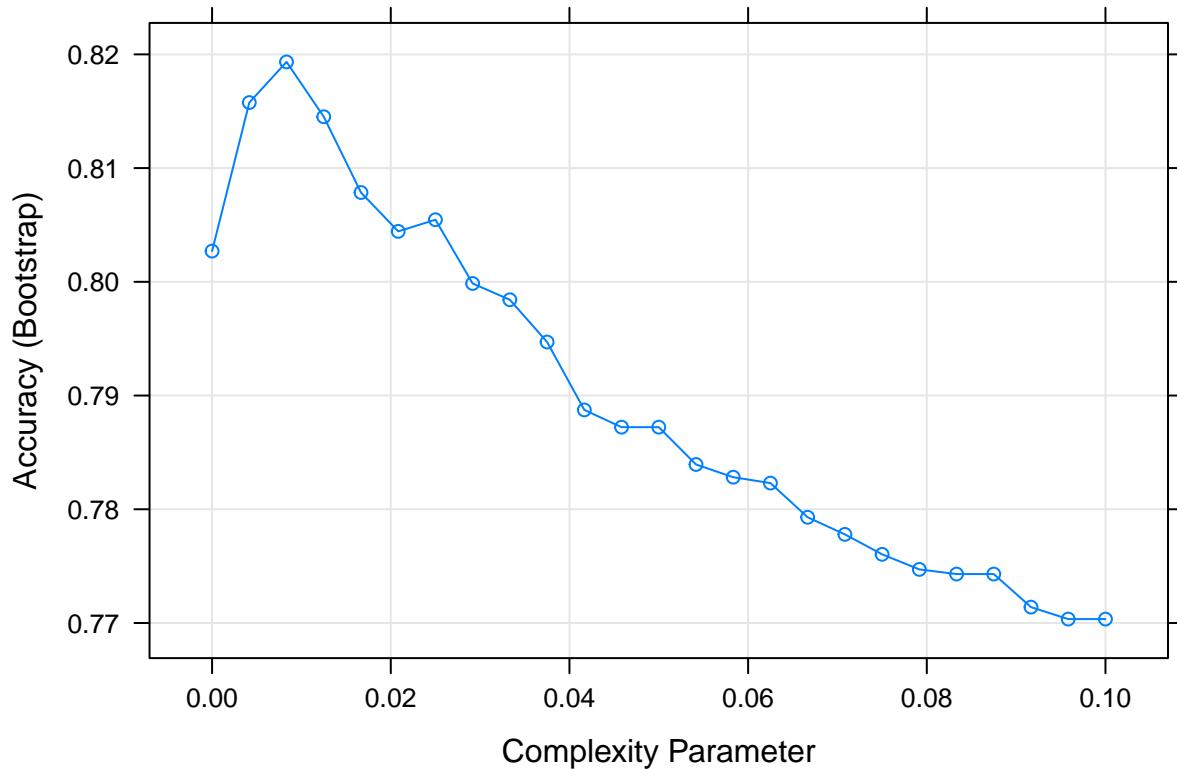
$$\text{Gini}(j) = \sum_{k=1}^K \hat{p}_{j,k} (1 - \hat{p}_{j,k})$$

$$\text{entropy}(j) = - \sum_{k=1}^K \hat{p}_{j,k} \log(\hat{p}_{j,k}), \text{with } 0 \times \log(0) \text{ defined as 0}$$

- 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)
```

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 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
```

```
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?

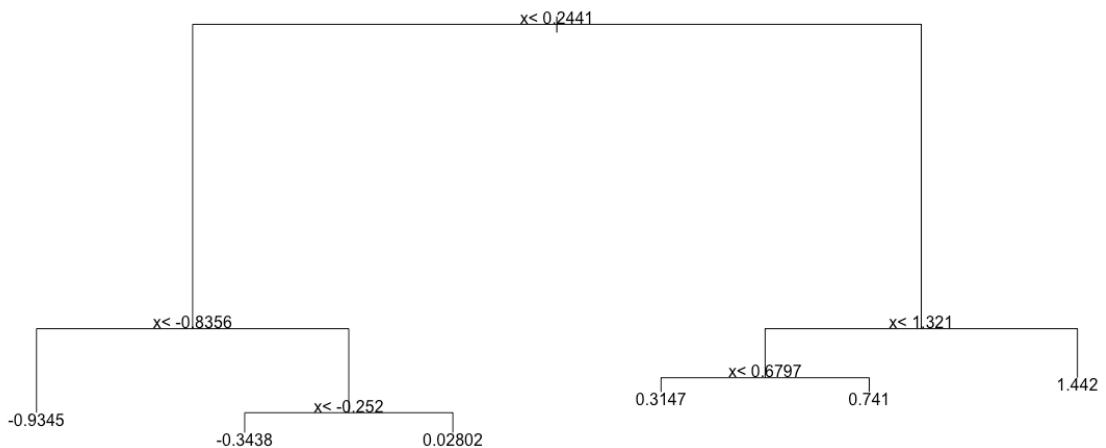
```
fit <- rpart(y ~ ., data = dat)
plot(fit)
text(fit)
```



- A.



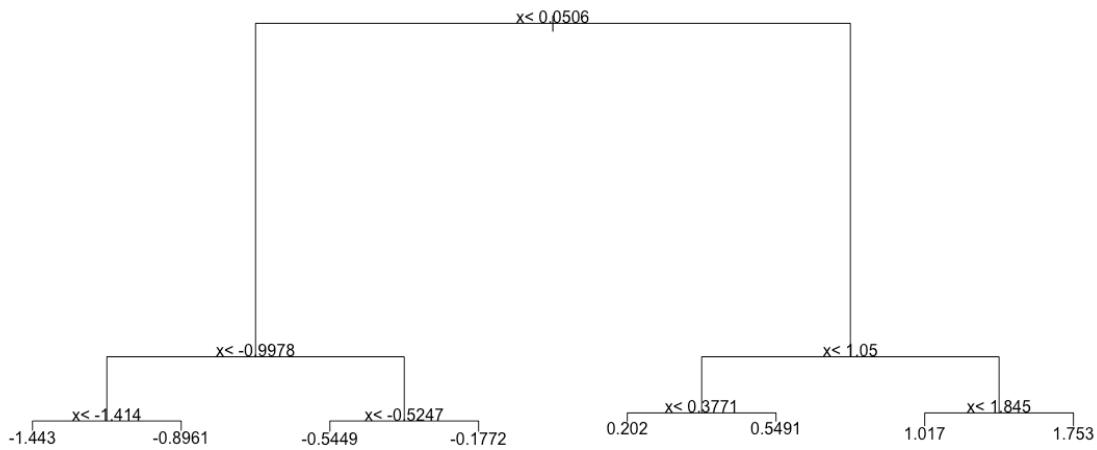
□ B.



□ 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)
```



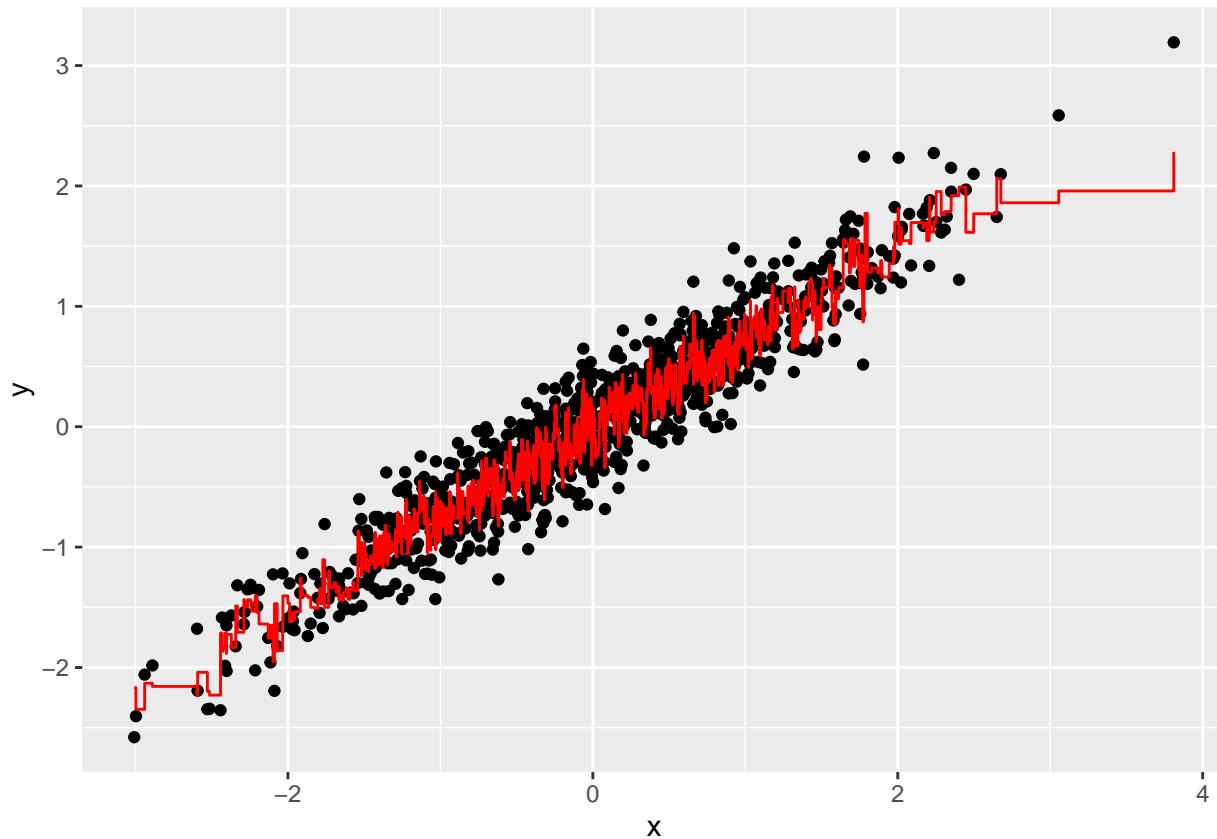
- A. `geom_step(aes(x, y_hat), col=2)`
- B. `geom_smooth(aes(y_hat, x), col=2)`
- C. `geom_quantile(aes(x, y_hat), col=2)`
- D. `geom_step(aes(y_hat, x), col=2)`

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.

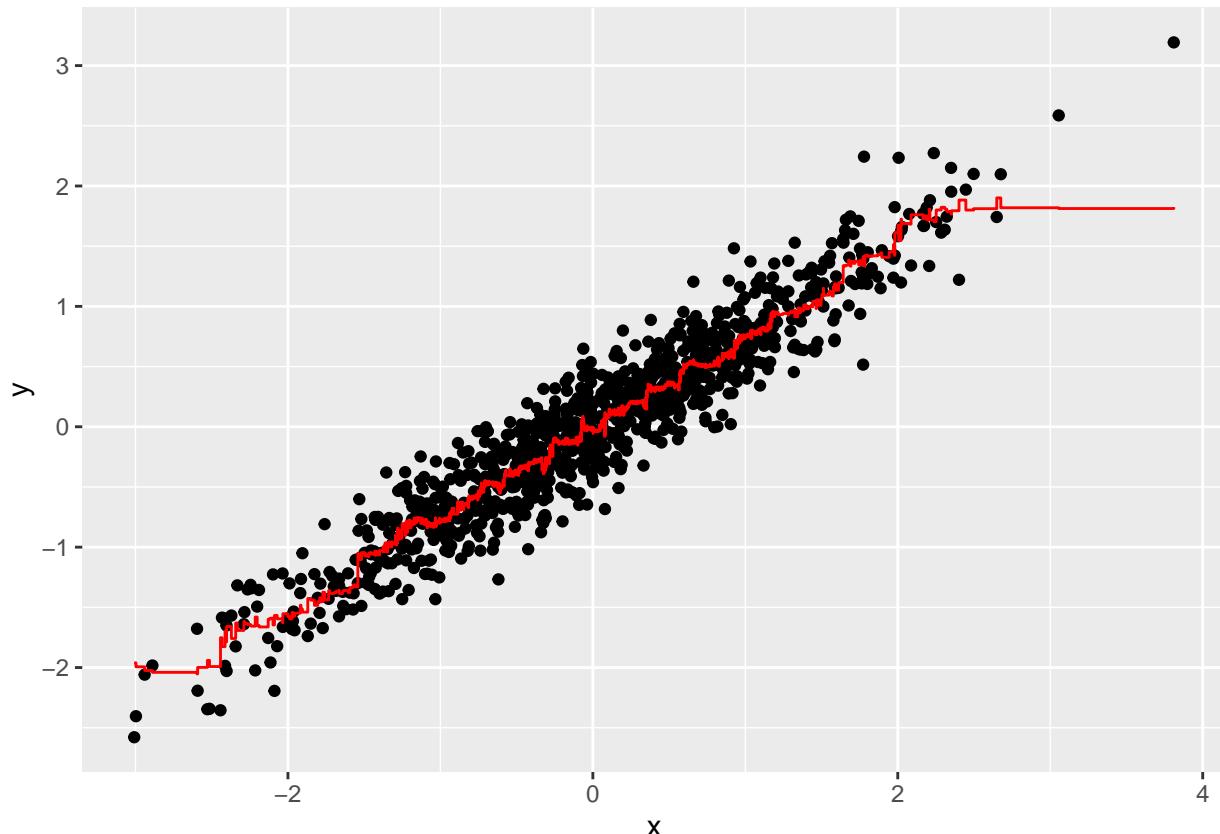
```
library(randomForest)
fit <- #BLANK
dat %>%
  mutate(y_hat = predict(fit)) %>%
  ggplot() +
  geom_point(aes(x, y)) +
  geom_step(aes(x, y_hat), col = "red")
```

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")

## $knn
## $knn$label
## [1] "k-Nearest Neighbors"
##
## $knn$library
## [1] "knn"
##
## $knn$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 = 1),
##                        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 = TRUE)
##   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 = TRUE)
##   predict(modelFit, newdata, type = "prob")
## }
##

```

```

## $knn$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")

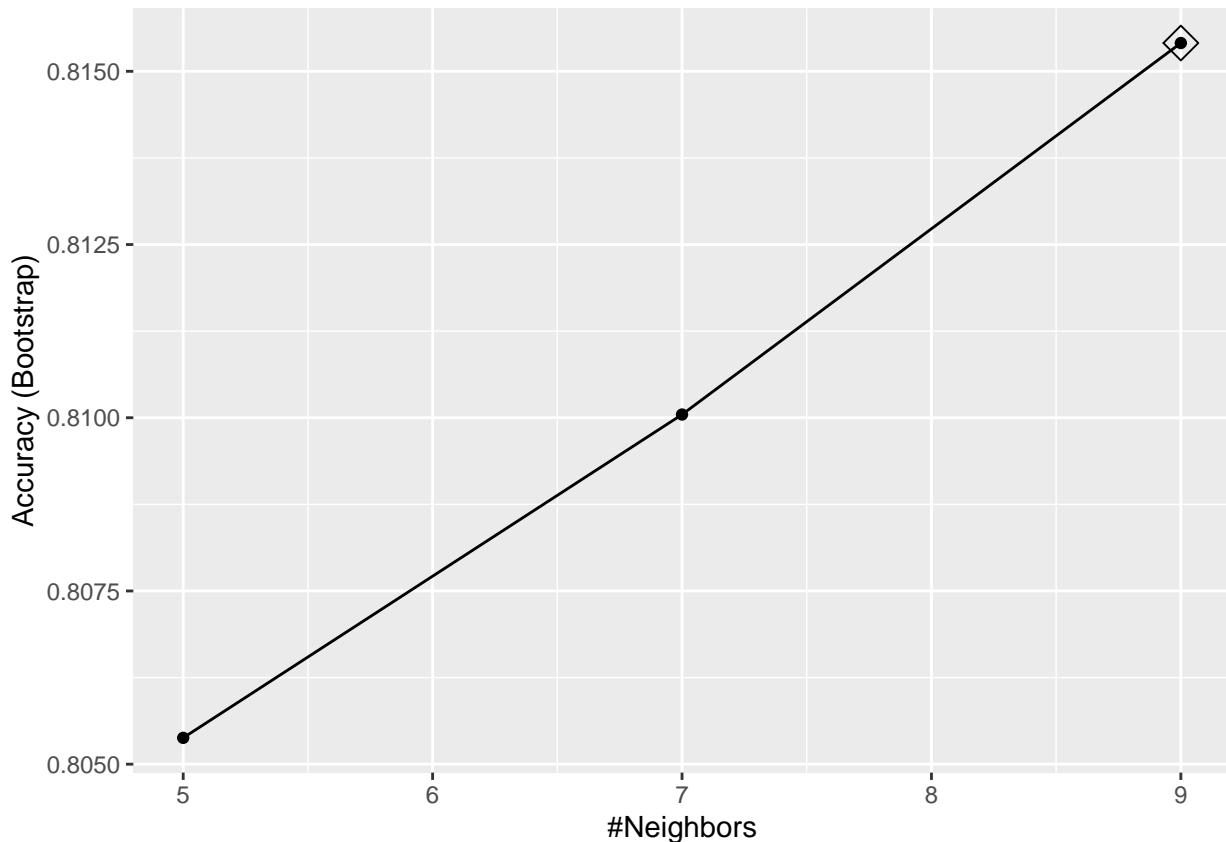
```

```

##   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)

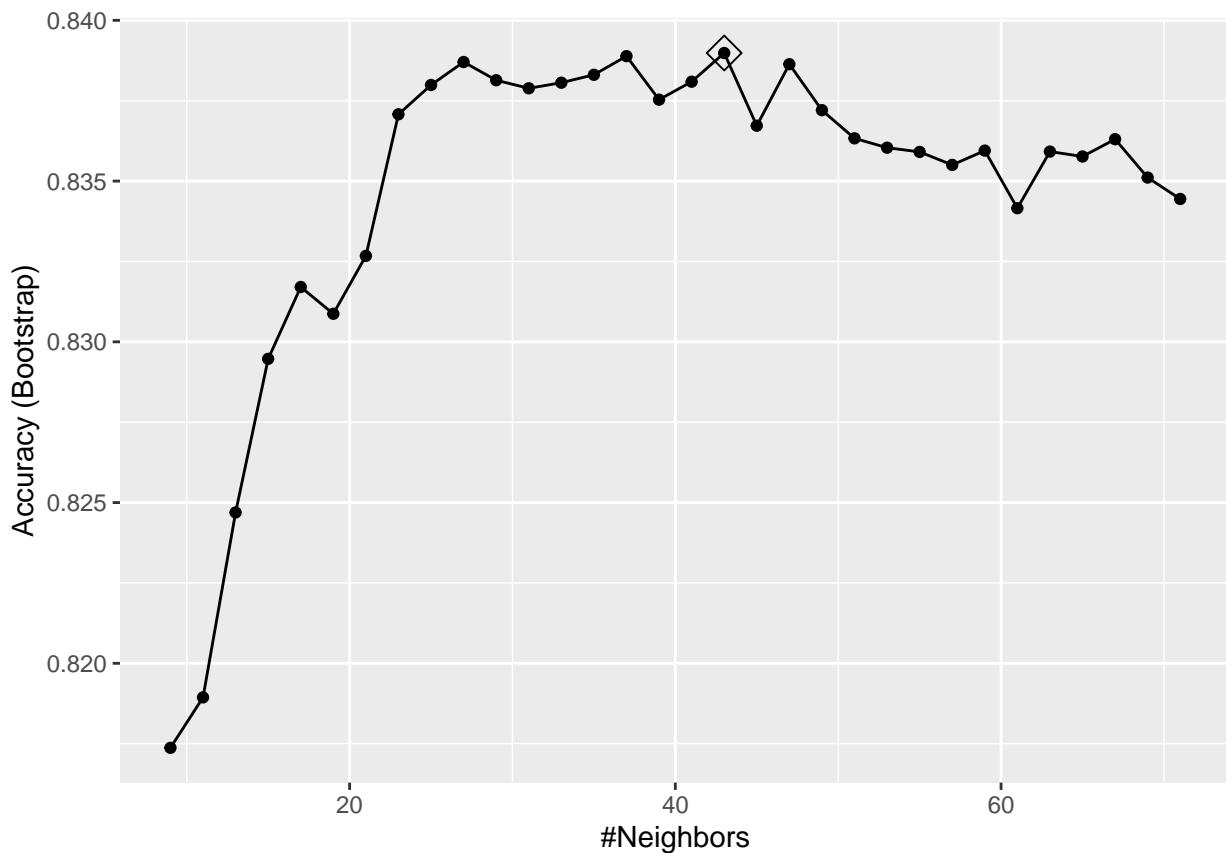
```



```

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"]

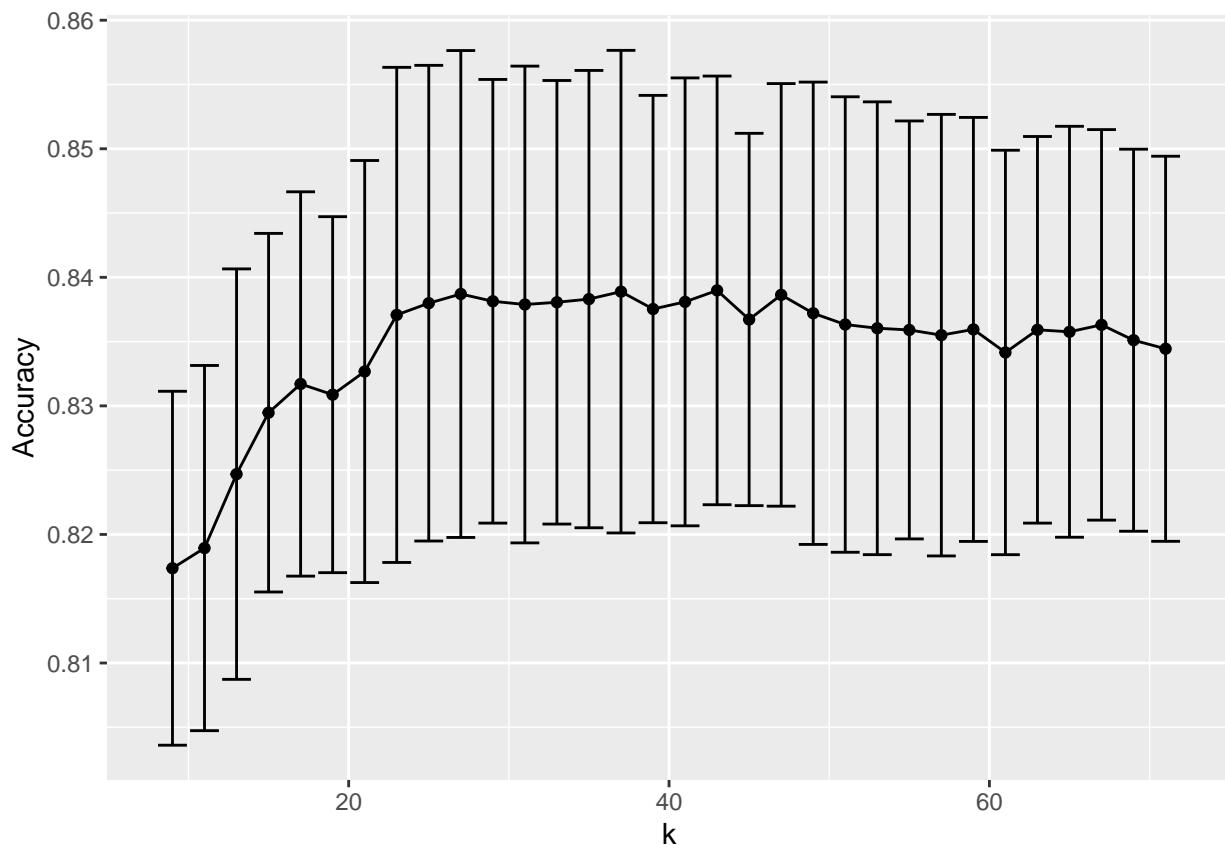
## Accuracy
## 0.855

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)

```

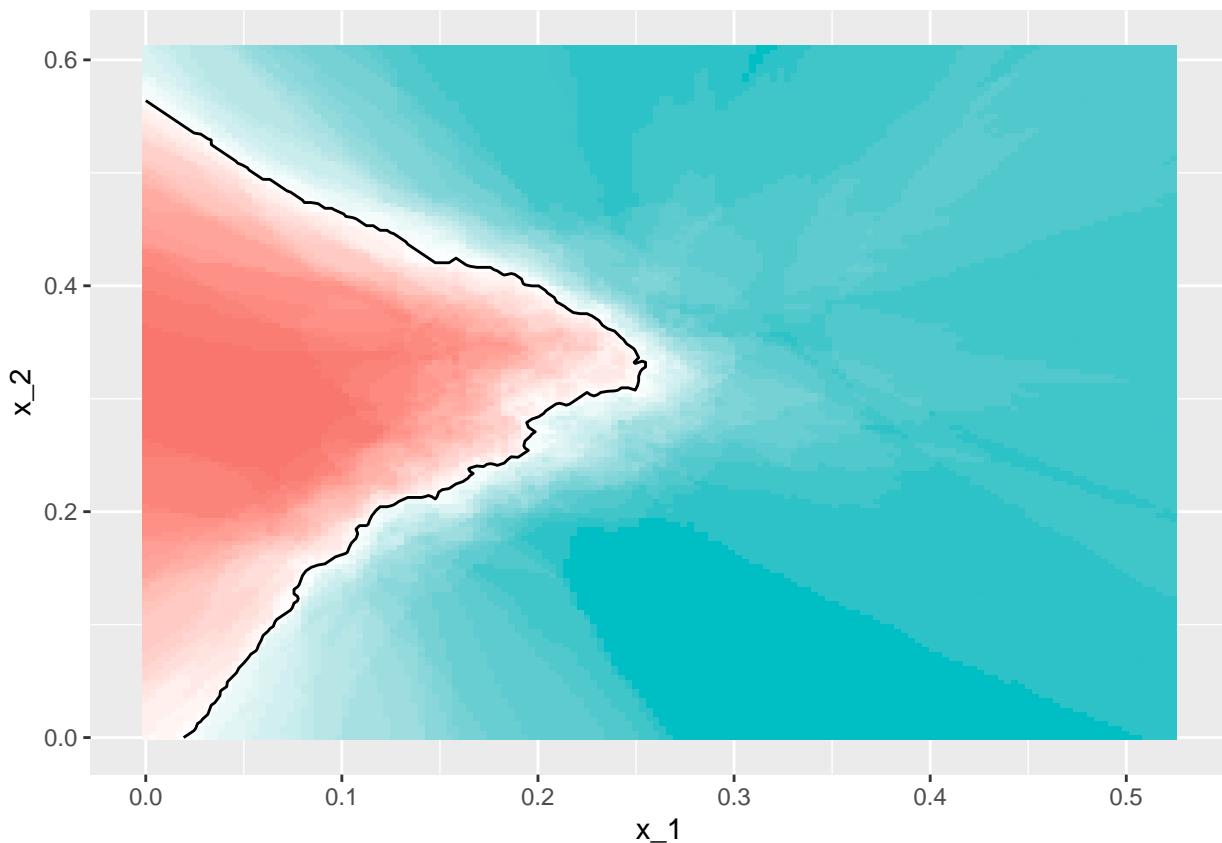


```
train_knn$results %>%
  ggplot(aes(x = k, y = Accuracy)) +
  geom_line() +
  geom_point() +
  geom_errorbar(aes(x = k,
                    ymin = Accuracy - AccuracySD,
                    ymax = Accuracy + AccuracySD))
```



```
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

- 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)

```



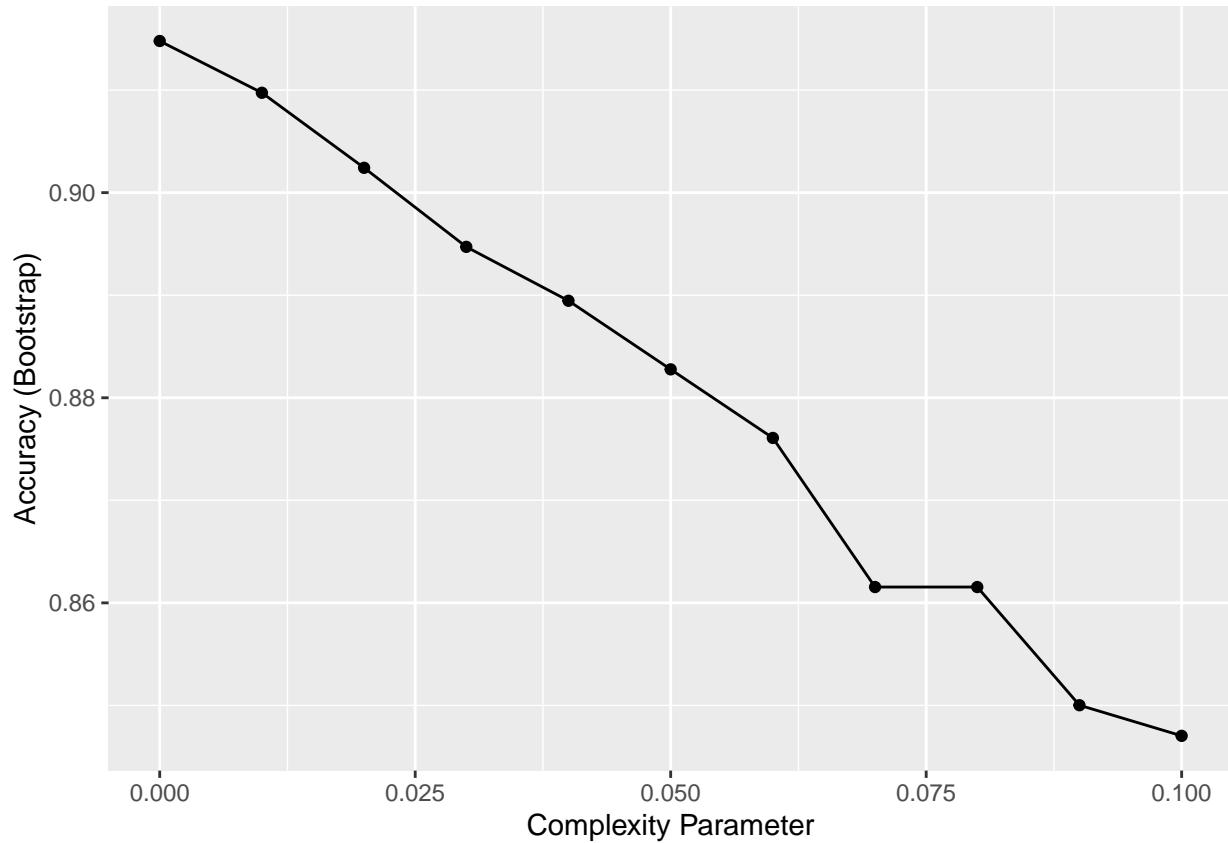
2. Note that there are only 6 placentas in the dataset. By default, `rpart` requires 20 observations before splitting a node. That means that it is difficult to have a node in which placentas are the majority. Rerun the analysis you did in Q1 with `caret::train()`, but this time with `method = "rpart"` 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

```