My Data Science Notes

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Contents

Intro

These notes are pulled from various classes, tutorials, books, etc. and are intended for my own consumption. If you are finding this on the internet, I hope it is useful to you, but you should know that I am just a student and there's a good chance whatever you're reading here is mistaken. In fact, that should probably be your null hypothesis… or your prior. Whatever.

Chapter 1

Probability

1.1 Principles

Here are three rules that come up all the time.

- $Pr(A \cup B) = Pr(A) + Pr(B) - Pr(AB)$. This rule generalizes to $Pr(A \cup B \cup C) = Pr(A) + Pr(B) + Pr(C) - Pr(AB) - Pr(AC) - Pr(BC) + Pr(ABC)$.
- $Pr(A|B) = \frac{P(AB)}{P(B)}$
- If A and B are independent, $Pr(A \cap B) = Pr(A)Pr(B)$, and $Pr(A|B) = Pr(A)$.

Uniform distributions on finite sample spaces often reduce to counting the elements of A and the sample space S, a process called combinatorics. Here are three important combinatorial rules.

Multiplication Rule. $|S| = |S_1| \cdots |S_k|$.

How many outcomes are possible from a sequence of 4 coin flips and 2 rolls of a die? $|S| = |S_1| \cdot |S_2| \ldots |S_6| = 2 \cdot 2 \cdot 2 \cdot 2 \cdot 6 \cdot 6 = 288$.

How many subsets are possible from a set of n=10 elements? In each subset, each element is either included or not, so there are $2^n = 1024$ subsets.

How many subsets are possible from a set of n=10 elements taken k at a time with replacement? Each experiment has n possible outcomes and is repeated k times, so there are n^k subsets.

Permutations. The number of *ordered* arrangements (permutations) of a set of $|S| = n$ items taken k at a time *without* replacement has $n(n-1) \ldots (n-k+1)$

subsets because each draw is one of k experiments with decreasing number of possible outcomes.

$$_nP_k = \frac{n!}{(n-k)!}$$

Notice that if $k = 0$ then there is 1 permutation; if $k = 1$ then there are n permutations; if $k = n$ then there are $n!$ permutations.

How many ways can you distribute 4 jackets among 4 people? $_nP_k = \frac{4!}{(4-4)!} = 4! = 24$

How many ways can you distribute 4 jackets among 2 people? $_nP_k = \frac{4!}{(4-2)!} = 12$

Subsets. The number of *unordered* arrangements (combinations) of a set of $|S| = n$ items taken k at a time *without* replacement has

$$_nC_k = \binom{n}{k} = \frac{n!}{k!(n-k)!}$$

combinations and is called the binomial coefficient. The binomial coefficient is the number of different subsets. Notice that if k=0 then there is 1 subset; if k=1 then there are n subsets; if k=n then there is 1 subset. The connection with the permutation rule is that there are $n!/(n-k)!$ permutations and each permutation has $k!$ permutations.

How many subsets of 7 people can be taken from a set of 12 persons? $_{12}C_7 = \binom{12}{7} = \frac{12!}{7!(12-7)!} = 792$

If you are dealt five cards, what is the probability of getting a "full-house" hand containing three kings and two aces (KKKAA)?

$$P(F) = \frac{\binom{4}{3}\binom{4}{2}}{\binom{52}{5}}$$

Distinguishable permutations. The number of *unordered* arrangements (distinguishable permutations) of a set of $|S| = n$ items in which n_1 are of one type, n_2 are of another type, etc., is

$$\binom{n}{n_1, n_2, \ldots, n_k} = \frac{n!}{n_1!n_2!\ldots n_k!}$$

How many ordered arrangements are there of the letters in the word PHILIPPINES? There are n=11 objects. $|P| = n_1 = 3$; $|H| = n_2 = 1$; $|I| = n_3 = 3$; $|L| = n_4 = 1$; $|N| = n_5 = 1$; $|E| = n_6 = 1$; $|S| = n_7 = 1$.

$$\binom{n}{n_1, n_2, \dots, n_k} = \frac{11!}{3!1!3!1!1!1!1!} = 1,108,800$$

How many ways can a research pool of 15 subjects be divided into three equally sized test groups?

$$\binom{n}{n_1, n_2, \dots, n_k} = \frac{15!}{5!5!5!} = 756,756$$

1.2 Discrete Distributions

1.2.1 Binomial

If X is the count of successful events in n identical and independent Bernoulli trials of success probability p, then X is a random variable with a binomial distribution $X \sim b(n, p)$ with mean $\mu = np$ and variance $\sigma^2 = np(1-p)$. The probability of $X = x$ successes in n trials is

$$P(X = x) = \frac{n!}{x!(n-x)!} p^x (1-p)^{n-x}.$$

What is the probability 2 out of 10 coin flips are heads if the probability of heads is 0.3?

Function `dbinom()` calculates the binomial probability.

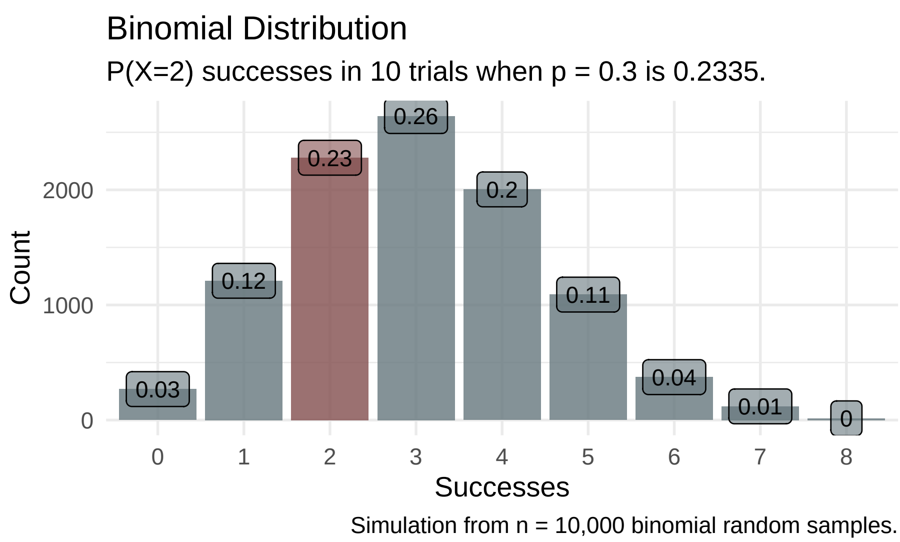
```
dbinom(x = 2, size = 10, prob = 0.3)
```

```
## [1] 0.2334744
```

A simulation of n = 10,000 random samples of size 10 gives a similar result. `rbinom()` generates a random sample of numbers from the binomial distribution.

```
library(tidyverse)

data.frame(cnt = rbinom(n = 10000, size = 10, prob = 0.3)) %>%
  count(cnt) %>%
  ungroup() %>%
  mutate(pct = n / sum(n),
         X_eq_x = cnt == 2) %>%
  ggplot(aes(x = as.factor(cnt), y = n, fill = X_eq_x, label = pct)) +
  geom_col(alpha = 0.8) +
```

```
  scale_fill_manual(values = c(my_colors$grey, my_colors$red)) +
  geom_label(aes(label = round(pct, 2)), size = 3, alpha = .6) +
  theme_minimal() +
  theme(legend.position = "none") +
  labs(title = "Binomial Distribution",
       subtitle = paste0("P(X=2) successes in 10 trials when p = 0.3 is ", round(dbinom
       x = "Successes",
       y = "Count",
       caption = "Simulation from n = 10,000 binomial random samples.")
```



What is the probability of <=2 heads in 10 coin flips where probability of heads is 0.3?

The cumulative probability is the sum of the first three bars in the simulation above. Function `pbinom()` calculates the *cumulative* binomial probability.

```
pbinom(q = 2, size = 10, prob = 0.3, lower.tail = TRUE)
```

```
## [1] 0.3827828
```

What is the expected number of heads in 25 coin flips if the probability of heads is 0.3?

The expected value, $\mu = np$, is 7.5. Here's an empirical test from 10,000 samples.

```
mean(rbinom(n = 10000, size = 25, prob = .3))
```

```
## [1] 7.5149
```

The variance, $\sigma^2 = np(1-p)$, is 5.25. Here's an empirical test.

```
var(rbinom(n = 10000, size = 25, prob = .3))
```

```
## [1] 5.185593
```

Suppose X and Y are independen random variables distributed $X \sim b(10, .6)$ and $Y \sim b(10, .7)$. What is the probability that either variable is <=4?

Let $P(A) = P(X <= 4)$ and $P(B) = P(Y <= 4)$. Then $P(A|B) = P(A) + P(B) - P(AB)$, and because the events are independent, $P(AB) = P(A)P(B)$.

```
p_a <- pbinom(q = 4, size = 10, prob = 0.6, lower.tail = TRUE)
p_b <- pbinom(q = 4, size = 10, prob = 0.7, lower.tail = TRUE)
p_a + p_b - (p_a * p_b)
```

```
## [1] 0.2057164
```

Here's an empirical test.

```
df <- data.frame(
  x = rbinom(10000, 10, 0.6),
  y = rbinom(10000, 10, 0.7)
  )
mean(if_else(df$x <= 4 | df$y <= 4, 1, 0))
```

```
## [1] 0.2061
```

1.2.2 Negative-Binomial

If X is the count of trials required to reach a target number r of successful events in identical and independent Bernoulli trials of success probability p, then X is a random variable with a negative-binomial distribution $X \sim nb(r, p)$ with mean $\mu = r/p$ and variance $\sigma^2 = r(1-p)/p^2$. The probability of $X = x$ trials prior to r successes is

$$P(X = x) = \binom{x-1}{r-1} p^r (1-p)^{x-r}.$$

An oil company has a p = 0.20 chance of striking oil when drilling a well. What is the probability the company drills x = 7 wells to strike oil r = 3 times?

$$P(X = 7) = \binom{7-1}{3-1}(0.2)^3(1-0.2)^{(7-3)} = 0.049.$$

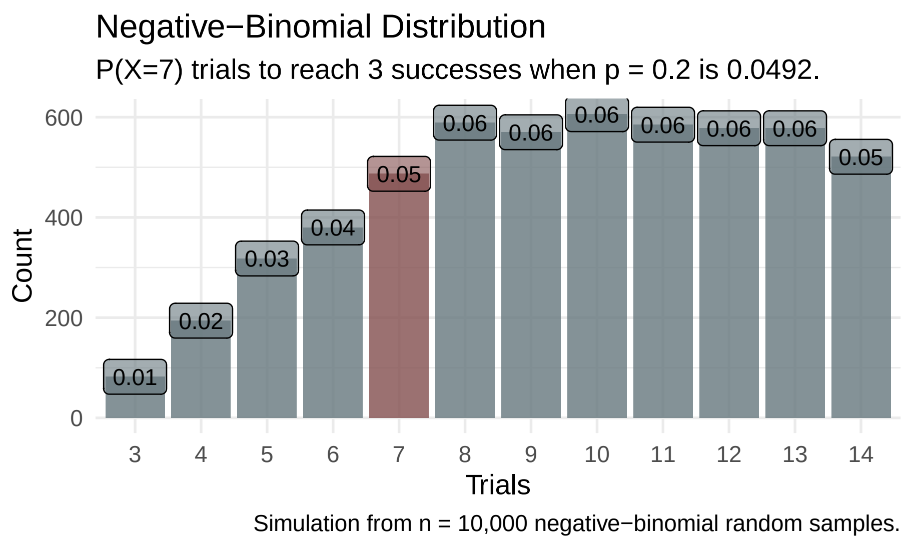
Function `dnbinom()` calculates the negative-binomial probability. Parameter `x` equals the number of failures, $x - r$.

```
dnbinom(x = 4, size = 3, prob = 0.2)
```

```
## [1] 0.049152
```

Here is a simulation of n = 10,000 random samples. `rnbinom()` generates a random sample of numbers from the negative-binomial distribution.

```
data.frame(cnt = rnbinom(n = 10000, size = 3, prob = 0.2)) %>%
  count(cnt) %>%
  ungroup() %>%
  mutate(pct = n / sum(n),
         X_eq_x = cnt == 7-3,
         cnt = cnt + 3) %>%
  filter(cnt < 15) %>%
  ggplot(aes(x = as.factor(cnt), y = n, fill = X_eq_x, label = pct)) +
  geom_col(alpha = 0.8) +
  scale_fill_manual(values = c(my_colors$grey, my_colors$red)) +
  geom_label(aes(label = round(pct, 2)), size = 3, alpha = .6, check_overlap = TRUE) +
  theme_minimal() +
  theme(legend.position = "none") +
  labs(title = "Negative-Binomial Distribution",
       subtitle = paste0("P(X=7) trials to reach 3 successes when p = 0.2 is ", round(d
       x = "Trials",
       y = "Count",
       caption = "Simulation from n = 10,000 negative-binomial random samples.")
```



1.2.3 Geometric

If X is the count of independent Bernoulli trials of success probability p required to achieve the first successful trial, then X is a random variable with a geometric distribution $X \sim G(p)$ with mean $\mu = \frac{n}{p}$ and variance $\sigma^2 = \frac{(1-p)}{p^2}$. The probability of $X = n$ trials is

$$f(X = n) = p(1-p)^{n-1}.$$

The probability of $X <= n$ trials is

$$F(X = n) = 1 - (1-p)^n.$$

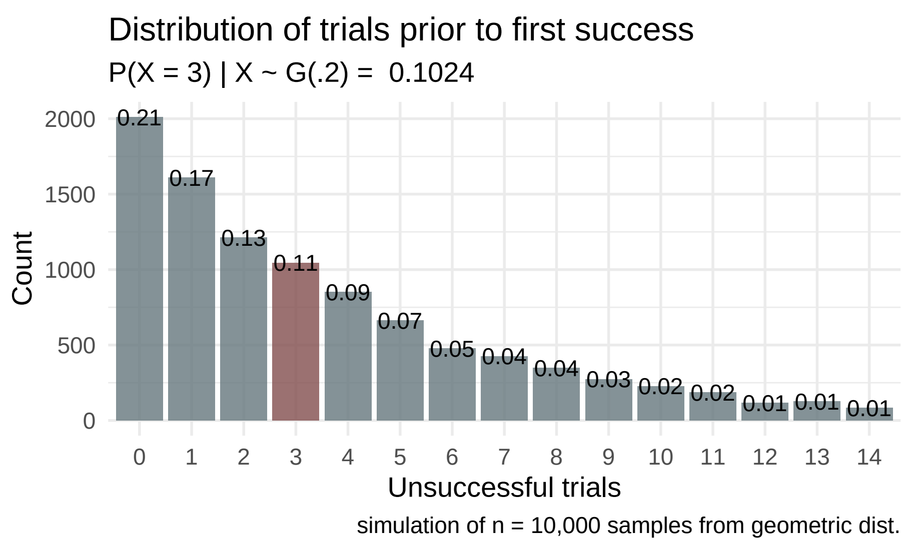
Example. A sports marketer randomly selects persons on the street until he encounters someone who attended a game last season. What is the probability the marketer encounters x = 3 people who did not attend a game before the first success if p = 0.20 of the population attended a game?

Function `pgeom()` calculates the geometric distribution probability.

```
dgeom(x = 3, prob = 0.20)
```

```
## [1] 0.1024
```

```
data.frame(cnt = rgeom(n = 10000, prob = 0.20)) %>%
  count(cnt) %>%
  top_n(n = 15, wt = n) %>%
  ungroup() %>%
  mutate(pct = round(n / sum(n), 2),
         X_eq_x = cnt == 3) %>%
  ggplot(aes(x = as.factor(cnt), y = n, fill = X_eq_x, label = pct)) +
  geom_col(alpha = 0.8) +
  scale_fill_manual(values = c(my_colors$grey, my_colors$red)) +
  geom_text(size = 3) +
  theme_minimal() +
  theme(legend.position = "none") +
  labs(title = "Distribution of trials prior to first success",
       subtitle = paste("P(X = 3) | X ~ G(.2) = ", round(dgeom(3, .2), 4)),
       x = "Unsuccessful trials",
       y = "Count",
       caption = "simulation of n = 10,000 samples from geometric dist.")
```



1.3 Continuous Distributions

1.3.1 Normal

Random variable X is distributed $X \sim N(\mu, \sigma^2)$ if

$$f(X) = \frac{1}{\sigma\sqrt{2\pi}} e^{-.5(\frac{x-\mu}{\sigma})^2}$$

.

Example

IQ scores are distributed $X \sim N(100, 16^2$. What is the probability a randomly selected person's IQ is <90?

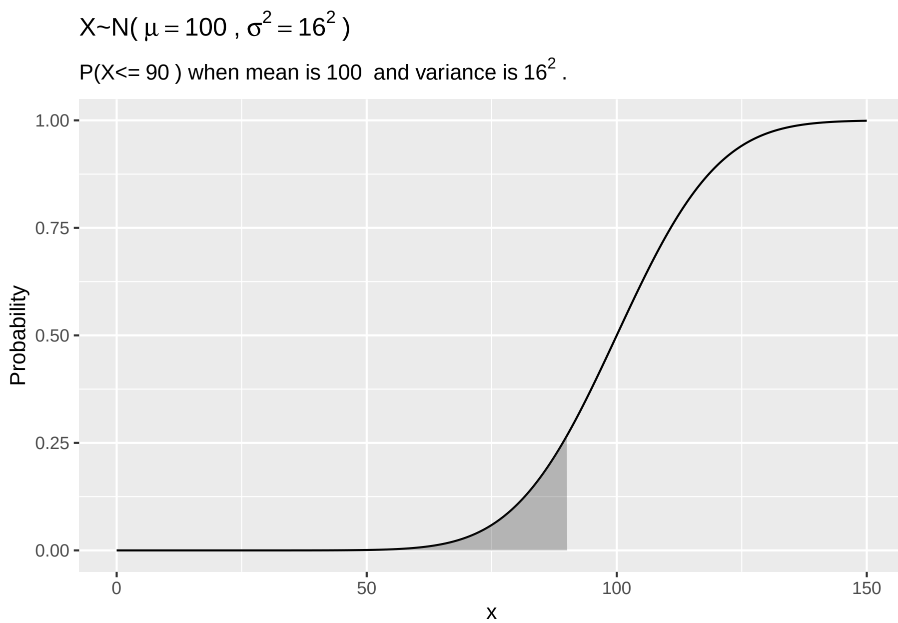
```
my_mean = 100
my_sd = 16
my_x = 90
# exact
pnorm(q = my_x, mean = my_mean, sd = my_sd, lower.tail = TRUE)
```

```
## [1] 0.2659855
```

```
# simulated
mean(rnorm(n = 10000, mean = my_mean, sd = my_sd) <= my_x)
```

```
## [1] 0.2599
```

```
library(dplyr)
library(ggplot2)

data.frame(x = 0:1500 / 10,
           prob = pnorm(q = 0:1500 / 10,
                        mean = my_mean,
                        sd = my_sd,
                        lower.tail = TRUE)) %>%
  mutate(cdf = ifelse(x > 0 & x <= my_x, prob, 0)) %>%
ggplot() +
  geom_line(aes(x = x, y = prob)) +
  geom_area(aes(x = x, y = cdf), alpha = 0.3) +
  labs(title = bquote('X~N('~mu==.(my_mean)~','~sigma^{2}==.(my_sd)^{2}~')'),
       subtitle = bquote('P(X<='~.(my_x)~') when mean is'~.(my_mean)~' and variance is'~.(my_sd)^
       x = "x",
       y = "Probability")
```



1.3.2 Example

IQ scores are distributed $X \sim N(100, 16^2$. What is the probability a randomly selected person's IQ is >140?

```
my_mean = 100
my_sd = 16
my_x = 140
# exact
pnorm(q = my_x, mean = my_mean, sd = my_sd, lower.tail = FALSE)
```

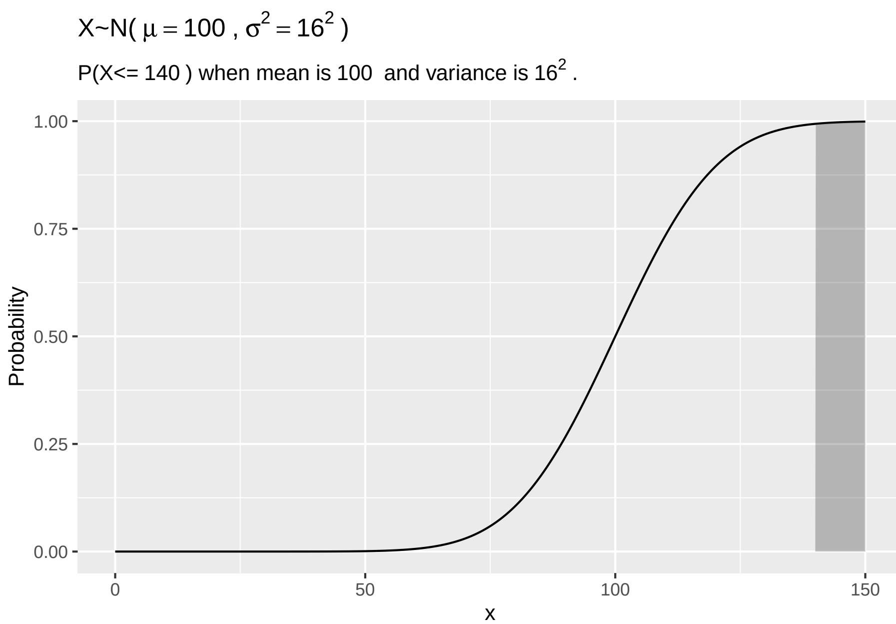
```
## [1] 0.006209665
```

```
# simulated
mean(rnorm(n = 10000, mean = my_mean, sd = my_sd) > my_x)
```

```
## [1] 0.0065
```

```
library(dplyr)
library(ggplot2)

data.frame(x = 0:1500 / 10,
```

```
           prob = pnorm(q = 0:1500 / 10,
                        mean = my_mean,
                        sd = my_sd,
                        lower.tail = TRUE)) %>%
  mutate(cdf = ifelse(x > my_x & x < 1000, prob, 0)) %>%
ggplot() +
  geom_line(aes(x = x, y = prob)) +
  geom_area(aes(x = x, y = cdf), alpha = 0.3) +
  labs(title = bquote('X~N('~mu==.(my_mean)~','~sigma^{2}==.(my_sd)^{2}~')'),
       subtitle = bquote('P(X<='~.(my_x)~') when mean is'~.(my_mean)~' and variance is'~.(my_sd)^
       x = "x",
       y = "Probability")
```



1.3.3 Example

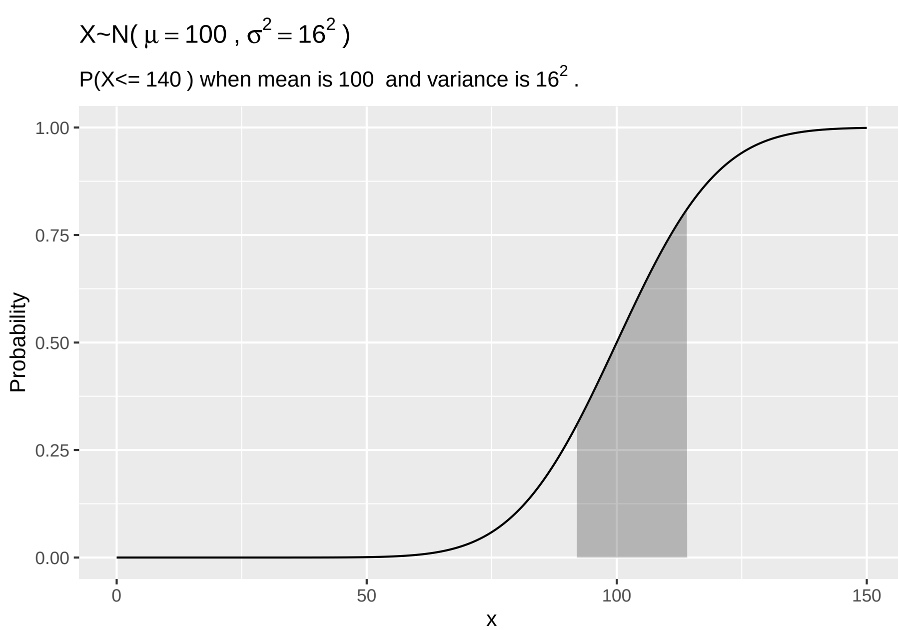
IQ scores are distributed $X \sim N(100, 16^2$. *What is the probability a randomly selected person's IQ is between 92 and 114?*

```
my_mean = 100
my_sd = 16
my_x_l = 92
my_x_h = 114
# exact
```

```
pnorm(q = my_x_h, mean = my_mean, sd = my_sd, lower.tail = TRUE) -
  pnorm(q = my_x_l, mean = my_mean, sd = my_sd, lower.tail = TRUE)
```

```
## [1] 0.5006755
```

```
library(dplyr)
library(ggplot2)

data.frame(x = 0:1500 / 10,
           prob = pnorm(q = 0:1500 / 10,
                        mean = my_mean,
                        sd = my_sd,
                        lower.tail = TRUE)) %>%
  mutate(cdf = ifelse(x > my_x_l & x <= my_x_h, prob, 0)) %>%
ggplot() +
  geom_line(aes(x = x, y = prob)) +
  geom_area(aes(x = x, y = cdf), alpha = 0.3) +
  labs(title = bquote('X~N('~mu==.(my_mean)~','~sigma^{2}==.(my_sd)^{2}~')'),
       subtitle = bquote('P(X<='~.(my_x)~') when mean is'~.(my_mean)~' and variance is
       x = "x",
       y = "Probability")
```



1.3.4 Example

Class scores are distributed $X \sim N(70, 10^2$. If the instructor wants to give A's to >=85th percentile and B's to 75th-85th percentile, what are the cutoffs?

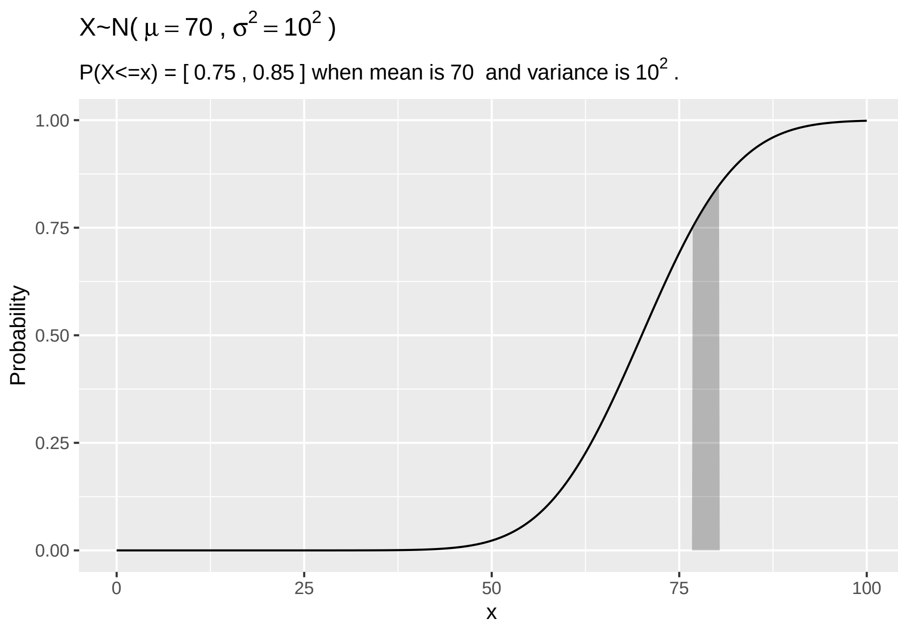
```
my_mean = 70
my_sd = 10
my_pct_l = .75
my_pct_h = .85

qnorm(p = my_pct_l, mean = my_mean, sd = my_sd, lower.tail = TRUE)
```

```
## [1] 76.7449
```

```
qnorm(p = my_pct_h, mean = my_mean, sd = my_sd, lower.tail = TRUE)
```

```
## [1] 80.36433
```

```
library(dplyr)
library(ggplot2)

data.frame(x = 0:1000 / 10,
           prob = pnorm(q = 0:1000 / 10,
                        mean = my_mean,
                        sd = my_sd,
                        lower.tail = TRUE)) %>%
  mutate(cdf = ifelse(prob > my_pct_l & prob <= my_pct_h, prob, 0)) %>%
ggplot() +
  geom_line(aes(x = x, y = prob)) +
  geom_area(aes(x = x, y = cdf), alpha = 0.3) +
  labs(title = bquote('X~N('~mu==.(my_mean)~','~sigma^{2}==.(my_sd)^{2}~')'),
       subtitle = bquote('P(X<=x) = ['~.(my_pct_l)~','~.(my_pct_h)~'] when mean is'~.(my_mean)~'
       x = "x",
       y = "Probability")
```



1.3.5 Normal Approximation to Binomial

The CLT implies that certain distributions can be approximated by the normal distribution.

The binomial distribution $X \sim B(n, p)$ is approximately normal with mean $\mu = np$ and variance $\sigma^2 = np(1-p)$. The approximation is useful when the expected number of successes and failures is at least 5: $np >= 5$ and $n(1-p) >= 5$.

1.3.6 Example

A measure requires p>=50% popular to pass. A sample of n=1,000 yields x=460 approvals. What is the probability that the overall population approves, P(X)>0.5?

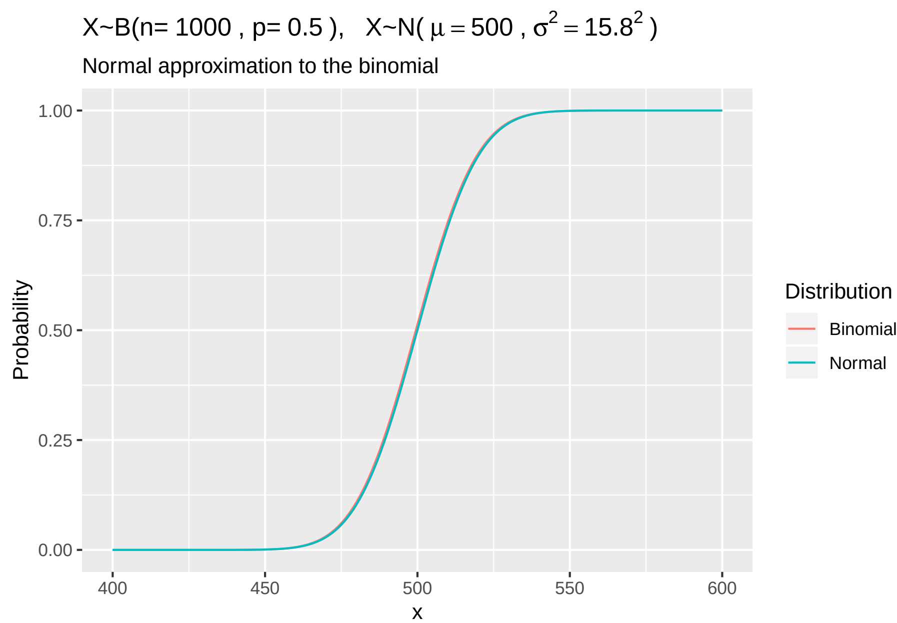
```
my_x = 460
my_p = 0.50
my_n = 1000

my_mean = my_p * my_n
my_sd = round(sqrt(my_n * my_p * (1 - my_p)), 1)

# Exact binomial
pbinom(q = my_x, size = my_n, prob = my_p, lower.tail = TRUE)
```

```
## [1] 0.006222073
```

```
# Normal approximation
pnorm(q = my_x, mean = my_p * my_n, sd = sqrt(my_n * my_p * (1 - my_p)), lower.tail = TRUE)
```

```
## [1] 0.005706018
```

```
library(dplyr)
library(ggplot2)
library(tidyr)

data.frame(x = 400:600,
           Normal = pnorm(q = 400:600,
                        mean = my_p * my_n,
                        sd = sqrt(my_n * my_p * (1 - my_p)),
                        lower.tail = TRUE),
           Binomial = pbinom(q = 400:600,
                        size = my_n,
                        prob = my_p,
                        lower.tail = TRUE)) %>%
  gather(key = "Distribution", value = "cdf", c(-x)) %>%
  ggplot(aes(x = x, y = cdf, color = Distribution)) +
  geom_line() +
  labs(title = bquote('X~B(n='~.(my_n)~', p='~.(my_p)~'),  '~'X~N('~mu==.(my_mean)~','~sigma^{2}=
       subtitle = "Normal approximation to the binomial",
       x = "x",
       y = "Probability")
```



The Poisson distribution $x\ P(\lambda)$ is approximately normal with mean $\mu = \lambda$ and variance $\sigma^2 = \lambda$, for large values of λ.

1.3.7 Example

*The annual number of earthquakes registering at least 2.5 on the Richter Scale and having an epicenter within 40 miles of downtown Memphis follows a Poisson distribution with mean $\lambda = 6.5$. What is the probability that at least $x >= 9$** such earthquakes will strike next year?*

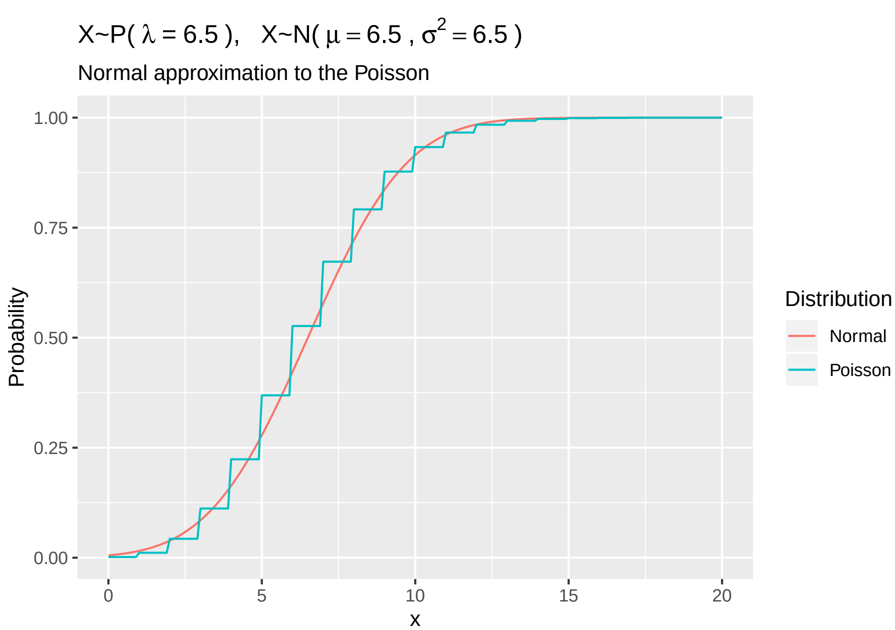
```
my_x = 9
my_lambda = 6.5
my_sd = round(sqrt(my_lambda), 2)

# Exact Poisson
ppois(q = my_x - 1, lambda = my_lambda, lower.tail = FALSE)
```

```
## [1] 0.208427
```

```
# Normal approximation
pnorm(q = my_x - 0.5, mean = my_lambda, sd = my_sd, lower.tail = FALSE)
```

```
## [1] 0.216428
```

```
library(dplyr)
library(ggplot2)
library(tidyr)

data.frame(x = 0:200 / 10,
           Normal = pnorm(q = 0:200 / 10,
                        mean = my_lambda,
                        sd = my_sd,
                        lower.tail = TRUE),
           Poisson = ppois(q = 0:200 / 10,
                         lambda = my_lambda,
                         lower.tail = TRUE)) %>%
  gather(key = "Distribution", value = "cdf", c(-x)) %>%
  ggplot(aes(x = x, y = cdf, color = Distribution)) +
  geom_line() +
  labs(title = bquote('X~P('~lambda~'='~.(my_lambda)~'),  '~'X~N('~mu==.(my_lambda)~','~sigma^{2
       subtitle = "Normal approximation to the Poisson",
       x = "x",
       y = "Probability")
```



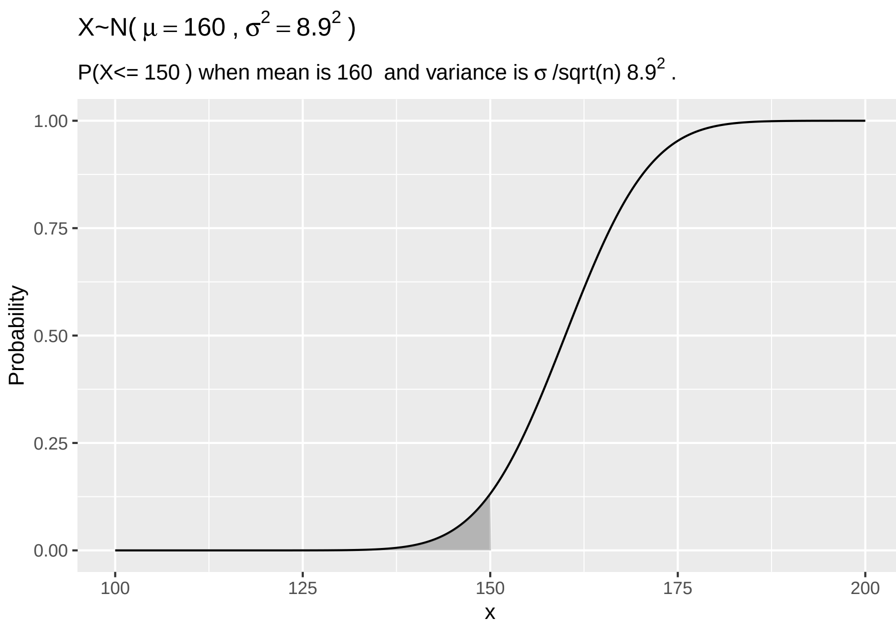
1.3.8 From Sample to Population

Suppose a person's blood pressure typically measures 160?20 mm. If one takes n=5 blood pressure readings, what is the probability the average will be <=150?

```
my_mu = 160
my_sigma = 20
my_n = 5
my_x = 150

my_se = round(my_sigma / sqrt(my_n), 1)

pnorm(q = my_x, mean = my_mu, sd = my_sigma / sqrt(my_n), lower.tail = TRUE)
```

```
## [1] 0.1317762
```

```
library(dplyr)
library(ggplot2)

data.frame(x = 1000:2000 / 10,
           prob = pnorm(q = 1000:2000 / 10,
                        mean = my_mu,
                        sd = my_sigma / sqrt(my_n),
                        lower.tail = TRUE)) %>%
  mutate(cdf = ifelse(x > 0 & x <= my_x, prob, 0)) %>%
ggplot() +
  geom_line(aes(x = x, y = prob)) +
  geom_area(aes(x = x, y = cdf), alpha = 0.3) +
  labs(title = bquote('X~N('~mu==.(my_mu)~','~sigma^{2}==.(my_se)^{2}~')'),
       subtitle = bquote('P(X<='~.(my_x)~') when mean is'~.(my_mu)~' and variance is'~
       x = "x",
       y = "Probability")
```




```
knitr::include_app("https://mpfoley73.shinyapps.io/shiny_dist/",
  height = "600px")
```

Chapter 2

Inference

Chapter 3

Experiments

Some *significant* applications are demonstrated in this chapter.

3.1 Example one

3.2 Example two

Chapter 4

Regression

Chapter 5

Generalized Linear Models

These notes are primarily from PSU Online course Analysis of Discrete Data which uses Alan Agresti's **Categorical Data Analysis** (which I have not yet purchased) (Agresti, 2013). I also reviewed:

Penn State University, STAT 501, "Lesson 15: Logistic, Poisson & Nonlinear Regression". https://newonlinecourses.science.psu.edu/stat501/lesson/15

"Generalized Linar Models in R". DataCamp. https://www.datacamp.com/courses/generalized-linear-models-in-r.

"Multiple and Logistic Regression". DataCamp. https://www.datacamp.com/courses/multiple-and-logistic-regression.

"The Difference Between Logistic and Probit Regression", The Analysis Factor. https://www.theanalysisfactor.com/the-difference-between-logistic-and-probit-regression/.

Molnar, Christoph. "Interpretable machine learning. A Guide for Making Black Box Models Explainable", 2019. https://christophm.github.io/interpretable-ml-book/.

In generalized linear models (GLMs), the modeled response is *a function* of the mean of y. There are three components to a GLM. The *random component* is the probability distribution of the response variable (normal, binomial, Poisson, etc.). The *systematic component* is the explanatory variables $X\beta$. The *link function* η specifies the link between random and systematic components. The link function converts the response value from a range $[0, 1]$ in logistic and probit and $[0, +\infty]$ for Poisson to a value ranging from $[-\infty, +\infty]$, and creates a linear relationship with the predictor variables.

For a standard linear regression, the link function is the identity function,

$$f(\mu_Y) = \mu_Y.$$

The standard linear regression is thus a special case of the GLM. For a logistic regression, the link function is

$$f(\mu_Y) = \ln(\frac{\pi}{1-\pi})$$

where π is the event probability. For a probit regression, the link function is

$$f(\mu_Y) = \Phi^{-1}(\pi).$$

The difference between logistic and probit link function is theoretical - the practical significance is slight. Logistic regression has the advantage that it can be back-transformed from log odds to odds ratios. For a Poisson regression, the link function is

$$f(\mu_Y) = \ln(\lambda)$$

where λ is the expected event rate.

GLM uses maximum likelihood estimation (MLE) rather than ordinary least squares (OLS) to estimate the parameters, and thus relies on large-sample approximations.

In R, specify a GLM just like an linear model, but with the `glm()` function, specifying the distribution with the `family` parameter.

- `family = "gaussian"`: linear regression
- `family = "binomial"`: logistic regression
- `family = binomial(link = "probit")`: probit regression
- `family = "poisson"`: Poisson regression

5.1 Logistic Regression

Logistic regression estimates the probability of a particular level of a categorical response variable given a set of predictors. The response levels can be binary, nominal (multiple categories), or ordinal (multiple levels).

The **binary** logistic regression model is

$$y_i = logit(\pi_i) = \log\left(\frac{\pi_i}{1-\pi_i}\right) = X_i\beta$$

where π_i is the "success probability" that observation i is in a specified category of the binary y variable. You can solve for π to get

$$\pi = \frac{\exp(X\beta)}{1 + \exp(X\beta)}.$$

The model predicts the *log odds* of the response variable. The maximum likelihood estimator maximizes the the likelihood function

$$L(\beta; y, X) = \prod_{i=1}^{n} \pi_i^{y_i}(1-\pi_i)^{(1-y_i)} = \prod_{i=1}^{n} \frac{\exp(y_i X_i \beta)}{1 + \exp(X_i \beta)}.$$

There is no closed-form solution, so GLM estimates coefficients with interatively reweighted least squares.

Example

Dataset `leuk` contains response variable `REMISS` indicating whether leukemia remission occurred (1|0) and several explanatory variables.

```
data_dir <- "C:/Users/mpfol/OneDrive/Documents/Data Science/Data/"
leuk <- read_tsv(paste(data_dir, "leukemia_remission.txt", sep = "/"))
```

```
## Parsed with column specification:
## cols(
##   REMISS = col_double(),
##   CELL = col_double(),
##   SMEAR = col_double(),
##   INFIL = col_double(),
##   LI = col_double(),
##   BLAST = col_double(),
##   TEMP = col_double()
## )
```

```
str(leuk)
```

```
## Classes 'spec_tbl_df', 'tbl_df', 'tbl' and 'data.frame': 27 obs. of  7 variables:
##  $ REMISS: num  1 1 0 0 1 0 1 0 0 0 ...
##  $ CELL  : num  0.8 0.9 0.8 1 0.9 1 0.95 0.95 1 0.95 ...
##  $ SMEAR : num  0.83 0.36 0.88 0.87 0.75 0.65 0.97 0.87 0.45 0.36 ...
##  $ INFIL : num  0.66 0.32 0.7 0.87 0.68 0.65 0.92 0.83 0.45 0.34 ...
##  $ LI    : num  1.9 1.4 0.8 0.7 1.3 0.6 1 1.9 0.8 0.5 ...
##  $ BLAST : num  1.1 0.74 0.18 1.05 0.52 0.52 1.23 1.35 0.32 0 ...
##  $ TEMP  : num  1 0.99 0.98 0.99 0.98 0.98 0.99 1.02 1 1.04 ...
##  - attr(*, "spec")=
```

```
##   .. cols(
##   ..   REMISS = col_double(),
##   ..   CELL = col_double(),
##   ..   SMEAR = col_double(),
##   ..   INFIL = col_double(),
##   ..   LI = col_double(),
##   ..   BLAST = col_double(),
##   ..   TEMP = col_double()
##   .. )
```

Fit a logistic regression in R using `glm(formula, data, family = binomial)` where `family = binomial` specifies a binomial error distribution.

```
m1 <- glm(REMISS ~ ., family = binomial, data = leuk)
m1
```

```
##
## Call:  glm(formula = REMISS ~ ., family = binomial, data = leuk)
##
## Coefficients:
## (Intercept)         CELL        SMEAR        INFIL           LI        BLAST
##    64.25808     30.83006     24.68632    -24.97447      4.36045     -0.01153
##        TEMP
##  -100.17340
##
## Degrees of Freedom: 26 Total (i.e. Null);  20 Residual
## Null Deviance:       34.37
## Residual Deviance: 21.59     AIC: 35.59
```

```
summary(m1)
```

```
##
## Call:
## glm(formula = REMISS ~ ., family = binomial, data = leuk)
##
## Deviance Residuals:
##      Min        1Q    Median        3Q       Max
## -1.95404  -0.66259  -0.02516   0.78184   1.57465
##
## Coefficients:
##              Estimate Std. Error z value Pr(>|z|)
## (Intercept)   64.25808   74.96480   0.857    0.391
## CELL          30.83006   52.13520   0.591    0.554
## SMEAR         24.68632   61.52601   0.401    0.688
```

```
## INFIL        -24.97447   65.28088  -0.383    0.702
## LI             4.36045    2.65798   1.641    0.101
## BLAST         -0.01153    2.26634  -0.005    0.996
## TEMP        -100.17340   77.75289  -1.288    0.198
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 34.372  on 26  degrees of freedom
## Residual deviance: 21.594  on 20  degrees of freedom
## AIC: 35.594
##
## Number of Fisher Scoring iterations: 8
```

The *predicted* value $\hat{y}$ is the estimated **log odds** of the response variable,

$$\hat{y} = X\hat{\beta} = \ln(\frac{\pi}{1-\pi}).$$

Suppose each predictor equals its mean value, then the log odds of `REMISS` is -2.684.

```
pred <- predict(m1, newdata = data.frame(CELL = mean(leuk$CELL),
                                         SMEAR = mean(leuk$SMEAR),
                                         INFIL = mean(leuk$INFIL),
                                         LI = mean(leuk$LI),
                                         BLAST = mean(leuk$BLAST),
                                         TEMP = mean(leuk$TEMP)))
```

Log odds are not easy to interpet, but it is convenient for updating prior probabilities in Bayesian analyses. *See this article in Statistics How To.* Exponentiate the log odds to get the more intuitive **odds**.

$$\exp(\hat{y}) = \exp(X\hat{\beta}) = \frac{\pi}{1-\pi}.$$

The odds of having achieved remission when each predictor equals its mean value is $\exp(\hat{y}) = 0.068$.

```
exp(pred)
```

```
##          1
## 0.06826334
```

You might express that more commonly as 1 / 0.068 = 15:1. So a person with average values of the predictors has an odds of "15 to 1" of having achieved remission.

```r
1/exp(pred)
```

```
##        1
## 14.64915
```

Or, solve for π to get the **probability**.

$$\pi = \frac{\exp(X\beta)}{1 + \exp(X\beta)}$$

The probability of having achieved remission when each predictor equals its mean value is $\pi = 0.064$. The `predict()` function for a logistic model returns log-odds, but can also return π by specifying parameter `type = "response"`.

```r
exp(pred) / (1 + exp(pred))
```

```
##          1
## 0.06390123
```

```r
prob <- predict(m1, newdata = data.frame(CELL = mean(leuk$CELL),
                                         SMEAR = mean(leuk$SMEAR),
                                         INFIL = mean(leuk$INFIL),
                                         LI = mean(leuk$LI),
                                         BLAST = mean(leuk$BLAST),
                                         TEMP = mean(leuk$TEMP)),
                type = "response")
```

It is common to express the results in terms of the **odds ratio**. The *odds ratio* is the ratio of the odds before and after an increment to the predictors. It tells you how much the odds would be multiplied after a $X_1 - X_0$ unit increase in X.

$$\theta = \frac{\pi/(1-\pi)|_{X=X_1}}{\pi/(1-\pi)|_{X=X_0}} = \frac{\exp(X_1\hat{\beta})}{\exp(X_0\hat{\beta})} = \exp((X_1 - X_0)\hat{\beta}) = \exp(\delta\hat{\beta})$$

For example, increasing `LI` by .01 increases the odds of remission by a factor of $\exp(0.1 \cdot 4.36) = 1.547$ (from 15:1 to 23:1).

```r
exp(.1 * m1$coefficients)
```

```
##  (Intercept)         CELL        SMEAR        INFIL           LI        BLAST
## 6.175799e+02 2.182391e+01 1.180628e+01 8.229480e-02 1.546579e+00 9.988476e-01
##         TEMP
## 4.461948e-05
```

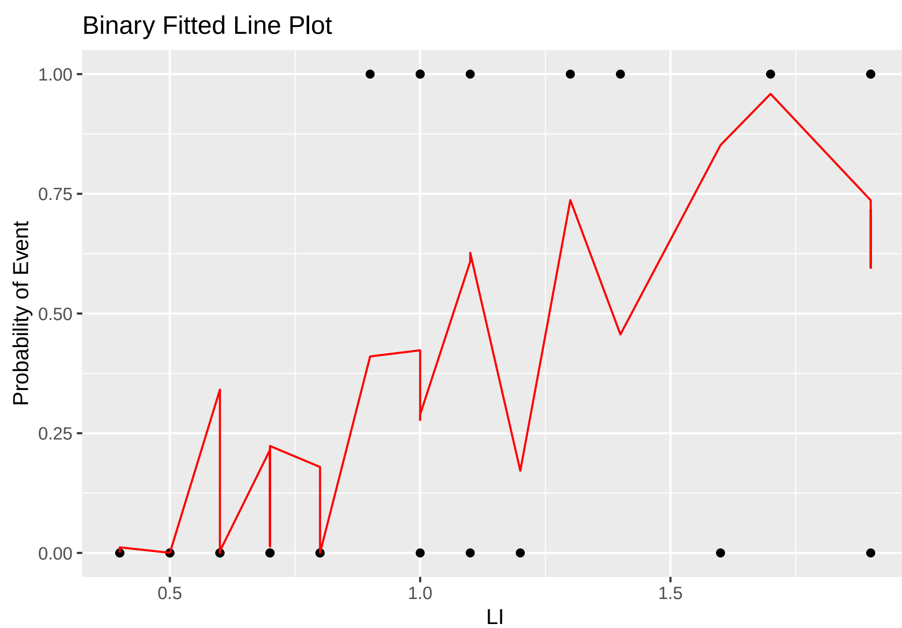
You can calculate an odds ratio using `oddsratio::or_glm()`.

```
library(oddsratio)
or_glm(data = leuk,
       model = m1,
       incr = list(CELL = 0.01,
                   SMEAR = 0.01,
                   INFIL = 5,
                   LI = 0.1,
                   BLAST = 1.0,
                   TEMP = 0.3))
```

```
## # A tibble: 6 x 5
##   predictor oddsratio `CI_low (2.5)` `CI_high (97.5)` increment
##   <chr>         <dbl>          <dbl>            <dbl> <chr>
## 1 CELL          1.36           0.747         4.64e  0 0.01
## 2 SMEAR         1.28           0.537         5.15e  0 0.01
## 3 INFIL         0              0             1.09e152 5
## 4 LI            1.55           1.04          2.99e  0 0.1
## 5 BLAST         0.989          0.009         9.10e  1 1
## 6 TEMP          0              0             1.10e  3 0.3
```

The predicted values can also be expressed as the probabilities π. This produces the familiar signmoidal shape of the binary relationship.

```
augment(m1, type.predict = "response") %>%
  ggplot(aes(x = LI, y = REMISS)) +
  geom_point() +
  geom_line(aes(y = .fitted), color = "red") +
  labs(x = "LI",
       y = "Probability of Event",
       title = "Binary Fitted Line Plot")
```



Whereas in linear regression the the coefficient p-values use the *t* test (*t* statistic), logistic regression coefficient p-values use the *Wald test* **Z*-statistic).

$$Z = \frac{\hat{\beta}_i}{SE(\hat{\beta}_i)}$$

```
round((z <- m1$coefficients / summary(m1)$coefficients[,"Std. Error"]), 3)
```

```
## (Intercept)        CELL       SMEAR       INFIL          LI       BLAST
##       0.857       0.591       0.401      -0.383       1.641      -0.005
##        TEMP
##      -1.288
```

```
round(pnorm(abs(z), lower.tail = FALSE) * 2, 3)
```

```
## (Intercept)        CELL       SMEAR       INFIL          LI       BLAST
##       0.391       0.554       0.688       0.702       0.101       0.996
##        TEMP
##       0.198
```

Evaluate a logistic model fit with an analysis of deviance. Deviance is defined as -2 times the log-likelihood $-2l(\beta)$. The null deviance is the deviance of the null model and is analagous to SST in ANOVA. The residual deviance is analagous to SSE in ANOVA.

```r
logLik(glm(REMISS ~ ., data = leuk, family = "binomial")) * (-2)
```

```
## 'log Lik.' 21.59385 (df=7)
```

```r
anova(m1)
```

```
## Analysis of Deviance Table
##
## Model: binomial, link: logit
##
## Response: REMISS
##
## Terms added sequentially (first to last)
##
##
##       Df Deviance Resid. Df Resid. Dev
## NULL                     26     34.372
## CELL   1   2.5800        25     31.792
## SMEAR  1   0.5188        24     31.273
## INFIL  1   0.2927        23     30.980
## LI     1   6.7818        22     24.199
## BLAST  1   0.3271        21     23.871
## TEMP   1   2.2775        20     21.594
```

```r
m1
```

```
##
## Call:  glm(formula = REMISS ~ ., family = binomial, data = leuk)
##
## Coefficients:
## (Intercept)         CELL        SMEAR        INFIL           LI        BLAST
##    64.25808     30.83006     24.68632    -24.97447      4.36045     -0.01153
##        TEMP
##  -100.17340
##
## Degrees of Freedom: 26 Total (i.e. Null);  20 Residual
## Null Deviance:       34.37
## Residual Deviance: 21.59     AIC: 35.59
```

```r
summary(m1)
```

```
##
## Call:
```

```
## glm(formula = REMISS ~ ., family = binomial, data = leuk)
##
## Deviance Residuals:
##      Min        1Q    Median        3Q       Max
## -1.95404  -0.66259  -0.02516   0.78184   1.57465
##
## Coefficients:
##               Estimate Std. Error z value Pr(>|z|)
## (Intercept)   64.25808   74.96480   0.857    0.391
## CELL          30.83006   52.13520   0.591    0.554
## SMEAR         24.68632   61.52601   0.401    0.688
## INFIL        -24.97447   65.28088  -0.383    0.702
## LI             4.36045    2.65798   1.641    0.101
## BLAST         -0.01153    2.26634  -0.005    0.996
## TEMP        -100.17340   77.75289  -1.288    0.198
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 34.372  on 26  degrees of freedom
## Residual deviance: 21.594  on 20  degrees of freedom
## AIC: 35.594
##
## Number of Fisher Scoring iterations: 8
```

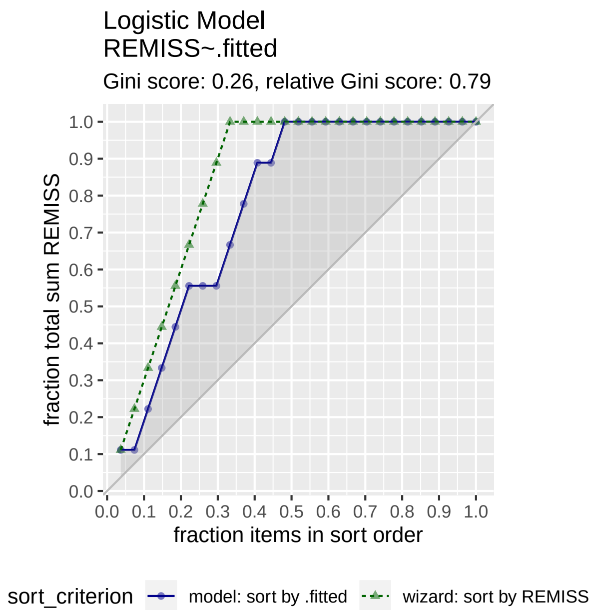
The deviance of the null model (no regressors) is 34.372. The deviance of the full model is 26.073.

```
glance(m1)
```

```
## # A tibble: 1 x 7
##   null.deviance df.null logLik   AIC   BIC deviance df.residual
##           <dbl>   <int>  <dbl> <dbl> <dbl>    <dbl>       <int>
## 1          34.4      26  -10.8  35.6  44.7     21.6          20
```

Use the `GainCurvePlot()` function to plot the gain curve (background on gain curve at Data Science Central from the model predictions. The x-axis is the fraction of items seen when sorted by the predicted value, and the y-axis is the cumulative summed true outcome. The “wizard” curve is the gain curve when the data is sorted by the true outcome. If the model’s gain curve is close to the wizard gain curve, then the model sorted the response variable well. The grey area is the gain over a random sorting.

```
augment(m1) %>% data.frame() %>%
  GainCurvePlot(xvar = ".fitted", truthVar = "REMISS", title = "Logistic Model")
```

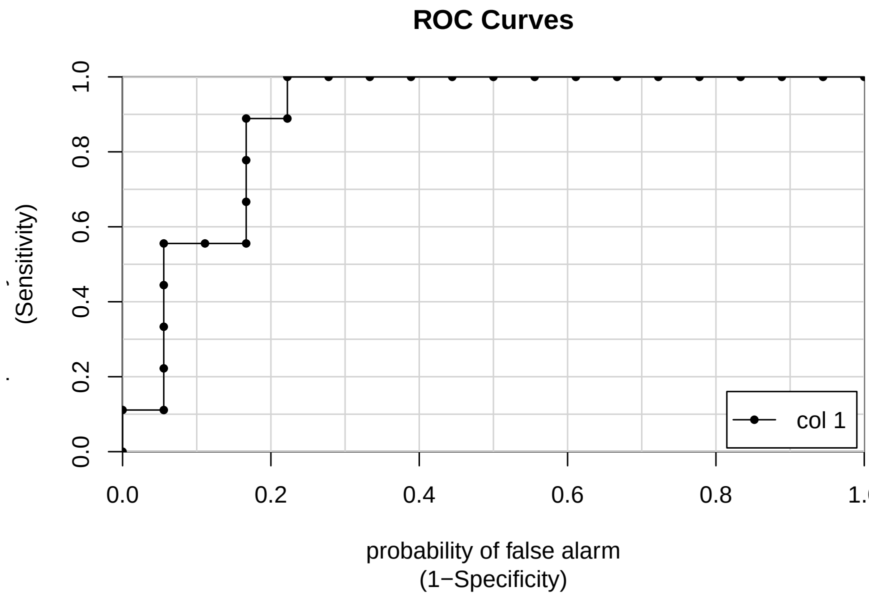


`REMISS` equals 1 in 9 of the 27 responses.

- The wizard curve shows that after sorting the responses it encounters all 9 1s (100%) after looking at 9 of the 27 response (33%).
- The bottom of the grey diagonal shows that after making random predictions and sorting the predictions, it encounters only 3 1s (33%) after looking at 9 of the 27 responses (33%). It has to look at all 27 responses (100%) to encounter all 9 1s (100%).
- The gain curve encounters 5 1s (55%) after looking at 9 of the 27 responses (33%). It has to look at 14 responses to encounter all 9 1s (100%).

Another way to evaluate the predictive model is the ROC curve. It evaluates all possible thresholds for splitting predicted probabilities into predicted classes. This is often a much more useful metric than simply ranking models by their accuracy at a set threshold, as different models might require different calibration steps (looking at a confusion matrix at each step) to find the optimal classification threshold for that model.

```
library(caTools)
colAUC(m1$fitted.values, m1$data$REMISS, plotROC = TRUE)
```




```
##              [,1]
## 0 vs. 1 0.8950617
```

5.2 Poisson Regression

Poisson models count data, like "traffic tickets per day", or "website hits per day". The response is an expected *rate* or intensity. For count data, specify the generalized model, this time with `family = poisson` or `family = quasipoisson`.

Recall that the probability of achieving a count y when the expected rate is λ is distributed

$$P(Y = y|\lambda) = \frac{e^{-\lambda}\lambda^y}{y!}.$$

The poisson regression model is

$$\lambda = \exp(X\beta).$$

You can solve this for y to get

$$y = X\beta = \ln(\lambda).$$

That is, the model predicts the log of the response rate. For a sample of size n, the likelihood function is

$$L(\beta; y, X) = \prod_{i=1}^{n} \frac{e^{-\exp(X_i\beta)} \exp(X_i\beta)^{y_i}}{y_i!}.$$

The log-likelihood is

$$l(\beta) = \sum_{i=1}^{n}(y_i X_i \beta - \sum_{i=1}^{n} \exp(X_i\beta) - \sum_{i=1}^{n} \log(y_i!).$$

Maximizing the log-likelihood has no closed-form solution, so the coefficient estimates are found through interatively reweighted least squares.

Poisson processes assume the variance of the response variable equals its mean. "Equals" means the mean and variance are of a similar order of magnitude. If that assumption does not hold, use the quasi-poisson. Use Poisson regression for large datasets. If the predicted counts are much greater than zero (>30), the linear regression will work fine. Whereas RMSE is not useful for logistic models, it is a good metric in Poisson.

Example

Dataset `fire` contains response variable `injuries` counting the number of injuries during the month and one explanatory variable, the month `mo`.

```
fire <- read_csv(file = "C:/Users/mpfol/OneDrive/Documents/Data Science/Data/CivilInjury_0.csv")
```

```
## Parsed with column specification:
## cols(
##   ID = col_double(),
##   `Injury Date` = col_datetime(format = ""),
##   `Total Injuries` = col_double()
## )
```

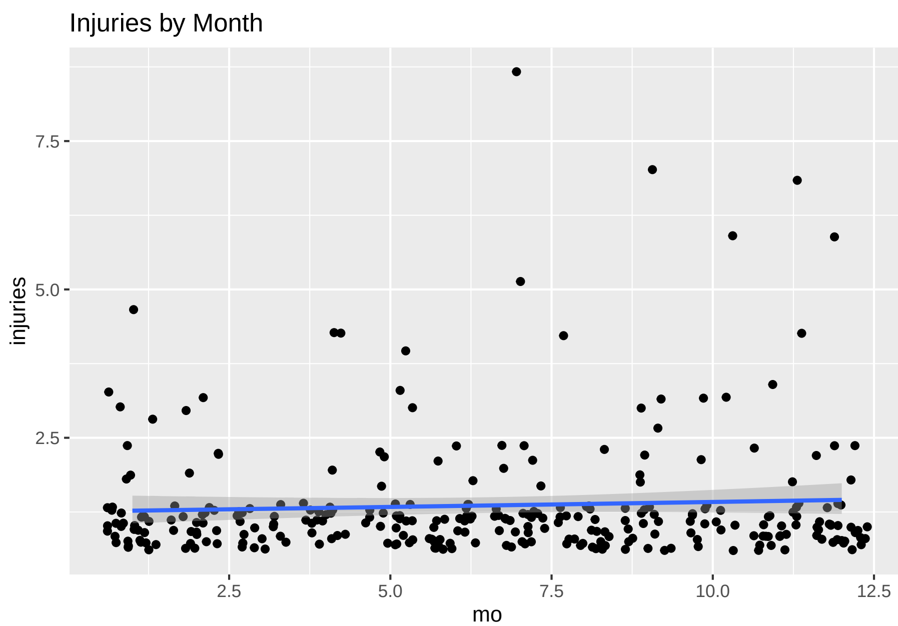
```
fire <- fire %>%
  mutate(mo = as.POSIXlt(`Injury Date`)$mon + 1) %>%
  rename(dt = `Injury Date`,
         injuries = `Total Injuries`)
str(fire)
```

```
## Classes 'spec_tbl_df', 'tbl_df', 'tbl' and 'data.frame': 300 obs. of  4 variables:
##  $ ID      : num  1 2 3 4 5 6 7 8 9 10 ...
```

```
## $ dt       : POSIXct, format: "2005-01-10" "2005-01-11" ...
## $ injuries: num 1 1 1 5 2 1 1 1 1 1 ...
## $ mo       : num 1 1 1 1 1 1 2 2 2 4 ...
```

In a situation like this where there the relationship is bivariate, start with a visualization.

```
ggplot(fire, aes(x = mo, y = injuries)) +
  geom_jitter() +
  geom_smooth(method = "glm", method.args = list(family = "poisson")) +
  labs(title = "Injuries by Month")
```



Fit a poisson regression in R using `glm(formula, data, family = poisson)`. But first, check whether the mean and variance of `injuries` are the same magnitude? If not, then use `family = quasipoisson`.

```
mean(fire$injuries)
```

```
## [1] 1.36
```

```
var(fire$injuries)
```

```
## [1] 1.020468
```

They are of the same magnitude, so fit the regression with `family = poisson`.

```
m2 <- glm(injuries ~ mo, family = poisson, data = fire)
summary(m2)
```

```
##
## Call:
## glm(formula = injuries ~ mo, family = poisson, data = fire)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -0.3987  -0.3473  -0.3034  -0.2502   4.3185
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  0.22805    0.10482   2.176   0.0296 *
## mo           0.01215    0.01397   0.870   0.3844
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for poisson family taken to be 1)
##
##     Null deviance: 139.87  on 299  degrees of freedom
## Residual deviance: 139.11  on 298  degrees of freedom
## AIC: 792.08
##
## Number of Fisher Scoring iterations: 5
```

The *predicted* value $\hat{y}$ is the estimated **log** of the response variable,

$$\hat{y} = X\hat{\beta} = \ln(\lambda).$$

Suppose `mo` is January (mo = `), then the log ofinjuries`' is $\hat{y} = 0.323787$. Or, more intuitively, the expected count of injuries is $\exp(0.323787) = 1.38$

```
predict(m2, newdata = data.frame(mo=1))
```

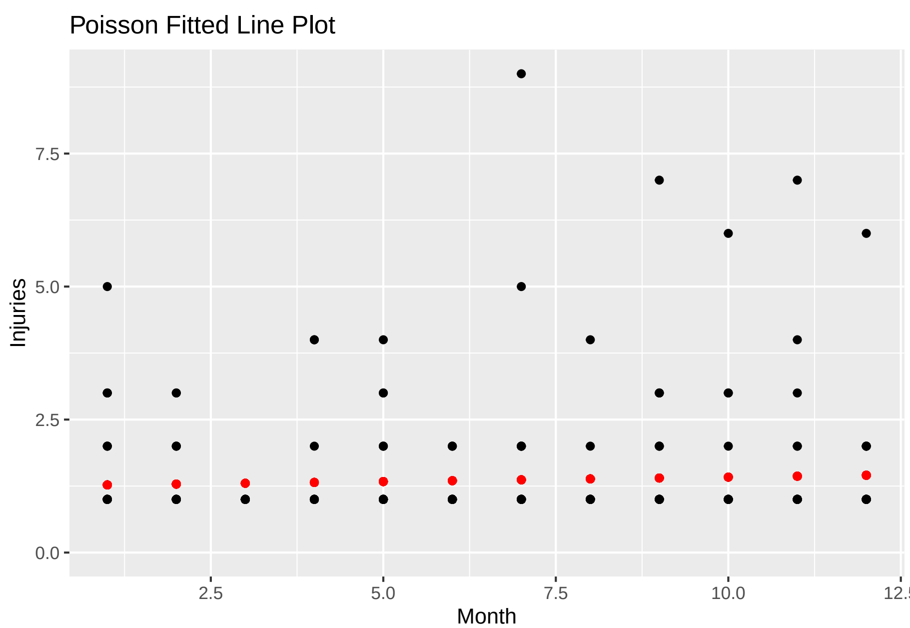
```
##         1
## 0.2401999
```

```
predict(m2, newdata = data.frame(mo=1), type = "response")
```

```
##        1
## 1.271503
```

Here is a plot of the predicted counts in red.

```
augment(m2, type.predict = "response") %>%
  ggplot(aes(x = mo, y = injuries)) +
  geom_point() +
  geom_point(aes(y = .fitted), color = "red") +
  scale_y_continuous(limits = c(0, NA)) +
  labs(x = "Month",
       y = "Injuries",
       title = "Poisson Fitted Line Plot")
```



Evaluate a logistic model fit with an analysis of deviance.

```
(perf <- glance(m2))
```

```
## # A tibble: 1 x 7
##   null.deviance df.null logLik   AIC   BIC deviance df.residual
##           <dbl>   <int>  <dbl> <dbl> <dbl>    <dbl>       <int>
## 1          140.     299  -394.  792.  799.     139.         298
```

```
(pseudoR2 <- 1 - perf$deviance / perf$null.deviance)
```

```
## [1] 0.005413723
```

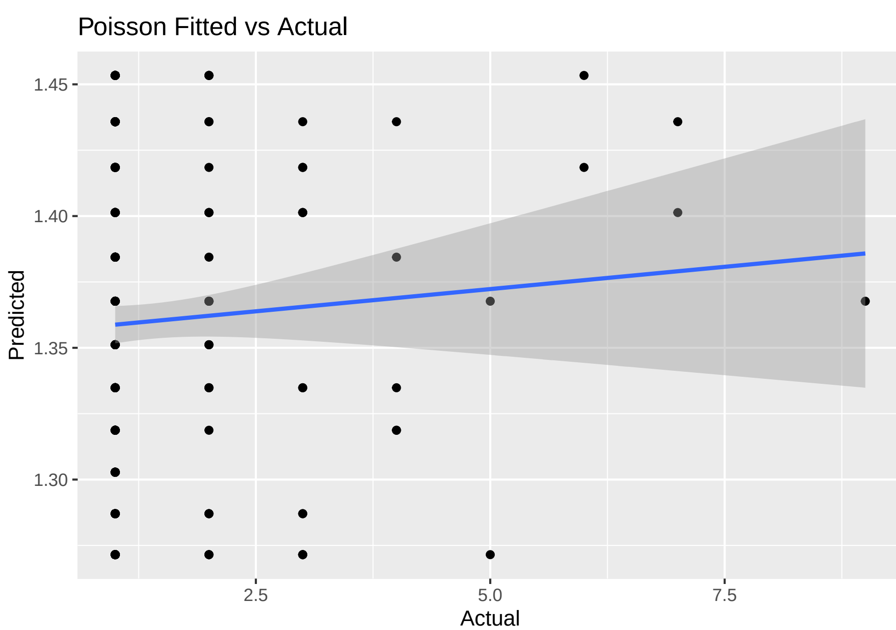
The deviance of the null model (no regressors) is 139.9. The deviance of the full model is 132.2. The psuedo-R2 is very low at .05. How about the RMSE?

```
RMSE(pred = predict(m2, type = "response"), obs = fire$injuries)
```

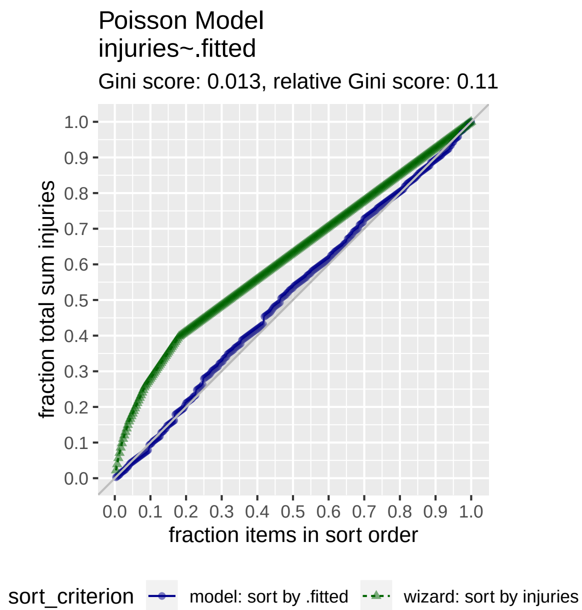
```
## [1] 1.006791
```

The average prediction error is about 0.99. That's almost as much as the variance of `injuries` - i.e., just predicting the mean of `injuries` would be almost as good! Use the `GainCurvePlot()` function to plot the gain curve.

```
augment(m2, type.predict = "response") %>%
  ggplot(aes(x = injuries, y = .fitted)) +
  geom_point() +
  geom_smooth(method ="lm") +
  labs(x = "Actual",
       y = "Predicted",
       title = "Poisson Fitted vs Actual")
```




```
augment(m2) %>% data.frame() %>%
  GainCurvePlot(xvar = ".fitted", truthVar = "injuries", title = "Poisson Model")
```



It seems that `mo` was a poor predictor of `injuries`.

Chapter 6

Classification

Chapter 7

Regularization

Chapter 8

Non-linear Models

Linear methods can model nonlinear relationships by including polynomial terms, interaction effects, and variable transformations. However, it is often difficult to identify how to formulate the model. Nonlinear models may be preferable because you do not need to know the the exact form of the nonlinearity prior to model training.

8.1 Splines

A regression spline fits a piecewise polynomial to the range of X partitioned by *knots* (K knots produce $K + 1$ piecewise polynomials) **James et al** (James et al., 2013). The polynomials can be of any degree d, but are usually in the range [0, 3], most commonly 3 (a cubic spline). To avoid discontinuities in the fit, a degree-d spline is constrained to have continuity in derivatives up to degree $d-1$ at each knot.

A cubic spline fit to a data set with K knots, performs least squares regression with an intercept and $3 + K$ predictors, of the form

$$y_i = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \beta_4 h(X, \xi_1) + \beta_5 h(X, \xi_2) + \dots + \beta_{K+3} h(X, \xi_K)$$

where $\xi_1, \dots, \xi_K$ are the knots are truncated power basis functions $h(X, \xi) = (X - \xi)^3$ if $X > \xi$, else 0.

Splines can have high variance at the outer range of the predictors. A **natural spline** is a regression spline additionally constrained to be linear at the boundaries.

How many knots should there be, and Where should the knots be placed? It is common to place knots in a uniform fashion, with equal numbers of points between each knot. The number of knots is typically chosen by trial and error using cross-validation to minimize the RSS. The number of knots is usually expressed in terms of degrees of freedom. A cubic spline will have $K + 3 + 1$ degrees of freedom. A natural spline has $K + 3 + 1$ - 5 degrees of freedom due to the constraints at the endpoints.

A further constraint can be added to reduce overfitting by enforcing smoothness in the spline. Instead of minimizing the loss function $\sum (y - g(x))^2$ where $g(x)$ is a natural spline, minimize a loss function with an additional penalty for variability:

$$L = \sum (y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt.$$

The function $g(x)$ that minimizes the loss function is a *natural cubic spline* with knots at each $x_1, \ldots, x_n$. This is called a **smoothing spline**. The larger g is, the greater the penalty on variation in the spline. In a smoothing spline, you do not optimize the number or location of the knots – there is a knot at each training observation. Instead, you optimize λ. One way to optimze λ is cross-validation to minimize RSS. Leave-one-out cross-validation (LOOCV) can be computed efficiently for smoothing splines.

8.2 MARS

Multivariate adaptive regression splines (MARS) is a non-parametric algorithm that creates a piecewise linear model to capture nonlinearities and interactions effects. The resulting model is a weighted sum of *basis* functions $B_i(X)$:

$$\hat{y} = \sum_{i=1}^{k} w_i B_i(x)$$

The basis functions are either a constant (for the intercept), a *hinge* function of the form $\max(0, x - x_0)$ or $\max(0, x_0 - x)$ (a more concise representation is $[\pm(x - x_0)]_+$), or products of two or more hinge functions (for interactions). MARS automatically selects which predictors to use and what predictor values to serve as the *knots* of the hinge functions.

MARS builds a model in two phases: the forward pass and the backward pass, similar to growing and pruning of tree models. MARS starts with a model consisting of just the intercept term equaling the mean of the response values. It then asseses every predictor to find a basis function pair consisting of opposing sides of a mirrored hinge function which produces the maximum improvement in the model error. MARS repeats the process until either it reaches a predefined limit of terms or the error improvement reaches a predefined limit.

MARS generalizes the model by removing terms according to the generalized cross validation (GCV) criterion. GCV is a form of regularization: it trades off goodness-of-fit against model complexity.

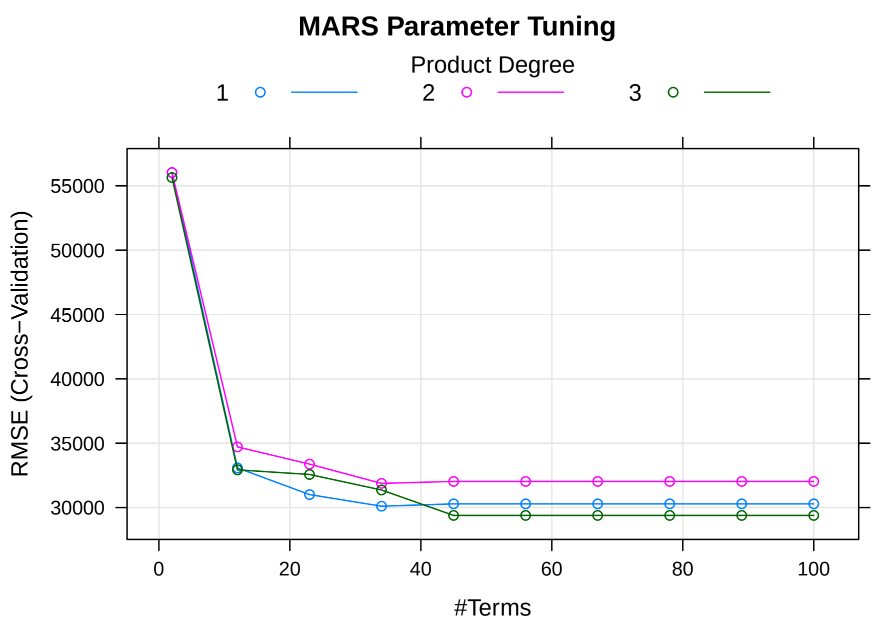
The `earth::earth()` function (documentation) performs the MARS algorithm (*the term "MARS" is trademarked, so open-source implementations use "Earth" instead*). The caret implementation tunes two parameters: `nprune` and `degree`. `nprune` is the maximum number of terms in the pruned model. `degree` is the maximum degree of interaction (default is 1 (no interactions)). However, there are other hyperparameters in the model that may improve performance, including `minspan` which regulates the number of knots in the predictors.

Here is an example using the Ames housing data set (following this tutorial.

```
library(tidyverse)
library(earth)
library(caret)

# set up
ames <- AmesHousing::make_ames()
set.seed(12345)
idx <- createDataPartition(ames$Sale_Price, p = 0.80, list = FALSE)
ames_train <- ames[idx, ] %>% as.data.frame()
ames_test  <- ames[-idx, ]

m <- train(
  x = subset(ames_train, select = -Sale_Price),
  y = ames_train$Sale_Price,
  method = "earth",
  metric = "RMSE",
  minspan = -15,
  trControl = trainControl(method = "cv", number = 10),
  tuneGrid = expand.grid(
    degree = 1:3,
    nprune = seq(2, 100, length.out = 10) %>% floor()
  )
)
```

The model plot shows the best tuning parameter combination.

```
plot(m, main = "MARS Parameter Tuning")
```




```
m$bestTune
```

```
##    nprune degree
## 25     45      3
```

How does this model perform against the holdout data?

```
caret::postResample(
  pred = log(predict(m, newdata = ames_test)),
  obs = log(ames_test$Sale_Price)
)
```

```
##       RMSE   Rsquared        MAE
## 0.16515620 0.85470300 0.09319503
```

8.3 GAM

Generalized additive models (GAM) allow for non-linear relationships between each feature and the response by replacing each linear component $\beta_j x_{ij}$ with a nonlinear function $f_j(x_{ij})$. The GAM model is of the form

$$y_i = \beta_0 + \sum f_j(x_{ij}) + \epsilon_i.$$

It is called an additive model because we calculate a separate f_j for each X_j, and then add together all of their contributions.

The advantage of GAMs is that they automatically model non-linear relationships so you do not need to manually try out many different transformations on each variable individually. And because the model is additive, you can still examine the effect of each X_j on Y individually while holding all of the other variables fixed. The main limitation of GAMs is that the model is restricted to be additive, so important interactions can be missed unless you explicitly add them.

Chapter 9

Decision Trees

Decision trees, also known as classification and regression tree (CART) models, are tree-based methods for supervised machine learning. Simple *classification trees* and *regression trees* are easy to use and interpret, but are not competitive with the best machine learning methods. However, they form the foundation for **bagged trees**, **random forests**, and **boosted trees** models, which although less interpretable, are very accurate.

CART models segment the predictor space into K non-overlapping terminal nodes (leaves), $A_1, A_2, \dots, A_K$. Each node is described by a set of rules which can be used to predict new responses. The predicted value $\hat{y}$ for each node is the mode (classification), or mean (regression).

CART models define the nodes through a *top-down greedy* process called *recursive binary splitting*. The process is *top-down* because it begins at the top of the tree with all observations in a single region and successively splits the predictor space. It is *greedy* because at each splitting step, the best split is made at that particular step without consideration to subsequent splits.

The best split is the predictor variable and cutpoint that minimizes a cost function. For a regression tree, the most common cost function is the sum of squared residuals,

$$RSS = \sum_{k=1}^{K} \sum_{i \in A_k} \left(y_i - \hat{y}_{A_k} \right)^2.$$

For a classification tree, the most common cost functions are the Gini index,

$$G = \sum_{c=1}^{C} \hat{p}_{kc}(1 - \hat{p}_{kc}),$$

or the entropy

$$D = -\sum_{c=1}^{C} \hat{p}_{kc} \log \hat{p}_{kc}$$

where $\hat{p}_{kc}$ is the proportion of training observations in node k node that are class c. A completely *pure* node in a binary tree will have $\hat{p} \in [0, 1]$ and $G = D = 0$. A completely impure node in a binary tree will have $\hat{p} = 0.5$ and $G = 0.5^2 \cdot 2 = 0.25$ and $D = -(0.5 \log(0.5)) \cdot 2 = 0.69$.

CART repeats the splitting process for each of the child nodes until a *stopping criterion* is satisfied, usually when no node size surpasses a predefined maximum, or continued splitting does not improve the model significantly. CART may also impose a minimum number of observations in each node.

The resulting tree likely over-fits the training data and therefore does not generalize well to test data, so CART *prunes* the tree, minimizing the cross-validated prediction error. Rather than cross-validating every possible subtree to find the one with minimum error, CART uses *cost-complexity pruning*. Cost-complexity is the tradeoff between error (cost) and tree size (complexity) where the tradeoff is quantified with cost-complexity parameter c_p. In the equation below, the cost complexity of the tree $R_{c_p}(T)$ is the sum of its risk (error) plus a "cost complexity" factor c_p multiple of the tree size $|T|$.

$$R_{c_p}(T) = R(T) + c_p|T|$$

c_p can take on any value from $[0..\infty]$, but it turns out there is an optimal tree for *ranges* of c_p values, so there are only a finite set of *interesting* values for c_p (James et al., 2013) (Therneau and Atkinson, 2019) (Kuhn and Johnson, 2016). A parametric algorithm identifies the interesting c_p values and their associated pruned trees, T_{c_p}.

CART uses cross-validation to determine which c_p is optimal.

9.1 Classification Tree

A simple classification tree is rarely performed on its own; the bagged, random forest, and gradient boosting methods build on this logic. However, it is good to start here to build understanding. I'll learn by example. Using the `ISLR::OJ` data set, I will predict which brand of orange juice, Citrus Hill (CH) or Minute Maid = (MM), customers `Purchase` using from the 17 feature variables. Load the libraries and data.

```
library(ISLR)  # OJ dataset
library(rpart)  # classification and regression trees
library(caret)  # modeling workflow
library(rpart.plot)  # better formatted plots than the ones in rpart
library(plotROC)  # ROC curves
library(ROCR)
library(tidyverse)
library(skimr)  # neat alternative to glance & summary

oj_dat <- OJ
#skim_with(numeric = list(p0 = NULL, p25 = NULL, p50 = NULL, p75 = NULL,
#                                 p100 = NULL, hist = NULL))
#skim(oj_dat)
```

I'll split `oj_dat` (n = 1,070) into `oj_train` (80%, n = 857) and `oj_test` (20%, n = 213). I'll fit a simple decision tree with `oj_train`, then later a bagged tree, a random forest, and a gradient boosting tree. I'll compare their predictive performance with `oj_test`.

```
set.seed(12345)
partition <- createDataPartition(y = oj_dat$Purchase, p = 0.8, list = FALSE)
oj_train <- oj_dat[partition, ]
oj_test <- oj_dat[-partition, ]
```

Function `rpart::rpart()` builds a full tree, minimizing the Gini index G by default (`parms = list(split = "gini")`), until the stopping criterion is satisfied. The default stopping criterion is

- only attempt a split if the current node as at least `minsplit = 20` observations,
- only accept a split if each of the two resulting nodes have at least `minbucket = round(minsplit/3)` observations, and
- only accept a split if the resulting overall fit improves by `cp = 0.01` (i.e., $\Delta G <= 0.01$).

```
set.seed(123)
oj_model_1 <- rpart(
   formula = Purchase ~ .,
   data = oj_train,
   method = "class"  # "class" for classification, "anova" for regression
   )
print(oj_model_1)
```

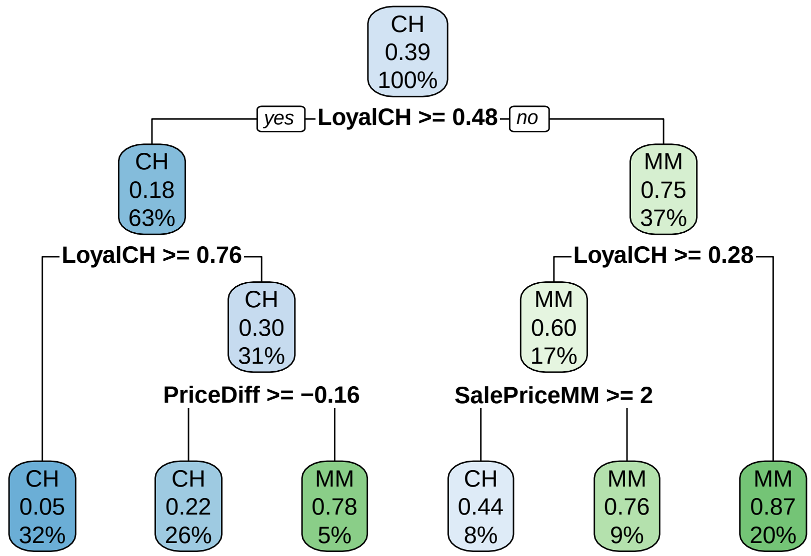
```
## n= 857
```

```
##
## node), split, n, loss, yval, (yprob)
##       * denotes terminal node
##
##  1) root 857 334 CH (0.61026838 0.38973162)
##    2) LoyalCH>=0.48285 537  94 CH (0.82495345 0.17504655)
##      4) LoyalCH>=0.7648795 271  13 CH (0.95202952 0.04797048) *
##      5) LoyalCH< 0.7648795 266  81 CH (0.69548872 0.30451128)
##       10) PriceDiff>=-0.165 226  50 CH (0.77876106 0.22123894) *
##       11) PriceDiff< -0.165 40   9 MM (0.22500000 0.77500000) *
##    3) LoyalCH< 0.48285 320  80 MM (0.25000000 0.75000000)
##      6) LoyalCH>=0.2761415 146  58 MM (0.39726027 0.60273973)
##       12) SalePriceMM>=2.04 71  31 CH (0.56338028 0.43661972) *
##       13) SalePriceMM< 2.04 75  18 MM (0.24000000 0.76000000) *
##      7) LoyalCH< 0.2761415 174  22 MM (0.12643678 0.87356322) *
```

The output starts with the root node. The predicted class at the root is `CH` and this prediction produces 334 errors on the 857 observations for a success rate of 0.61026838 and an error rate of 0.38973162. The child nodes of node "x" are labeled 2x) and 2x+1), so the child nodes of 1) are 2) and 3), and the child nodes of 2) are 4) and 5). Terminal nodes are labeled with an asterisk (*).

Surprisingly, only 3 of the 17 features were used the in full tree: `LoyalCH` (Customer brand loyalty for CH), `PriceDiff` (relative price of MM over CH), and `SalePriceMM` (absolute price of MM). The first split is at `LoyalCH` = 0.48285. Here is what the full (unpruned) tree looks like.

```r
rpart.plot(oj_model_1, yesno = TRUE)
```



The boxes show the node classification (based on mode), the proportion of observations that are *not* `CH`, and the proportion of observations included in the node.

`rpart()` not only grew the full tree, it identified the set of cost complexity parameters, and measured the model performance of each corresponding tree using cross-validation. `printcp()` displays the candidate c_p values. You can use this table to decide how to prune the tree.

```
printcp(oj_model_1)
```

```
##
## Classification tree:
## rpart(formula = Purchase ~ ., data = oj_train, method = "class")
##
## Variables actually used in tree construction:
## [1] LoyalCH     PriceDiff   SalePriceMM
##
## Root node error: 334/857 = 0.38973
##
## n= 857
##
##         CP nsplit rel error  xerror     xstd
## 1 0.479042      0   1.00000 1.00000 0.042745
## 2 0.032934      1   0.52096 0.54192 0.035775
```

```
## 3 0.013473      3   0.45509 0.47006 0.033905
## 4 0.010000      5   0.42814 0.46407 0.033736
```

There are 4 c_p values in this model. The model with the smallest complexity parameter allows the most splits (`nsplit`). The highest complexity parameter corresponds to a tree with just a root node. `rel error` is the error rate relative to the root node. The root node absolute error is 0.38973162 (the proportion of MM), so its `rel error` is 0.38973162/0.38973162 = 1.0. That means the absolute error of the full tree (at CP = 0.01) is 0.42814 * 0.38973162 = 0.1669. You can verify that by calculating the error rate of the predicted values:

```
data.frame(pred = predict(oj_model_1, newdata = oj_train, type = "class")) %>%
   mutate(obs = oj_train$Purchase,
          err = if_else(pred != obs, 1, 0)) %>%
   summarize(mean_err = mean(err))
```

```
##    mean_err
## 1 0.1668611
```

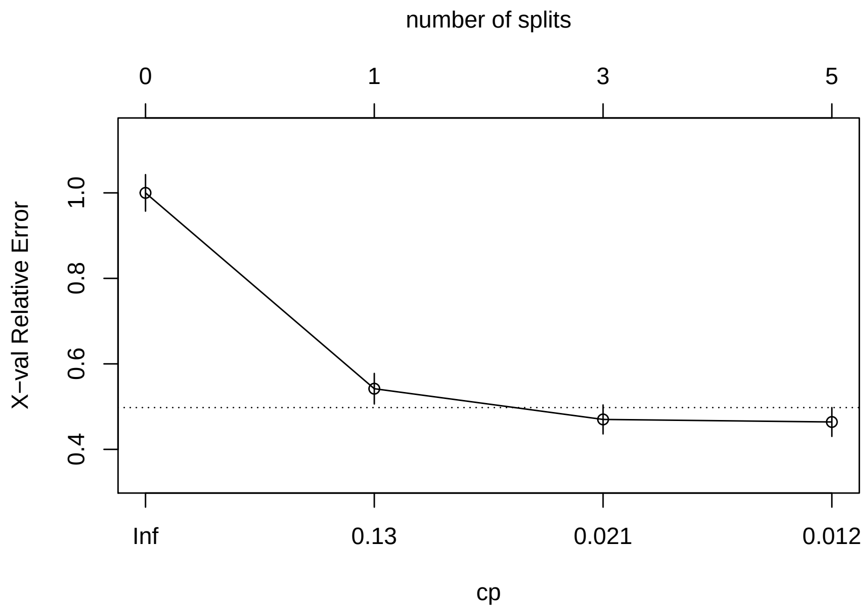
Finishing the CP table tour, `xerror` is the relative cross-validated error rate and `xstd` is its standard error. If you want the lowest possible error, then prune to the tree with the smallest relative CV error (`xerror`) ($c_p = 0.01$, CV error = 0.1809). If you want to balance predictive power with simplicity, prune to the smallest tree within 1 SE of the one with the smallest relative error. The CP table is not super-helpful for finding that tree. I'll add a column to find it.

```
oj_model_1$cptable %>%
   data.frame() %>%
   mutate(min_xerror_idx = which.min(oj_model_1$cptable[, "xerror"]),
          rownum = row_number(),
          xerror_cap = oj_model_1$cptable[min_xerror_idx, "xerror"] +
             oj_model_1$cptable[min_xerror_idx, "xstd"],
          eval = case_when(rownum == min_xerror_idx ~ "min xerror",
                           xerror < xerror_cap ~ "under cap",
                           TRUE ~ "")) %>%
   select(-rownum, -min_xerror_idx)
```

```
##           CP nsplit rel.error    xerror       xstd xerror_cap       eval
## 1 0.47904192      0 1.0000000 1.0000000 0.04274518  0.4978082
## 2 0.03293413      1 0.5209581 0.5419162 0.03577468  0.4978082
## 3 0.01347305      3 0.4550898 0.4700599 0.03390486  0.4978082  under cap
## 4 0.01000000      5 0.4281437 0.4640719 0.03373631  0.4978082 min xerror
```

The simplest tree using the 1-SE rule is $c_p = 0.01347305, CV error = 0.1832). Fortunately, `plotcp()` presents a nice graphical representation of the relationship between `xerror` and `cp`.

```
plotcp(oj_model_1, upper = "splits")
```



The dashed line is set at the minimum `xerror` + `xstd`. The top axis shows the number of splits in the tree. I'm not sure why the CP values are not the same as in the table (they are close, but not the same). The figure suggests I should prune to 5 or 3 splits. I see this curve never really hits a minimum - it is still decreasing at 5 splits. The default tuning parameter value `cp = 0.01` may be too small, so I'll set it to `cp = 0.001` and start over.

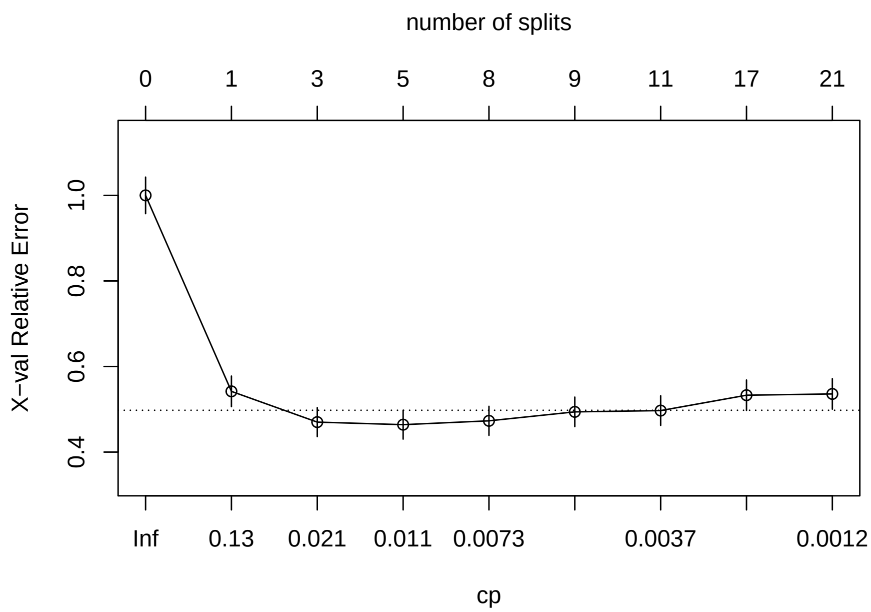
```
set.seed(123)
oj_model_1b <- rpart(
   formula = Purchase ~ .,
   data = oj_train,
   method = "class",
   cp = 0.001
   )
print(oj_model_1b)
```

```
## n= 857
##
## node), split, n, loss, yval, (yprob)
##       * denotes terminal node
##
##   1) root 857 334 CH (0.61026838 0.38973162)
```

```
##     2) LoyalCH>=0.48285 537  94 CH (0.82495345 0.17504655)
##       4) LoyalCH>=0.7648795 271  13 CH (0.95202952 0.04797048) *
##       5) LoyalCH< 0.7648795 266  81 CH (0.69548872 0.30451128)
##        10) PriceDiff>=-0.165 226  50 CH (0.77876106 0.22123894)
##          20) ListPriceDiff>=0.255 115  11 CH (0.90434783 0.09565217) *
##          21) ListPriceDiff< 0.255 111  39 CH (0.64864865 0.35135135)
##            42) PriceMM>=2.155 19   2 CH (0.89473684 0.10526316) *
##            43) PriceMM< 2.155 92  37 CH (0.59782609 0.40217391)
##              86) DiscCH>=0.115 7   0 CH (1.00000000 0.00000000) *
##              87) DiscCH< 0.115 85  37 CH (0.56470588 0.43529412)
##               174) ListPriceDiff>=0.215 45  15 CH (0.66666667 0.33333333) *
##               175) ListPriceDiff< 0.215 40  18 MM (0.45000000 0.55000000)
##                 350) LoyalCH>=0.527571 28  13 CH (0.53571429 0.46428571)
##                   700) WeekofPurchase< 266.5 21   8 CH (0.61904762 0.38095238) *
##                   701) WeekofPurchase>=266.5 7   2 MM (0.28571429 0.71428571) *
##                 351) LoyalCH< 0.527571 12   3 MM (0.25000000 0.75000000) *
##        11) PriceDiff< -0.165 40   9 MM (0.22500000 0.77500000) *
##     3) LoyalCH< 0.48285 320  80 MM (0.25000000 0.75000000)
##       6) LoyalCH>=0.2761415 146  58 MM (0.39726027 0.60273973)
##        12) SalePriceMM>=2.04 71  31 CH (0.56338028 0.43661972)
##          24) LoyalCH< 0.303104 7   0 CH (1.00000000 0.00000000) *
##          25) LoyalCH>=0.303104 64  31 CH (0.51562500 0.48437500)
##            50) WeekofPurchase>=246.5 52  22 CH (0.57692308 0.42307692)
##             100) PriceCH< 1.94 35  11 CH (0.68571429 0.31428571)
##               200) StoreID< 1.5 9   1 CH (0.88888889 0.11111111) *
##               201) StoreID>=1.5 26  10 CH (0.61538462 0.38461538)
##                 402) LoyalCH< 0.410969 17   4 CH (0.76470588 0.23529412) *
##                 403) LoyalCH>=0.410969 9   3 MM (0.33333333 0.66666667) *
##             101) PriceCH>=1.94 17   6 MM (0.35294118 0.64705882) *
##            51) WeekofPurchase< 246.5 12   3 MM (0.25000000 0.75000000) *
##        13) SalePriceMM< 2.04 75  18 MM (0.24000000 0.76000000)
##          26) SpecialCH>=0.5 14   6 CH (0.57142857 0.42857143) *
##          27) SpecialCH< 0.5 61  10 MM (0.16393443 0.83606557) *
##       7) LoyalCH< 0.2761415 174  22 MM (0.12643678 0.87356322)
##        14) LoyalCH>=0.035047 117  21 MM (0.17948718 0.82051282)
##          28) WeekofPurchase< 273.5 104  21 MM (0.20192308 0.79807692)
##            56) PriceCH>=1.875 20   9 MM (0.45000000 0.55000000)
##             112) WeekofPurchase>=252.5 12   5 CH (0.58333333 0.41666667) *
##             113) WeekofPurchase< 252.5 8   2 MM (0.25000000 0.75000000) *
##            57) PriceCH< 1.875 84  12 MM (0.14285714 0.85714286) *
##          29) WeekofPurchase>=273.5 13   0 MM (0.00000000 1.00000000) *
##        15) LoyalCH< 0.035047 57   1 MM (0.01754386 0.98245614) *
```

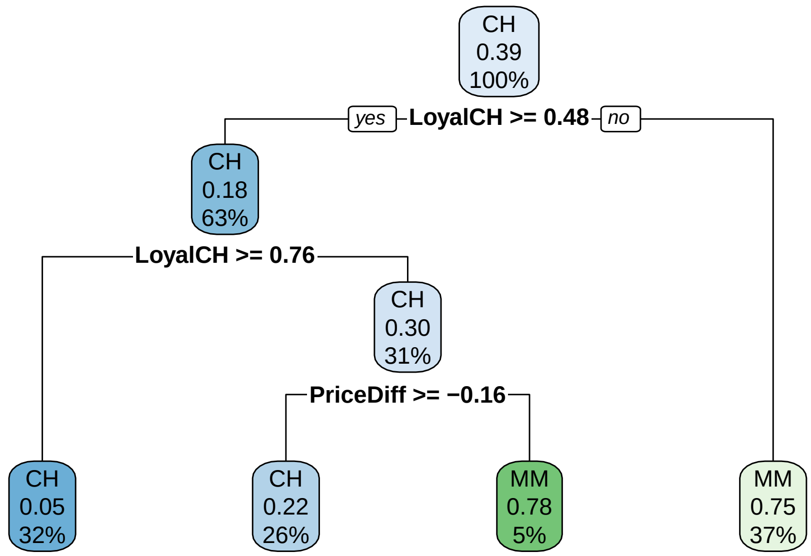
This is a much larger tree. Did I find a `cp` value that produces a local min?

```r
plotcp(oj_model_1b, upper = "splits")
```



Yes, the min is at CP = 0.011 with 5 splits. The min + 1 SE is at CP = 0.021 with 3 splits. I'll prune the tree to 3 splits.

```r
oj_model_1b_pruned <- prune(
   oj_model_1b,
   cp = oj_model_1b$cptable[oj_model_1b$cptable[, 2] == 3, "CP"]
)
rpart.plot(oj_model_1b_pruned, yesno = TRUE)
```



The most "important" indicator of `Purchase` appears to be `LoyalCH`. From the **rpart** vignette (page 12),

> "An overall measure of variable importance is the sum of the goodness of split measures for each split for which it was the primary variable, plus goodness (adjusted agreement) for all splits in which it was a surrogate."

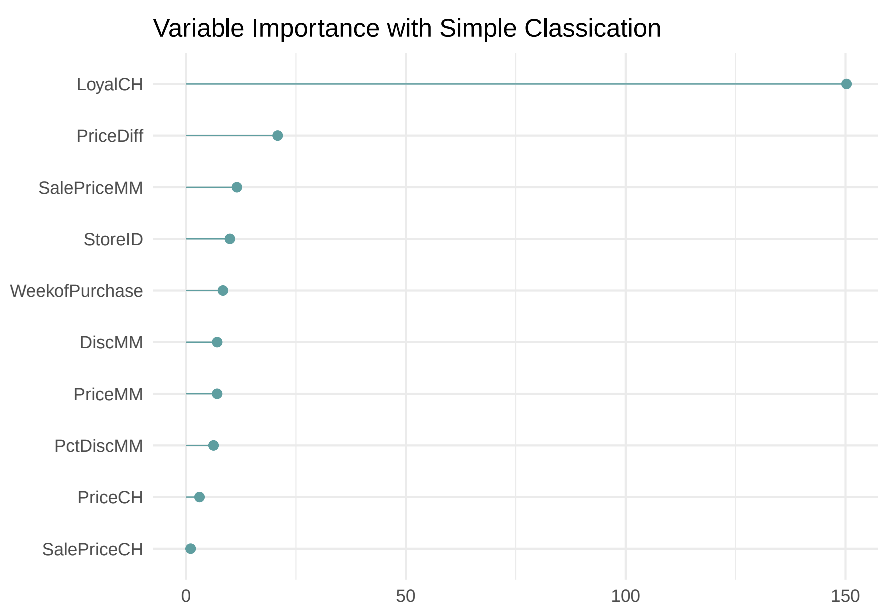
Surrogates refer to alternative features for a node to handle missing data. For each split, CART evaluates a variety of alternative "surrogate" splits to use when the feature value for the primary split is NA. Surrogate splits are splits that produce results similar to the original split.

A variable's importance is the sum of the improvement in the overall Gini (or RMSE) measure produced by the nodes in which it appears. Here is the variable importance for this model.

```
oj_model_1b_pruned$variable.importance
```

```
##       LoyalCH      PriceDiff    SalePriceMM        StoreID WeekofPurchase
##    150.237336      20.843067      11.567443       9.965419       8.386282
##        DiscMM        PriceMM      PctDiscMM        PriceCH    SalePriceCH
##      7.081470       7.065493       6.252920       3.055594       1.042153
```

```
oj_model_1b_pruned$variable.importance %>%
  data.frame() %>%
  rownames_to_column(var = "Feature") %>%
  rename(Overall = '.') %>%
  ggplot(aes(x = fct_reorder(Feature, Overall), y = Overall)) +
  geom_pointrange(aes(ymin = 0, ymax = Overall), color = "cadetblue", size = .3) +
  theme_minimal() +
  coord_flip() +
  labs(x = "", y = "", title = "Variable Importance with Simple Classication")
```



LoyalCH is by far the most important variable, as expected from its position at the top of the tree, and one level down.

You can see how the surrogates appear in the model with the summary() function.

```
summary(oj_model_1b_pruned)
```

```
## Call:
## rpart(formula = Purchase ~ ., data = oj_train, method = "class",
##     cp = 0.001)
##   n= 857
##
##            CP nsplit rel error    xerror       xstd
```

```
## 1 0.47904192      0 1.0000000 1.0000000 0.04274518
## 2 0.03293413      1 0.5209581 0.5419162 0.03577468
## 3 0.01347305      3 0.4550898 0.4700599 0.03390486
##
## Variable importance
##       LoyalCH      PriceDiff    SalePriceMM        StoreID WeekofPurchase
##            67              9              5              4              4
##        DiscMM        PriceMM      PctDiscMM        PriceCH
##             3              3              3              1
##
## Node number 1: 857 observations,    complexity param=0.4790419
##   predicted class=CH  expected loss=0.3897316  P(node) =1
##     class counts:   523   334
##    probabilities: 0.610 0.390
##   left son=2 (537 obs) right son=3 (320 obs)
##   Primary splits:
##       LoyalCH       < 0.48285   to the right, improve=132.56800, (0 missing)
##       StoreID       < 3.5       to the right, improve= 40.12097, (0 missing)
##       PriceDiff     < 0.015     to the right, improve= 24.26552, (0 missing)
##       ListPriceDiff < 0.255     to the right, improve= 22.79117, (0 missing)
##       SalePriceMM   < 1.84      to the right, improve= 20.16447, (0 missing)
##   Surrogate splits:
##       StoreID        < 3.5       to the right, agree=0.646, adj=0.053, (0 split)
##       PriceMM        < 1.89      to the right, agree=0.638, adj=0.031, (0 split)
##       WeekofPurchase < 229.5     to the right, agree=0.632, adj=0.016, (0 split)
##       DiscMM         < 0.77      to the left,  agree=0.629, adj=0.006, (0 split)
##       SalePriceMM    < 1.385     to the right, agree=0.629, adj=0.006, (0 split)
##
## Node number 2: 537 observations,    complexity param=0.03293413
##   predicted class=CH  expected loss=0.1750466  P(node) =0.6266044
##     class counts:   443    94
##    probabilities: 0.825 0.175
##   left son=4 (271 obs) right son=5 (266 obs)
##   Primary splits:
##       LoyalCH       < 0.7648795 to the right, improve=17.669310, (0 missing)
##       PriceDiff     < 0.015     to the right, improve=15.475200, (0 missing)
##       SalePriceMM   < 1.84      to the right, improve=13.951730, (0 missing)
##       ListPriceDiff < 0.255     to the right, improve=11.407560, (0 missing)
##       DiscMM        < 0.15      to the left,  improve= 7.795122, (0 missing)
##   Surrogate splits:
##       WeekofPurchase < 257.5     to the right, agree=0.594, adj=0.180, (0 split)
##       PriceCH        < 1.775     to the right, agree=0.590, adj=0.173, (0 split)
##       StoreID        < 3.5       to the right, agree=0.587, adj=0.165, (0 split)
##       PriceMM        < 2.04      to the right, agree=0.587, adj=0.165, (0 split)
##       SalePriceMM    < 2.04      to the right, agree=0.587, adj=0.165, (0 split)
##
```

```
## Node number 3: 320 observations
##   predicted class=MM  expected loss=0.25  P(node) =0.3733956
##     class counts:    80   240
##    probabilities: 0.250 0.750
##
## Node number 4: 271 observations
##   predicted class=CH  expected loss=0.04797048  P(node) =0.3162194
##     class counts:   258    13
##    probabilities: 0.952 0.048
##
## Node number 5: 266 observations,    complexity param=0.03293413
##   predicted class=CH  expected loss=0.3045113  P(node) =0.3103851
##     class counts:   185    81
##    probabilities: 0.695 0.305
##   left son=10 (226 obs) right son=11 (40 obs)
##   Primary splits:
##       PriceDiff     < -0.165    to the right, improve=20.84307, (0 missing)
##       ListPriceDiff < 0.235     to the right, improve=20.82404, (0 missing)
##       SalePriceMM   < 1.84      to the right, improve=16.80587, (0 missing)
##       DiscMM        < 0.15      to the left,  improve=10.05120, (0 missing)
##       PctDiscMM     < 0.0729725 to the left,  improve=10.05120, (0 missing)
##   Surrogate splits:
##       SalePriceMM    < 1.585     to the right, agree=0.906, adj=0.375, (0 split)
##       DiscMM         < 0.57      to the left,  agree=0.895, adj=0.300, (0 split)
##       PctDiscMM      < 0.264375  to the left,  agree=0.895, adj=0.300, (0 split)
##       WeekofPurchase < 274.5     to the left,  agree=0.872, adj=0.150, (0 split)
##       SalePriceCH    < 2.075     to the left,  agree=0.857, adj=0.050, (0 split)
##
## Node number 10: 226 observations
##   predicted class=CH  expected loss=0.2212389  P(node) =0.2637106
##     class counts:   176    50
##    probabilities: 0.779 0.221
##
## Node number 11: 40 observations
##   predicted class=MM  expected loss=0.225  P(node) =0.04667445
##     class counts:     9    31
##    probabilities: 0.225 0.775
```

The last step is to make predictions on the validation data set. For a classification tree, set argument `type = "class"`.

```
oj_model_1b_preds <- predict(oj_model_1b_pruned, oj_test, type = "class")
```

I'll evaluate the predictions and record the accuracy (correct classification percentage) for comparison to other models. Two ways to evaluate the model are the confusion matrix, and the ROC curve.

9.1.1 Confusion Matrix

Print the confusion matrix with `caret::confusionMatrix()` to see how well does this model performs against the test data set.

```
oj_model_1b_cm <- confusionMatrix(data = oj_model_1b_preds, reference = oj_test$Purchas
oj_model_1b_cm
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  CH  MM
##         CH 113  13
##         MM  17  70
##
##                Accuracy : 0.8592
##                  95% CI : (0.8051, 0.9029)
##     No Information Rate : 0.6103
##     P-Value [Acc > NIR] : 1.265e-15
##
##                   Kappa : 0.7064
##
##  Mcnemar's Test P-Value : 0.5839
##
##             Sensitivity : 0.8692
##             Specificity : 0.8434
##          Pos Pred Value : 0.8968
##          Neg Pred Value : 0.8046
##              Prevalence : 0.6103
##          Detection Rate : 0.5305
##    Detection Prevalence : 0.5915
##       Balanced Accuracy : 0.8563
##
##        'Positive' Class : CH
##
```

The confusion matrix is at the top. It also includes a lot of statistics. It's worth getting familiar with the stats. The model accuracy and 95% CI are calculated from the binomial test.

```
binom.test(x = 113 + 70, n = 213)
```

```
##
##  Exact binomial test
```

```
##
## data:  113 + 70 and 213
## number of successes = 183, number of trials = 213, p-value < 2.2e-16
## alternative hypothesis: true probability of success is not equal to 0.5
## 95 percent confidence interval:
##  0.8050785 0.9029123
## sample estimates:
## probability of success
##              0.8591549
```

The "No Information Rate" (NIR) statistic is the class rate for the largest class. In this case CH is the largest class, so NIR = 130/213 = 0.6103. "P-Value [Acc > NIR]" is the binomial test that the model accuracy is significantly better than the NIR (i.e., significantly better than just always guessing CH).

```
binom.test(x = 113 + 70, n = 213, p = 130/213, alternative = "greater")
```

```
##
##  Exact binomial test
##
## data:  113 + 70 and 213
## number of successes = 183, number of trials = 213, p-value = 1.265e-15
## alternative hypothesis: true probability of success is greater than 0.6103286
## 95 percent confidence interval:
##  0.8138446 1.0000000
## sample estimates:
## probability of success
##              0.8591549
```

The "Accuracy" statistic indicates the model predicts 0.8590 of the observations correctly. That's good, but less impressive when you consider the prevalence of CH is 0.6103 - you could achieve 61% accuracy just by predicting CH every time. A measure that controls for the prevalence is Cohen's kappa statistic. The kappa statistic is explained here. It compares the accuracy to the accuracy of a "random system". It is defined as

$$\kappa = \frac{Acc - RA}{1 - RA}$$

where

$$RA = \frac{ActFalse \times PredFalse + ActTrue \times PredTrue}{Total \times Total}$$

is the hypotheical probability of a chance agreement. ActFalse will be the number of "MM" ($13 + 70 = 83$) and actual true will be the number of "CH" ($113 + 17 = 130$). The predicted counts are

```
table(oj_model_1b_preds)
```

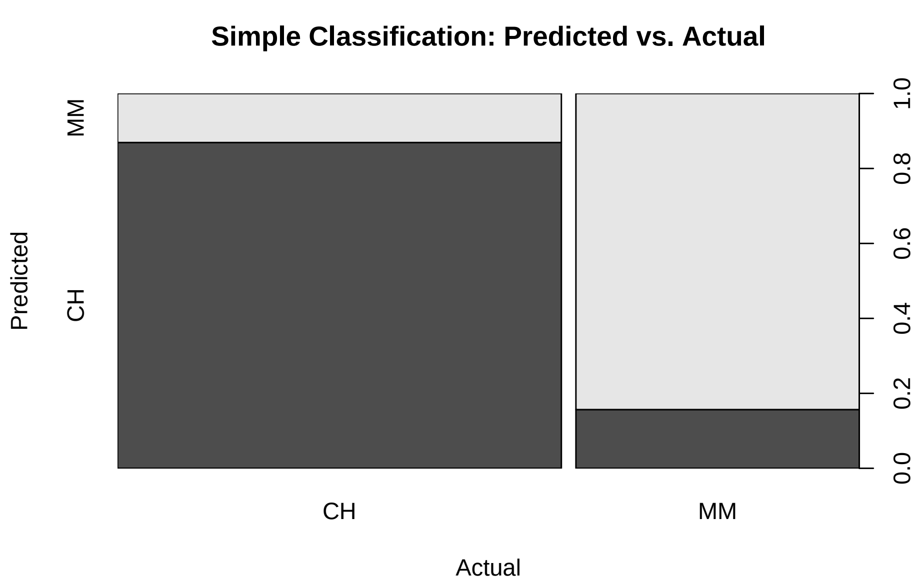
```
## oj_model_1b_preds
##  CH  MM
## 126  87
```

So, $RA = (83 * 87 + 130 * 126)/213^2 = 0.5202$ and $\kappa = (0.8592 - 0.5202)/(1 - 0.5202) = 0.7064$. The kappa statistic varies from 0 to 1 where 0 means accurate predictions occur merely by chance, and 1 means the predictions are in perfect agreement with the observations. In this case, a kappa statistic of 0.7064 is "substantial". See chart here.

The other measures from the `confusionMatrix()` output are various proportions and you can remind yourself of their definitions in the documentation with `?confusionMatrix`.

Visuals are almost always helpful. Here is a plot of the confusion matrix.

```
plot(oj_test$Purchase, oj_model_1b_preds,
     main = "Simple Classification: Predicted vs. Actual",
     xlab = "Actual",
     ylab = "Predicted")
```



By the way, how does the validation set accuracy ()

```
oj_model_1b_train_preds <- predict(oj_model_1b_pruned, oj_train, type = "class")
oj_model_1b_train_cm <- confusionMatrix(data = oj_model_1b_train_preds, reference = oj_train$Purc
oj_model_1b_train_cm$overall
```

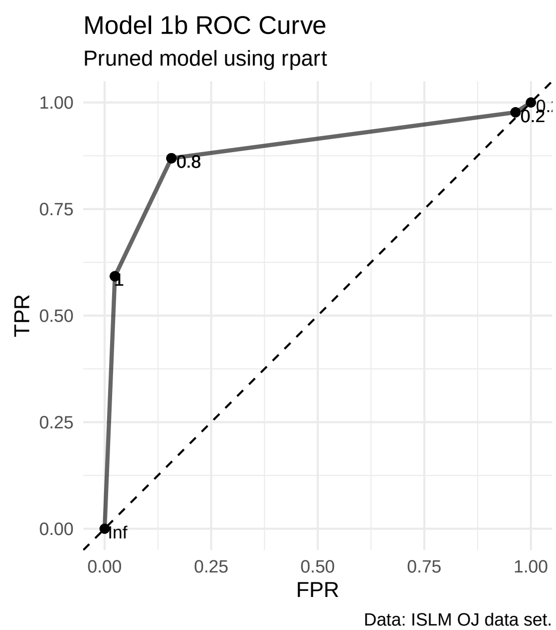
```
##       Accuracy          Kappa  AccuracyLower  AccuracyUpper   AccuracyNull
##   8.226371e-01   6.323113e-01   7.953840e-01   8.476497e-01   6.102684e-01
## AccuracyPValue  McnemarPValue
##   1.859617e-41   4.258396e-02
```

The accuracy on the training data set was a little lower than on the test data set. I though it would be higher, not lower.

9.1.2 ROC Curve

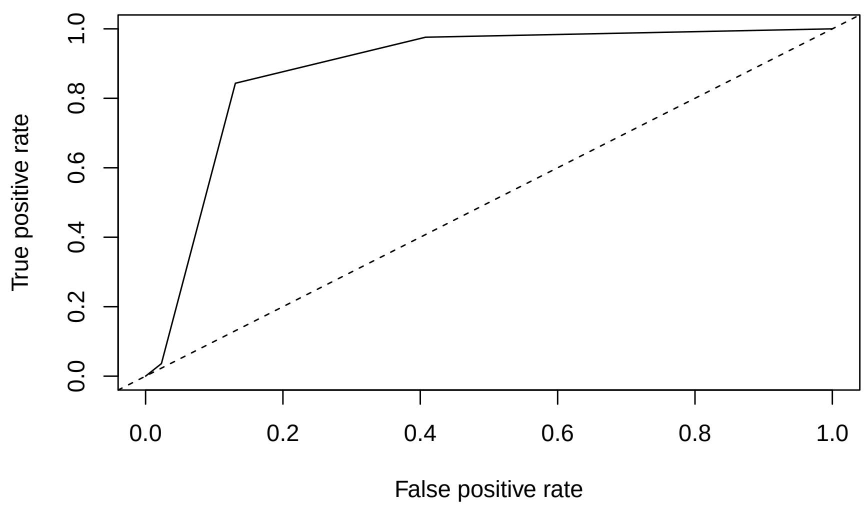
Another measure of accuracy is the ROC (receiver operating characteristics) curve (Fawcett, 2005). The ROC curve is a plot of the true positive rate (TPR, sensitivity) versus the false positive rate (FPR, 1 - specificity) for a set of thresholds. By default, the threshold for predicting the default classification is 0.50, but it could be any threshold. The ROC curves varies the thresholds. (I'll use the `geom_roc` geom from **plotROC**.

```
data.frame(M = predict(oj_model_1b_pruned, oj_test, "prob")[, 1],
           D = if_else(oj_test$Purchase == "CH", 1, 0)) %>%
   ggplot() +
   geom_roc(aes(m = M, d = D), hjust = -0.4, vjust = 1.5, linealpha = 0.6, labelsize = 3, n.cuts
   geom_abline(intercept = 0, slope = 1, linetype = 2) +
   coord_equal() +
   theme_minimal() +
   labs(x = "FPR", y = "TPR",
        title = "Model 1b ROC Curve",
        subtitle = "Pruned model using rpart",
        caption = "Data: ISLM OJ data set.")
```



You can also use `prediction()` and `plot.prediction()` from the **ROCR** package.

```
pred <- prediction(predict(oj_model_1b_pruned, newdata = oj_test, type = "prob")[, 2],
plot(performance(pred, "tpr", "fpr"))
abline(0, 1, lty = 2)
```



Hmm, not quite the same…

A few points on the ROC space are helpful for understanding how to use it.

- The lower left point (0, 0) is the result of *always* predicting "negative" or in this case "MM" if "CH" is taken as the default class. Sure, your false positive rate is zero, but since you never predict a positive, your true positive rate is also zero.

- The upper right point (1, 1) is the results of *always* predicting "positive" (or "CH" here). You catch all the positives, but you miss all the negatives.
- The upper left point (0, 1) is the result of perfect accuracy. You catch all the positives and all the negatives.
- The lower right point (1, 0) is the result of perfect imbecility. You made the exact wrong prediction every time.
- The 45 degree diagonal is the result of randomly guessing positive (CH) X percent of the time. If you guess positive 90% of the time and the prevalence is 50%, your TPR will be 90% and your FPR will also be 90%, etc.

From the last bullet, it is evident that any point below and to the right of the 45 degree diagonal represents an instance where the model would have been better off just predicting entirely one way or the other. The goal is for all nodes to bunch up in the upper left.

Points to the left of the diagonal with a low TPR can be thought of as "conservative" predicters - they only make positive (CH) predictions with strong evidence. Points to the left of the diagonal with a high TPR can be thought of as “liberal” predicters - they make positive (CH) predictions with weak evidence.

9.1.3 Caret Approach

I can also fit the model with `caret::train()`. There are two ways to tune hyperparameters in `train()`:

- set the number of tuning parameter values to consider by setting `tuneLength`, or
- set particular values to consider for each parameter by defining a `tuneGrid`.

I’ll build the model using 10-fold cross-validation to optimize the hyperparameter CP. If you don’t have any idea what the tuning parameter ought to look like, use `tuneLength` to get close, then fine-tune with `tuneGrid`. That’s what I’ll do. I’ll create a training control object that I can re-use in other model builds.

```
oj_trControl = trainControl(
   method = "cv",  # k-fold cross validation
   number = 10,  # 10 folds
   savePredictions = "final",       # save predictions for the optimal tuning paramete
   classProbs = TRUE  # return class probabilities in addition to predicted values
#   summaryFunction = twoClassSummary  # computes sensitivity, specificity and the are
   )
```

Now fit the model.

```
set.seed(1234)
oj_model_2 = train(
   Purchase ~ .,
   data = oj_train,
   method = "rpart",
   tuneLength = 5,
   metric = "Accuracy",
   trControl = oj_trControl
   )
```

`caret` built a full tree using `rpart`’s default parameters: gini splitting index, at least 20 observations in a node in order to consider splitting it, and at least 6 observations in each node. Caret then calculated the accuracy for each candidate value of α. Here is the results.

```
print(oj_model_2)
```

```
## CART
##
## 857 samples
##  17 predictor
##   2 classes: 'CH', 'MM'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 772, 772, 771, 770, 771, 771, ...
## Resampling results across tuning parameters:
##
##   cp           Accuracy   Kappa
##   0.005988024  0.8085999  0.5931149
##   0.008982036  0.8086267  0.5943277
##   0.013473054  0.8051657  0.5885521
##   0.032934132  0.7841798  0.5371171
##   0.479041916  0.6603904  0.1774773
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was cp = 0.008982036.
```

The second `cp` (0.008982036) produced the highest accuracy. I can drill into the best value of `cp` using a tuning grid. I'll try that now.

```
set.seed(1234)
oj_model_3 = train(
   Purchase ~ .,
   data = oj_train,
   method = "rpart",
   tuneGrid = expand.grid(cp = seq(from = 0.001, to = 0.010, length = 11)),
   metric='Accuracy',
   trControl = oj_trControl
   )
print(oj_model_3)
```

```
## CART
##
## 857 samples
##  17 predictor
##   2 classes: 'CH', 'MM'
##
## No pre-processing
```

```
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 772, 772, 771, 770, 771, 771, ...
## Resampling results across tuning parameters:
##
##   cp      Accuracy   Kappa
##   0.0010  0.8004874  0.5753480
##   0.0019  0.8016502  0.5785232
##   0.0028  0.8039758  0.5845653
##   0.0037  0.8085999  0.5955198
##   0.0046  0.8039351  0.5851273
##   0.0055  0.8085863  0.5937949
##   0.0064  0.8085999  0.5931149
##   0.0073  0.8120883  0.6011446
##   0.0082  0.8120883  0.6011446
##   0.0091  0.8086267  0.5943277
##   0.0100  0.8086540  0.5953150
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was cp = 0.0082.
```

The beset model is at cp = 0.009. Here are the rules in the final model.

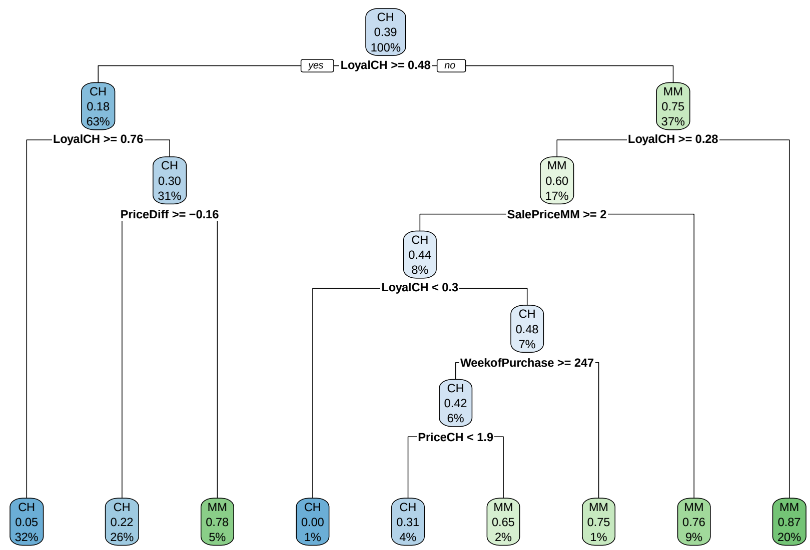
```
oj_model_3$finalModel
```

```
## n= 857
##
## node), split, n, loss, yval, (yprob)
##       * denotes terminal node
##
##   1) root 857 334 CH (0.61026838 0.38973162)
##     2) LoyalCH>=0.48285 537  94 CH (0.82495345 0.17504655)
##       4) LoyalCH>=0.7648795 271  13 CH (0.95202952 0.04797048) *
##       5) LoyalCH< 0.7648795 266  81 CH (0.69548872 0.30451128)
##        10) PriceDiff>=-0.165 226  50 CH (0.77876106 0.22123894) *
##        11) PriceDiff< -0.165 40   9 MM (0.22500000 0.77500000) *
##     3) LoyalCH< 0.48285 320  80 MM (0.25000000 0.75000000)
##       6) LoyalCH>=0.2761415 146  58 MM (0.39726027 0.60273973)
##        12) SalePriceMM>=2.04 71  31 CH (0.56338028 0.43661972)
##          24) LoyalCH< 0.303104 7   0 CH (1.00000000 0.00000000) *
##          25) LoyalCH>=0.303104 64  31 CH (0.51562500 0.48437500)
##            50) WeekofPurchase>=246.5 52  22 CH (0.57692308 0.42307692)
##             100) PriceCH< 1.94 35  11 CH (0.68571429 0.31428571) *
##             101) PriceCH>=1.94 17   6 MM (0.35294118 0.64705882) *
##            51) WeekofPurchase< 246.5 12   3 MM (0.25000000 0.75000000) *
##        13) SalePriceMM< 2.04 75  18 MM (0.24000000 0.76000000) *
```

```
##       7) LoyalCH< 0.2761415 174  22 MM (0.12643678 0.87356322) *
```

Here is the tree.

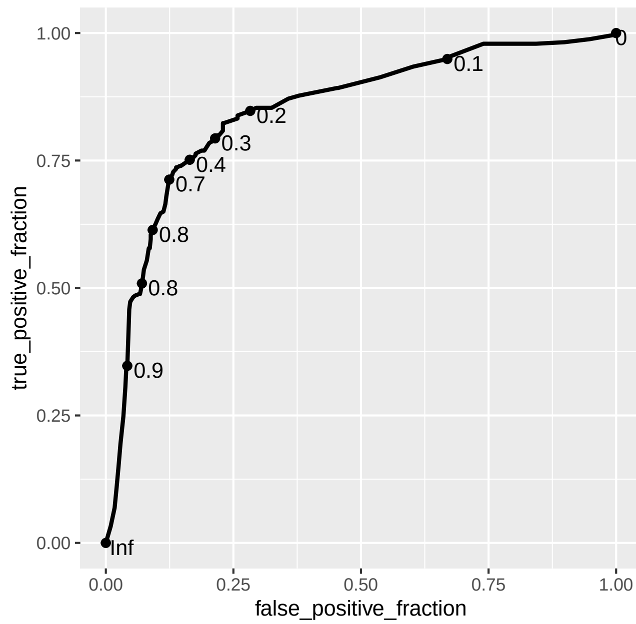
```
rpart.plot(oj_model_3$finalModel)
```



Here is the ROC curve.

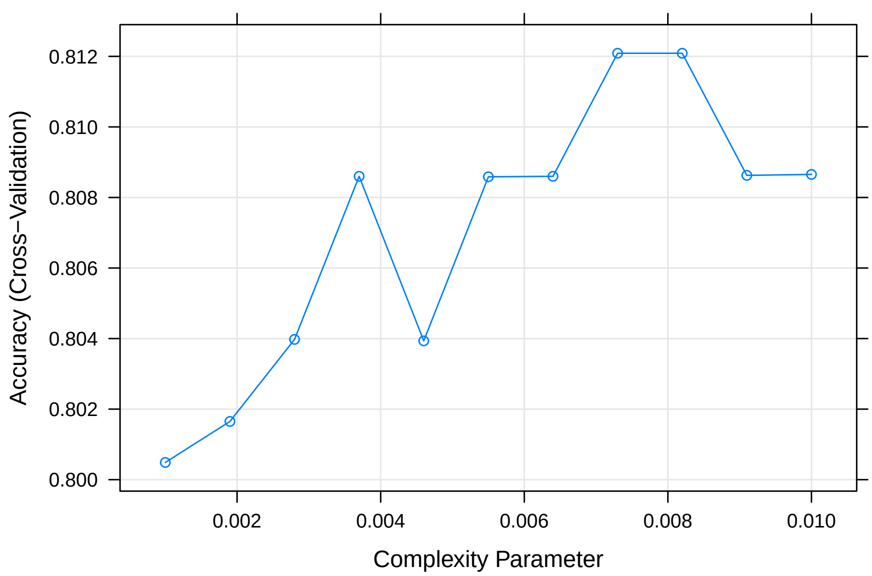
```
library(plotROC)
ggplot(oj_model_3$pred) +
    geom_roc(
       aes(
          m = MM,
          d = factor(obs, levels = c("CH", "MM"))
       ),
       hjust = -0.4, vjust = 1.5
    ) +
   coord_equal()
```

```
## Warning in verify_d(data$d): D not labeled 0/1, assuming CH = 0 and MM = 1!
```



Here are the cross-validated Accuracy for each candidate cp value.

```
plot(oj_model_3)
```



Evaluate the model by making predictions with the test data set.

```
oj_model_3_preds <- predict(oj_model_3, oj_test, type = "raw")
```

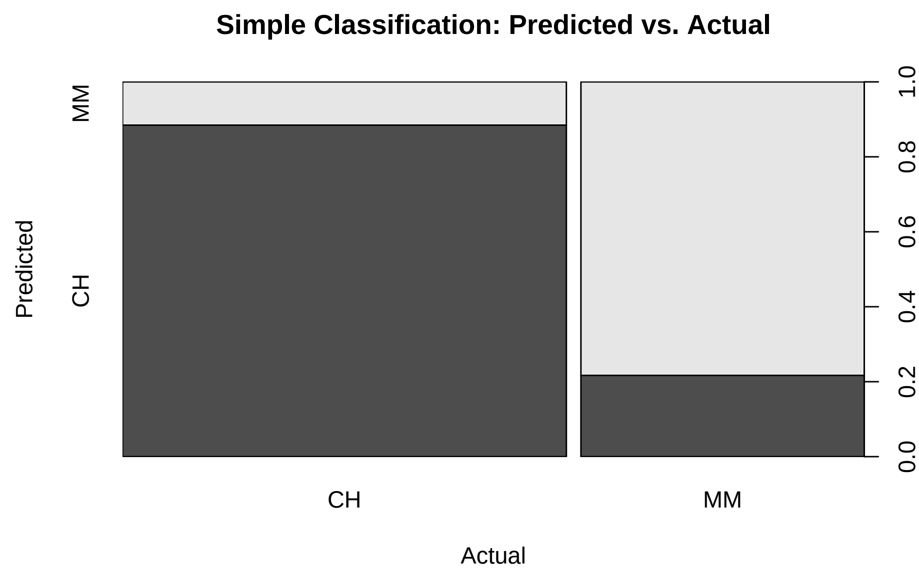
The confusion matrix shows the true positives and true negatives.

```
oj_model_3_cm <- confusionMatrix(
   data = oj_model_3_preds,
   reference = oj_test$Purchase
)
oj_model_3_cm
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  CH  MM
##         CH 115  18
##         MM  15  65
##
##                Accuracy : 0.8451
##                  95% CI : (0.7894, 0.8909)
##     No Information Rate : 0.6103
##     P-Value [Acc > NIR] : 6.311e-14
##
##                   Kappa : 0.6721
##
##  Mcnemar's Test P-Value : 0.7277
##
##             Sensitivity : 0.8846
##             Specificity : 0.7831
##          Pos Pred Value : 0.8647
##          Neg Pred Value : 0.8125
##              Prevalence : 0.6103
##          Detection Rate : 0.5399
##    Detection Prevalence : 0.6244
##       Balanced Accuracy : 0.8339
##
##        'Positive' Class : CH
##
```

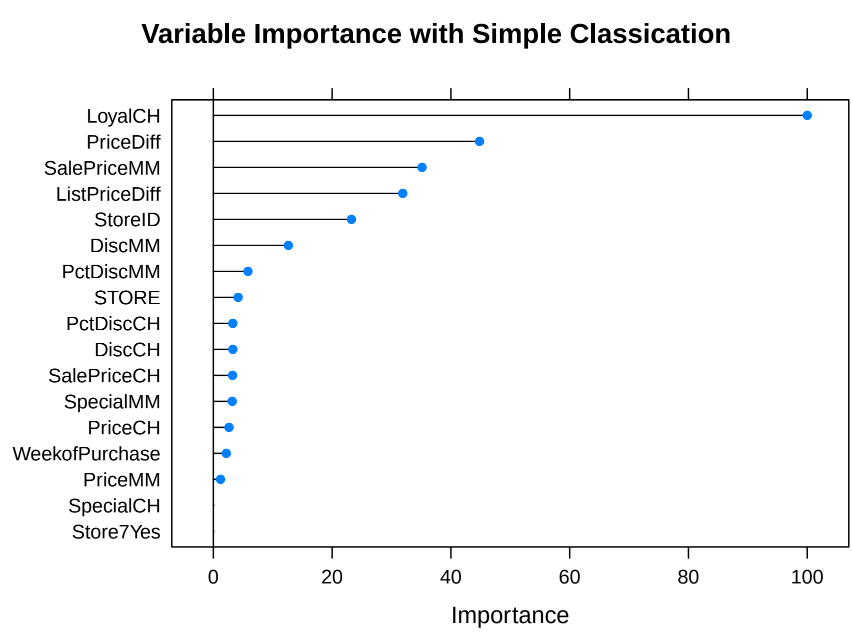
The accuracy metric is the slightly worse than in my previous model. Here is a graphical representation of the confusion matrix.

```
plot(oj_test$Purchase, oj_model_3_preds,
     main = "Simple Classification: Predicted vs. Actual",
     xlab = "Actual",
     ylab = "Predicted")
```



Finally, here is the variable importance plot.

```
plot(varImp(oj_model_3), main="Variable Importance with Simple Classication")
```



Looks like the manual effort faired best. Here is a summary the accuracy rates of the three models.

```
rbind(data.frame(model = "Manual Class", Acc = round(oj_model_1b_cm$overall["Accuracy"], 5)),
      data.frame(model = "Caret w/tuneGrid", Acc = round(oj_model_3_cm$overall["Accuracy"], 5))
)
```

```
##                        model     Acc
## Accuracy      Manual Class 0.85915
## Accuracy1 Caret w/tuneGrid 0.84507
```

9.2 Regression Trees

A simple regression tree is built in a manner similar to a simple classificatioon tree, and like the simple classification tree, it is rarely invoked on its own; the bagged, random forest, and gradient boosting methods build on this logic. I'll learn by example again. Using the `ISLR::Carseats` data set, I will predict `Sales` using from the 10 feature variables. Load the data.

```
carseats_dat <- Carseats
#skim_with(numeric = list(p0 = NULL, p25 = NULL, p50 = NULL, p75 = NULL,
#                                 p100 = NULL, hist = NULL))
#skim(carseats_dat)
```

I'll split `careseats_dat` (n = 400) into `carseats_train` (80%, n = 321) and `carseats_test` (20%, n = 79). I'll fit a simple decision tree with `carseats_train`, then later a bagged tree, a random forest, and a gradient boosting tree. I'll compare their predictive performance with `carseats_test`.

```
set.seed(12345)
partition <- createDataPartition(y = carseats_dat$Sales, p = 0.8, list = FALSE)
carseats_train <- carseats_dat[partition, ]
carseats_test <- carseats_dat[-partition, ]
```

The first step is to build a full tree, then perform k-fold cross-validation to help select the optimal cost complexity (cp). The only difference here is the `rpart()` parameter `method = "anova"` to produce a regression tree.

```
set.seed(1234)
carseats_model_1 <- rpart(
   formula = Sales ~ .,
   data = carseats_train,
   method = "anova",
```

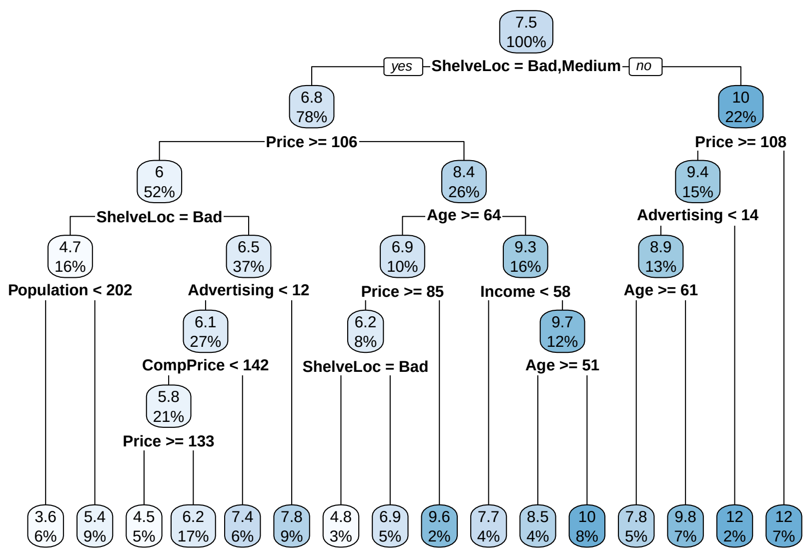
```
    xval = 10,
    model = TRUE  # to plot splits with factor variables.
)
print(carseats_model_1)
```

```
## n= 321
##
## node), split, n, deviance, yval
##       * denotes terminal node
##
##  1) root 321 2567.76800  7.535950
##    2) ShelveLoc=Bad,Medium 251 1474.14100  6.770359
##      4) Price>=105.5 168  719.70630  5.987024
##        8) ShelveLoc=Bad 50  165.70160  4.693600
##         16) Population< 201.5 20   48.35505  3.646500 *
##         17) Population>=201.5 30   80.79922  5.391667 *
##        9) ShelveLoc=Medium 118  434.91370  6.535085
##         18) Advertising< 11.5 88  290.05490  6.113068
##           36) CompPrice< 142 69  193.86340  5.769420
##             72) Price>=132.5 16   50.75440  4.455000 *
##             73) Price< 132.5 53  107.12060  6.166226 *
##           37) CompPrice>=142 19   58.45118  7.361053 *
##         19) Advertising>=11.5 30   83.21323  7.773000 *
##      5) Price< 105.5 83  442.68920  8.355904
##       10) Age>=63.5 32  153.42300  6.922500
##         20) Price>=85 25   66.89398  6.160800
##           40) ShelveLoc=Bad 9   18.39396  4.772222 *
##           41) ShelveLoc=Medium 16   21.38544  6.941875 *
##         21) Price< 85 7   20.22194  9.642857 *
##       11) Age< 63.5 51  182.26350  9.255294
##         22) Income< 57.5 12   28.03042  7.707500 *
##         23) Income>=57.5 39  116.63950  9.731538
##           46) Age>=50.5 14   21.32597  8.451429 *
##           47) Age< 50.5 25   59.52474 10.448400 *
##    3) ShelveLoc=Good 70  418.98290 10.281140
##      6) Price>=107.5 49  242.58730  9.441633
##       12) Advertising< 13.5 41  162.47820  8.926098
##         24) Age>=61 17   53.37051  7.757647 *
##         25) Age< 61 24   69.45776  9.753750 *
##       13) Advertising>=13.5 8   13.36599 12.083750 *
##      7) Price< 107.5 21   61.28200 12.240000 *
```

The output starts with the root node. The predicted `Sales` at the root is the mean `Sales` for the training data set, 7.535950 (values are \$000s). The deviance at the root is the SSE, 2567.768. The child nodes of node "x" are labeled 2x) and 2x+1), so the child nodes of 1) are 2) and 3), and the child nodes of 2) are 4) and 5). Terminal nodes are labeled with an asterisk (*).

The first split is at `ShelveLoc` = [Bad, Medium] vs Good. Here is what the full (unpruned) tree looks like.

```
rpart.plot(carseats_model_1, yesno = TRUE)
```



The boxes show the node predicted value (mean) and the proportion of observations that are in the node (or child nodes).

`rpart()` not only grew the full tree, it also used cross-validation to test the performance of the possible complexity hyperparameters. `printcp()` displays the candidate cp values. You can use this table to decide how to prune the tree.

```
printcp(carseats_model_1)
```

```
##
## Regression tree:
## rpart(formula = Sales ~ ., data = carseats_train, method = "anova",
##     model = TRUE, xval = 10)
##
## Variables actually used in tree construction:
## [1] Advertising Age         CompPrice   Income      Population  Price
## [7] ShelveLoc
```

```
##
## Root node error: 2567.8/321 = 7.9993
##
## n= 321
##
##          CP nsplit rel error  xerror     xstd
## 1  0.262736      0   1.00000 1.00635 0.076664
## 2  0.121407      1   0.73726 0.74888 0.058981
## 3  0.046379      2   0.61586 0.65278 0.050839
## 4  0.044830      3   0.56948 0.67245 0.051638
## 5  0.041671      4   0.52465 0.66230 0.051065
## 6  0.025993      5   0.48298 0.62345 0.049368
## 7  0.025823      6   0.45698 0.61980 0.048026
## 8  0.024007      7   0.43116 0.62058 0.048213
## 9  0.015441      8   0.40715 0.58061 0.041738
## 10 0.014698      9   0.39171 0.56413 0.041368
## 11 0.014641     10   0.37701 0.56277 0.041271
## 12 0.014233     11   0.36237 0.56081 0.041097
## 13 0.014015     12   0.34814 0.55647 0.038308
## 14 0.013938     13   0.33413 0.55647 0.038308
## 15 0.010560     14   0.32019 0.57110 0.038872
## 16 0.010000     15   0.30963 0.56676 0.038090
```

There are 16 possible cp values in this model. The model with the smallest complexity parameter allows the most splits (`nsplit`). The highest complexity parameter corresponds to a tree with just a root node. `rel error` is the SSE relative to the root node. The root node SSE is 2567.76800, so its `rel error` is 2567.76800/2567.76800 = 1.0. That means the absolute error of the full tree (at CP = 0.01) is 0.30963 * 2567.76800 = 795.058. You can verify that by calculating the SSE of the model predicted values:

```
data.frame(pred = predict(carseats_model_1, newdata = carseats_train)) %>%
  mutate(obs = carseats_train$Sales,
         sq_err = (obs - pred)^2) %>%
  summarize(sse = sum(sq_err))
```

```
##        sse
## 1 795.0525
```

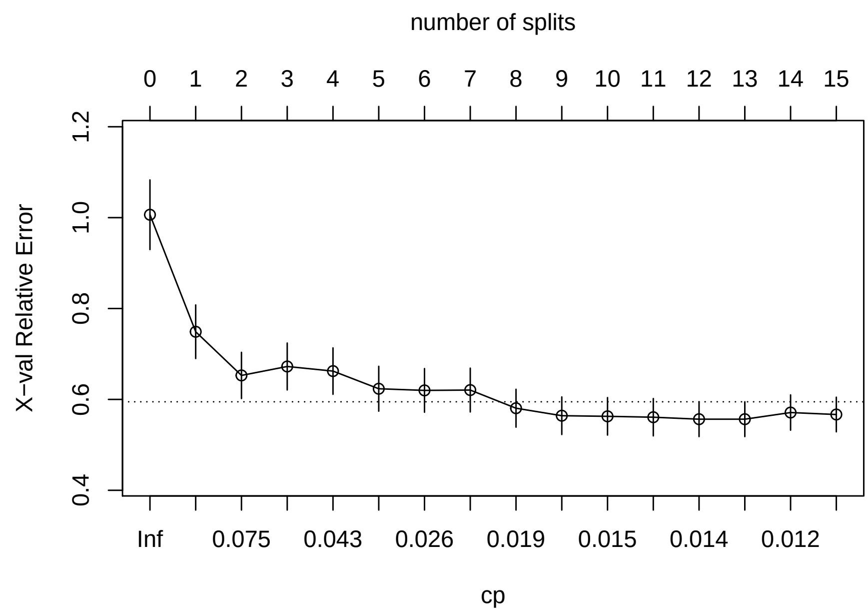
Finishing the CP table tour, `xerror` is the cross-validated SSE and `xstd` is its standard error. If you want the lowest possible error, then prune to the tree with the smallest relative SSE (`xerror`). If you want to balance predictive power with simplicity, prune to the smallest tree within 1 SE of the one with the smallest relative SSE. The CP table is not super-helpful for finding that tree. I'll add a column to find it.

```
carseats_model_1$cptable %>%
  data.frame() %>%
  mutate(min_xerror_idx = which.min(carseats_model_1$cptable[, "xerror"]),
         rownum = row_number(),
         xerror_cap = carseats_model_1$cptable[min_xerror_idx, "xerror"] +
           carseats_model_1$cptable[min_xerror_idx, "xstd"],
         eval = case_when(rownum == min_xerror_idx ~ "min xerror",
                          xerror < xerror_cap ~ "under cap",
                          TRUE ~ "")) %>%
  select(-rownum, -min_xerror_idx)
```

```
##            CP nsplit rel.error    xerror       xstd xerror_cap       eval
## 1  0.26273578      0 1.0000000 1.0063530 0.07666355  0.5947744
## 2  0.12140705      1 0.7372642 0.7488767 0.05898146  0.5947744
## 3  0.04637919      2 0.6158572 0.6527823 0.05083938  0.5947744
## 4  0.04483023      3 0.5694780 0.6724529 0.05163819  0.5947744
## 5  0.04167149      4 0.5246478 0.6623028 0.05106530  0.5947744
## 6  0.02599265      5 0.4829763 0.6234457 0.04936799  0.5947744
## 7  0.02582284      6 0.4569836 0.6198034 0.04802643  0.5947744
## 8  0.02400748      7 0.4311608 0.6205756 0.04821332  0.5947744
## 9  0.01544139      8 0.4071533 0.5806072 0.04173785  0.5947744  under cap
## 10 0.01469771      9 0.3917119 0.5641331 0.04136793  0.5947744  under cap
## 11 0.01464055     10 0.3770142 0.5627713 0.04127139  0.5947744  under cap
## 12 0.01423309     11 0.3623736 0.5608073 0.04109662  0.5947744  under cap
## 13 0.01401541     12 0.3481405 0.5564663 0.03830810  0.5947744 min xerror
## 14 0.01393771     13 0.3341251 0.5564663 0.03830810  0.5947744  under cap
## 15 0.01055959     14 0.3201874 0.5710951 0.03887227  0.5947744  under cap
## 16 0.01000000     15 0.3096278 0.5667561 0.03808991  0.5947744  under cap
```

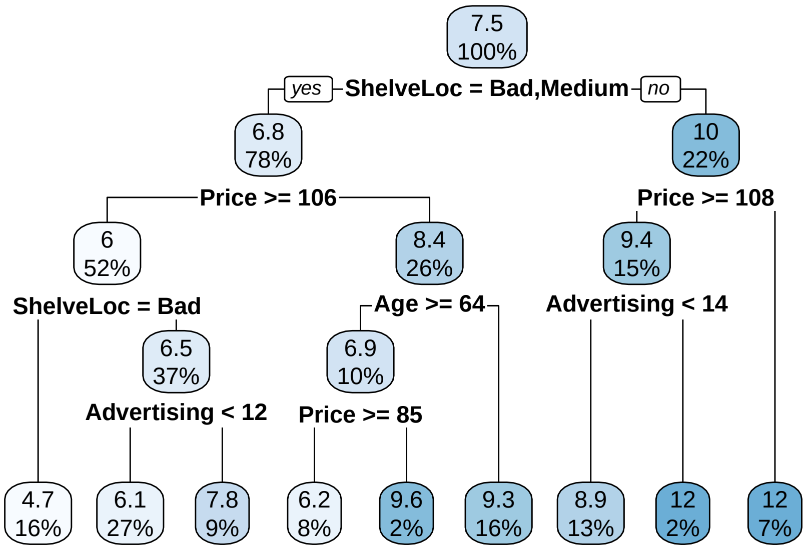
Okay, so the simplest tree is the one with CP = 0.01544139 (8 splits). Fortunately, `plotcp()` presents a nice graphical representation of the relationship between `xerror` and `cp`.

```
plotcp(carseats_model_1, upper = "splits")
```



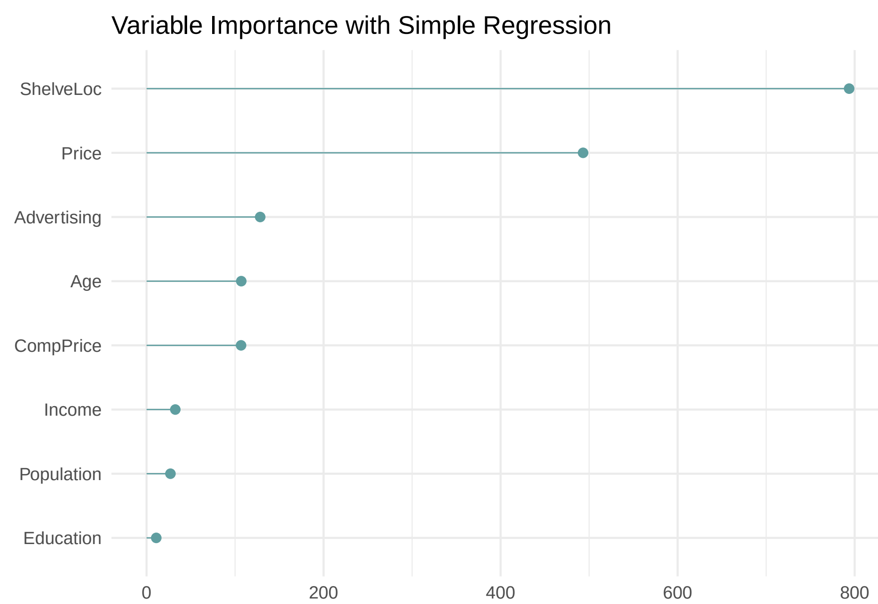
The dashed line is set at the minimum `xerror` + `xstd`. The top axis shows the number of splits in the tree. I'm not sure why the CP values are not the same as in the table (they are close, but not the same). The smallest relative error is at 0.0140154, but the maximum CP below the dashed line (one standard deviation above the mimimum error) is at CP = .019 (8 splits). Use the `prune()` function to prune the tree by specifying the associated cost-complexity `cp`.

```
carseats_model_1_pruned <- prune(
   carseats_model_1,
   cp = carseats_model_1$cptable[carseats_model_1$cptable[, 2] == 8, "CP"]
)
rpart.plot(carseats_model_1_pruned, yesno = TRUE)
```



The most "important" indicator of `Sales` is `ShelveLoc`. Here are the importance values from the model.

```
carseats_model_1_pruned$variable.importance %>%
   data.frame() %>%
   rownames_to_column(var = "Feature") %>%
   rename(Overall = '.') %>%
   ggplot(aes(x = fct_reorder(Feature, Overall), y = Overall)) +
   geom_pointrange(aes(ymin = 0, ymax = Overall), color = "cadetblue", size = .3) +
   theme_minimal() +
   coord_flip() +
   labs(x = "", y = "", title = "Variable Importance with Simple Regression")
```



The most important indicator of `Sales` is `ShelveLoc`, then `Price`, then `Age`, all of which appear in the final model. `CompPrice` was also important.

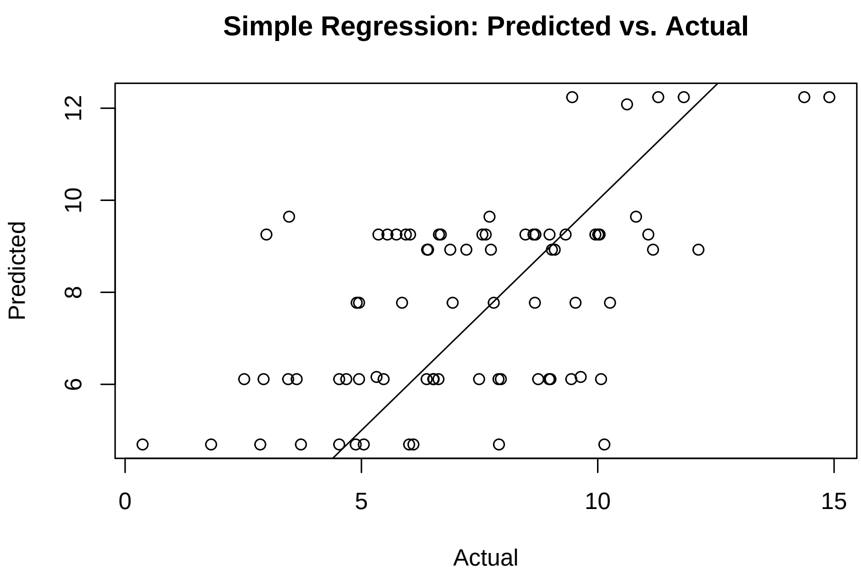
The last step is to make predictions on the validation data set. The root mean squared error ($RMSE = \sqrt{(1/2)\sum(actual - pred)^2}$) and mean absolute error ($MAE = (1/n)\sum|actual - pred|$) are the two most common measures of predictive accuracy. The key difference is that RMSE punishes large errors more harshly. For a regression tree, set argument `type = "vector"` (or do not specify at all).

```
carseats_model_1_preds <- predict(
   carseats_model_1_pruned,
   carseats_test,
   type = "vector"
)

carseats_model_1_pruned_rmse <- RMSE(
   pred = carseats_model_1_preds,
   obs = carseats_test$Sales
)
carseats_model_1_pruned_rmse
```

```
## [1] 2.388059
```

The pruning process leads to an average prediction error of 2.388 in the test data set. Not too bad considering the standard deviation of `Sales` is 2.801. Here is a predicted vs actual plot.

```
plot(carseats_test$Sales, carseats_model_1_preds,
     main = "Simple Regression: Predicted vs. Actual",
     xlab = "Actual",
     ylab = "Predicted")
abline(0, 1)
```



The 6 possible predicted values do a decent job of binning the observations.

9.2.1 Caret Approach

I can also fit the model with `caret::train()`, specifying `method = "rpart"`.

I'll build the model using 10-fold cross-validation to optimize the hyperparameter CP.

```
carseats_trControl = trainControl(
   method = "cv",  # k-fold cross validation
   number = 10,  # 10 folds
   savePredictions = "final"       # save predictions for the optimal tuning parameter
)
```

I'll let the model look for the best CP tuning parameter with `tuneLength` to get close, then fine-tune with `tuneGrid`.

```
set.seed(1234)
carseats_model_2 = train(
   Sales ~ .,
   data = carseats_train,
   method = "rpart",  # for classification tree
   tuneLength = 5,  # choose up to 5 combinations of tuning parameters (cp)
   metric = "RMSE",  # evaluate hyperparamter combinations with RMSE
   trControl = carseats_trControl
)
```

```
## Warning in nominalTrainWorkflow(x = x, y = y, wts = weights, info = trainInfo, :
## There were missing values in resampled performance measures.
```

```
print(carseats_model_2)
```

```
## CART
##
## 321 samples
##  10 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 289, 289, 289, 289, 289, 289, ...
## Resampling results across tuning parameters:
##
##   cp          RMSE      Rsquared   MAE
##   0.04167149  2.209383  0.4065251  1.778797
##   0.04483023  2.243618  0.3849728  1.805027
##   0.04637919  2.275563  0.3684309  1.808814
##   0.12140705  2.400455  0.2942663  1.936927
##   0.26273578  2.692867  0.1898998  2.192774
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was cp = 0.04167149.
```

The first `cp` (0.04167149) produced the smallest RMSE. I can drill into the best value of `cp` using a tuning grid. I'll try that now.

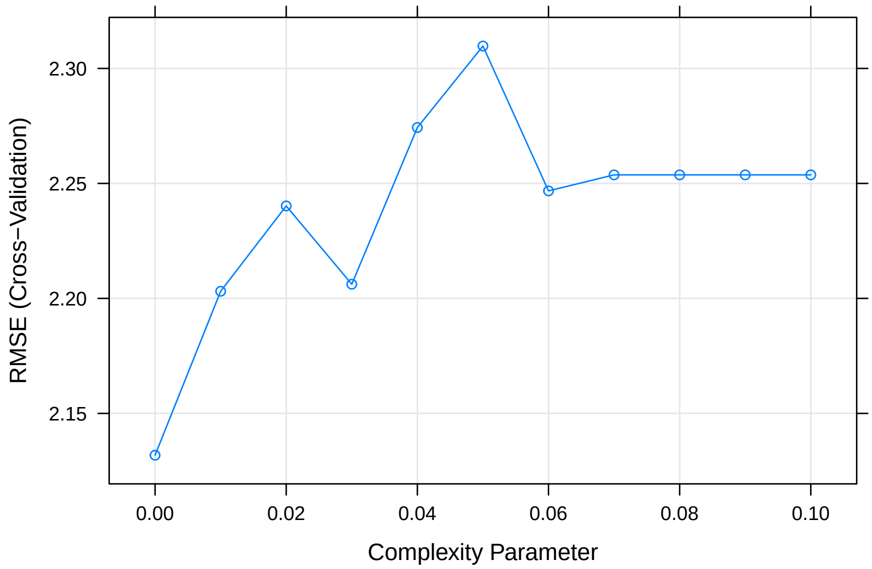
```
myGrid <-  expand.grid(cp = seq(from = 0, to = 0.1, by = 0.01))
carseats_model_3 = train(
   Sales ~ .,
```

```
  data = carseats_train,
  method = "rpart",  # for classification tree
  tuneGrid = myGrid,  # choose up to 5 combinations of tuning parameters (cp)
  metric = "RMSE",  # evaluate hyperparamter combinations with RMSE
  trControl = carseats_trControl
)
print(carseats_model_3)
```

```
## CART
##
## 321 samples
##  10 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 289, 289, 289, 289, 288, 289, ...
## Resampling results across tuning parameters:
##
##   cp    RMSE      Rsquared   MAE
##   0.00  2.131814  0.4578761  1.725960
##   0.01  2.203111  0.4294647  1.790050
##   0.02  2.240209  0.3948080  1.834786
##   0.03  2.206168  0.4139717  1.762170
##   0.04  2.274313  0.3686176  1.795154
##   0.05  2.309746  0.3405228  1.830556
##   0.06  2.246757  0.3703977  1.780266
##   0.07  2.253725  0.3679986  1.794485
##   0.08  2.253725  0.3679986  1.794485
##   0.09  2.253725  0.3679986  1.794485
##   0.10  2.253725  0.3679986  1.794485
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was cp = 0.
```

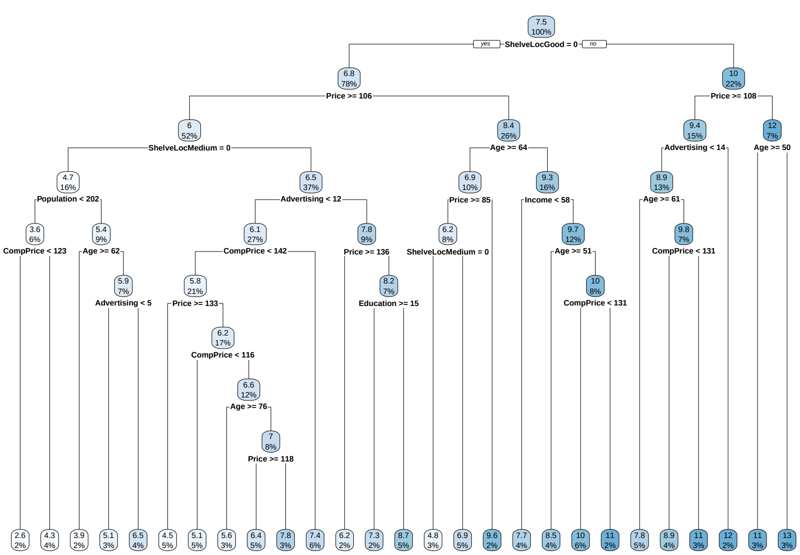
It looks like the best performing tree is the unpruned one.

```
plot(carseats_model_3)
```



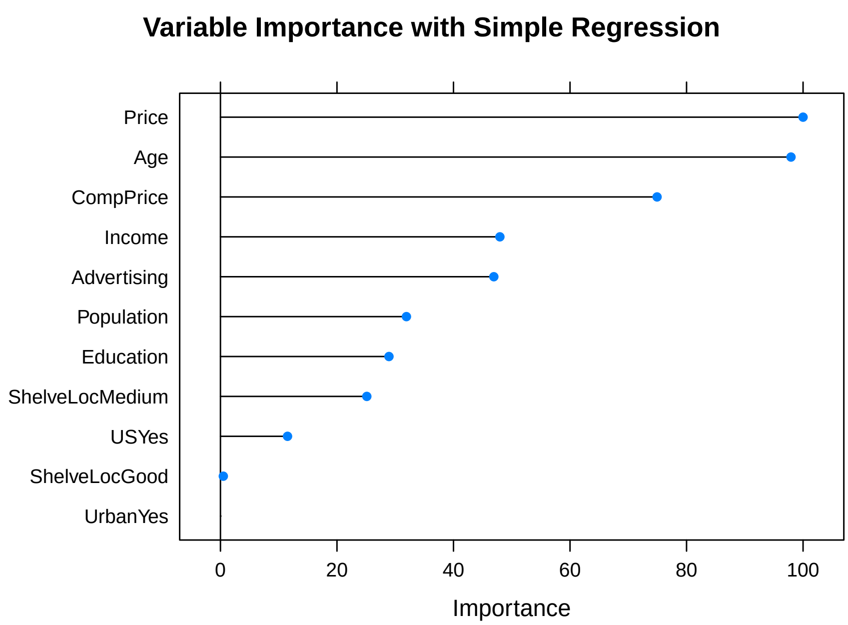
Lets's see the final model.

```
rpart.plot(carseats_model_3$finalModel)
```



What were the most important variables?

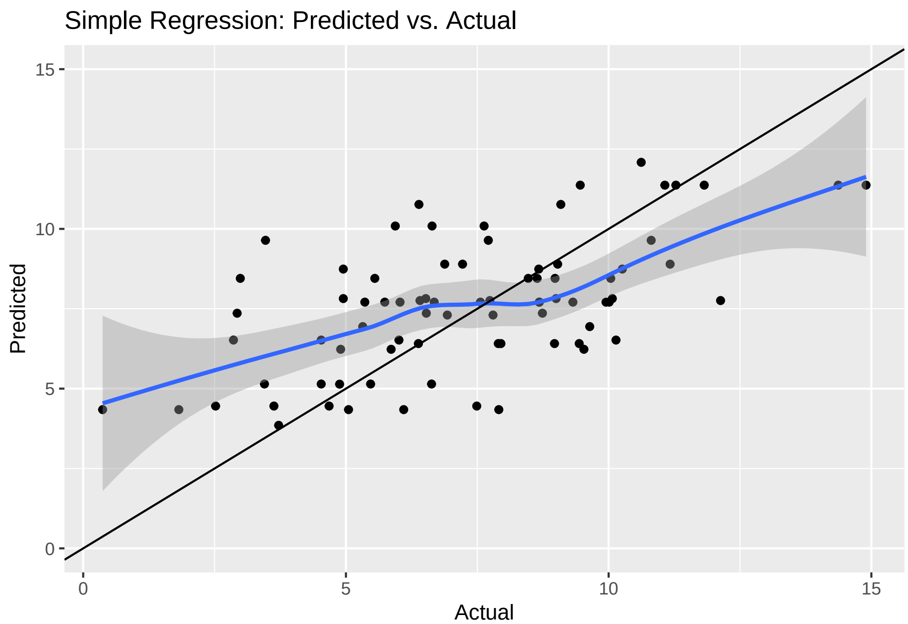
```
plot(varImp(carseats_model_3), main="Variable Importance with Simple Regression")
```



Evaluate the model by making predictions with the test data set.

```
carseats_model_3_preds <- predict(carseats_model_3, carseats_test, type = "raw")
data.frame(Actual = carseats_test$Sales, Predicted = carseats_model_3_preds) %>%
ggplot(aes(x = Actual, y = Predicted)) +
   geom_point() +
   geom_smooth() +
   geom_abline(slope = 1, intercept = 0) +
   scale_y_continuous(limits = c(0, 15)) +
   labs(title = "Simple Regression: Predicted vs. Actual")
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```



Looks like the model over-estimates at the low end and undestimates at the high end. Calculate the test data set RMSE.

```
carseats_model_3_pruned_rmse <- RMSE(
   pred = carseats_model_3_preds,
   obs = carseats_test$Sales
)
carseats_model_3_pruned_rmse
```

```
## [1] 2.298331
```

Caret faired better in this model. Here is a summary the RMSE values of the two models.

```
rbind(data.frame(model = "Manual ANOVA",
                 RMSE = round(carseats_model_1_pruned_rmse, 5)),
      data.frame(model = "Caret",
                 RMSE = round(carseats_model_3_pruned_rmse, 5))
)
```

```
##          model    RMSE
## 1 Manual ANOVA 2.38806
## 2        Caret 2.29833
```

9.3 Bagging

Bootstrap aggregation, or *bagging*, is a general-purpose procedure for reducing the variance of a statistical learning method. The algorithm constructs B regression trees using B bootstrapped training sets, and averages the resulting predictions. These trees are grown deep, and are not pruned. Hence each individual tree has high variance, but low bias. Averaging these B trees reduces the variance. For classification trees, bagging takes the "majority vote" for the prediction. Use a value of B sufficiently large that the error has settled down.

To test the model accuracy, the out-of-bag observations are predicted from the models that do not use them. If B/3 of observations are in-bag, there are *B/3* predictions per observation. These predictions are averaged for the test prediction. Again, for classification trees, a majority vote is taken.

The downside to bagging is that it improves accuracy at the expense of interpretability. There is no longer a single tree to interpret, so it is no longer clear which variables are more important than others.

Bagged trees are a special case of random forests, so see the next section for an example.

9.4 Random Forests

Random forests improve bagged trees by way of a small tweak that de-correlates the trees. As in bagging, the algorithm builds a number of decision trees on bootstrapped training samples. But when building these decision trees, each time a split in a tree is considered, a random sample of *mtry* predictors is chosen as split candidates from the full set of p predictors. A fresh sample of *mtry* predictors is taken at each split. Typically $mtry \sim \sqrt{b}$. Bagged trees are thus a special case of random forests where $mtry = p$.

9.4.0.1 Bagging Classification Example

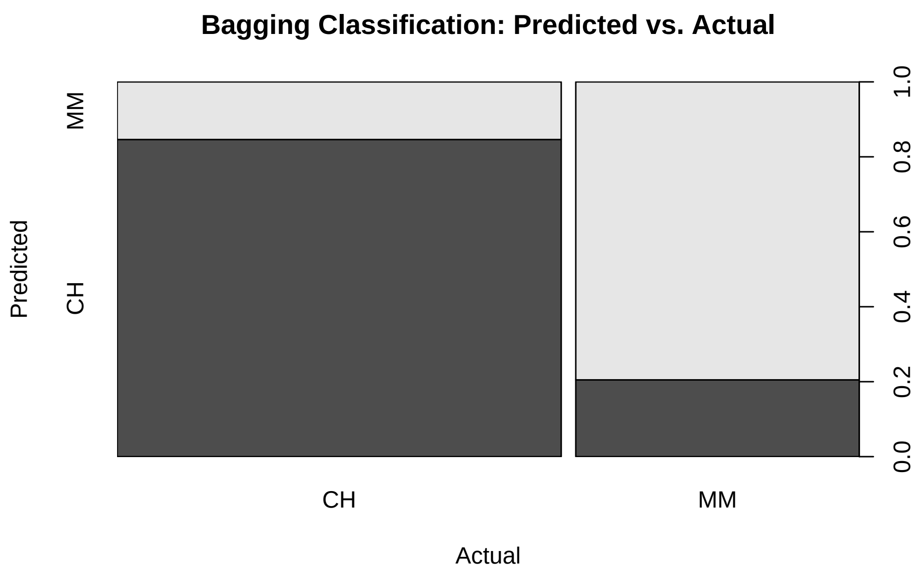
Again using the `OJ` data set to predict `Purchase`, this time I'll use the bagging method by specifying `method = "treebag"`. I'll use `tuneLength = 5` and not worry about `tuneGrid` anymore. Caret has no hyperparameters to tune with this model.

```
oj.bag = train(Purchase ~ .,
               data = oj_train,
               method = "treebag",  # for bagging
               tuneLength = 5,  # choose up to 5 combinations of tuning parameters
               metric = "ROC",  # evaluate hyperparamter combinations with ROC
```

```
               trControl = trainControl(
                 method = "cv",  # k-fold cross validation
                 number = 10,  # k=10 folds
                 savePredictions = "final",       # save predictions for the optimal t
                      classProbs = TRUE,  # return class probabilities in addition to p
                      summaryFunction = twoClassSummary  # for binary response variabl
                      )
                    )
oj.bag
```

```
## Bagged CART
##
## 857 samples
##  17 predictor
##   2 classes: 'CH', 'MM'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 771, 772, 771, 771, 771, 772, ...
## Resampling results:
##
##   ROC        Sens       Spec
##   0.8524038  0.8165094  0.7217469
```

```
#plot(oj.bag$)
oj.pred <- predict(oj.bag, oj_test, type = "raw")
plot(oj_test$Purchase, oj.pred,
     main = "Bagging Classification: Predicted vs. Actual",
     xlab = "Actual",
     ylab = "Predicted")
```

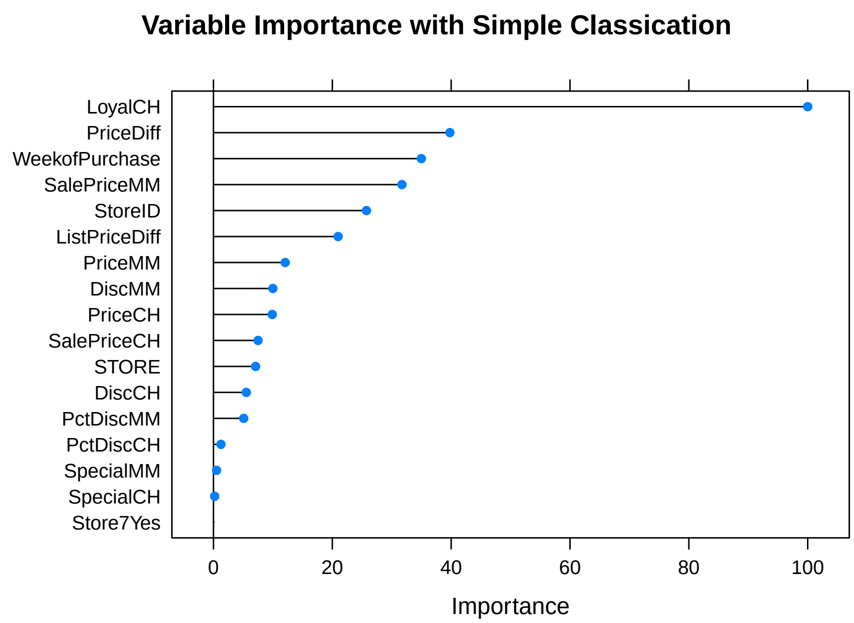



```r
(oj.conf <- confusionMatrix(data = oj.pred,
                            reference = oj_test$Purchase))
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  CH  MM
##         CH 110  17
##         MM  20  66
##
##                Accuracy : 0.8263
##                  95% CI : (0.7686, 0.8746)
##     No Information Rate : 0.6103
##     P-Value [Acc > NIR] : 7.121e-12
##
##                   Kappa : 0.6372
##
##  Mcnemar's Test P-Value : 0.7423
##
##             Sensitivity : 0.8462
##             Specificity : 0.7952
##          Pos Pred Value : 0.8661
##          Neg Pred Value : 0.7674
##              Prevalence : 0.6103
```

```
##          Detection Rate : 0.5164
##    Detection Prevalence : 0.5962
##       Balanced Accuracy : 0.8207
##
##        'Positive' Class : CH
##
```

```
oj.bag.acc <- as.numeric(oj.conf$overall[1])
rm(oj.pred)
rm(oj.conf)
#plot(oj.bag$, oj.bag$finalModel$y)
plot(varImp(oj.bag), main="Variable Importance with Simple Classication")
```



9.4.0.2 Random Forest Classification Example

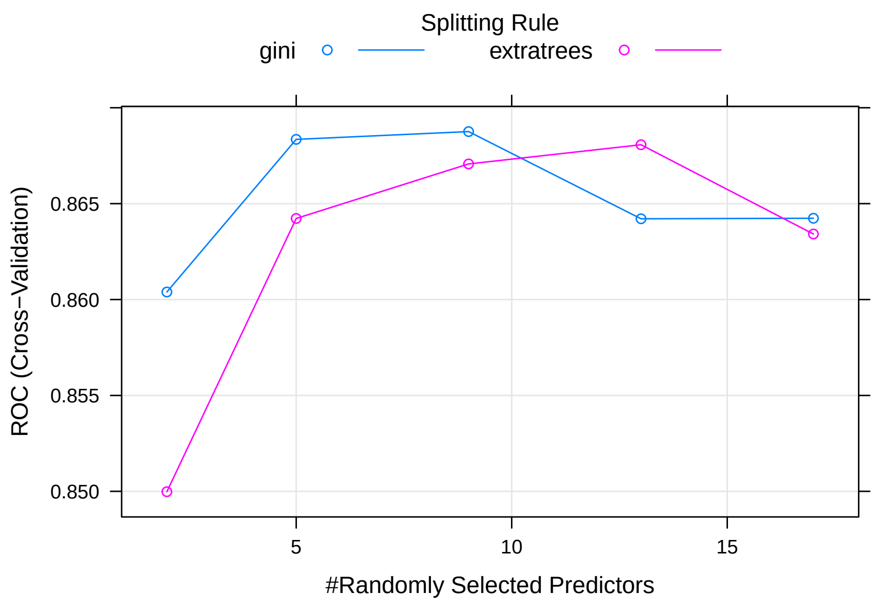
Now I'll try it with the random forest method by specifying `method = "ranger"`. I'll stick with `tuneLength = 5`. Caret tunes three hyperparameters:

- `mtry`: number of randomly selected predictors. Default is sqrt(p).
- `splitrule`: splitting rule. For classification, options are "gini" (default) and "extratrees".
- `min.node.size`: minimal node size. Default is 1 for classification.

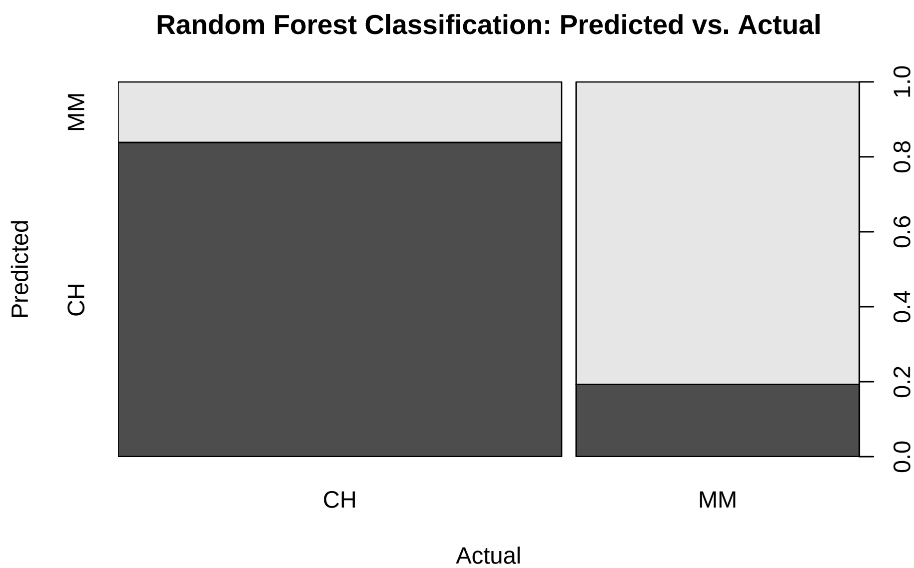
```
oj.frst = train(Purchase ~ .,
               data = oj_train,
               method = "ranger",  # for random forest
               tuneLength = 5,  # choose up to 5 combinations of tuning parameters
               metric = "ROC",  # evaluate hyperparamter combinations with ROC
               trControl = trainControl(
                 method = "cv",  # k-fold cross validation
                 number = 10,  # 10 folds
                 savePredictions = "final",       # save predictions for the optimal tuning param
                 classProbs = TRUE,  # return class probabilities in addition to predicted values
                 summaryFunction = twoClassSummary  # for binary response variable
                 )
               )
oj.frst
```

```
## Random Forest
##
## 857 samples
##  17 predictor
##   2 classes: 'CH', 'MM'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 772, 771, 772, 770, 772, 772, ...
## Resampling results across tuning parameters:
##
##   mtry  splitrule   ROC        Sens       Spec
##    2    gini        0.8603930  0.8719158  0.6946524
##    2    extratrees  0.8499806  0.8814586  0.6287879
##    5    gini        0.8683505  0.8470247  0.7246881
##    5    extratrees  0.8642275  0.8584543  0.6886809
##    9    gini        0.8687568  0.8374456  0.7272727
##    9    extratrees  0.8670702  0.8451379  0.6858289
##   13    gini        0.8642114  0.8297896  0.7361854
##   13    extratrees  0.8680705  0.8298258  0.7064171
##   17    gini        0.8642378  0.8145501  0.7423351
##   17    extratrees  0.8634162  0.8260160  0.7093583
##
## Tuning parameter 'min.node.size' was held constant at a value of 1
## ROC was used to select the optimal model using the largest value.
## The final values used for the model were mtry = 9, splitrule = gini
##  and min.node.size = 1.
```

```
plot(oj.frst)
```




```
oj.pred <- predict(oj.frst, oj_test, type = "raw")
plot(oj_test$Purchase, oj.pred,
     main = "Random Forest Classification: Predicted vs. Actual",
     xlab = "Actual",
     ylab = "Predicted")
```




```r
(oj.conf <- confusionMatrix(data = oj.pred,
                            reference = oj_test$Purchase))
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  CH  MM
##         CH 109  16
##         MM  21  67
##
##                Accuracy : 0.8263
##                  95% CI : (0.7686, 0.8746)
##     No Information Rate : 0.6103
##     P-Value [Acc > NIR] : 7.121e-12
##
##                   Kappa : 0.6387
##
##  Mcnemar's Test P-Value : 0.5108
##
##             Sensitivity : 0.8385
##             Specificity : 0.8072
##          Pos Pred Value : 0.8720
##          Neg Pred Value : 0.7614
##              Prevalence : 0.6103
```

```
##          Detection Rate : 0.5117
##    Detection Prevalence : 0.5869
##       Balanced Accuracy : 0.8228
##
##        'Positive' Class : CH
##
```

```
oj.frst.acc <- as.numeric(oj.conf$overall[1])
rm(oj.pred)
rm(oj.conf)
#plot(oj.bag$, oj.bag$finalModel$y)
#plot(varImp(oj.frst), main="Variable Importance with Simple Classication")
```

The model algorithm explains *"ROC was used to select the optimal model using the largest value. The final values used for the model were mtry = 9, splitrule = extratrees and min.node.size = 1."* You can see the results of tuning grid combinations in the associated plot of ROC AUC vs mtry grouped by splitting rule.

The bagging (accuracy = 0.80751) and random forest (accuracy = 0.81690) models faired pretty well, but the manual classification tree is still in first place. There's still gradient boosting to investigate!

```
rbind(data.frame(model = "Manual Class", Accuracy = round(oj_model_1b_cm$overall["Accu
      data.frame(model = "Caret w.tuneGrid", Accuracy = round(oj_model_3_cm$overall["Ac
      data.frame(model = "Bagging", Accuracy = round(oj.bag.acc, 5)),
      data.frame(model = "Random Forest", Accuracy = round(oj.frst.acc, 5))
) %>% arrange(desc(Accuracy))
```

```
##              model Accuracy
## 1     Manual Class  0.85915
## 2 Caret w.tuneGrid  0.84507
## 3          Bagging  0.82629
## 4    Random Forest  0.82629
```

9.4.0.3 Bagging Regression Example

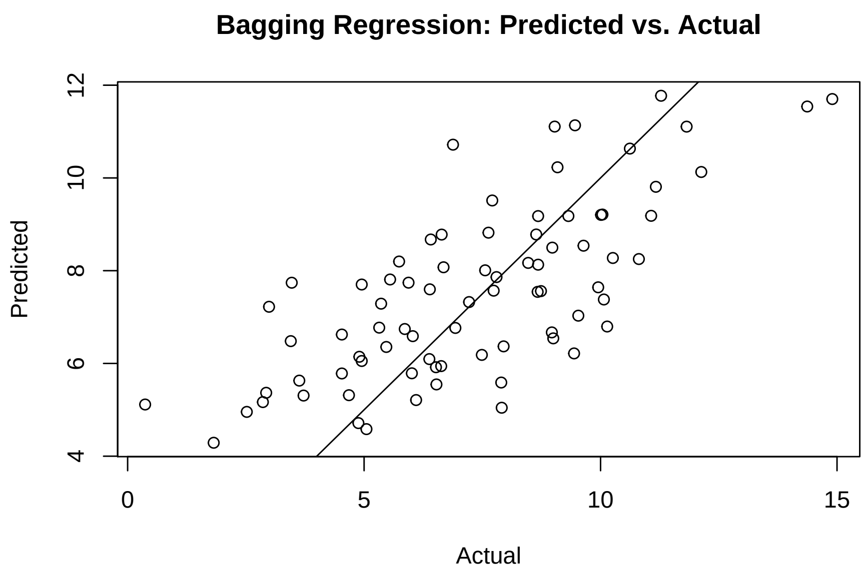
Again using the `Carseats` data set to predict `Sales`, this time I'll use the bagging method by specifying `method = "treebag"`. I'll use `tuneLength = 5` and not worry about `tuneGrid` anymore. Caret has no hyperparameters to tune with this model.

```
carseats.bag = train(Sales ~ .,
                     data = carseats_train,
```

```
               method = "treebag",  # for bagging
               tuneLength = 5,  # choose up to 5 combinations of tuning parameters
               metric = "RMSE",  # evaluate hyperparamter combinations with RMSE
               trControl = trainControl(
                 method = "cv",  # k-fold cross validation
                 number = 10,  # 10 folds
                 savePredictions = "final"       # save predictions for the optimal tuning parame
                 )
               )
carseats.bag
```

```
## Bagged CART
##
## 321 samples
##  10 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 289, 289, 289, 288, 289, 289, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
##   1.709371  0.6532837  1.374155
```

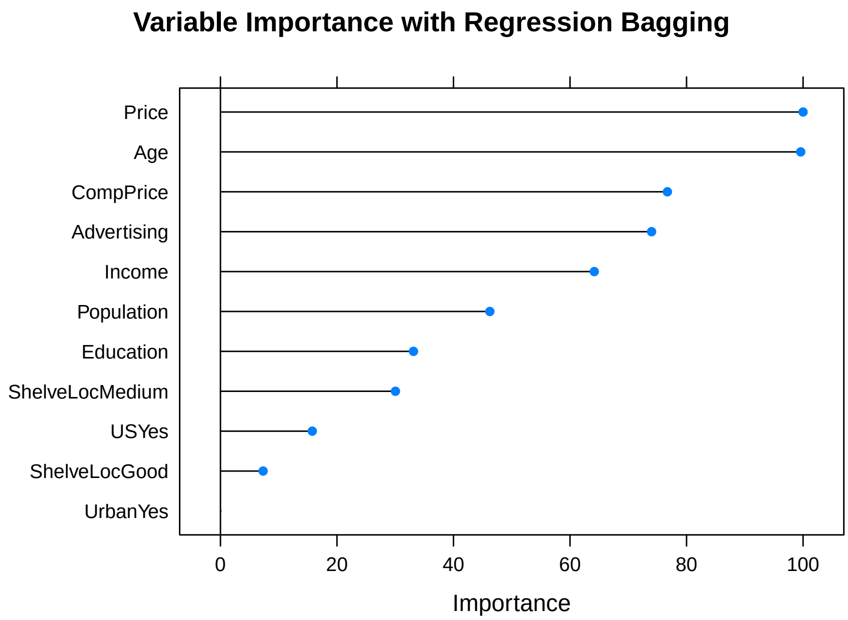
```
#plot(carseats.bag$finalModel)
carseats.pred <- predict(carseats.bag, carseats_test, type = "raw")
plot(carseats_test$Sales, carseats.pred,
     main = "Bagging Regression: Predicted vs. Actual",
     xlab = "Actual",
     ylab = "Predicted")
abline(0, 1)
```




```
(carseats.bag.rmse <- RMSE(pred = carseats.pred,
                           obs = carseats_test$Sales))
```

```
## [1] 1.932792
```

```
rm(carseats.pred)
plot(varImp(carseats.bag), main="Variable Importance with Regression Bagging")
```



9.4.0.4 Random Forest Regression Example

Now I'll try it with the random forest method by specifying `method = "ranger"`. I'll stick with `tuneLength = 5`. Caret tunes three hyperparameters:

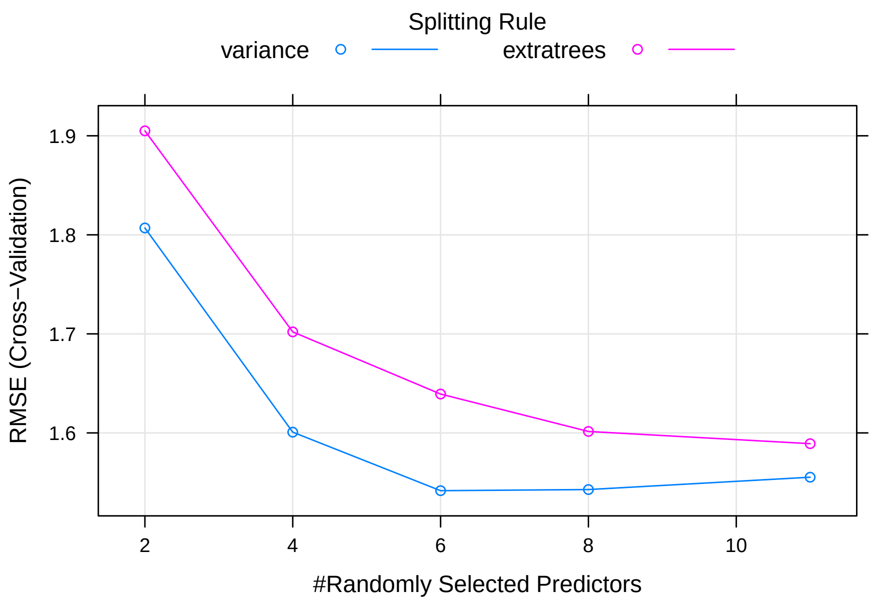
- `mtry`: number of randomly selected predictors
- `splitrule`: splitting rule. For regression, options are "variance" (default), "extratrees", and "maxstat".
- `min.node.size`: minimal node size

```
carseats.frst = train(Sales ~ .,
                data = carseats_train,
                method = "ranger",  # for random forest
                tuneLength = 5,  # choose up to 5 combinations of tuning parameters
                metric = "RMSE",  # evaluate hyperparamter combinations with RMSE
                trControl = trainControl(
                  method = "cv",  # k-fold cross validation
                  number = 10,  # 10 folds
                  savePredictions = "final"       # save predictions for the optimal tuning parame
                  )
                )
carseats.frst
```

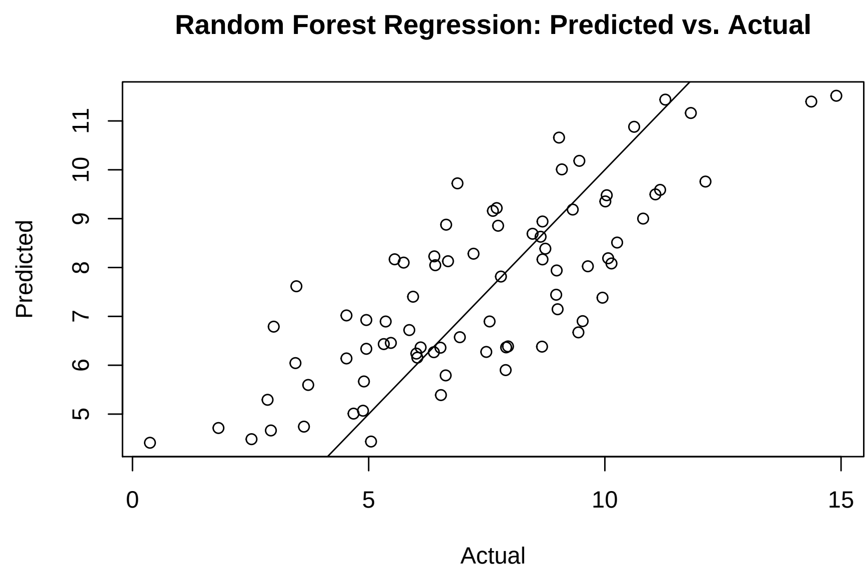
```
## Random Forest
```

```
##
## 321 samples
##  10 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 289, 289, 289, 289, 289, 288, ...
## Resampling results across tuning parameters:
##
##   mtry  splitrule   RMSE      Rsquared   MAE
##    2    variance    1.806943  0.6957452  1.446420
##    2    extratrees  1.905011  0.6466527  1.539096
##    4    variance    1.600763  0.7288625  1.266868
##    4    extratrees  1.702009  0.6862545  1.357981
##    6    variance    1.541675  0.7336448  1.217061
##    6    extratrees  1.639248  0.6966549  1.302159
##    8    variance    1.542806  0.7236085  1.221671
##    8    extratrees  1.601484  0.7053834  1.269484
##   11    variance    1.555271  0.7168108  1.230252
##   11    extratrees  1.589152  0.7058982  1.255090
##
## Tuning parameter 'min.node.size' was held constant at a value of 5
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were mtry = 6, splitrule = variance
##  and min.node.size = 5.
```

```r
plot(carseats.frst)
```




```r
carseats.pred <- predict(carseats.frst, carseats_test, type = "raw")
plot(carseats_test$Sales, carseats.pred,
     main = "Random Forest Regression: Predicted vs. Actual",
     xlab = "Actual",
     ylab = "Predicted")
abline(0, 1)
```




```
(carseats.frst.rmse <- RMSE(pred = carseats.pred,
                            obs = carseats_test$Sales))
```

```
## [1] 1.758112
```

```
rm(carseats.pred)
#plot(varImp(carseats.frst), main="Variable Importance with Regression Random Forest")
```

The model algorithm explains *"RMSE was used to select the optimal model using the smallest value. The final values used for the model were mtry = 11, splitrule = variance and min.node.size = 5."* You can see the results of tuning grid combinations in the associated plot of ROC AUC vs mtry grouped by splitting rule.

The bagging and random forest models faired very well - they took over the first and second place!

```
rbind(data.frame(model = "Manual ANOVA", RMSE = round(carseats_model_1_pruned_rmse, 5)
      data.frame(model = "ANOVA w.tuneGrid", RMSE = round(carseats_model_3_pruned_rmse
      data.frame(model = "Bagging", RMSE = round(carseats.bag.rmse, 5)),
      data.frame(model = "Random Forest", RMSE = round(carseats.frst.rmse, 5))
) %>% arrange(RMSE)
```

```
##              model    RMSE
```

```
## 1    Random Forest 1.75811
## 2          Bagging 1.93279
## 3 ANOVA w.tuneGrid 2.29833
## 4     Manual ANOVA 2.38806
```

9.5 Gradient Boosting

Boosting is a method to improve (boost) the week learners sequentially and increase the model accuracy with a combined model. There are several boosting algorithms. One of the earliest was AdaBoost (adaptive boost). A more recent innovation is gradient boosting.

Adaboost creates a single split tree (decision stump) then weights the observations by how well the initial tree performed, putting more weight on the difficult observations. It then creates a second tree using the weights so that it focuses on the difficult observations. Observations that are difficult to classify receive increasing larger weights until the algorithm identifies a model that correctly classifies them. The final model returns predictions that are a majority vode. (*I think Adaboost applies only to classification problems, not regressions*).

Gradient boosting generalizes the AdaBoost method, so that the object is to minimize a loss function. In the case of classification problems, the loss function is the log-loss; for regression problems, the loss function is mean squared error. The regression trees are addative, so that the successive models can be added together to correct the residuals in the earlier models. Gradient boosting constructs its trees in a "greedy" manner, meaning it chooses the best splits based on purity scores like Gini or minimizing the loss. It is common to constrain the weak learners by setting maximum tree size parameters. Gradient boosting continues until it reaches maximum number of trees or an acceptible error level. This can result in overfitting, so it is common to employ regularization methods that penalize aspects of the model.

Tree Constraints. In general the more constrained the tree, the more trees need to be grown. Parameters to optimize include number of trees, tree depth, number of nodes, minimmum observations per split, and minimum improvement to loss.

Learning Rate. Each successive tree can be weighted to slow down the learning rate. Decreasing the learning rate increases the number of required trees. Common growth rates are 0.1 to 0.3.

The gradient boosting algorithm fits a shallow tree T_1 to the data, $M_1 = T_1$. Then it fits a tree T_2 to the residuals and adds a weighted sum of the tree to the original tree as $M_2 = M_1 + \gamma T_2$. For regularized boosting, include a learning rate factor $\eta \in (0..1)$, $M_2 = M_1 + \eta\gamma T_2$. A larger η produces faster learning, but risks overfitting. The process repeats until the residuals are small enough, or until it reaches the maximum iterations. Because overfitting is a risk, use cross-validation to select the appropriate number of trees (the number of trees producing the lowest RMSE).

9.5.0.1 Gradient Boosting Classification Example

Again using the `OJ` data set to predict `Purchase`, this time I'll use the gradient boosting method by specifying `method = "gbm"`. I'll use `tuneLength = 5` and not worry about `tuneGrid` anymore. Caret tunes the following hyperparameters (see `modelLookup("gbm")`).

- `n.trees`: number of boosting iterations
- `interaction.depth`: maximum tree depth
- `shrinkage`: shrinkage
- `n.minobsinnode`: mimimum terminal node size

```
oj.gbm <- train(Purchase ~ .,
               data = oj_train,
               method = "gbm",  # for bagged tree
               tuneLength = 5,  # choose up to 5 combinations of tuning parameters
               metric = "ROC",  # evaluate hyperparamter combinations with ROC
               trControl = trainControl(
                 method = "cv",  # k-fold cross validation
                 number = 10,  # 10 folds
                 savePredictions = "final",       # save predictions for the optimal t
                      classProbs = TRUE,  # return class probabilities in addition to 
                      summaryFunction = twoClassSummary  # for binary response variabl
                      )
                    )
```

```
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2789             nan     0.1000    0.0273
##      2        1.2286             nan     0.1000    0.0245
##      3        1.1929             nan     0.1000    0.0175
##      4        1.1613             nan     0.1000    0.0148
##      5        1.1263             nan     0.1000    0.0146
##      6        1.0991             nan     0.1000    0.0105
##      7        1.0752             nan     0.1000    0.0102
##      8        1.0579             nan     0.1000    0.0087
##      9        1.0433             nan     0.1000    0.0047
##     10        1.0280             nan     0.1000    0.0082
##     20        0.9233             nan     0.1000    0.0026
##     40        0.8226             nan     0.1000    0.0010
##     60        0.7809             nan     0.1000   -0.0001
##     80        0.7595             nan     0.1000   -0.0002
```

```
##    100        0.7506             nan     0.1000   -0.0008
##    120        0.7407             nan     0.1000   -0.0005
##    140        0.7317             nan     0.1000   -0.0005
##    160        0.7277             nan     0.1000   -0.0009
##    180        0.7232             nan     0.1000   -0.0004
##    200        0.7181             nan     0.1000   -0.0007
##    220        0.7115             nan     0.1000   -0.0008
##    240        0.7096             nan     0.1000   -0.0010
##    250        0.7081             nan     0.1000   -0.0015
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2695             nan     0.1000    0.0319
##      2        1.2150             nan     0.1000    0.0260
##      3        1.1702             nan     0.1000    0.0225
##      4        1.1260             nan     0.1000    0.0186
##      5        1.0913             nan     0.1000    0.0147
##      6        1.0586             nan     0.1000    0.0160
##      7        1.0276             nan     0.1000    0.0146
##      8        1.0045             nan     0.1000    0.0109
##      9        0.9836             nan     0.1000    0.0099
##     10        0.9624             nan     0.1000    0.0068
##     20        0.8337             nan     0.1000    0.0027
##     40        0.7525             nan     0.1000   -0.0005
##     60        0.7240             nan     0.1000   -0.0005
##     80        0.7063             nan     0.1000   -0.0006
##    100        0.6879             nan     0.1000   -0.0011
##    120        0.6751             nan     0.1000   -0.0018
##    140        0.6605             nan     0.1000   -0.0012
##    160        0.6477             nan     0.1000   -0.0013
##    180        0.6359             nan     0.1000   -0.0010
##    200        0.6274             nan     0.1000   -0.0018
##    220        0.6166             nan     0.1000   -0.0005
##    240        0.6078             nan     0.1000   -0.0011
##    250        0.6014             nan     0.1000   -0.0019
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2548             nan     0.1000    0.0377
##      2        1.1905             nan     0.1000    0.0294
##      3        1.1343             nan     0.1000    0.0258
##      4        1.0935             nan     0.1000    0.0180
##      5        1.0529             nan     0.1000    0.0168
##      6        1.0172             nan     0.1000    0.0159
##      7        0.9824             nan     0.1000    0.0151
##      8        0.9534             nan     0.1000    0.0127
##      9        0.9277             nan     0.1000    0.0109
##     10        0.9066             nan     0.1000    0.0088
```

```
##     20        0.7870             nan     0.1000    0.0023
##     40        0.7150             nan     0.1000   -0.0008
##     60        0.6799             nan     0.1000   -0.0023
##     80        0.6520             nan     0.1000   -0.0012
##    100        0.6298             nan     0.1000   -0.0005
##    120        0.6117             nan     0.1000   -0.0024
##    140        0.5973             nan     0.1000   -0.0016
##    160        0.5849             nan     0.1000   -0.0023
##    180        0.5670             nan     0.1000   -0.0015
##    200        0.5548             nan     0.1000   -0.0006
##    220        0.5440             nan     0.1000   -0.0024
##    240        0.5290             nan     0.1000   -0.0020
##    250        0.5228             nan     0.1000   -0.0016
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2554             nan     0.1000    0.0399
##      2        1.1847             nan     0.1000    0.0346
##      3        1.1321             nan     0.1000    0.0199
##      4        1.0823             nan     0.1000    0.0224
##      5        1.0392             nan     0.1000    0.0208
##      6        1.0067             nan     0.1000    0.0145
##      7        0.9768             nan     0.1000    0.0139
##      8        0.9462             nan     0.1000    0.0123
##      9        0.9238             nan     0.1000    0.0095
##     10        0.8966             nan     0.1000    0.0090
##     20        0.7681             nan     0.1000    0.0007
##     40        0.6937             nan     0.1000   -0.0004
##     60        0.6552             nan     0.1000   -0.0017
##     80        0.6202             nan     0.1000   -0.0018
##    100        0.5887             nan     0.1000   -0.0027
##    120        0.5653             nan     0.1000   -0.0012
##    140        0.5434             nan     0.1000   -0.0017
##    160        0.5275             nan     0.1000   -0.0008
##    180        0.5068             nan     0.1000   -0.0012
##    200        0.4935             nan     0.1000   -0.0016
##    220        0.4801             nan     0.1000   -0.0018
##    240        0.4665             nan     0.1000   -0.0010
##    250        0.4603             nan     0.1000   -0.0012
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2513             nan     0.1000    0.0375
##      2        1.1795             nan     0.1000    0.0320
##      3        1.1264             nan     0.1000    0.0254
##      4        1.0742             nan     0.1000    0.0225
##      5        1.0282             nan     0.1000    0.0196
##      6        0.9888             nan     0.1000    0.0177
```

```
##      7        0.9547             nan     0.1000    0.0136
##      8        0.9303             nan     0.1000    0.0103
##      9        0.9008             nan     0.1000    0.0121
##     10        0.8803             nan     0.1000    0.0073
##     20        0.7563             nan     0.1000    0.0003
##     40        0.6715             nan     0.1000   -0.0012
##     60        0.6253             nan     0.1000   -0.0016
##     80        0.5868             nan     0.1000   -0.0021
##    100        0.5538             nan     0.1000   -0.0015
##    120        0.5285             nan     0.1000   -0.0034
##    140        0.5070             nan     0.1000   -0.0025
##    160        0.4872             nan     0.1000   -0.0012
##    180        0.4736             nan     0.1000   -0.0023
##    200        0.4566             nan     0.1000   -0.0015
##    220        0.4407             nan     0.1000   -0.0011
##    240        0.4262             nan     0.1000   -0.0013
##    250        0.4186             nan     0.1000   -0.0024
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2743             nan     0.1000    0.0307
##      2        1.2220             nan     0.1000    0.0240
##      3        1.1885             nan     0.1000    0.0165
##      4        1.1522             nan     0.1000    0.0177
##      5        1.1186             nan     0.1000    0.0136
##      6        1.0912             nan     0.1000    0.0111
##      7        1.0693             nan     0.1000    0.0106
##      8        1.0492             nan     0.1000    0.0089
##      9        1.0309             nan     0.1000    0.0093
##     10        1.0172             nan     0.1000    0.0069
##     20        0.9206             nan     0.1000    0.0030
##     40        0.8357             nan     0.1000   -0.0002
##     60        0.7936             nan     0.1000   -0.0000
##     80        0.7764             nan     0.1000   -0.0009
##    100        0.7682             nan     0.1000   -0.0004
##    120        0.7620             nan     0.1000   -0.0008
##    140        0.7582             nan     0.1000   -0.0011
##    160        0.7536             nan     0.1000   -0.0005
##    180        0.7501             nan     0.1000   -0.0006
##    200        0.7448             nan     0.1000   -0.0008
##    220        0.7409             nan     0.1000   -0.0006
##    240        0.7385             nan     0.1000   -0.0011
##    250        0.7368             nan     0.1000   -0.0007
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2697             nan     0.1000    0.0323
##      2        1.2121             nan     0.1000    0.0276
```

```
##        3        1.1636             nan     0.1000    0.0251
##        4        1.1220             nan     0.1000    0.0166
##        5        1.0826             nan     0.1000    0.0131
##        6        1.0537             nan     0.1000    0.0134
##        7        1.0269             nan     0.1000    0.0104
##        8        1.0061             nan     0.1000    0.0084
##        9        0.9858             nan     0.1000    0.0082
##       10        0.9678             nan     0.1000    0.0066
##       20        0.8429             nan     0.1000    0.0024
##       40        0.7685             nan     0.1000   -0.0010
##       60        0.7422             nan     0.1000   -0.0006
##       80        0.7228             nan     0.1000   -0.0009
##      100        0.7073             nan     0.1000   -0.0013
##      120        0.6937             nan     0.1000   -0.0024
##      140        0.6836             nan     0.1000   -0.0014
##      160        0.6703             nan     0.1000   -0.0022
##      180        0.6607             nan     0.1000   -0.0009
##      200        0.6529             nan     0.1000   -0.0011
##      220        0.6438             nan     0.1000   -0.0017
##      240        0.6370             nan     0.1000   -0.0015
##      250        0.6311             nan     0.1000   -0.0011
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##        1        1.2569             nan     0.1000    0.0361
##        2        1.1946             nan     0.1000    0.0301
##        3        1.1386             nan     0.1000    0.0266
##        4        1.0954             nan     0.1000    0.0205
##        5        1.0524             nan     0.1000    0.0204
##        6        1.0186             nan     0.1000    0.0149
##        7        0.9847             nan     0.1000    0.0126
##        8        0.9618             nan     0.1000    0.0086
##        9        0.9344             nan     0.1000    0.0114
##       10        0.9135             nan     0.1000    0.0095
##       20        0.8003             nan     0.1000    0.0027
##       40        0.7353             nan     0.1000   -0.0011
##       60        0.7042             nan     0.1000   -0.0027
##       80        0.6800             nan     0.1000   -0.0017
##      100        0.6602             nan     0.1000   -0.0008
##      120        0.6393             nan     0.1000   -0.0017
##      140        0.6231             nan     0.1000   -0.0016
##      160        0.6077             nan     0.1000   -0.0028
##      180        0.5977             nan     0.1000   -0.0012
##      200        0.5863             nan     0.1000   -0.0014
##      220        0.5749             nan     0.1000   -0.0013
##      240        0.5618             nan     0.1000   -0.0022
##      250        0.5577             nan     0.1000   -0.0022
```

```
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2495             nan     0.1000    0.0419
##      2        1.1884             nan     0.1000    0.0265
##      3        1.1279             nan     0.1000    0.0248
##      4        1.0820             nan     0.1000    0.0208
##      5        1.0426             nan     0.1000    0.0166
##      6        1.0089             nan     0.1000    0.0146
##      7        0.9799             nan     0.1000    0.0126
##      8        0.9474             nan     0.1000    0.0140
##      9        0.9225             nan     0.1000    0.0079
##     10        0.9066             nan     0.1000    0.0048
##     20        0.7815             nan     0.1000    0.0014
##     40        0.7028             nan     0.1000   -0.0019
##     60        0.6661             nan     0.1000   -0.0011
##     80        0.6386             nan     0.1000   -0.0006
##    100        0.6075             nan     0.1000   -0.0005
##    120        0.5861             nan     0.1000   -0.0019
##    140        0.5674             nan     0.1000   -0.0020
##    160        0.5467             nan     0.1000   -0.0016
##    180        0.5318             nan     0.1000   -0.0020
##    200        0.5200             nan     0.1000   -0.0025
##    220        0.5050             nan     0.1000   -0.0009
##    240        0.4930             nan     0.1000   -0.0020
##    250        0.4883             nan     0.1000   -0.0016
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2558             nan     0.1000    0.0336
##      2        1.1856             nan     0.1000    0.0326
##      3        1.1172             nan     0.1000    0.0305
##      4        1.0713             nan     0.1000    0.0222
##      5        1.0313             nan     0.1000    0.0171
##      6        0.9965             nan     0.1000    0.0164
##      7        0.9613             nan     0.1000    0.0156
##      8        0.9354             nan     0.1000    0.0103
##      9        0.9089             nan     0.1000    0.0111
##     10        0.8859             nan     0.1000    0.0059
##     20        0.7690             nan     0.1000    0.0006
##     40        0.6889             nan     0.1000   -0.0004
##     60        0.6452             nan     0.1000   -0.0021
##     80        0.6127             nan     0.1000   -0.0021
##    100        0.5811             nan     0.1000   -0.0032
##    120        0.5557             nan     0.1000   -0.0011
##    140        0.5332             nan     0.1000   -0.0012
##    160        0.5118             nan     0.1000   -0.0014
##    180        0.4879             nan     0.1000   -0.0012
```

```
##    200        0.4737             nan     0.1000   -0.0020
##    220        0.4591             nan     0.1000   -0.0024
##    240        0.4460             nan     0.1000   -0.0030
##    250        0.4386             nan     0.1000   -0.0013
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2717             nan     0.1000    0.0320
##      2        1.2209             nan     0.1000    0.0250
##      3        1.1751             nan     0.1000    0.0208
##      4        1.1404             nan     0.1000    0.0149
##      5        1.1056             nan     0.1000    0.0119
##      6        1.0782             nan     0.1000    0.0125
##      7        1.0569             nan     0.1000    0.0081
##      8        1.0356             nan     0.1000    0.0098
##      9        1.0176             nan     0.1000    0.0080
##     10        1.0042             nan     0.1000    0.0066
##     20        0.9023             nan     0.1000    0.0021
##     40        0.8156             nan     0.1000    0.0006
##     60        0.7793             nan     0.1000    0.0004
##     80        0.7609             nan     0.1000   -0.0014
##    100        0.7514             nan     0.1000   -0.0006
##    120        0.7448             nan     0.1000   -0.0005
##    140        0.7406             nan     0.1000   -0.0008
##    160        0.7353             nan     0.1000   -0.0007
##    180        0.7329             nan     0.1000   -0.0008
##    200        0.7281             nan     0.1000   -0.0014
##    220        0.7239             nan     0.1000   -0.0008
##    240        0.7211             nan     0.1000   -0.0011
##    250        0.7203             nan     0.1000   -0.0010
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2647             nan     0.1000    0.0368
##      2        1.2060             nan     0.1000    0.0275
##      3        1.1558             nan     0.1000    0.0232
##      4        1.1207             nan     0.1000    0.0178
##      5        1.0787             nan     0.1000    0.0172
##      6        1.0478             nan     0.1000    0.0141
##      7        1.0178             nan     0.1000    0.0117
##      8        0.9963             nan     0.1000    0.0099
##      9        0.9749             nan     0.1000    0.0107
##     10        0.9514             nan     0.1000    0.0095
##     20        0.8341             nan     0.1000    0.0029
##     40        0.7601             nan     0.1000   -0.0015
##     60        0.7335             nan     0.1000   -0.0010
##     80        0.7131             nan     0.1000   -0.0011
##    100        0.7006             nan     0.1000   -0.0018
```

```
##    120        0.6886             nan     0.1000   -0.0008
##    140        0.6740             nan     0.1000   -0.0014
##    160        0.6628             nan     0.1000   -0.0017
##    180        0.6522             nan     0.1000   -0.0010
##    200        0.6423             nan     0.1000   -0.0005
##    220        0.6353             nan     0.1000   -0.0020
##    240        0.6251             nan     0.1000   -0.0017
##    250        0.6211             nan     0.1000   -0.0013
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2533             nan     0.1000    0.0369
##      2        1.1914             nan     0.1000    0.0304
##      3        1.1304             nan     0.1000    0.0280
##      4        1.0808             nan     0.1000    0.0214
##      5        1.0411             nan     0.1000    0.0177
##      6        1.0095             nan     0.1000    0.0131
##      7        0.9791             nan     0.1000    0.0118
##      8        0.9487             nan     0.1000    0.0146
##      9        0.9234             nan     0.1000    0.0114
##     10        0.9050             nan     0.1000    0.0081
##     20        0.7868             nan     0.1000   -0.0018
##     40        0.7190             nan     0.1000   -0.0002
##     60        0.6929             nan     0.1000   -0.0013
##     80        0.6706             nan     0.1000   -0.0012
##    100        0.6511             nan     0.1000   -0.0008
##    120        0.6313             nan     0.1000   -0.0028
##    140        0.6161             nan     0.1000   -0.0010
##    160        0.6016             nan     0.1000   -0.0019
##    180        0.5875             nan     0.1000   -0.0013
##    200        0.5754             nan     0.1000   -0.0021
##    220        0.5613             nan     0.1000   -0.0011
##    240        0.5456             nan     0.1000   -0.0014
##    250        0.5423             nan     0.1000   -0.0016
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2526             nan     0.1000    0.0406
##      2        1.1845             nan     0.1000    0.0346
##      3        1.1309             nan     0.1000    0.0246
##      4        1.0809             nan     0.1000    0.0250
##      5        1.0380             nan     0.1000    0.0205
##      6        1.0017             nan     0.1000    0.0164
##      7        0.9661             nan     0.1000    0.0146
##      8        0.9372             nan     0.1000    0.0130
##      9        0.9115             nan     0.1000    0.0105
##     10        0.8921             nan     0.1000    0.0084
##     20        0.7698             nan     0.1000    0.0014
```

```
##     40        0.6902             nan     0.1000   -0.0016
##     60        0.6501             nan     0.1000   -0.0019
##     80        0.6200             nan     0.1000   -0.0006
##    100        0.5995             nan     0.1000   -0.0026
##    120        0.5766             nan     0.1000   -0.0019
##    140        0.5576             nan     0.1000   -0.0020
##    160        0.5428             nan     0.1000   -0.0027
##    180        0.5276             nan     0.1000   -0.0026
##    200        0.5091             nan     0.1000   -0.0011
##    220        0.4954             nan     0.1000   -0.0014
##    240        0.4801             nan     0.1000   -0.0028
##    250        0.4748             nan     0.1000   -0.0021
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2578             nan     0.1000    0.0379
##      2        1.1876             nan     0.1000    0.0342
##      3        1.1214             nan     0.1000    0.0297
##      4        1.0650             nan     0.1000    0.0254
##      5        1.0182             nan     0.1000    0.0188
##      6        0.9812             nan     0.1000    0.0172
##      7        0.9484             nan     0.1000    0.0116
##      8        0.9182             nan     0.1000    0.0116
##      9        0.8929             nan     0.1000    0.0068
##     10        0.8704             nan     0.1000    0.0085
##     20        0.7522             nan     0.1000    0.0002
##     40        0.6778             nan     0.1000   -0.0019
##     60        0.6318             nan     0.1000   -0.0015
##     80        0.5982             nan     0.1000   -0.0011
##    100        0.5669             nan     0.1000   -0.0032
##    120        0.5451             nan     0.1000   -0.0012
##    140        0.5224             nan     0.1000   -0.0002
##    160        0.5005             nan     0.1000   -0.0027
##    180        0.4834             nan     0.1000   -0.0015
##    200        0.4693             nan     0.1000   -0.0009
##    220        0.4530             nan     0.1000   -0.0016
##    240        0.4419             nan     0.1000   -0.0035
##    250        0.4324             nan     0.1000   -0.0016
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2761             nan     0.1000    0.0283
##      2        1.2243             nan     0.1000    0.0231
##      3        1.1816             nan     0.1000    0.0192
##      4        1.1477             nan     0.1000    0.0158
##      5        1.1174             nan     0.1000    0.0122
##      6        1.0930             nan     0.1000    0.0116
##      7        1.0704             nan     0.1000    0.0102
```

```
##      8        1.0499             nan     0.1000    0.0083
##      9        1.0340             nan     0.1000    0.0078
##     10        1.0167             nan     0.1000    0.0082
##     20        0.9152             nan     0.1000    0.0021
##     40        0.8226             nan     0.1000    0.0007
##     60        0.7895             nan     0.1000    0.0000
##     80        0.7690             nan     0.1000   -0.0008
##    100        0.7612             nan     0.1000   -0.0010
##    120        0.7541             nan     0.1000   -0.0004
##    140        0.7491             nan     0.1000   -0.0012
##    160        0.7443             nan     0.1000   -0.0006
##    180        0.7405             nan     0.1000   -0.0009
##    200        0.7369             nan     0.1000   -0.0009
##    220        0.7329             nan     0.1000   -0.0007
##    240        0.7287             nan     0.1000   -0.0014
##    250        0.7268             nan     0.1000   -0.0011
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2642             nan     0.1000    0.0359
##      2        1.2066             nan     0.1000    0.0279
##      3        1.1624             nan     0.1000    0.0237
##      4        1.1213             nan     0.1000    0.0202
##      5        1.0853             nan     0.1000    0.0162
##      6        1.0560             nan     0.1000    0.0116
##      7        1.0275             nan     0.1000    0.0125
##      8        1.0040             nan     0.1000    0.0109
##      9        0.9823             nan     0.1000    0.0077
##     10        0.9612             nan     0.1000    0.0105
##     20        0.8409             nan     0.1000    0.0026
##     40        0.7578             nan     0.1000   -0.0007
##     60        0.7294             nan     0.1000   -0.0007
##     80        0.7095             nan     0.1000   -0.0026
##    100        0.6965             nan     0.1000   -0.0012
##    120        0.6857             nan     0.1000   -0.0022
##    140        0.6751             nan     0.1000   -0.0004
##    160        0.6650             nan     0.1000   -0.0018
##    180        0.6581             nan     0.1000   -0.0017
##    200        0.6520             nan     0.1000   -0.0009
##    220        0.6436             nan     0.1000   -0.0011
##    240        0.6351             nan     0.1000   -0.0009
##    250        0.6312             nan     0.1000   -0.0016
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2577             nan     0.1000    0.0367
##      2        1.1908             nan     0.1000    0.0288
##      3        1.1314             nan     0.1000    0.0257
```

```
##      4        1.0832             nan     0.1000    0.0231
##      5        1.0473             nan     0.1000    0.0147
##      6        1.0104             nan     0.1000    0.0174
##      7        0.9743             nan     0.1000    0.0139
##      8        0.9460             nan     0.1000    0.0113
##      9        0.9236             nan     0.1000    0.0105
##     10        0.9026             nan     0.1000    0.0077
##     20        0.7942             nan     0.1000    0.0009
##     40        0.7292             nan     0.1000   -0.0018
##     60        0.6933             nan     0.1000   -0.0013
##     80        0.6650             nan     0.1000   -0.0008
##    100        0.6458             nan     0.1000   -0.0020
##    120        0.6252             nan     0.1000   -0.0018
##    140        0.6106             nan     0.1000   -0.0010
##    160        0.5953             nan     0.1000   -0.0009
##    180        0.5810             nan     0.1000   -0.0014
##    200        0.5683             nan     0.1000   -0.0016
##    220        0.5544             nan     0.1000   -0.0009
##    240        0.5425             nan     0.1000   -0.0010
##    250        0.5367             nan     0.1000   -0.0012
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2542             nan     0.1000    0.0373
##      2        1.1874             nan     0.1000    0.0310
##      3        1.1277             nan     0.1000    0.0279
##      4        1.0765             nan     0.1000    0.0231
##      5        1.0393             nan     0.1000    0.0179
##      6        1.0012             nan     0.1000    0.0141
##      7        0.9658             nan     0.1000    0.0139
##      8        0.9421             nan     0.1000    0.0101
##      9        0.9187             nan     0.1000    0.0088
##     10        0.8966             nan     0.1000    0.0095
##     20        0.7715             nan     0.1000    0.0019
##     40        0.6966             nan     0.1000   -0.0017
##     60        0.6516             nan     0.1000   -0.0010
##     80        0.6206             nan     0.1000   -0.0015
##    100        0.5991             nan     0.1000   -0.0028
##    120        0.5818             nan     0.1000   -0.0019
##    140        0.5644             nan     0.1000   -0.0018
##    160        0.5476             nan     0.1000   -0.0016
##    180        0.5329             nan     0.1000   -0.0016
##    200        0.5212             nan     0.1000   -0.0016
##    220        0.5055             nan     0.1000   -0.0032
##    240        0.4926             nan     0.1000   -0.0013
##    250        0.4850             nan     0.1000   -0.0006
##
```

```
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2523             nan     0.1000    0.0397
##      2        1.1844             nan     0.1000    0.0301
##      3        1.1269             nan     0.1000    0.0263
##      4        1.0773             nan     0.1000    0.0216
##      5        1.0310             nan     0.1000    0.0211
##      6        0.9902             nan     0.1000    0.0176
##      7        0.9582             nan     0.1000    0.0119
##      8        0.9338             nan     0.1000    0.0106
##      9        0.9054             nan     0.1000    0.0120
##     10        0.8869             nan     0.1000    0.0083
##     20        0.7620             nan     0.1000   -0.0001
##     40        0.6734             nan     0.1000   -0.0010
##     60        0.6333             nan     0.1000   -0.0004
##     80        0.5982             nan     0.1000   -0.0023
##    100        0.5685             nan     0.1000   -0.0013
##    120        0.5436             nan     0.1000   -0.0024
##    140        0.5196             nan     0.1000   -0.0012
##    160        0.5010             nan     0.1000   -0.0031
##    180        0.4832             nan     0.1000   -0.0032
##    200        0.4677             nan     0.1000   -0.0014
##    220        0.4504             nan     0.1000   -0.0016
##    240        0.4333             nan     0.1000   -0.0013
##    250        0.4273             nan     0.1000   -0.0022
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2726             nan     0.1000    0.0321
##      2        1.2186             nan     0.1000    0.0259
##      3        1.1770             nan     0.1000    0.0190
##      4        1.1350             nan     0.1000    0.0186
##      5        1.1017             nan     0.1000    0.0147
##      6        1.0810             nan     0.1000    0.0096
##      7        1.0570             nan     0.1000    0.0105
##      8        1.0375             nan     0.1000    0.0098
##      9        1.0188             nan     0.1000    0.0081
##     10        1.0020             nan     0.1000    0.0072
##     20        0.9034             nan     0.1000    0.0023
##     40        0.8070             nan     0.1000   -0.0001
##     60        0.7671             nan     0.1000   -0.0003
##     80        0.7500             nan     0.1000   -0.0007
##    100        0.7415             nan     0.1000   -0.0008
##    120        0.7349             nan     0.1000   -0.0008
##    140        0.7282             nan     0.1000   -0.0006
##    160        0.7222             nan     0.1000   -0.0006
##    180        0.7190             nan     0.1000   -0.0003
##    200        0.7160             nan     0.1000   -0.0013
```

```
##    220        0.7128             nan     0.1000   -0.0008
##    240        0.7092             nan     0.1000   -0.0012
##    250        0.7066             nan     0.1000   -0.0005
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2597             nan     0.1000    0.0362
##      2        1.2019             nan     0.1000    0.0279
##      3        1.1504             nan     0.1000    0.0230
##      4        1.1084             nan     0.1000    0.0168
##      5        1.0702             nan     0.1000    0.0184
##      6        1.0378             nan     0.1000    0.0136
##      7        1.0090             nan     0.1000    0.0131
##      8        0.9848             nan     0.1000    0.0115
##      9        0.9632             nan     0.1000    0.0078
##     10        0.9410             nan     0.1000    0.0094
##     20        0.8215             nan     0.1000    0.0037
##     40        0.7478             nan     0.1000   -0.0001
##     60        0.7184             nan     0.1000   -0.0008
##     80        0.6985             nan     0.1000   -0.0007
##    100        0.6799             nan     0.1000   -0.0013
##    120        0.6660             nan     0.1000    0.0002
##    140        0.6534             nan     0.1000   -0.0009
##    160        0.6423             nan     0.1000   -0.0016
##    180        0.6325             nan     0.1000   -0.0016
##    200        0.6226             nan     0.1000   -0.0011
##    220        0.6139             nan     0.1000   -0.0010
##    240        0.6043             nan     0.1000   -0.0017
##    250        0.6016             nan     0.1000   -0.0012
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2549             nan     0.1000    0.0413
##      2        1.1843             nan     0.1000    0.0345
##      3        1.1274             nan     0.1000    0.0245
##      4        1.0809             nan     0.1000    0.0213
##      5        1.0418             nan     0.1000    0.0178
##      6        1.0056             nan     0.1000    0.0128
##      7        0.9797             nan     0.1000    0.0122
##      8        0.9562             nan     0.1000    0.0083
##      9        0.9288             nan     0.1000    0.0116
##     10        0.9070             nan     0.1000    0.0088
##     20        0.7819             nan     0.1000    0.0013
##     40        0.7119             nan     0.1000   -0.0008
##     60        0.6706             nan     0.1000   -0.0013
##     80        0.6482             nan     0.1000   -0.0018
##    100        0.6271             nan     0.1000   -0.0027
##    120        0.6065             nan     0.1000   -0.0013
```

```
##     140        0.5901             nan     0.1000   -0.0021
##     160        0.5709             nan     0.1000   -0.0009
##     180        0.5563             nan     0.1000   -0.0005
##     200        0.5427             nan     0.1000   -0.0025
##     220        0.5333             nan     0.1000   -0.0012
##     240        0.5239             nan     0.1000   -0.0015
##     250        0.5186             nan     0.1000   -0.0018
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##        1        1.2503             nan     0.1000    0.0405
##        2        1.1806             nan     0.1000    0.0343
##        3        1.1211             nan     0.1000    0.0276
##        4        1.0676             nan     0.1000    0.0242
##        5        1.0226             nan     0.1000    0.0193
##        6        0.9842             nan     0.1000    0.0164
##        7        0.9549             nan     0.1000    0.0120
##        8        0.9274             nan     0.1000    0.0125
##        9        0.8994             nan     0.1000    0.0100
##       10        0.8810             nan     0.1000    0.0068
##       20        0.7641             nan     0.1000    0.0015
##       40        0.6902             nan     0.1000   -0.0013
##       60        0.6497             nan     0.1000   -0.0026
##       80        0.6225             nan     0.1000   -0.0020
##      100        0.5898             nan     0.1000   -0.0009
##      120        0.5662             nan     0.1000   -0.0014
##      140        0.5460             nan     0.1000   -0.0015
##      160        0.5293             nan     0.1000   -0.0029
##      180        0.5142             nan     0.1000   -0.0018
##      200        0.5021             nan     0.1000   -0.0021
##      220        0.4850             nan     0.1000   -0.0025
##      240        0.4738             nan     0.1000   -0.0010
##      250        0.4697             nan     0.1000   -0.0025
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##        1        1.2510             nan     0.1000    0.0400
##        2        1.1788             nan     0.1000    0.0356
##        3        1.1185             nan     0.1000    0.0284
##        4        1.0652             nan     0.1000    0.0255
##        5        1.0228             nan     0.1000    0.0209
##        6        0.9819             nan     0.1000    0.0175
##        7        0.9467             nan     0.1000    0.0146
##        8        0.9149             nan     0.1000    0.0133
##        9        0.8872             nan     0.1000    0.0105
##       10        0.8681             nan     0.1000    0.0067
##       20        0.7435             nan     0.1000    0.0013
##       40        0.6620             nan     0.1000   -0.0012
```

```
##     60        0.6096             nan     0.1000   -0.0011
##     80        0.5775             nan     0.1000   -0.0017
##    100        0.5491             nan     0.1000   -0.0016
##    120        0.5248             nan     0.1000   -0.0030
##    140        0.5082             nan     0.1000   -0.0016
##    160        0.4873             nan     0.1000   -0.0022
##    180        0.4700             nan     0.1000   -0.0020
##    200        0.4543             nan     0.1000   -0.0013
##    220        0.4388             nan     0.1000   -0.0031
##    240        0.4269             nan     0.1000   -0.0013
##    250        0.4237             nan     0.1000   -0.0015
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2737             nan     0.1000    0.0306
##      2        1.2188             nan     0.1000    0.0241
##      3        1.1752             nan     0.1000    0.0184
##      4        1.1384             nan     0.1000    0.0168
##      5        1.1052             nan     0.1000    0.0134
##      6        1.0800             nan     0.1000    0.0103
##      7        1.0601             nan     0.1000    0.0106
##      8        1.0416             nan     0.1000    0.0097
##      9        1.0234             nan     0.1000    0.0070
##     10        1.0079             nan     0.1000    0.0055
##     20        0.9090             nan     0.1000    0.0034
##     40        0.8145             nan     0.1000    0.0004
##     60        0.7708             nan     0.1000    0.0003
##     80        0.7528             nan     0.1000   -0.0009
##    100        0.7433             nan     0.1000   -0.0010
##    120        0.7366             nan     0.1000   -0.0002
##    140        0.7317             nan     0.1000   -0.0007
##    160        0.7262             nan     0.1000   -0.0009
##    180        0.7217             nan     0.1000   -0.0005
##    200        0.7172             nan     0.1000   -0.0013
##    220        0.7141             nan     0.1000   -0.0012
##    240        0.7102             nan     0.1000   -0.0002
##    250        0.7086             nan     0.1000   -0.0012
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2660             nan     0.1000    0.0361
##      2        1.2076             nan     0.1000    0.0275
##      3        1.1575             nan     0.1000    0.0247
##      4        1.1197             nan     0.1000    0.0178
##      5        1.0845             nan     0.1000    0.0173
##      6        1.0529             nan     0.1000    0.0131
##      7        1.0259             nan     0.1000    0.0123
##      8        0.9969             nan     0.1000    0.0117
```

```
##      9        0.9748             nan     0.1000    0.0082
##     10        0.9535             nan     0.1000    0.0076
##     20        0.8305             nan     0.1000    0.0033
##     40        0.7475             nan     0.1000   -0.0002
##     60        0.7207             nan     0.1000   -0.0018
##     80        0.7037             nan     0.1000   -0.0017
##    100        0.6882             nan     0.1000   -0.0014
##    120        0.6802             nan     0.1000   -0.0010
##    140        0.6709             nan     0.1000   -0.0015
##    160        0.6613             nan     0.1000   -0.0014
##    180        0.6523             nan     0.1000   -0.0004
##    200        0.6449             nan     0.1000   -0.0011
##    220        0.6367             nan     0.1000   -0.0014
##    240        0.6286             nan     0.1000   -0.0013
##    250        0.6233             nan     0.1000   -0.0019
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2551             nan     0.1000    0.0346
##      2        1.1931             nan     0.1000    0.0315
##      3        1.1316             nan     0.1000    0.0272
##      4        1.0872             nan     0.1000    0.0204
##      5        1.0437             nan     0.1000    0.0187
##      6        1.0098             nan     0.1000    0.0139
##      7        0.9818             nan     0.1000    0.0107
##      8        0.9579             nan     0.1000    0.0111
##      9        0.9321             nan     0.1000    0.0129
##     10        0.9121             nan     0.1000    0.0066
##     20        0.7838             nan     0.1000    0.0022
##     40        0.7153             nan     0.1000   -0.0001
##     60        0.6832             nan     0.1000   -0.0011
##     80        0.6612             nan     0.1000   -0.0019
##    100        0.6415             nan     0.1000   -0.0020
##    120        0.6252             nan     0.1000   -0.0020
##    140        0.6084             nan     0.1000   -0.0017
##    160        0.5936             nan     0.1000   -0.0009
##    180        0.5834             nan     0.1000   -0.0021
##    200        0.5669             nan     0.1000   -0.0009
##    220        0.5568             nan     0.1000   -0.0011
##    240        0.5467             nan     0.1000   -0.0027
##    250        0.5422             nan     0.1000   -0.0015
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2574             nan     0.1000    0.0391
##      2        1.1858             nan     0.1000    0.0330
##      3        1.1308             nan     0.1000    0.0237
##      4        1.0768             nan     0.1000    0.0205
```

```
##      5        1.0311             nan     0.1000    0.0203
##      6        0.9934             nan     0.1000    0.0175
##      7        0.9643             nan     0.1000    0.0121
##      8        0.9342             nan     0.1000    0.0118
##      9        0.9061             nan     0.1000    0.0104
##     10        0.8869             nan     0.1000    0.0078
##     20        0.7608             nan     0.1000    0.0000
##     40        0.6861             nan     0.1000   -0.0012
##     60        0.6452             nan     0.1000   -0.0007
##     80        0.6147             nan     0.1000   -0.0020
##    100        0.5919             nan     0.1000   -0.0015
##    120        0.5685             nan     0.1000   -0.0015
##    140        0.5516             nan     0.1000   -0.0007
##    160        0.5322             nan     0.1000   -0.0024
##    180        0.5188             nan     0.1000   -0.0013
##    200        0.5045             nan     0.1000   -0.0011
##    220        0.4913             nan     0.1000   -0.0012
##    240        0.4791             nan     0.1000   -0.0021
##    250        0.4735             nan     0.1000   -0.0011
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2526             nan     0.1000    0.0413
##      2        1.1759             nan     0.1000    0.0342
##      3        1.1130             nan     0.1000    0.0286
##      4        1.0692             nan     0.1000    0.0198
##      5        1.0244             nan     0.1000    0.0208
##      6        0.9858             nan     0.1000    0.0160
##      7        0.9512             nan     0.1000    0.0156
##      8        0.9230             nan     0.1000    0.0086
##      9        0.8945             nan     0.1000    0.0128
##     10        0.8741             nan     0.1000    0.0071
##     20        0.7489             nan     0.1000    0.0012
##     40        0.6645             nan     0.1000   -0.0017
##     60        0.6174             nan     0.1000   -0.0018
##     80        0.5875             nan     0.1000   -0.0022
##    100        0.5620             nan     0.1000   -0.0009
##    120        0.5374             nan     0.1000   -0.0026
##    140        0.5202             nan     0.1000   -0.0017
##    160        0.5003             nan     0.1000   -0.0014
##    180        0.4829             nan     0.1000   -0.0021
##    200        0.4660             nan     0.1000   -0.0024
##    220        0.4560             nan     0.1000   -0.0024
##    240        0.4425             nan     0.1000   -0.0020
##    250        0.4349             nan     0.1000   -0.0021
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
```

```
##      1        1.2722             nan     0.1000    0.0322
##      2        1.2256             nan     0.1000    0.0203
##      3        1.1806             nan     0.1000    0.0216
##      4        1.1444             nan     0.1000    0.0179
##      5        1.1141             nan     0.1000    0.0147
##      6        1.0890             nan     0.1000    0.0118
##      7        1.0707             nan     0.1000    0.0085
##      8        1.0493             nan     0.1000    0.0108
##      9        1.0332             nan     0.1000    0.0069
##     10        1.0157             nan     0.1000    0.0086
##     20        0.9131             nan     0.1000    0.0039
##     40        0.8200             nan     0.1000    0.0010
##     60        0.7820             nan     0.1000    0.0004
##     80        0.7654             nan     0.1000   -0.0014
##    100        0.7561             nan     0.1000   -0.0009
##    120        0.7476             nan     0.1000   -0.0011
##    140        0.7412             nan     0.1000   -0.0003
##    160        0.7365             nan     0.1000   -0.0004
##    180        0.7340             nan     0.1000   -0.0005
##    200        0.7299             nan     0.1000   -0.0007
##    220        0.7266             nan     0.1000   -0.0008
##    240        0.7237             nan     0.1000   -0.0008
##    250        0.7234             nan     0.1000   -0.0005
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2651             nan     0.1000    0.0334
##      2        1.2070             nan     0.1000    0.0269
##      3        1.1557             nan     0.1000    0.0231
##      4        1.1153             nan     0.1000    0.0171
##      5        1.0815             nan     0.1000    0.0155
##      6        1.0482             nan     0.1000    0.0152
##      7        1.0172             nan     0.1000    0.0130
##      8        0.9922             nan     0.1000    0.0112
##      9        0.9735             nan     0.1000    0.0078
##     10        0.9545             nan     0.1000    0.0083
##     20        0.8345             nan     0.1000    0.0033
##     40        0.7573             nan     0.1000   -0.0001
##     60        0.7333             nan     0.1000   -0.0011
##     80        0.7105             nan     0.1000   -0.0006
##    100        0.6966             nan     0.1000   -0.0011
##    120        0.6815             nan     0.1000   -0.0012
##    140        0.6641             nan     0.1000   -0.0008
##    160        0.6482             nan     0.1000   -0.0016
##    180        0.6413             nan     0.1000   -0.0012
##    200        0.6329             nan     0.1000   -0.0008
##    220        0.6240             nan     0.1000   -0.0015
```

```
##    240        0.6160             nan     0.1000   -0.0011
##    250        0.6111             nan     0.1000   -0.0017
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2637             nan     0.1000    0.0352
##      2        1.1913             nan     0.1000    0.0330
##      3        1.1333             nan     0.1000    0.0254
##      4        1.0844             nan     0.1000    0.0231
##      5        1.0391             nan     0.1000    0.0195
##      6        1.0021             nan     0.1000    0.0152
##      7        0.9729             nan     0.1000    0.0118
##      8        0.9513             nan     0.1000    0.0086
##      9        0.9272             nan     0.1000    0.0096
##     10        0.9064             nan     0.1000    0.0085
##     20        0.7931             nan     0.1000    0.0041
##     40        0.7237             nan     0.1000   -0.0004
##     60        0.6981             nan     0.1000   -0.0012
##     80        0.6718             nan     0.1000   -0.0026
##    100        0.6529             nan     0.1000   -0.0016
##    120        0.6396             nan     0.1000   -0.0010
##    140        0.6233             nan     0.1000   -0.0013
##    160        0.6101             nan     0.1000   -0.0011
##    180        0.5932             nan     0.1000   -0.0015
##    200        0.5794             nan     0.1000   -0.0010
##    220        0.5645             nan     0.1000   -0.0011
##    240        0.5498             nan     0.1000   -0.0018
##    250        0.5448             nan     0.1000   -0.0012
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2583             nan     0.1000    0.0380
##      2        1.1835             nan     0.1000    0.0345
##      3        1.1231             nan     0.1000    0.0268
##      4        1.0730             nan     0.1000    0.0218
##      5        1.0329             nan     0.1000    0.0173
##      6        0.9952             nan     0.1000    0.0161
##      7        0.9630             nan     0.1000    0.0130
##      8        0.9348             nan     0.1000    0.0126
##      9        0.9109             nan     0.1000    0.0108
##     10        0.8940             nan     0.1000    0.0058
##     20        0.7714             nan     0.1000    0.0009
##     40        0.6915             nan     0.1000   -0.0022
##     60        0.6527             nan     0.1000   -0.0006
##     80        0.6232             nan     0.1000   -0.0011
##    100        0.6008             nan     0.1000   -0.0018
##    120        0.5783             nan     0.1000   -0.0017
##    140        0.5562             nan     0.1000   -0.0023
```

```
##    160        0.5375             nan     0.1000   -0.0014
##    180        0.5165             nan     0.1000   -0.0019
##    200        0.5043             nan     0.1000   -0.0021
##    220        0.4907             nan     0.1000   -0.0022
##    240        0.4783             nan     0.1000   -0.0019
##    250        0.4728             nan     0.1000   -0.0022
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2435             nan     0.1000    0.0421
##      2        1.1748             nan     0.1000    0.0315
##      3        1.1147             nan     0.1000    0.0294
##      4        1.0672             nan     0.1000    0.0236
##      5        1.0265             nan     0.1000    0.0188
##      6        0.9873             nan     0.1000    0.0165
##      7        0.9555             nan     0.1000    0.0151
##      8        0.9289             nan     0.1000    0.0100
##      9        0.9030             nan     0.1000    0.0085
##     10        0.8836             nan     0.1000    0.0077
##     20        0.7615             nan     0.1000    0.0016
##     40        0.6861             nan     0.1000   -0.0016
##     60        0.6393             nan     0.1000   -0.0017
##     80        0.6022             nan     0.1000   -0.0021
##    100        0.5787             nan     0.1000   -0.0023
##    120        0.5532             nan     0.1000   -0.0024
##    140        0.5303             nan     0.1000   -0.0017
##    160        0.5079             nan     0.1000   -0.0015
##    180        0.4894             nan     0.1000   -0.0017
##    200        0.4716             nan     0.1000   -0.0019
##    220        0.4537             nan     0.1000   -0.0017
##    240        0.4389             nan     0.1000   -0.0007
##    250        0.4327             nan     0.1000   -0.0013
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2786             nan     0.1000    0.0297
##      2        1.2244             nan     0.1000    0.0249
##      3        1.1873             nan     0.1000    0.0203
##      4        1.1524             nan     0.1000    0.0140
##      5        1.1216             nan     0.1000    0.0141
##      6        1.0961             nan     0.1000    0.0125
##      7        1.0730             nan     0.1000    0.0103
##      8        1.0536             nan     0.1000    0.0086
##      9        1.0376             nan     0.1000    0.0067
##     10        1.0208             nan     0.1000    0.0083
##     20        0.9191             nan     0.1000    0.0025
##     40        0.8304             nan     0.1000    0.0006
##     60        0.7967             nan     0.1000   -0.0009
```

```
##      80        0.7809             nan     0.1000   -0.0007
##     100        0.7724             nan     0.1000   -0.0012
##     120        0.7661             nan     0.1000   -0.0004
##     140        0.7613             nan     0.1000   -0.0012
##     160        0.7558             nan     0.1000   -0.0004
##     180        0.7511             nan     0.1000   -0.0004
##     200        0.7460             nan     0.1000   -0.0006
##     220        0.7421             nan     0.1000   -0.0013
##     240        0.7388             nan     0.1000   -0.0007
##     250        0.7365             nan     0.1000   -0.0009
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##       1        1.2662             nan     0.1000    0.0324
##       2        1.2096             nan     0.1000    0.0223
##       3        1.1565             nan     0.1000    0.0234
##       4        1.1199             nan     0.1000    0.0184
##       5        1.0844             nan     0.1000    0.0144
##       6        1.0520             nan     0.1000    0.0153
##       7        1.0254             nan     0.1000    0.0130
##       8        1.0023             nan     0.1000    0.0091
##       9        0.9789             nan     0.1000    0.0100
##      10        0.9608             nan     0.1000    0.0074
##      20        0.8450             nan     0.1000    0.0015
##      40        0.7728             nan     0.1000   -0.0010
##      60        0.7478             nan     0.1000   -0.0011
##      80        0.7312             nan     0.1000   -0.0005
##     100        0.7193             nan     0.1000   -0.0008
##     120        0.7053             nan     0.1000   -0.0015
##     140        0.6952             nan     0.1000   -0.0006
##     160        0.6855             nan     0.1000   -0.0007
##     180        0.6758             nan     0.1000   -0.0013
##     200        0.6663             nan     0.1000   -0.0011
##     220        0.6599             nan     0.1000   -0.0008
##     240        0.6511             nan     0.1000   -0.0015
##     250        0.6471             nan     0.1000   -0.0012
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##       1        1.2605             nan     0.1000    0.0359
##       2        1.1990             nan     0.1000    0.0295
##       3        1.1393             nan     0.1000    0.0250
##       4        1.0933             nan     0.1000    0.0198
##       5        1.0564             nan     0.1000    0.0142
##       6        1.0189             nan     0.1000    0.0153
##       7        0.9922             nan     0.1000    0.0114
##       8        0.9677             nan     0.1000    0.0095
##       9        0.9451             nan     0.1000    0.0105
```

```
##     10        0.9247             nan     0.1000    0.0070
##     20        0.8103             nan     0.1000    0.0028
##     40        0.7386             nan     0.1000   -0.0008
##     60        0.7043             nan     0.1000   -0.0029
##     80        0.6768             nan     0.1000   -0.0006
##    100        0.6509             nan     0.1000   -0.0012
##    120        0.6340             nan     0.1000   -0.0015
##    140        0.6159             nan     0.1000   -0.0020
##    160        0.6042             nan     0.1000   -0.0015
##    180        0.5892             nan     0.1000   -0.0009
##    200        0.5800             nan     0.1000   -0.0015
##    220        0.5693             nan     0.1000   -0.0015
##    240        0.5583             nan     0.1000   -0.0014
##    250        0.5545             nan     0.1000   -0.0009
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2535             nan     0.1000    0.0373
##      2        1.1854             nan     0.1000    0.0315
##      3        1.1321             nan     0.1000    0.0243
##      4        1.0809             nan     0.1000    0.0232
##      5        1.0425             nan     0.1000    0.0193
##      6        1.0039             nan     0.1000    0.0155
##      7        0.9741             nan     0.1000    0.0124
##      8        0.9470             nan     0.1000    0.0120
##      9        0.9198             nan     0.1000    0.0119
##     10        0.9026             nan     0.1000    0.0068
##     20        0.7913             nan     0.1000    0.0012
##     40        0.7186             nan     0.1000   -0.0003
##     60        0.6837             nan     0.1000   -0.0016
##     80        0.6483             nan     0.1000   -0.0009
##    100        0.6236             nan     0.1000   -0.0014
##    120        0.5982             nan     0.1000   -0.0024
##    140        0.5790             nan     0.1000   -0.0015
##    160        0.5596             nan     0.1000   -0.0035
##    180        0.5411             nan     0.1000   -0.0007
##    200        0.5267             nan     0.1000   -0.0020
##    220        0.5139             nan     0.1000   -0.0012
##    240        0.4973             nan     0.1000   -0.0021
##    250        0.4919             nan     0.1000   -0.0009
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2535             nan     0.1000    0.0388
##      2        1.1840             nan     0.1000    0.0318
##      3        1.1232             nan     0.1000    0.0262
##      4        1.0698             nan     0.1000    0.0244
##      5        1.0285             nan     0.1000    0.0185
```

```
##       6        0.9955             nan     0.1000    0.0134
##       7        0.9661             nan     0.1000    0.0146
##       8        0.9362             nan     0.1000    0.0139
##       9        0.9138             nan     0.1000    0.0090
##      10        0.8958             nan     0.1000    0.0069
##      20        0.7770             nan     0.1000    0.0004
##      40        0.7015             nan     0.1000   -0.0011
##      60        0.6610             nan     0.1000   -0.0024
##      80        0.6300             nan     0.1000   -0.0035
##     100        0.5995             nan     0.1000   -0.0016
##     120        0.5673             nan     0.1000   -0.0024
##     140        0.5459             nan     0.1000   -0.0038
##     160        0.5245             nan     0.1000   -0.0029
##     180        0.5053             nan     0.1000   -0.0016
##     200        0.4902             nan     0.1000   -0.0012
##     220        0.4748             nan     0.1000   -0.0026
##     240        0.4577             nan     0.1000   -0.0022
##     250        0.4513             nan     0.1000   -0.0027
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##       1        1.2725             nan     0.1000    0.0315
##       2        1.2219             nan     0.1000    0.0246
##       3        1.1809             nan     0.1000    0.0195
##       4        1.1501             nan     0.1000    0.0136
##       5        1.1172             nan     0.1000    0.0151
##       6        1.0930             nan     0.1000    0.0122
##       7        1.0669             nan     0.1000    0.0116
##       8        1.0449             nan     0.1000    0.0093
##       9        1.0285             nan     0.1000    0.0066
##      10        1.0180             nan     0.1000    0.0038
##      20        0.9148             nan     0.1000    0.0024
##      40        0.8255             nan     0.1000   -0.0002
##      60        0.7874             nan     0.1000    0.0005
##      80        0.7699             nan     0.1000   -0.0002
##     100        0.7627             nan     0.1000   -0.0013
##     120        0.7552             nan     0.1000   -0.0003
##     140        0.7490             nan     0.1000   -0.0009
##     160        0.7430             nan     0.1000   -0.0010
##     180        0.7382             nan     0.1000   -0.0008
##     200        0.7349             nan     0.1000   -0.0005
##     220        0.7314             nan     0.1000   -0.0013
##     240        0.7268             nan     0.1000   -0.0007
##     250        0.7253             nan     0.1000   -0.0006
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##       1        1.2623             nan     0.1000    0.0345
```

```
##      2        1.2026             nan     0.1000    0.0294
##      3        1.1548             nan     0.1000    0.0218
##      4        1.1129             nan     0.1000    0.0177
##      5        1.0812             nan     0.1000    0.0157
##      6        1.0509             nan     0.1000    0.0147
##      7        1.0280             nan     0.1000    0.0099
##      8        1.0037             nan     0.1000    0.0104
##      9        0.9810             nan     0.1000    0.0097
##     10        0.9609             nan     0.1000    0.0089
##     20        0.8459             nan     0.1000    0.0019
##     40        0.7693             nan     0.1000   -0.0002
##     60        0.7363             nan     0.1000   -0.0008
##     80        0.7162             nan     0.1000   -0.0023
##    100        0.7052             nan     0.1000   -0.0015
##    120        0.6917             nan     0.1000   -0.0028
##    140        0.6756             nan     0.1000   -0.0020
##    160        0.6652             nan     0.1000   -0.0003
##    180        0.6557             nan     0.1000   -0.0014
##    200        0.6468             nan     0.1000   -0.0006
##    220        0.6353             nan     0.1000   -0.0006
##    240        0.6277             nan     0.1000   -0.0007
##    250        0.6244             nan     0.1000   -0.0011
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2566             nan     0.1000    0.0386
##      2        1.1937             nan     0.1000    0.0297
##      3        1.1355             nan     0.1000    0.0258
##      4        1.0909             nan     0.1000    0.0201
##      5        1.0509             nan     0.1000    0.0179
##      6        1.0145             nan     0.1000    0.0162
##      7        0.9840             nan     0.1000    0.0123
##      8        0.9551             nan     0.1000    0.0122
##      9        0.9369             nan     0.1000    0.0088
##     10        0.9164             nan     0.1000    0.0072
##     20        0.8017             nan     0.1000    0.0007
##     40        0.7255             nan     0.1000   -0.0002
##     60        0.6940             nan     0.1000   -0.0009
##     80        0.6684             nan     0.1000   -0.0008
##    100        0.6504             nan     0.1000   -0.0011
##    120        0.6325             nan     0.1000   -0.0013
##    140        0.6140             nan     0.1000   -0.0013
##    160        0.5974             nan     0.1000   -0.0002
##    180        0.5833             nan     0.1000   -0.0010
##    200        0.5666             nan     0.1000   -0.0011
##    220        0.5550             nan     0.1000   -0.0020
##    240        0.5451             nan     0.1000   -0.0023
```

```
##      250        0.5372             nan     0.1000   -0.0015
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##        1        1.2498             nan     0.1000    0.0417
##        2        1.1832             nan     0.1000    0.0281
##        3        1.1271             nan     0.1000    0.0244
##        4        1.0777             nan     0.1000    0.0218
##        5        1.0407             nan     0.1000    0.0151
##        6        1.0058             nan     0.1000    0.0141
##        7        0.9753             nan     0.1000    0.0148
##        8        0.9445             nan     0.1000    0.0133
##        9        0.9192             nan     0.1000    0.0115
##       10        0.9036             nan     0.1000    0.0060
##       20        0.7800             nan     0.1000    0.0017
##       40        0.7027             nan     0.1000   -0.0018
##       60        0.6571             nan     0.1000   -0.0015
##       80        0.6285             nan     0.1000   -0.0028
##      100        0.6088             nan     0.1000   -0.0028
##      120        0.5816             nan     0.1000   -0.0033
##      140        0.5649             nan     0.1000   -0.0020
##      160        0.5430             nan     0.1000   -0.0012
##      180        0.5294             nan     0.1000   -0.0016
##      200        0.5109             nan     0.1000   -0.0021
##      220        0.4943             nan     0.1000   -0.0027
##      240        0.4793             nan     0.1000   -0.0010
##      250        0.4732             nan     0.1000   -0.0016
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##        1        1.2514             nan     0.1000    0.0374
##        2        1.1825             nan     0.1000    0.0323
##        3        1.1249             nan     0.1000    0.0244
##        4        1.0758             nan     0.1000    0.0248
##        5        1.0288             nan     0.1000    0.0205
##        6        0.9950             nan     0.1000    0.0151
##        7        0.9607             nan     0.1000    0.0120
##        8        0.9307             nan     0.1000    0.0132
##        9        0.9071             nan     0.1000    0.0100
##       10        0.8828             nan     0.1000    0.0094
##       20        0.7598             nan     0.1000    0.0013
##       40        0.6744             nan     0.1000   -0.0017
##       60        0.6343             nan     0.1000   -0.0018
##       80        0.5947             nan     0.1000   -0.0013
##      100        0.5667             nan     0.1000   -0.0019
##      120        0.5457             nan     0.1000   -0.0029
##      140        0.5235             nan     0.1000   -0.0024
##      160        0.5036             nan     0.1000   -0.0019
```

```
##    180        0.4856             nan     0.1000   -0.0030
##    200        0.4678             nan     0.1000   -0.0020
##    220        0.4534             nan     0.1000   -0.0023
##    240        0.4412             nan     0.1000   -0.0018
##    250        0.4336             nan     0.1000   -0.0019
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2803             nan     0.1000    0.0300
##      2        1.2282             nan     0.1000    0.0252
##      3        1.1859             nan     0.1000    0.0212
##      4        1.1515             nan     0.1000    0.0150
##      5        1.1195             nan     0.1000    0.0146
##      6        1.0928             nan     0.1000    0.0127
##      7        1.0679             nan     0.1000    0.0107
##      8        1.0480             nan     0.1000    0.0092
##      9        1.0320             nan     0.1000    0.0078
##     10        1.0185             nan     0.1000    0.0060
##     20        0.9144             nan     0.1000    0.0035
##     40        0.8227             nan     0.1000    0.0009
##     60        0.7776             nan     0.1000   -0.0003
##     80        0.7595             nan     0.1000   -0.0005
##    100        0.7498             nan     0.1000   -0.0002
##    120        0.7441             nan     0.1000   -0.0002
##    140        0.7392             nan     0.1000   -0.0006
##    160        0.7347             nan     0.1000   -0.0004
##    180        0.7323             nan     0.1000   -0.0013
##    200        0.7259             nan     0.1000   -0.0003
##    220        0.7226             nan     0.1000   -0.0003
##    240        0.7204             nan     0.1000   -0.0004
##    250        0.7180             nan     0.1000   -0.0010
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2639             nan     0.1000    0.0365
##      2        1.2041             nan     0.1000    0.0277
##      3        1.1555             nan     0.1000    0.0224
##      4        1.1135             nan     0.1000    0.0190
##      5        1.0741             nan     0.1000    0.0174
##      6        1.0444             nan     0.1000    0.0128
##      7        1.0172             nan     0.1000    0.0120
##      8        0.9928             nan     0.1000    0.0114
##      9        0.9698             nan     0.1000    0.0105
##     10        0.9523             nan     0.1000    0.0071
##     20        0.8290             nan     0.1000    0.0023
##     40        0.7563             nan     0.1000   -0.0012
##     60        0.7274             nan     0.1000   -0.0011
##     80        0.7078             nan     0.1000   -0.0014
```

```
##    100        0.6940             nan     0.1000   -0.0008
##    120        0.6795             nan     0.1000   -0.0015
##    140        0.6698             nan     0.1000   -0.0008
##    160        0.6585             nan     0.1000   -0.0011
##    180        0.6453             nan     0.1000   -0.0002
##    200        0.6358             nan     0.1000   -0.0007
##    220        0.6313             nan     0.1000   -0.0019
##    240        0.6263             nan     0.1000   -0.0020
##    250        0.6222             nan     0.1000   -0.0013
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2566             nan     0.1000    0.0352
##      2        1.1939             nan     0.1000    0.0309
##      3        1.1369             nan     0.1000    0.0252
##      4        1.0871             nan     0.1000    0.0217
##      5        1.0427             nan     0.1000    0.0188
##      6        1.0083             nan     0.1000    0.0132
##      7        0.9772             nan     0.1000    0.0138
##      8        0.9496             nan     0.1000    0.0146
##      9        0.9264             nan     0.1000    0.0103
##     10        0.9027             nan     0.1000    0.0097
##     20        0.7804             nan     0.1000    0.0026
##     40        0.7150             nan     0.1000   -0.0014
##     60        0.6814             nan     0.1000   -0.0023
##     80        0.6575             nan     0.1000   -0.0021
##    100        0.6395             nan     0.1000   -0.0021
##    120        0.6198             nan     0.1000   -0.0014
##    140        0.6030             nan     0.1000   -0.0016
##    160        0.5852             nan     0.1000   -0.0013
##    180        0.5747             nan     0.1000   -0.0017
##    200        0.5616             nan     0.1000   -0.0014
##    220        0.5461             nan     0.1000   -0.0019
##    240        0.5350             nan     0.1000   -0.0025
##    250        0.5289             nan     0.1000   -0.0008
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2508             nan     0.1000    0.0399
##      2        1.1799             nan     0.1000    0.0327
##      3        1.1202             nan     0.1000    0.0267
##      4        1.0681             nan     0.1000    0.0230
##      5        1.0267             nan     0.1000    0.0188
##      6        0.9903             nan     0.1000    0.0144
##      7        0.9579             nan     0.1000    0.0146
##      8        0.9311             nan     0.1000    0.0122
##      9        0.9093             nan     0.1000    0.0100
##     10        0.8920             nan     0.1000    0.0071
```

```
##     20        0.7669             nan     0.1000    0.0027
##     40        0.6912             nan     0.1000   -0.0021
##     60        0.6458             nan     0.1000   -0.0026
##     80        0.6124             nan     0.1000   -0.0004
##    100        0.5870             nan     0.1000   -0.0014
##    120        0.5656             nan     0.1000   -0.0013
##    140        0.5518             nan     0.1000   -0.0023
##    160        0.5341             nan     0.1000   -0.0011
##    180        0.5194             nan     0.1000   -0.0010
##    200        0.5076             nan     0.1000   -0.0026
##    220        0.4978             nan     0.1000   -0.0018
##    240        0.4803             nan     0.1000   -0.0012
##    250        0.4720             nan     0.1000   -0.0022
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2479             nan     0.1000    0.0415
##      2        1.1762             nan     0.1000    0.0296
##      3        1.1123             nan     0.1000    0.0268
##      4        1.0657             nan     0.1000    0.0197
##      5        1.0210             nan     0.1000    0.0199
##      6        0.9815             nan     0.1000    0.0159
##      7        0.9479             nan     0.1000    0.0105
##      8        0.9197             nan     0.1000    0.0126
##      9        0.8955             nan     0.1000    0.0088
##     10        0.8742             nan     0.1000    0.0090
##     20        0.7586             nan     0.1000    0.0012
##     40        0.6843             nan     0.1000   -0.0018
##     60        0.6355             nan     0.1000   -0.0027
##     80        0.5939             nan     0.1000   -0.0014
##    100        0.5648             nan     0.1000   -0.0014
##    120        0.5434             nan     0.1000   -0.0016
##    140        0.5223             nan     0.1000   -0.0021
##    160        0.5026             nan     0.1000   -0.0021
##    180        0.4889             nan     0.1000   -0.0021
##    200        0.4758             nan     0.1000   -0.0012
##    220        0.4520             nan     0.1000   -0.0008
##    240        0.4417             nan     0.1000   -0.0027
##    250        0.4358             nan     0.1000   -0.0023
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        1.2643             nan     0.1000    0.0332
##      2        1.2100             nan     0.1000    0.0272
##      3        1.1593             nan     0.1000    0.0240
##      4        1.1180             nan     0.1000    0.0196
##      5        1.0825             nan     0.1000    0.0170
##      6        1.0508             nan     0.1000    0.0135
```

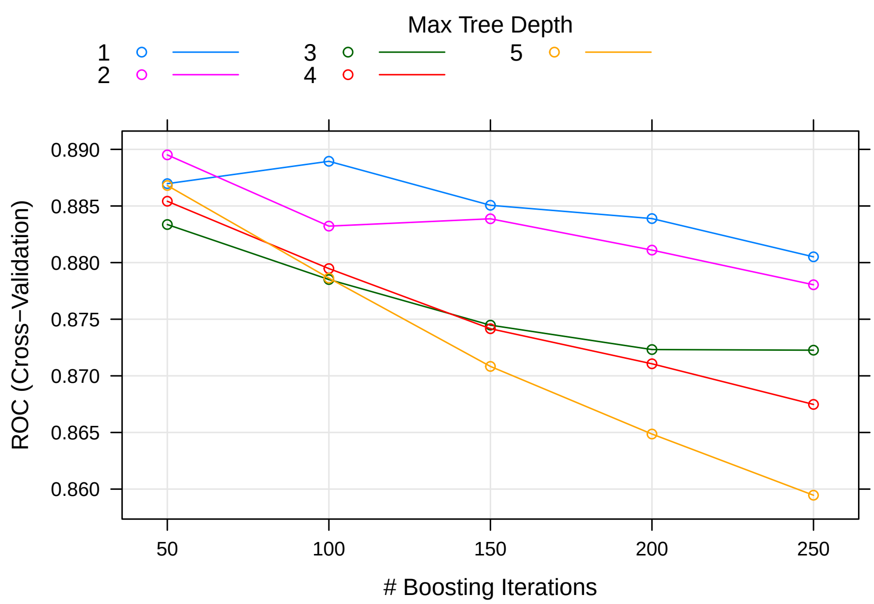
```
##      7        1.0219             nan     0.1000    0.0112
##      8        0.9984             nan     0.1000    0.0118
##      9        0.9778             nan     0.1000    0.0072
##     10        0.9565             nan     0.1000    0.0096
##     20        0.8389             nan     0.1000    0.0025
##     40        0.7624             nan     0.1000   -0.0009
##     50        0.7453             nan     0.1000   -0.0006
```

```
oj.gbm
```

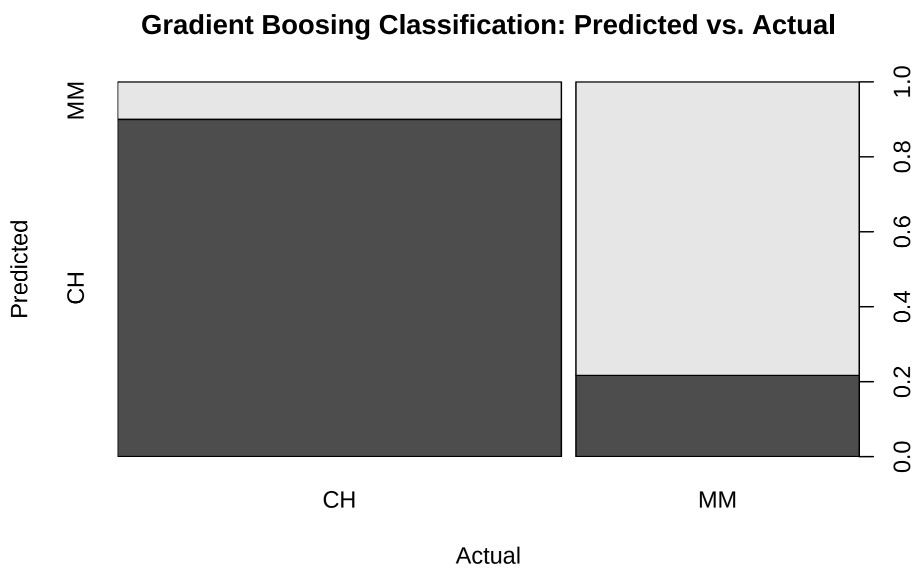
```
## Stochastic Gradient Boosting
##
## 857 samples
##  17 predictor
##   2 classes: 'CH', 'MM'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 772, 770, 771, 771, 772, 771, ...
## Resampling results across tuning parameters:
##
##   interaction.depth  n.trees  ROC        Sens       Spec
##   1                   50      0.8869715  0.8720247  0.7245098
##   1                  100      0.8889466  0.8738389  0.7302139
##   1                  150      0.8850612  0.8680697  0.7303030
##   1                  200      0.8838868  0.8738026  0.7213012
##   1                  250      0.8805090  0.8622642  0.7275401
##   2                   50      0.8895139  0.8719521  0.7451872
##   2                  100      0.8832208  0.8623367  0.7334225
##   2                  150      0.8838687  0.8679971  0.7394831
##   2                  200      0.8811028  0.8642598  0.7245989
##   2                  250      0.8780432  0.8489840  0.7336898
##   3                   50      0.8833620  0.8700290  0.7245989
##   3                  100      0.8785063  0.8604862  0.7454545
##   3                  150      0.8744782  0.8470972  0.7156863
##   3                  200      0.8723217  0.8414731  0.7246881
##   3                  250      0.8722653  0.8337446  0.7217469
##   4                   50      0.8854180  0.8604862  0.7605169
##   4                  100      0.8794721  0.8413280  0.7336898
##   4                  150      0.8741609  0.8432511  0.7308378
##   4                  200      0.8710638  0.8470972  0.7249554
##   4                  250      0.8674771  0.8490203  0.7218360
##   5                   50      0.8868076  0.8585994  0.7574866
##   5                  100      0.8786285  0.8471698  0.7486631
##   5                  150      0.8708328  0.8395138  0.7458111
```

```
##   5                  200      0.8648622  0.8452467  0.7455437
##   5                  250      0.8594578  0.8375544  0.7336007
##
## Tuning parameter 'shrinkage' was held constant at a value of 0.1
##
## Tuning parameter 'n.minobsinnode' was held constant at a value of 10
## ROC was used to select the optimal model using the largest value.
## The final values used for the model were n.trees = 50, interaction.depth =
##  2, shrinkage = 0.1 and n.minobsinnode = 10.
```

```
plot(oj.gbm)
```




```
oj.pred <- predict(oj.gbm, oj_test, type = "raw")
plot(oj_test$Purchase, oj.pred,
     main = "Gradient Boosing Classification: Predicted vs. Actual",
     xlab = "Actual",
     ylab = "Predicted")
```




```
(oj.conf <- confusionMatrix(data = oj.pred,
                            reference = oj_test$Purchase))
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  CH  MM
##         CH 117  18
##         MM  13  65
##
##                Accuracy : 0.8545
##                  95% CI : (0.7998, 0.8989)
##     No Information Rate : 0.6103
##     P-Value [Acc > NIR] : 4.83e-15
##
##                   Kappa : 0.6907
##
##  Mcnemar's Test P-Value : 0.4725
##
##             Sensitivity : 0.9000
##             Specificity : 0.7831
##          Pos Pred Value : 0.8667
##          Neg Pred Value : 0.8333
##              Prevalence : 0.6103
```

```
##          Detection Rate : 0.5493
##    Detection Prevalence : 0.6338
##       Balanced Accuracy : 0.8416
##
##        'Positive' Class : CH
##
```

```
oj.gbm.acc <- as.numeric(oj.conf$overall[1])
rm(oj.pred)
rm(oj.conf)
#plot(oj.bag$, oj.bag$finalModel$y)
#plot(varImp(oj.gbm), main="Variable Importance with Gradient Boosting")
```

9.5.0.2 Gradient Boosting Regression Example

Again using the `Carseats` data set to predict `Sales`, this time I'll use the gradient boosting method by specifying `method = "gbm"`. I'll use `tuneLength = 5` and not worry about `tuneGrid` anymore. Caret tunes the following hyperparameters.

- `n.trees`: number of boosting iterations (increasing `n.trees` reduces the error on training set, but may lead to over-fitting)
- `interaction.depth`: maximum tree depth (the default six - node tree appears to do an excellent job)
- `shrinkage`: learning rate (reduces the impact of each additional fitted base-learner (tree) by reducing the size of incremental steps and thus penalizes the importance of each consecutive iteration. The intuition is that it is better to improve a model by taking many small steps than by taking fewer large steps. If one of the boosting iterations turns out to be erroneous, its negative impact can be easily corrected in subsequent steps.)
- `n.minobsinnode`: mimimum terminal node size

```
carseats.gbm <- train(Sales ~ .,
                      data = carseats_train,
                      method = "gbm",  # for bagged tree
                      tuneLength = 5,  # choose up to 5 combinations of tuning parameters
                      metric = "RMSE",  # evaluate hyperparamter combinations with ROC
                      trControl = trainControl(
                        method = "cv",  # k-fold cross validation
                        number = 10,  # 10 folds
                        savePredictions = "final",       # save predictions for the optimal tunin
                        verboseIter = FALSE,
                        returnData = FALSE
                        )
                      )
```

```
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1         7.6155             nan     0.1000    0.3126
##      2         7.3677             nan     0.1000    0.2471
##      3         7.1383             nan     0.1000    0.1559
##      4         6.8796             nan     0.1000    0.3000
##      5         6.6084             nan     0.1000    0.2696
##      6         6.3846             nan     0.1000    0.1575
##      7         6.1551             nan     0.1000    0.2016
##      8         5.9837             nan     0.1000    0.1171
##      9         5.7969             nan     0.1000    0.1558
##     10         5.6503             nan     0.1000    0.1243
##     20         4.5758             nan     0.1000    0.0472
##     40         3.3276             nan     0.1000    0.0043
##     60         2.6161             nan     0.1000    0.0154
##     80         2.1215             nan     0.1000   -0.0029
##    100         1.7822             nan     0.1000   -0.0166
##    120         1.5354             nan     0.1000   -0.0016
##    140         1.3313             nan     0.1000    0.0067
##    160         1.2074             nan     0.1000   -0.0030
##    180         1.0966             nan     0.1000    0.0005
##    200         1.0083             nan     0.1000   -0.0019
##    220         0.9572             nan     0.1000   -0.0008
##    240         0.9048             nan     0.1000   -0.0052
##    250         0.8922             nan     0.1000   -0.0051
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1         7.4939             nan     0.1000    0.5303
##      2         6.9609             nan     0.1000    0.4503
##      3         6.5646             nan     0.1000    0.3312
##      4         6.2135             nan     0.1000    0.2836
##      5         5.9347             nan     0.1000    0.2472
##      6         5.6654             nan     0.1000    0.2045
##      7         5.3757             nan     0.1000    0.2134
##      8         5.1883             nan     0.1000    0.1810
##      9         5.0431             nan     0.1000    0.1205
##     10         4.8440             nan     0.1000    0.0749
##     20         3.4421             nan     0.1000    0.1291
##     40         2.0285             nan     0.1000    0.0246
##     60         1.4136             nan     0.1000    0.0003
##     80         1.0839             nan     0.1000    0.0003
##    100         0.9011             nan     0.1000    0.0052
##    120         0.8195             nan     0.1000   -0.0075
##    140         0.7664             nan     0.1000   -0.0036
##    160         0.7243             nan     0.1000   -0.0010
##    180         0.6839             nan     0.1000   -0.0028
##    200         0.6448             nan     0.1000   -0.0048
```

```
##    220        0.6123             nan     0.1000   -0.0035
##    240        0.5897             nan     0.1000   -0.0038
##    250        0.5767             nan     0.1000   -0.0050
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.3122             nan     0.1000    0.5956
##      2        6.7737             nan     0.1000    0.4295
##      3        6.3033             nan     0.1000    0.4215
##      4        5.9081             nan     0.1000    0.2966
##      5        5.5342             nan     0.1000    0.3320
##      6        5.1666             nan     0.1000    0.2748
##      7        4.9365             nan     0.1000    0.1688
##      8        4.6557             nan     0.1000    0.2144
##      9        4.4412             nan     0.1000    0.1072
##     10        4.2075             nan     0.1000    0.1861
##     20        2.7722             nan     0.1000    0.0107
##     40        1.4659             nan     0.1000    0.0203
##     60        1.0163             nan     0.1000   -0.0055
##     80        0.8430             nan     0.1000   -0.0074
##    100        0.7427             nan     0.1000   -0.0031
##    120        0.6731             nan     0.1000   -0.0078
##    140        0.6151             nan     0.1000   -0.0080
##    160        0.5814             nan     0.1000   -0.0074
##    180        0.5452             nan     0.1000   -0.0054
##    200        0.5023             nan     0.1000   -0.0071
##    220        0.4697             nan     0.1000   -0.0058
##    240        0.4340             nan     0.1000   -0.0022
##    250        0.4207             nan     0.1000   -0.0088
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.3508             nan     0.1000    0.7012
##      2        6.7011             nan     0.1000    0.5533
##      3        6.1585             nan     0.1000    0.5138
##      4        5.7274             nan     0.1000    0.3542
##      5        5.2438             nan     0.1000    0.3597
##      6        4.9357             nan     0.1000    0.2545
##      7        4.6359             nan     0.1000    0.2195
##      8        4.3960             nan     0.1000    0.2294
##      9        4.1786             nan     0.1000    0.1539
##     10        3.9850             nan     0.1000    0.1414
##     20        2.4927             nan     0.1000    0.0532
##     40        1.2882             nan     0.1000    0.0112
##     60        0.8551             nan     0.1000   -0.0074
##     80        0.6752             nan     0.1000   -0.0044
##    100        0.5795             nan     0.1000   -0.0097
##    120        0.4983             nan     0.1000   -0.0038
```

```
##    140        0.4440             nan     0.1000   -0.0032
##    160        0.4044             nan     0.1000   -0.0056
##    180        0.3666             nan     0.1000   -0.0076
##    200        0.3337             nan     0.1000   -0.0065
##    220        0.3066             nan     0.1000   -0.0022
##    240        0.2736             nan     0.1000   -0.0039
##    250        0.2608             nan     0.1000   -0.0038
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.2719             nan     0.1000    0.7029
##      2        6.5623             nan     0.1000    0.5180
##      3        6.0426             nan     0.1000    0.4144
##      4        5.5613             nan     0.1000    0.4419
##      5        5.1070             nan     0.1000    0.2878
##      6        4.7641             nan     0.1000    0.2383
##      7        4.4677             nan     0.1000    0.2141
##      8        4.2399             nan     0.1000    0.0706
##      9        3.9751             nan     0.1000    0.1927
##     10        3.7100             nan     0.1000    0.1701
##     20        2.2565             nan     0.1000    0.0859
##     40        1.1000             nan     0.1000   -0.0080
##     60        0.7464             nan     0.1000   -0.0020
##     80        0.5790             nan     0.1000   -0.0024
##    100        0.4941             nan     0.1000   -0.0054
##    120        0.4290             nan     0.1000   -0.0030
##    140        0.3723             nan     0.1000   -0.0052
##    160        0.3330             nan     0.1000   -0.0042
##    180        0.2951             nan     0.1000   -0.0056
##    200        0.2627             nan     0.1000   -0.0038
##    220        0.2336             nan     0.1000   -0.0018
##    240        0.2089             nan     0.1000   -0.0017
##    250        0.1964             nan     0.1000   -0.0029
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.8758             nan     0.1000    0.1611
##      2        7.4638             nan     0.1000    0.4117
##      3        7.1509             nan     0.1000    0.2868
##      4        6.8550             nan     0.1000    0.2921
##      5        6.6144             nan     0.1000    0.2482
##      6        6.4519             nan     0.1000    0.1654
##      7        6.3108             nan     0.1000    0.0792
##      8        6.1631             nan     0.1000    0.1260
##      9        6.0160             nan     0.1000    0.1119
##     10        5.8043             nan     0.1000    0.1567
##     20        4.6275             nan     0.1000    0.0715
##     40        3.4435             nan     0.1000   -0.0080
```

```
##     60        2.6905             nan     0.1000    0.0048
##     80        2.1544             nan     0.1000    0.0127
##    100        1.7772             nan     0.1000   -0.0062
##    120        1.4927             nan     0.1000   -0.0058
##    140        1.3013             nan     0.1000    0.0010
##    160        1.1609             nan     0.1000    0.0023
##    180        1.0670             nan     0.1000   -0.0058
##    200        0.9890             nan     0.1000   -0.0088
##    220        0.9407             nan     0.1000    0.0000
##    240        0.9016             nan     0.1000   -0.0042
##    250        0.8853             nan     0.1000   -0.0037
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.6412             nan     0.1000    0.5298
##      2        7.0819             nan     0.1000    0.4917
##      3        6.5521             nan     0.1000    0.3297
##      4        6.1791             nan     0.1000    0.2744
##      5        5.9412             nan     0.1000    0.1842
##      6        5.6434             nan     0.1000    0.2504
##      7        5.3703             nan     0.1000    0.2167
##      8        5.1224             nan     0.1000    0.1739
##      9        4.9715             nan     0.1000    0.1184
##     10        4.7654             nan     0.1000    0.1615
##     20        3.3795             nan     0.1000    0.0636
##     40        2.0395             nan     0.1000    0.0080
##     60        1.4605             nan     0.1000   -0.0029
##     80        1.1344             nan     0.1000   -0.0025
##    100        0.9495             nan     0.1000   -0.0087
##    120        0.8562             nan     0.1000   -0.0037
##    140        0.7855             nan     0.1000   -0.0043
##    160        0.7298             nan     0.1000   -0.0057
##    180        0.6813             nan     0.1000   -0.0010
##    200        0.6441             nan     0.1000   -0.0027
##    220        0.6118             nan     0.1000   -0.0040
##    240        0.5838             nan     0.1000   -0.0071
##    250        0.5734             nan     0.1000   -0.0007
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.4922             nan     0.1000    0.6088
##      2        6.9029             nan     0.1000    0.5644
##      3        6.4669             nan     0.1000    0.4526
##      4        5.9980             nan     0.1000    0.4160
##      5        5.5505             nan     0.1000    0.2603
##      6        5.2643             nan     0.1000    0.2640
##      7        5.0169             nan     0.1000    0.1944
##      8        4.8024             nan     0.1000    0.1732
```

```
##      9        4.5720             nan     0.1000    0.1124
##     10        4.3508             nan     0.1000    0.1700
##     20        2.8015             nan     0.1000    0.0839
##     40        1.5058             nan     0.1000    0.0041
##     60        1.0433             nan     0.1000   -0.0028
##     80        0.8409             nan     0.1000   -0.0038
##    100        0.7262             nan     0.1000   -0.0091
##    120        0.6504             nan     0.1000   -0.0011
##    140        0.5944             nan     0.1000   -0.0082
##    160        0.5390             nan     0.1000   -0.0053
##    180        0.5004             nan     0.1000   -0.0058
##    200        0.4655             nan     0.1000   -0.0034
##    220        0.4306             nan     0.1000   -0.0051
##    240        0.4014             nan     0.1000   -0.0052
##    250        0.3922             nan     0.1000   -0.0045
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.5384             nan     0.1000    0.6216
##      2        6.8492             nan     0.1000    0.5668
##      3        6.2425             nan     0.1000    0.4236
##      4        5.7761             nan     0.1000    0.4459
##      5        5.3374             nan     0.1000    0.3815
##      6        5.0229             nan     0.1000    0.2852
##      7        4.7392             nan     0.1000    0.2818
##      8        4.4323             nan     0.1000    0.1682
##      9        4.2010             nan     0.1000    0.2173
##     10        3.9190             nan     0.1000    0.1539
##     20        2.3973             nan     0.1000    0.0126
##     40        1.2163             nan     0.1000    0.0078
##     60        0.8634             nan     0.1000   -0.0088
##     80        0.7010             nan     0.1000   -0.0174
##    100        0.6125             nan     0.1000   -0.0047
##    120        0.5409             nan     0.1000   -0.0043
##    140        0.4880             nan     0.1000   -0.0087
##    160        0.4416             nan     0.1000   -0.0077
##    180        0.4022             nan     0.1000   -0.0087
##    200        0.3700             nan     0.1000   -0.0066
##    220        0.3326             nan     0.1000   -0.0048
##    240        0.3010             nan     0.1000   -0.0020
##    250        0.2897             nan     0.1000   -0.0057
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.4641             nan     0.1000    0.6228
##      2        6.7842             nan     0.1000    0.6612
##      3        6.2574             nan     0.1000    0.5100
##      4        5.6693             nan     0.1000    0.5417
```

```
##      5        5.2506             nan     0.1000    0.3664
##      6        4.8195             nan     0.1000    0.3499
##      7        4.4803             nan     0.1000    0.2959
##      8        4.1807             nan     0.1000    0.1964
##      9        3.9058             nan     0.1000    0.1460
##     10        3.6831             nan     0.1000    0.1246
##     20        2.1373             nan     0.1000    0.0659
##     40        1.0923             nan     0.1000    0.0073
##     60        0.7575             nan     0.1000   -0.0129
##     80        0.6127             nan     0.1000   -0.0132
##    100        0.5130             nan     0.1000   -0.0123
##    120        0.4313             nan     0.1000   -0.0060
##    140        0.3732             nan     0.1000   -0.0102
##    160        0.3229             nan     0.1000   -0.0040
##    180        0.2862             nan     0.1000   -0.0015
##    200        0.2556             nan     0.1000   -0.0035
##    220        0.2289             nan     0.1000   -0.0049
##    240        0.2066             nan     0.1000   -0.0024
##    250        0.1957             nan     0.1000   -0.0030
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        8.0133             nan     0.1000    0.2136
##      2        7.6170             nan     0.1000    0.3813
##      3        7.2757             nan     0.1000    0.3566
##      4        6.9741             nan     0.1000    0.2780
##      5        6.7490             nan     0.1000    0.2272
##      6        6.6030             nan     0.1000    0.0955
##      7        6.3914             nan     0.1000    0.1949
##      8        6.2217             nan     0.1000    0.1345
##      9        6.0156             nan     0.1000    0.1629
##     10        5.8483             nan     0.1000    0.1217
##     20        4.7672             nan     0.1000    0.0084
##     40        3.5325             nan     0.1000    0.0072
##     60        2.7373             nan     0.1000    0.0204
##     80        2.2393             nan     0.1000    0.0177
##    100        1.8533             nan     0.1000   -0.0056
##    120        1.5588             nan     0.1000   -0.0006
##    140        1.3684             nan     0.1000   -0.0059
##    160        1.2137             nan     0.1000   -0.0029
##    180        1.0929             nan     0.1000    0.0053
##    200        1.0225             nan     0.1000   -0.0018
##    220        0.9612             nan     0.1000   -0.0014
##    240        0.9268             nan     0.1000   -0.0089
##    250        0.9073             nan     0.1000   -0.0005
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
```

```
##      1         7.6769             nan     0.1000    0.4910
##      2         7.1336             nan     0.1000    0.4624
##      3         6.7130             nan     0.1000    0.3977
##      4         6.3914             nan     0.1000    0.2512
##      5         6.0813             nan     0.1000    0.3267
##      6         5.8205             nan     0.1000    0.1912
##      7         5.5575             nan     0.1000    0.1760
##      8         5.3300             nan     0.1000    0.1566
##      9         5.1406             nan     0.1000    0.0895
##     10         4.9999             nan     0.1000    0.0993
##     20         3.4990             nan     0.1000    0.1416
##     40         2.1301             nan     0.1000    0.0205
##     60         1.4553             nan     0.1000   -0.0010
##     80         1.1386             nan     0.1000   -0.0129
##    100         0.9532             nan     0.1000   -0.0062
##    120         0.8461             nan     0.1000   -0.0020
##    140         0.7941             nan     0.1000   -0.0103
##    160         0.7479             nan     0.1000   -0.0069
##    180         0.7076             nan     0.1000   -0.0046
##    200         0.6764             nan     0.1000   -0.0034
##    220         0.6375             nan     0.1000   -0.0039
##    240         0.6118             nan     0.1000   -0.0084
##    250         0.5967             nan     0.1000   -0.0038
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1         7.5573             nan     0.1000    0.6889
##      2         6.9522             nan     0.1000    0.5641
##      3         6.4789             nan     0.1000    0.3647
##      4         6.1178             nan     0.1000    0.1990
##      5         5.7289             nan     0.1000    0.3137
##      6         5.4295             nan     0.1000    0.1935
##      7         5.0791             nan     0.1000    0.2922
##      8         4.8212             nan     0.1000    0.2147
##      9         4.5435             nan     0.1000    0.1970
##     10         4.3324             nan     0.1000    0.1800
##     20         2.8598             nan     0.1000    0.0779
##     40         1.5947             nan     0.1000    0.0099
##     60         1.0802             nan     0.1000   -0.0061
##     80         0.8896             nan     0.1000   -0.0082
##    100         0.7621             nan     0.1000   -0.0069
##    120         0.6690             nan     0.1000   -0.0080
##    140         0.6158             nan     0.1000   -0.0050
##    160         0.5707             nan     0.1000   -0.0019
##    180         0.5336             nan     0.1000   -0.0046
##    200         0.4984             nan     0.1000   -0.0062
##    220         0.4607             nan     0.1000   -0.0045
```

```
##    240        0.4323             nan     0.1000   -0.0052
##    250        0.4196             nan     0.1000   -0.0041
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.4906             nan     0.1000    0.6789
##      2        6.9506             nan     0.1000    0.3624
##      3        6.3953             nan     0.1000    0.4020
##      4        5.9823             nan     0.1000    0.3891
##      5        5.5966             nan     0.1000    0.2061
##      6        5.1879             nan     0.1000    0.2865
##      7        4.8319             nan     0.1000    0.2808
##      8        4.5432             nan     0.1000    0.2153
##      9        4.2635             nan     0.1000    0.2355
##     10        3.9960             nan     0.1000    0.1091
##     20        2.4108             nan     0.1000    0.1056
##     40        1.2650             nan     0.1000    0.0002
##     60        0.8721             nan     0.1000    0.0013
##     80        0.6979             nan     0.1000   -0.0035
##    100        0.5984             nan     0.1000   -0.0062
##    120        0.5296             nan     0.1000   -0.0059
##    140        0.4772             nan     0.1000   -0.0068
##    160        0.4300             nan     0.1000   -0.0125
##    180        0.3866             nan     0.1000   -0.0057
##    200        0.3463             nan     0.1000   -0.0064
##    220        0.3136             nan     0.1000   -0.0027
##    240        0.2853             nan     0.1000   -0.0041
##    250        0.2719             nan     0.1000   -0.0052
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.4823             nan     0.1000    0.6726
##      2        6.8225             nan     0.1000    0.6054
##      3        6.2303             nan     0.1000    0.4431
##      4        5.7262             nan     0.1000    0.3136
##      5        5.2917             nan     0.1000    0.3020
##      6        4.9481             nan     0.1000    0.2905
##      7        4.5620             nan     0.1000    0.2910
##      8        4.3225             nan     0.1000    0.1791
##      9        4.0699             nan     0.1000    0.2349
##     10        3.8179             nan     0.1000    0.1849
##     20        2.3059             nan     0.1000    0.0418
##     40        1.1688             nan     0.1000   -0.0035
##     60        0.7851             nan     0.1000    0.0072
##     80        0.6170             nan     0.1000   -0.0038
##    100        0.5177             nan     0.1000   -0.0026
##    120        0.4381             nan     0.1000   -0.0056
##    140        0.3801             nan     0.1000   -0.0035
```

```
##    160        0.3340             nan     0.1000   -0.0031
##    180        0.2933             nan     0.1000   -0.0080
##    200        0.2558             nan     0.1000   -0.0058
##    220        0.2289             nan     0.1000   -0.0028
##    240        0.2021             nan     0.1000   -0.0050
##    250        0.1882             nan     0.1000   -0.0018
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.4102             nan     0.1000    0.3839
##      2        7.0494             nan     0.1000    0.3040
##      3        6.8614             nan     0.1000    0.1707
##      4        6.6267             nan     0.1000    0.2365
##      5        6.4159             nan     0.1000    0.2192
##      6        6.2072             nan     0.1000    0.1818
##      7        5.9995             nan     0.1000    0.1441
##      8        5.8238             nan     0.1000    0.1470
##      9        5.6784             nan     0.1000    0.0881
##     10        5.5111             nan     0.1000    0.1191
##     20        4.4453             nan     0.1000    0.0629
##     40        3.2797             nan     0.1000    0.0303
##     60        2.5893             nan     0.1000    0.0080
##     80        2.1025             nan     0.1000   -0.0054
##    100        1.7328             nan     0.1000    0.0016
##    120        1.5056             nan     0.1000    0.0039
##    140        1.3304             nan     0.1000   -0.0021
##    160        1.2081             nan     0.1000   -0.0085
##    180        1.1043             nan     0.1000    0.0002
##    200        1.0182             nan     0.1000    0.0011
##    220        0.9519             nan     0.1000   -0.0138
##    240        0.9161             nan     0.1000   -0.0036
##    250        0.9019             nan     0.1000   -0.0080
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.3296             nan     0.1000    0.5238
##      2        6.8236             nan     0.1000    0.4935
##      3        6.4024             nan     0.1000    0.3814
##      4        6.0460             nan     0.1000    0.3352
##      5        5.7799             nan     0.1000    0.2079
##      6        5.5073             nan     0.1000    0.2249
##      7        5.2509             nan     0.1000    0.1626
##      8        5.0841             nan     0.1000    0.0927
##      9        4.8799             nan     0.1000    0.1436
##     10        4.7477             nan     0.1000    0.0329
##     20        3.3287             nan     0.1000    0.0705
##     40        2.0283             nan     0.1000    0.0048
##     60        1.3816             nan     0.1000    0.0072
```

```
##     80        1.0728             nan     0.1000   -0.0016
##    100        0.9094             nan     0.1000    0.0076
##    120        0.8114             nan     0.1000   -0.0058
##    140        0.7446             nan     0.1000   -0.0069
##    160        0.7042             nan     0.1000   -0.0008
##    180        0.6679             nan     0.1000   -0.0038
##    200        0.6315             nan     0.1000   -0.0026
##    220        0.6063             nan     0.1000   -0.0076
##    240        0.5797             nan     0.1000   -0.0034
##    250        0.5662             nan     0.1000   -0.0046
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.2648             nan     0.1000    0.6118
##      2        6.7163             nan     0.1000    0.5338
##      3        6.2474             nan     0.1000    0.4288
##      4        5.8703             nan     0.1000    0.2640
##      5        5.5532             nan     0.1000    0.3193
##      6        5.2463             nan     0.1000    0.3198
##      7        4.9416             nan     0.1000    0.1943
##      8        4.6990             nan     0.1000    0.1722
##      9        4.4949             nan     0.1000    0.1469
##     10        4.2995             nan     0.1000    0.1804
##     20        2.7721             nan     0.1000    0.0861
##     40        1.4803             nan     0.1000    0.0123
##     60        1.0423             nan     0.1000   -0.0095
##     80        0.8424             nan     0.1000    0.0072
##    100        0.7137             nan     0.1000   -0.0079
##    120        0.6440             nan     0.1000   -0.0074
##    140        0.5827             nan     0.1000   -0.0044
##    160        0.5432             nan     0.1000   -0.0097
##    180        0.5079             nan     0.1000   -0.0044
##    200        0.4749             nan     0.1000   -0.0006
##    220        0.4448             nan     0.1000   -0.0068
##    240        0.4197             nan     0.1000   -0.0041
##    250        0.4073             nan     0.1000   -0.0040
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.1301             nan     0.1000    0.6518
##      2        6.4611             nan     0.1000    0.5540
##      3        5.8979             nan     0.1000    0.4264
##      4        5.4531             nan     0.1000    0.3997
##      5        5.0649             nan     0.1000    0.2551
##      6        4.7495             nan     0.1000    0.2099
##      7        4.4799             nan     0.1000    0.2317
##      8        4.1899             nan     0.1000    0.2269
##      9        4.0084             nan     0.1000    0.0679
```

```
##     10        3.8183             nan     0.1000    0.0965
##     20        2.3118             nan     0.1000    0.0409
##     40        1.2467             nan     0.1000    0.0054
##     60        0.8880             nan     0.1000   -0.0007
##     80        0.7226             nan     0.1000   -0.0048
##    100        0.6209             nan     0.1000   -0.0051
##    120        0.5444             nan     0.1000   -0.0087
##    140        0.4935             nan     0.1000   -0.0049
##    160        0.4445             nan     0.1000   -0.0053
##    180        0.3989             nan     0.1000   -0.0063
##    200        0.3638             nan     0.1000   -0.0079
##    220        0.3337             nan     0.1000   -0.0052
##    240        0.3055             nan     0.1000   -0.0048
##    250        0.2926             nan     0.1000   -0.0020
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.1126             nan     0.1000    0.7800
##      2        6.4349             nan     0.1000    0.5736
##      3        5.8711             nan     0.1000    0.5557
##      4        5.4355             nan     0.1000    0.3727
##      5        5.0058             nan     0.1000    0.2490
##      6        4.5813             nan     0.1000    0.2892
##      7        4.2200             nan     0.1000    0.3013
##      8        3.8990             nan     0.1000    0.2893
##      9        3.6677             nan     0.1000    0.1964
##     10        3.4290             nan     0.1000    0.1762
##     20        2.1135             nan     0.1000    0.0418
##     40        1.0761             nan     0.1000   -0.0015
##     60        0.7465             nan     0.1000   -0.0119
##     80        0.6002             nan     0.1000   -0.0082
##    100        0.4915             nan     0.1000   -0.0042
##    120        0.4217             nan     0.1000   -0.0055
##    140        0.3558             nan     0.1000   -0.0027
##    160        0.3103             nan     0.1000   -0.0039
##    180        0.2649             nan     0.1000   -0.0052
##    200        0.2323             nan     0.1000   -0.0017
##    220        0.2076             nan     0.1000   -0.0018
##    240        0.1858             nan     0.1000   -0.0025
##    250        0.1740             nan     0.1000   -0.0033
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.3456             nan     0.1000    0.2909
##      2        7.1114             nan     0.1000    0.1263
##      3        6.7570             nan     0.1000    0.2751
##      4        6.5482             nan     0.1000    0.1337
##      5        6.3257             nan     0.1000    0.2345
```

```
##      6        6.1206             nan     0.1000    0.1383
##      7        5.9301             nan     0.1000    0.1914
##      8        5.7797             nan     0.1000    0.1295
##      9        5.6019             nan     0.1000    0.1135
##     10        5.4685             nan     0.1000    0.0847
##     20        4.4722             nan     0.1000    0.0460
##     40        3.3338             nan     0.1000    0.0101
##     60        2.6477             nan     0.1000    0.0048
##     80        2.1648             nan     0.1000    0.0153
##    100        1.7916             nan     0.1000   -0.0011
##    120        1.5267             nan     0.1000    0.0018
##    140        1.3281             nan     0.1000   -0.0029
##    160        1.1995             nan     0.1000   -0.0011
##    180        1.1018             nan     0.1000    0.0001
##    200        1.0288             nan     0.1000   -0.0059
##    220        0.9667             nan     0.1000   -0.0033
##    240        0.9174             nan     0.1000   -0.0045
##    250        0.8974             nan     0.1000   -0.0025
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.1892             nan     0.1000    0.5473
##      2        6.7512             nan     0.1000    0.4586
##      3        6.4426             nan     0.1000    0.2760
##      4        6.1358             nan     0.1000    0.2140
##      5        5.8079             nan     0.1000    0.2639
##      6        5.5512             nan     0.1000    0.2127
##      7        5.3613             nan     0.1000    0.1317
##      8        5.0590             nan     0.1000    0.2354
##      9        4.9117             nan     0.1000    0.1361
##     10        4.7130             nan     0.1000    0.1626
##     20        3.4020             nan     0.1000    0.0257
##     40        2.0751             nan     0.1000    0.0224
##     60        1.4101             nan     0.1000   -0.0005
##     80        1.1014             nan     0.1000    0.0065
##    100        0.9405             nan     0.1000   -0.0067
##    120        0.8391             nan     0.1000   -0.0066
##    140        0.7718             nan     0.1000   -0.0054
##    160        0.7291             nan     0.1000   -0.0095
##    180        0.6810             nan     0.1000   -0.0036
##    200        0.6457             nan     0.1000   -0.0071
##    220        0.6189             nan     0.1000   -0.0034
##    240        0.5895             nan     0.1000   -0.0023
##    250        0.5794             nan     0.1000   -0.0084
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.1359             nan     0.1000    0.6309
```

```
##      2        6.5967             nan     0.1000    0.4591
##      3        6.1698             nan     0.1000    0.4132
##      4        5.7599             nan     0.1000    0.3928
##      5        5.4519             nan     0.1000    0.3237
##      6        5.1401             nan     0.1000    0.2872
##      7        4.9050             nan     0.1000    0.1392
##      8        4.6196             nan     0.1000    0.2846
##      9        4.3738             nan     0.1000    0.1828
##     10        4.1835             nan     0.1000    0.1700
##     20        2.8099             nan     0.1000    0.0580
##     40        1.6151             nan     0.1000   -0.0065
##     60        1.1301             nan     0.1000    0.0002
##     80        0.8944             nan     0.1000   -0.0077
##    100        0.7517             nan     0.1000   -0.0139
##    120        0.6730             nan     0.1000   -0.0085
##    140        0.6057             nan     0.1000   -0.0038
##    160        0.5547             nan     0.1000   -0.0097
##    180        0.5094             nan     0.1000   -0.0103
##    200        0.4766             nan     0.1000   -0.0066
##    220        0.4450             nan     0.1000   -0.0040
##    240        0.4151             nan     0.1000   -0.0027
##    250        0.4013             nan     0.1000   -0.0047
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.0294             nan     0.1000    0.7373
##      2        6.4316             nan     0.1000    0.6149
##      3        5.9113             nan     0.1000    0.3359
##      4        5.5546             nan     0.1000    0.3535
##      5        5.1917             nan     0.1000    0.2802
##      6        4.8371             nan     0.1000    0.3563
##      7        4.5468             nan     0.1000    0.2089
##      8        4.3248             nan     0.1000    0.1893
##      9        4.0651             nan     0.1000    0.1052
##     10        3.8138             nan     0.1000    0.1666
##     20        2.3320             nan     0.1000    0.0422
##     40        1.2332             nan     0.1000    0.0086
##     60        0.8464             nan     0.1000    0.0058
##     80        0.6737             nan     0.1000   -0.0128
##    100        0.5934             nan     0.1000   -0.0097
##    120        0.5242             nan     0.1000   -0.0050
##    140        0.4705             nan     0.1000   -0.0050
##    160        0.4233             nan     0.1000   -0.0078
##    180        0.3867             nan     0.1000   -0.0076
##    200        0.3531             nan     0.1000   -0.0040
##    220        0.3242             nan     0.1000   -0.0039
##    240        0.3013             nan     0.1000   -0.0036
```

```
##     250        0.2843             nan     0.1000   -0.0029
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.0098             nan     0.1000    0.5845
##      2        6.3343             nan     0.1000    0.4158
##      3        5.8514             nan     0.1000    0.3832
##      4        5.3437             nan     0.1000    0.4617
##      5        4.9793             nan     0.1000    0.3545
##      6        4.6111             nan     0.1000    0.3660
##      7        4.2957             nan     0.1000    0.2518
##      8        3.9570             nan     0.1000    0.2273
##      9        3.7320             nan     0.1000    0.1854
##     10        3.5140             nan     0.1000    0.1503
##     20        2.1057             nan     0.1000    0.0764
##     40        1.0592             nan     0.1000    0.0046
##     60        0.7323             nan     0.1000   -0.0010
##     80        0.5881             nan     0.1000   -0.0058
##    100        0.4956             nan     0.1000   -0.0051
##    120        0.4248             nan     0.1000   -0.0025
##    140        0.3718             nan     0.1000   -0.0073
##    160        0.3294             nan     0.1000   -0.0062
##    180        0.2819             nan     0.1000   -0.0026
##    200        0.2497             nan     0.1000   -0.0034
##    220        0.2233             nan     0.1000   -0.0058
##    240        0.1990             nan     0.1000   -0.0018
##    250        0.1871             nan     0.1000   -0.0021
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.5868             nan     0.1000    0.4115
##      2        7.2833             nan     0.1000    0.2331
##      3        7.0345             nan     0.1000    0.2570
##      4        6.8101             nan     0.1000    0.1071
##      5        6.5893             nan     0.1000    0.1563
##      6        6.3092             nan     0.1000    0.1664
##      7        6.1025             nan     0.1000    0.1476
##      8        5.9663             nan     0.1000    0.0749
##      9        5.7474             nan     0.1000    0.1445
##     10        5.5960             nan     0.1000    0.0876
##     20        4.4901             nan     0.1000    0.0532
##     40        3.2925             nan     0.1000    0.0364
##     60        2.6190             nan     0.1000    0.0090
##     80        2.1208             nan     0.1000    0.0132
##    100        1.7732             nan     0.1000   -0.0007
##    120        1.5132             nan     0.1000    0.0046
##    140        1.3283             nan     0.1000    0.0031
##    160        1.1925             nan     0.1000   -0.0002
```

```
##    180        1.0847             nan     0.1000   -0.0013
##    200        0.9981             nan     0.1000   -0.0003
##    220        0.9475             nan     0.1000   -0.0035
##    240        0.9021             nan     0.1000   -0.0047
##    250        0.8843             nan     0.1000   -0.0029
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.3282             nan     0.1000    0.5172
##      2        6.9512             nan     0.1000    0.3872
##      3        6.5318             nan     0.1000    0.3539
##      4        6.1978             nan     0.1000    0.2757
##      5        5.9066             nan     0.1000    0.2460
##      6        5.6366             nan     0.1000    0.2517
##      7        5.3731             nan     0.1000    0.1878
##      8        5.1982             nan     0.1000    0.1405
##      9        5.0115             nan     0.1000    0.1659
##     10        4.8495             nan     0.1000    0.1095
##     20        3.3891             nan     0.1000    0.1033
##     40        2.0749             nan     0.1000    0.0310
##     60        1.4400             nan     0.1000    0.0118
##     80        1.1141             nan     0.1000    0.0030
##    100        0.9360             nan     0.1000    0.0034
##    120        0.8234             nan     0.1000   -0.0051
##    140        0.7648             nan     0.1000   -0.0025
##    160        0.7108             nan     0.1000   -0.0075
##    180        0.6698             nan     0.1000   -0.0052
##    200        0.6366             nan     0.1000   -0.0069
##    220        0.6020             nan     0.1000   -0.0060
##    240        0.5770             nan     0.1000   -0.0049
##    250        0.5640             nan     0.1000   -0.0035
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.2616             nan     0.1000    0.6773
##      2        6.8094             nan     0.1000    0.2167
##      3        6.3219             nan     0.1000    0.4713
##      4        5.9148             nan     0.1000    0.3566
##      5        5.5959             nan     0.1000    0.2337
##      6        5.2724             nan     0.1000    0.3200
##      7        4.9638             nan     0.1000    0.1900
##      8        4.7283             nan     0.1000    0.1678
##      9        4.5198             nan     0.1000    0.1260
##     10        4.3024             nan     0.1000    0.1451
##     20        2.7404             nan     0.1000    0.0379
##     40        1.5392             nan     0.1000   -0.0055
##     60        1.0399             nan     0.1000    0.0123
##     80        0.8192             nan     0.1000    0.0004
```

```
##    100        0.7016             nan     0.1000   -0.0083
##    120        0.6325             nan     0.1000   -0.0080
##    140        0.5744             nan     0.1000   -0.0063
##    160        0.5259             nan     0.1000   -0.0054
##    180        0.4819             nan     0.1000   -0.0111
##    200        0.4502             nan     0.1000   -0.0055
##    220        0.4164             nan     0.1000   -0.0031
##    240        0.3874             nan     0.1000   -0.0056
##    250        0.3749             nan     0.1000   -0.0012
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.4180             nan     0.1000    0.3827
##      2        6.7805             nan     0.1000    0.4994
##      3        6.2576             nan     0.1000    0.4550
##      4        5.8389             nan     0.1000    0.2288
##      5        5.4627             nan     0.1000    0.3687
##      6        5.1119             nan     0.1000    0.3303
##      7        4.7963             nan     0.1000    0.3248
##      8        4.5143             nan     0.1000    0.2401
##      9        4.2403             nan     0.1000    0.1986
##     10        4.0630             nan     0.1000    0.1325
##     20        2.4827             nan     0.1000    0.0652
##     40        1.2766             nan     0.1000    0.0153
##     60        0.8585             nan     0.1000   -0.0103
##     80        0.6931             nan     0.1000   -0.0009
##    100        0.5966             nan     0.1000   -0.0085
##    120        0.5283             nan     0.1000   -0.0111
##    140        0.4718             nan     0.1000   -0.0106
##    160        0.4263             nan     0.1000   -0.0058
##    180        0.3870             nan     0.1000   -0.0051
##    200        0.3533             nan     0.1000   -0.0027
##    220        0.3194             nan     0.1000   -0.0032
##    240        0.2922             nan     0.1000   -0.0019
##    250        0.2785             nan     0.1000   -0.0040
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.1462             nan     0.1000    0.6854
##      2        6.5338             nan     0.1000    0.3961
##      3        6.0020             nan     0.1000    0.4159
##      4        5.5196             nan     0.1000    0.3879
##      5        5.0940             nan     0.1000    0.3601
##      6        4.7927             nan     0.1000    0.2963
##      7        4.4249             nan     0.1000    0.2827
##      8        4.1084             nan     0.1000    0.2133
##      9        3.8253             nan     0.1000    0.1881
##     10        3.6343             nan     0.1000    0.1233
```

```
##     20        2.1522             nan     0.1000    0.0354
##     40        1.0580             nan     0.1000    0.0161
##     60        0.7191             nan     0.1000    0.0018
##     80        0.5670             nan     0.1000   -0.0057
##    100        0.4832             nan     0.1000   -0.0050
##    120        0.4124             nan     0.1000   -0.0054
##    140        0.3602             nan     0.1000   -0.0078
##    160        0.3179             nan     0.1000   -0.0036
##    180        0.2778             nan     0.1000   -0.0047
##    200        0.2450             nan     0.1000   -0.0059
##    220        0.2183             nan     0.1000   -0.0040
##    240        0.1929             nan     0.1000   -0.0048
##    250        0.1839             nan     0.1000   -0.0040
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.4540             nan     0.1000    0.3641
##      2        7.1373             nan     0.1000    0.3291
##      3        6.8416             nan     0.1000    0.2730
##      4        6.5864             nan     0.1000    0.1830
##      5        6.3867             nan     0.1000    0.1603
##      6        6.1413             nan     0.1000    0.2019
##      7        5.9610             nan     0.1000    0.1395
##      8        5.8194             nan     0.1000    0.1027
##      9        5.6546             nan     0.1000    0.0827
##     10        5.4631             nan     0.1000    0.0971
##     20        4.3922             nan     0.1000    0.0188
##     40        3.2426             nan     0.1000    0.0345
##     60        2.5668             nan     0.1000    0.0223
##     80        2.0713             nan     0.1000    0.0088
##    100        1.7438             nan     0.1000   -0.0065
##    120        1.4921             nan     0.1000    0.0043
##    140        1.3219             nan     0.1000    0.0085
##    160        1.1951             nan     0.1000    0.0011
##    180        1.1011             nan     0.1000   -0.0045
##    200        1.0331             nan     0.1000   -0.0013
##    220        0.9765             nan     0.1000   -0.0020
##    240        0.9362             nan     0.1000   -0.0053
##    250        0.9130             nan     0.1000    0.0009
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.2752             nan     0.1000    0.5651
##      2        6.7895             nan     0.1000    0.4457
##      3        6.4533             nan     0.1000    0.2484
##      4        6.1292             nan     0.1000    0.3299
##      5        5.8643             nan     0.1000    0.2757
##      6        5.6456             nan     0.1000    0.1455
```

```
##      7        5.3780             nan     0.1000    0.2465
##      8        5.1363             nan     0.1000    0.1833
##      9        4.9400             nan     0.1000    0.1011
##     10        4.7344             nan     0.1000    0.1801
##     20        3.2834             nan     0.1000    0.0459
##     40        2.0454             nan     0.1000    0.0186
##     60        1.4428             nan     0.1000    0.0008
##     80        1.0931             nan     0.1000    0.0050
##    100        0.9245             nan     0.1000   -0.0066
##    120        0.8152             nan     0.1000   -0.0040
##    140        0.7456             nan     0.1000   -0.0028
##    160        0.6979             nan     0.1000   -0.0052
##    180        0.6573             nan     0.1000   -0.0035
##    200        0.6239             nan     0.1000   -0.0037
##    220        0.5949             nan     0.1000   -0.0042
##    240        0.5695             nan     0.1000   -0.0039
##    250        0.5578             nan     0.1000   -0.0039
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.2004             nan     0.1000    0.5575
##      2        6.6875             nan     0.1000    0.5080
##      3        6.1988             nan     0.1000    0.4364
##      4        5.7727             nan     0.1000    0.3191
##      5        5.4082             nan     0.1000    0.3497
##      6        5.1722             nan     0.1000    0.1589
##      7        4.8592             nan     0.1000    0.1847
##      8        4.6133             nan     0.1000    0.2159
##      9        4.3824             nan     0.1000    0.2002
##     10        4.1895             nan     0.1000    0.1182
##     20        2.7390             nan     0.1000    0.0733
##     40        1.5162             nan     0.1000   -0.0008
##     60        1.0207             nan     0.1000    0.0026
##     80        0.8292             nan     0.1000   -0.0016
##    100        0.7057             nan     0.1000   -0.0089
##    120        0.6346             nan     0.1000   -0.0085
##    140        0.5675             nan     0.1000   -0.0056
##    160        0.5176             nan     0.1000   -0.0074
##    180        0.4752             nan     0.1000   -0.0050
##    200        0.4333             nan     0.1000   -0.0054
##    220        0.4032             nan     0.1000   -0.0070
##    240        0.3743             nan     0.1000   -0.0022
##    250        0.3642             nan     0.1000   -0.0062
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.1706             nan     0.1000    0.6334
##      2        6.5472             nan     0.1000    0.5452
```

```
##      3        5.9610             nan     0.1000    0.4332
##      4        5.5223             nan     0.1000    0.3950
##      5        5.1475             nan     0.1000    0.2716
##      6        4.8185             nan     0.1000    0.2069
##      7        4.5333             nan     0.1000    0.2125
##      8        4.2886             nan     0.1000    0.2125
##      9        4.0286             nan     0.1000    0.1507
##     10        3.8317             nan     0.1000    0.1457
##     20        2.3895             nan     0.1000    0.0665
##     40        1.2552             nan     0.1000    0.0223
##     60        0.8795             nan     0.1000    0.0039
##     80        0.7069             nan     0.1000   -0.0107
##    100        0.6120             nan     0.1000   -0.0067
##    120        0.5331             nan     0.1000   -0.0065
##    140        0.4731             nan     0.1000   -0.0091
##    160        0.4256             nan     0.1000   -0.0038
##    180        0.3789             nan     0.1000   -0.0053
##    200        0.3447             nan     0.1000   -0.0045
##    220        0.3123             nan     0.1000   -0.0067
##    240        0.2807             nan     0.1000   -0.0018
##    250        0.2696             nan     0.1000   -0.0060
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.1181             nan     0.1000    0.6333
##      2        6.4637             nan     0.1000    0.5209
##      3        5.8982             nan     0.1000    0.5202
##      4        5.4003             nan     0.1000    0.3026
##      5        4.9882             nan     0.1000    0.2926
##      6        4.6393             nan     0.1000    0.2601
##      7        4.3294             nan     0.1000    0.2207
##      8        4.0488             nan     0.1000    0.2276
##      9        3.7542             nan     0.1000    0.2489
##     10        3.5442             nan     0.1000    0.1313
##     20        2.0640             nan     0.1000    0.0561
##     40        1.0503             nan     0.1000    0.0116
##     60        0.7338             nan     0.1000   -0.0011
##     80        0.5913             nan     0.1000   -0.0046
##    100        0.4891             nan     0.1000   -0.0047
##    120        0.4050             nan     0.1000   -0.0044
##    140        0.3428             nan     0.1000   -0.0083
##    160        0.2935             nan     0.1000   -0.0027
##    180        0.2561             nan     0.1000    0.0005
##    200        0.2280             nan     0.1000   -0.0051
##    220        0.1969             nan     0.1000   -0.0034
##    240        0.1764             nan     0.1000   -0.0047
##    250        0.1670             nan     0.1000   -0.0035
```

```
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.9913             nan     0.1000    0.3761
##      2        7.7852             nan     0.1000    0.1808
##      3        7.4353             nan     0.1000    0.3342
##      4        7.2002             nan     0.1000    0.1743
##      5        6.8764             nan     0.1000    0.3014
##      6        6.7249             nan     0.1000    0.1377
##      7        6.5608             nan     0.1000    0.0969
##      8        6.3857             nan     0.1000    0.1119
##      9        6.2081             nan     0.1000    0.2099
##     10        6.0676             nan     0.1000    0.0350
##     20        4.8481             nan     0.1000    0.0326
##     40        3.5311             nan     0.1000    0.0243
##     60        2.7637             nan     0.1000   -0.0042
##     80        2.2298             nan     0.1000    0.0035
##    100        1.8541             nan     0.1000    0.0040
##    120        1.5720             nan     0.1000   -0.0142
##    140        1.3723             nan     0.1000    0.0089
##    160        1.2296             nan     0.1000   -0.0073
##    180        1.1206             nan     0.1000   -0.0095
##    200        1.0353             nan     0.1000   -0.0009
##    220        0.9629             nan     0.1000   -0.0014
##    240        0.9290             nan     0.1000   -0.0011
##    250        0.9156             nan     0.1000   -0.0036
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.7709             nan     0.1000    0.4607
##      2        7.2930             nan     0.1000    0.4519
##      3        6.7154             nan     0.1000    0.2983
##      4        6.4052             nan     0.1000    0.2385
##      5        6.0937             nan     0.1000    0.2545
##      6        5.7996             nan     0.1000    0.2344
##      7        5.6159             nan     0.1000    0.1053
##      8        5.4356             nan     0.1000    0.1415
##      9        5.2146             nan     0.1000    0.1220
##     10        5.0671             nan     0.1000    0.1222
##     20        3.5111             nan     0.1000    0.0306
##     40        2.0860             nan     0.1000    0.0249
##     60        1.4474             nan     0.1000    0.0088
##     80        1.1308             nan     0.1000   -0.0062
##    100        0.9648             nan     0.1000    0.0020
##    120        0.8736             nan     0.1000   -0.0089
##    140        0.8043             nan     0.1000   -0.0064
##    160        0.7498             nan     0.1000   -0.0083
##    180        0.7018             nan     0.1000    0.0001
```

```
##    200        0.6598             nan     0.1000   -0.0037
##    220        0.6329             nan     0.1000   -0.0035
##    240        0.6049             nan     0.1000   -0.0068
##    250        0.5905             nan     0.1000   -0.0046
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.5947             nan     0.1000    0.5713
##      2        6.9919             nan     0.1000    0.5903
##      3        6.5417             nan     0.1000    0.4225
##      4        6.0968             nan     0.1000    0.3213
##      5        5.7124             nan     0.1000    0.3371
##      6        5.3694             nan     0.1000    0.2772
##      7        5.0464             nan     0.1000    0.2062
##      8        4.7692             nan     0.1000    0.2608
##      9        4.6153             nan     0.1000    0.0811
##     10        4.4195             nan     0.1000    0.0977
##     20        2.9502             nan     0.1000    0.1132
##     40        1.5511             nan     0.1000    0.0204
##     60        1.0570             nan     0.1000    0.0142
##     80        0.8503             nan     0.1000   -0.0047
##    100        0.7300             nan     0.1000   -0.0177
##    120        0.6452             nan     0.1000   -0.0077
##    140        0.5915             nan     0.1000   -0.0082
##    160        0.5400             nan     0.1000   -0.0058
##    180        0.5009             nan     0.1000   -0.0040
##    200        0.4669             nan     0.1000   -0.0059
##    220        0.4400             nan     0.1000   -0.0040
##    240        0.4131             nan     0.1000   -0.0079
##    250        0.4039             nan     0.1000   -0.0059
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.6580             nan     0.1000    0.6541
##      2        7.0177             nan     0.1000    0.5653
##      3        6.4657             nan     0.1000    0.5278
##      4        5.9869             nan     0.1000    0.4523
##      5        5.5715             nan     0.1000    0.3559
##      6        5.1874             nan     0.1000    0.2871
##      7        4.8558             nan     0.1000    0.2317
##      8        4.5402             nan     0.1000    0.2236
##      9        4.3011             nan     0.1000    0.1610
##     10        4.0022             nan     0.1000    0.2235
##     20        2.4352             nan     0.1000    0.0364
##     40        1.2432             nan     0.1000    0.0032
##     60        0.8629             nan     0.1000   -0.0036
##     80        0.7137             nan     0.1000   -0.0020
##    100        0.6171             nan     0.1000   -0.0102
```

```
##    120        0.5389             nan     0.1000   -0.0066
##    140        0.4772             nan     0.1000   -0.0067
##    160        0.4290             nan     0.1000   -0.0091
##    180        0.3873             nan     0.1000   -0.0116
##    200        0.3411             nan     0.1000   -0.0052
##    220        0.3122             nan     0.1000   -0.0030
##    240        0.2868             nan     0.1000   -0.0020
##    250        0.2726             nan     0.1000   -0.0027
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.4799             nan     0.1000    0.8543
##      2        6.8255             nan     0.1000    0.5990
##      3        6.2454             nan     0.1000    0.4987
##      4        5.7558             nan     0.1000    0.3832
##      5        5.3790             nan     0.1000    0.3350
##      6        5.0578             nan     0.1000    0.2406
##      7        4.7324             nan     0.1000    0.1941
##      8        4.3901             nan     0.1000    0.2642
##      9        4.0528             nan     0.1000    0.2389
##     10        3.7874             nan     0.1000    0.2426
##     20        2.1952             nan     0.1000    0.0768
##     40        1.1025             nan     0.1000   -0.0081
##     60        0.7689             nan     0.1000   -0.0002
##     80        0.6122             nan     0.1000   -0.0061
##    100        0.5200             nan     0.1000   -0.0109
##    120        0.4400             nan     0.1000   -0.0069
##    140        0.3837             nan     0.1000   -0.0055
##    160        0.3328             nan     0.1000   -0.0034
##    180        0.2920             nan     0.1000   -0.0077
##    200        0.2544             nan     0.1000   -0.0035
##    220        0.2241             nan     0.1000   -0.0036
##    240        0.1988             nan     0.1000   -0.0047
##    250        0.1865             nan     0.1000   -0.0028
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.2748             nan     0.1000    0.3849
##      2        6.9549             nan     0.1000    0.3086
##      3        6.6188             nan     0.1000    0.2131
##      4        6.3662             nan     0.1000    0.2414
##      5        6.1655             nan     0.1000    0.1744
##      6        5.9621             nan     0.1000    0.1800
##      7        5.7756             nan     0.1000    0.1729
##      8        5.6347             nan     0.1000    0.1348
##      9        5.5429             nan     0.1000    0.0634
##     10        5.3761             nan     0.1000    0.0928
##     20        4.3688             nan     0.1000    0.0591
```

```
##     40        3.2068             nan     0.1000    0.0402
##     60        2.5475             nan     0.1000    0.0114
##     80        2.0354             nan     0.1000    0.0023
##    100        1.7011             nan     0.1000   -0.0072
##    120        1.4362             nan     0.1000   -0.0015
##    140        1.2570             nan     0.1000   -0.0034
##    160        1.1369             nan     0.1000    0.0021
##    180        1.0223             nan     0.1000   -0.0062
##    200        0.9563             nan     0.1000   -0.0038
##    220        0.8991             nan     0.1000   -0.0058
##    240        0.8598             nan     0.1000   -0.0059
##    250        0.8460             nan     0.1000   -0.0086
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.1432             nan     0.1000    0.5851
##      2        6.7241             nan     0.1000    0.4090
##      3        6.2802             nan     0.1000    0.3640
##      4        5.9965             nan     0.1000    0.1559
##      5        5.7218             nan     0.1000    0.2864
##      6        5.4669             nan     0.1000    0.2326
##      7        5.1666             nan     0.1000    0.2190
##      8        4.9344             nan     0.1000    0.2265
##      9        4.7538             nan     0.1000    0.1466
##     10        4.5570             nan     0.1000    0.1311
##     20        3.2524             nan     0.1000    0.1132
##     40        1.9609             nan     0.1000    0.0491
##     60        1.3733             nan     0.1000   -0.0028
##     80        1.0764             nan     0.1000   -0.0083
##    100        0.8912             nan     0.1000   -0.0043
##    120        0.7917             nan     0.1000   -0.0084
##    140        0.7298             nan     0.1000   -0.0027
##    160        0.6894             nan     0.1000   -0.0061
##    180        0.6543             nan     0.1000   -0.0077
##    200        0.6175             nan     0.1000   -0.0009
##    220        0.5885             nan     0.1000   -0.0089
##    240        0.5540             nan     0.1000   -0.0036
##    250        0.5386             nan     0.1000   -0.0019
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.0286             nan     0.1000    0.5874
##      2        6.5422             nan     0.1000    0.4614
##      3        6.0807             nan     0.1000    0.4788
##      4        5.6220             nan     0.1000    0.3139
##      5        5.3339             nan     0.1000    0.1849
##      6        4.9990             nan     0.1000    0.2584
##      7        4.7023             nan     0.1000    0.2324
```

```
##      8        4.4521             nan     0.1000    0.2002
##      9        4.2254             nan     0.1000    0.1721
##     10        4.0158             nan     0.1000    0.1061
##     20        2.5603             nan     0.1000    0.0649
##     40        1.4633             nan     0.1000    0.0221
##     60        1.0126             nan     0.1000    0.0040
##     80        0.8089             nan     0.1000   -0.0011
##    100        0.6913             nan     0.1000   -0.0016
##    120        0.6212             nan     0.1000   -0.0039
##    140        0.5555             nan     0.1000    0.0013
##    160        0.5178             nan     0.1000   -0.0070
##    180        0.4779             nan     0.1000   -0.0062
##    200        0.4357             nan     0.1000   -0.0056
##    220        0.4076             nan     0.1000   -0.0034
##    240        0.3838             nan     0.1000   -0.0051
##    250        0.3724             nan     0.1000   -0.0045
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.0052             nan     0.1000    0.7357
##      2        6.3136             nan     0.1000    0.6391
##      3        5.8579             nan     0.1000    0.3395
##      4        5.4261             nan     0.1000    0.4118
##      5        5.0380             nan     0.1000    0.2541
##      6        4.7502             nan     0.1000    0.2364
##      7        4.5107             nan     0.1000    0.1393
##      8        4.2559             nan     0.1000    0.2325
##      9        4.0139             nan     0.1000    0.1431
##     10        3.7788             nan     0.1000    0.1690
##     20        2.2976             nan     0.1000    0.0670
##     40        1.1641             nan     0.1000    0.0258
##     60        0.7945             nan     0.1000   -0.0042
##     80        0.6385             nan     0.1000   -0.0010
##    100        0.5468             nan     0.1000   -0.0065
##    120        0.4711             nan     0.1000   -0.0070
##    140        0.4186             nan     0.1000   -0.0051
##    160        0.3792             nan     0.1000   -0.0062
##    180        0.3426             nan     0.1000   -0.0072
##    200        0.3149             nan     0.1000   -0.0066
##    220        0.2897             nan     0.1000   -0.0081
##    240        0.2642             nan     0.1000   -0.0020
##    250        0.2526             nan     0.1000   -0.0020
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.0074             nan     0.1000    0.6779
##      2        6.3049             nan     0.1000    0.6277
##      3        5.7428             nan     0.1000    0.5037
```

```
##      4        5.3843             nan     0.1000    0.2738
##      5        4.9412             nan     0.1000    0.4013
##      6        4.5370             nan     0.1000    0.2175
##      7        4.2296             nan     0.1000    0.2194
##      8        3.9306             nan     0.1000    0.2566
##      9        3.6976             nan     0.1000    0.1642
##     10        3.4742             nan     0.1000    0.1155
##     20        2.0717             nan     0.1000    0.0554
##     40        1.0961             nan     0.1000    0.0158
##     60        0.7387             nan     0.1000   -0.0071
##     80        0.5947             nan     0.1000   -0.0086
##    100        0.4878             nan     0.1000   -0.0035
##    120        0.4191             nan     0.1000   -0.0069
##    140        0.3558             nan     0.1000   -0.0047
##    160        0.3193             nan     0.1000   -0.0029
##    180        0.2757             nan     0.1000   -0.0060
##    200        0.2412             nan     0.1000   -0.0011
##    220        0.2154             nan     0.1000   -0.0022
##    240        0.1911             nan     0.1000   -0.0019
##    250        0.1798             nan     0.1000   -0.0025
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.5373             nan     0.1000    0.3255
##      2        7.2302             nan     0.1000    0.3081
##      3        7.0287             nan     0.1000    0.0792
##      4        6.8235             nan     0.1000    0.1648
##      5        6.5846             nan     0.1000    0.2528
##      6        6.3572             nan     0.1000    0.2142
##      7        6.2170             nan     0.1000    0.0731
##      8        6.0241             nan     0.1000    0.1693
##      9        5.8911             nan     0.1000    0.1379
##     10        5.7890             nan     0.1000    0.0396
##     20        4.6672             nan     0.1000    0.0610
##     40        3.3823             nan     0.1000    0.0241
##     60        2.6081             nan     0.1000    0.0076
##     80        2.1083             nan     0.1000    0.0027
##    100        1.7823             nan     0.1000   -0.0038
##    120        1.5329             nan     0.1000    0.0083
##    140        1.3371             nan     0.1000   -0.0004
##    160        1.1999             nan     0.1000   -0.0035
##    180        1.0969             nan     0.1000   -0.0001
##    200        1.0178             nan     0.1000   -0.0020
##    220        0.9601             nan     0.1000   -0.0065
##    240        0.9259             nan     0.1000   -0.0059
##    250        0.9093             nan     0.1000   -0.0037
##
```

```
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.3367             nan     0.1000    0.5068
##      2        6.8403             nan     0.1000    0.4133
##      3        6.4575             nan     0.1000    0.3430
##      4        6.1040             nan     0.1000    0.2802
##      5        5.9071             nan     0.1000    0.1333
##      6        5.6534             nan     0.1000    0.2078
##      7        5.4050             nan     0.1000    0.2252
##      8        5.2113             nan     0.1000    0.1294
##      9        4.9828             nan     0.1000    0.1934
##     10        4.8171             nan     0.1000    0.1146
##     20        3.3732             nan     0.1000    0.0232
##     40        2.0529             nan     0.1000    0.0254
##     60        1.4630             nan     0.1000    0.0107
##     80        1.1301             nan     0.1000   -0.0184
##    100        0.9347             nan     0.1000   -0.0020
##    120        0.8346             nan     0.1000   -0.0053
##    140        0.7561             nan     0.1000   -0.0116
##    160        0.7038             nan     0.1000   -0.0083
##    180        0.6608             nan     0.1000   -0.0050
##    200        0.6231             nan     0.1000   -0.0062
##    220        0.5885             nan     0.1000   -0.0053
##    240        0.5666             nan     0.1000   -0.0073
##    250        0.5537             nan     0.1000   -0.0016
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.3914             nan     0.1000    0.5561
##      2        6.7379             nan     0.1000    0.5924
##      3        6.1931             nan     0.1000    0.3638
##      4        5.7353             nan     0.1000    0.2706
##      5        5.4272             nan     0.1000    0.2604
##      6        5.1269             nan     0.1000    0.1462
##      7        4.9406             nan     0.1000    0.0649
##      8        4.7122             nan     0.1000    0.1369
##      9        4.5181             nan     0.1000    0.1104
##     10        4.3030             nan     0.1000    0.1313
##     20        2.8485             nan     0.1000    0.0934
##     40        1.6130             nan     0.1000   -0.0081
##     60        1.1086             nan     0.1000   -0.0165
##     80        0.8744             nan     0.1000   -0.0020
##    100        0.7519             nan     0.1000   -0.0066
##    120        0.6638             nan     0.1000   -0.0039
##    140        0.5997             nan     0.1000   -0.0044
##    160        0.5553             nan     0.1000   -0.0082
##    180        0.5230             nan     0.1000   -0.0054
##    200        0.4907             nan     0.1000   -0.0056
```

```
##    220        0.4566             nan     0.1000   -0.0051
##    240        0.4234             nan     0.1000   -0.0047
##    250        0.4103             nan     0.1000   -0.0062
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.3959             nan     0.1000    0.5344
##      2        6.7840             nan     0.1000    0.6032
##      3        6.2042             nan     0.1000    0.5214
##      4        5.7561             nan     0.1000    0.3567
##      5        5.3542             nan     0.1000    0.3154
##      6        5.0748             nan     0.1000    0.2697
##      7        4.6856             nan     0.1000    0.3381
##      8        4.4209             nan     0.1000    0.2125
##      9        4.1834             nan     0.1000    0.1959
##     10        3.9558             nan     0.1000    0.1757
##     20        2.5107             nan     0.1000    0.0757
##     40        1.3385             nan     0.1000    0.0197
##     60        0.9193             nan     0.1000    0.0067
##     80        0.7247             nan     0.1000   -0.0105
##    100        0.6080             nan     0.1000   -0.0060
##    120        0.5370             nan     0.1000   -0.0086
##    140        0.4808             nan     0.1000   -0.0094
##    160        0.4331             nan     0.1000   -0.0018
##    180        0.3896             nan     0.1000   -0.0076
##    200        0.3487             nan     0.1000   -0.0060
##    220        0.3156             nan     0.1000   -0.0044
##    240        0.2857             nan     0.1000   -0.0023
##    250        0.2735             nan     0.1000   -0.0045
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.2002             nan     0.1000    0.7128
##      2        6.5508             nan     0.1000    0.5996
##      3        5.9803             nan     0.1000    0.5293
##      4        5.5269             nan     0.1000    0.4154
##      5        5.1301             nan     0.1000    0.3923
##      6        4.7897             nan     0.1000    0.2007
##      7        4.4224             nan     0.1000    0.2482
##      8        4.1528             nan     0.1000    0.1840
##      9        3.8740             nan     0.1000    0.1938
##     10        3.6367             nan     0.1000    0.1894
##     20        2.1725             nan     0.1000    0.0933
##     40        1.0934             nan     0.1000    0.0063
##     60        0.7734             nan     0.1000   -0.0003
##     80        0.6267             nan     0.1000   -0.0113
##    100        0.5248             nan     0.1000   -0.0115
##    120        0.4509             nan     0.1000   -0.0086
```

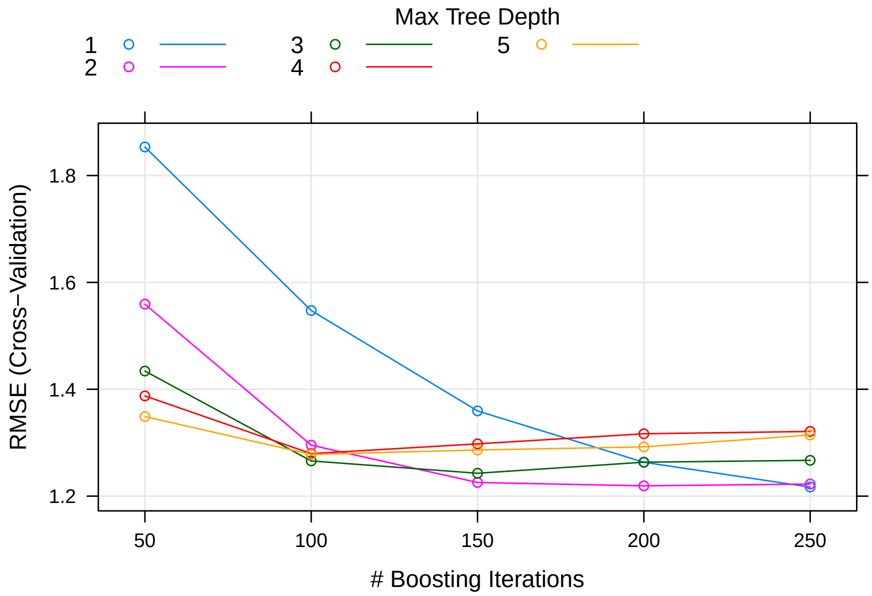
```
##    140        0.3909             nan     0.1000   -0.0042
##    160        0.3417             nan     0.1000   -0.0095
##    180        0.2979             nan     0.1000   -0.0010
##    200        0.2641             nan     0.1000   -0.0051
##    220        0.2324             nan     0.1000   -0.0048
##    240        0.2065             nan     0.1000   -0.0029
##    250        0.1944             nan     0.1000   -0.0033
##
## Iter   TrainDeviance   ValidDeviance   StepSize   Improve
##      1        7.5853             nan     0.1000    0.4622
##      2        7.2268             nan     0.1000    0.2276
##      3        6.9725             nan     0.1000    0.2317
##      4        6.7255             nan     0.1000    0.1945
##      5        6.5310             nan     0.1000    0.1967
##      6        6.3548             nan     0.1000    0.1452
##      7        6.1331             nan     0.1000    0.1877
##      8        6.0205             nan     0.1000    0.0816
##      9        5.8651             nan     0.1000    0.1151
##     10        5.7272             nan     0.1000    0.0983
##     20        4.5797             nan     0.1000    0.0457
##     40        3.3805             nan     0.1000    0.0281
##     60        2.6821             nan     0.1000   -0.0024
##     80        2.1887             nan     0.1000    0.0083
##    100        1.8328             nan     0.1000    0.0108
##    120        1.5572             nan     0.1000   -0.0039
##    140        1.3454             nan     0.1000    0.0011
##    160        1.2090             nan     0.1000   -0.0017
##    180        1.0998             nan     0.1000    0.0009
##    200        1.0155             nan     0.1000   -0.0061
##    220        0.9510             nan     0.1000   -0.0040
##    240        0.9159             nan     0.1000   -0.0058
##    250        0.8952             nan     0.1000   -0.0036
```

```
carseats.gbm
```

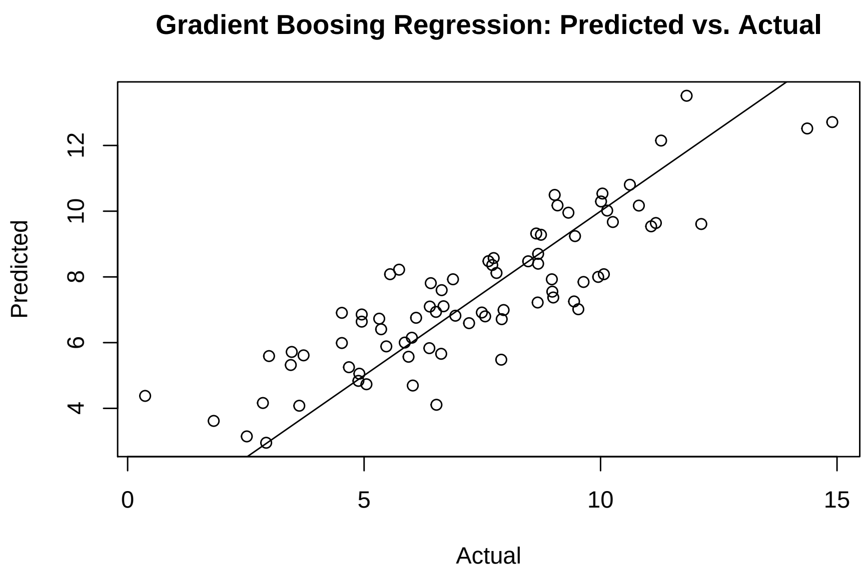
```
## Stochastic Gradient Boosting
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 289, 289, 289, 289, 289, 289, ...
## Resampling results across tuning parameters:
##
##   interaction.depth  n.trees  RMSE      Rsquared   MAE
##   1                   50      1.853439  0.6550573  1.4985804
##   1                  100      1.547356  0.7484921  1.2635775
```

```
##   1                   150      1.359464  0.7941783  1.1116649
##   1                   200      1.263360  0.8152576  1.0273078
##   1                   250      1.216972  0.8238354  0.9842987
##   2                    50      1.559349  0.7549692  1.2703898
##   2                   100      1.295349  0.8121515  1.0550231
##   2                   150      1.225522  0.8259530  0.9949898
##   2                   200      1.219263  0.8282347  0.9847772
##   2                   250      1.222610  0.8269006  0.9882843
##   3                    50      1.434103  0.7828979  1.1618345
##   3                   100      1.265869  0.8154077  1.0207212
##   3                   150      1.242808  0.8187860  0.9946575
##   3                   200      1.263512  0.8139170  1.0132197
##   3                   250      1.266998  0.8123660  1.0169904
##   4                    50      1.387541  0.7897254  1.1230060
##   4                   100      1.279528  0.8095927  1.0299009
##   4                   150      1.297827  0.8045587  1.0399179
##   4                   200      1.316687  0.7979882  1.0556691
##   4                   250      1.321038  0.7972775  1.0621347
##   5                    50      1.348922  0.7980728  1.0974910
##   5                   100      1.277990  0.8108521  1.0389748
##   5                   150      1.286355  0.8066147  1.0393349
##   5                   200      1.292184  0.8042104  1.0372671
##   5                   250      1.314433  0.7973539  1.0572041
##
## Tuning parameter 'shrinkage' was held constant at a value of 0.1
##
## Tuning parameter 'n.minobsinnode' was held constant at a value of 10
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were n.trees = 250, interaction.depth =
##  1, shrinkage = 0.1 and n.minobsinnode = 10.
```

```
plot(carseats.gbm)
```




```
carseats.pred <- predict(carseats.gbm, carseats_test, type = "raw")
plot(carseats_test$Sales, carseats.pred,
     main = "Gradient Boosing Regression: Predicted vs. Actual",
     xlab = "Actual",
     ylab = "Predicted")
abline(0,1)
```




```
(carseats.gbm.rmse <- RMSE(pred = carseats.pred,
                           obs = carseats_test$Sales))
```

```
## [1] 1.402428
```

```
rm(carseats.pred)

#plot(varImp(carseats.gbm), main="Variable Importance with Gradient Boosting")
```

9.6 Summary

Okay, I'm going to tally up the results! For the classification division, the winner is the manual classification tree! Gradient boosting made a valiant run at it, but came up just a little short.

```
rbind(data.frame(model = "Manual Class", Acc = round(oj_model_1b_cm$overall["Accuracy"]
      data.frame(model = "Class w.tuneGrid", Acc = round(oj_model_3_cm$overall["Accura
      data.frame(model = "Bagging", Acc = round(oj.bag.acc, 5)),
      data.frame(model = "Random Forest", Acc = round(oj.frst.acc, 5)),
      data.frame(model = "Gradient Boosting", Acc = round(oj.gbm.acc, 5))
) %>% arrange(desc(Acc))
```

```
##                model     Acc
## 1      Manual Class 0.85915
## 2 Gradient Boosting 0.85446
## 3  Class w.tuneGrid 0.84507
## 4           Bagging 0.82629
## 5     Random Forest 0.82629
```

And now for the regression division, the winnner is… gradient boosting!

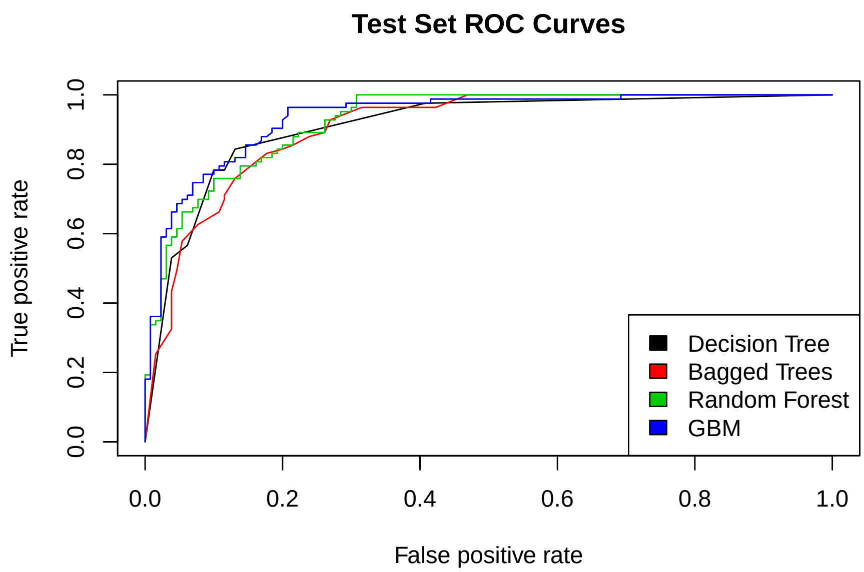
```
rbind(data.frame(model = "Manual ANOVA", RMSE = round(carseats_model_1_pruned_rmse, 5)),
      data.frame(model = "ANOVA w.tuneGrid", RMSE = round(carseats_model_3_pruned_rmse, 5)),
      data.frame(model = "Bagging", RMSE = round(carseats.bag.rmse, 5)),
      data.frame(model = "Random Forest", RMSE = round(carseats.frst.rmse, 5)),
      data.frame(model = "Gradient Boosting", RMSE = round(carseats.gbm.rmse, 5))
) %>% arrange(RMSE)
```

```
##                model    RMSE
## 1 Gradient Boosting 1.40243
## 2     Random Forest 1.75811
## 3           Bagging 1.93279
## 4  ANOVA w.tuneGrid 2.29833
## 5      Manual ANOVA 2.38806
```

Here are plots of the ROC curves for all the models (one from each chapter) on the same graph. The ROCR package provides the prediction() and performance() functions which generate the data required for plotting the ROC curve, given a set of predictions and actual (true) values. The more "up and to the left" the ROC curve of a model is, the better the model. The AUC performance metric is literally the "Area Under the ROC Curve", so the greater the area under this curve, the higher the AUC, and the better-performing the model is.

```
library(ROCR)
# List of predictions
oj.class.pred <- predict(oj_model_3, oj_test, type = "prob")[,2]
oj.bag.pred <- predict(oj.bag, oj_test, type = "prob")[,2]
oj.frst.pred <- predict(oj.frst, oj_test, type = "prob")[,2]
oj.gbm.pred <- predict(oj.gbm, oj_test, type = "prob")[,2]

preds_list <- list(oj.class.pred, oj.bag.pred, oj.frst.pred, oj.gbm.pred)
#preds_list <- list(oj.class.pred)

# List of actual values (same for all)
m <- length(preds_list)
actuals_list <- rep(list(oj_test$Purchase), m)
```

```
# Plot the ROC curves
pred <- prediction(preds_list, actuals_list)
#pred <- prediction(oj.class.pred[,2], oj_test$Purchase)
rocs <- performance(pred, "tpr", "fpr")
plot(rocs, col = as.list(1:m), main = "Test Set ROC Curves")
legend(x = "bottomright",
       legend = c("Decision Tree", "Bagged Trees", "Random Forest", "GBM"),
       fill = 1:m)
```



9.7 Reference

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Chapter 10

Support Vector Machines

These notes rely on (James et al., 2013), (Hastie et al., 2017), and (Kuhn and Johnson, 2016). I also reviewed the material in PSU's Applied Data Mining and Statistical Learning (STAT 508), and the *e1071* Support Vector Machines vignette.

The Support Vector Machines (SVM) algorithm finds the optimal separating hyperplane between members of two classes using an appropriate nonlinear mapping to a sufficiently high dimension. The hyperplane is defined by the observations that lie within a margin optimized by a cost hyperparameter. These observations are called the *support vectors*.

SVM is an extension of the *support vector classifier* which in turn is a generalization of the simple and intuitive *maximal margin classifier*.

10.1 Maximal Margin Classifier

The maximal margin classifier is the optimal hyperplane defined in the (rare) case where two classes are *linearly separable*. Given an $n \times p$ data matrix X with binary response variable defined as $y \in [-1, 1]$ it *may* be possible to define a p-dimensional hyperplane $h(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 \cdots + \beta_p X_p = x_i^T \beta + \beta_0 = 0$ such that all observations of each class fall on opposite sides of the hyperplane. This "separating hyperplane" has the property that if β is constrained to be a unit vector, $||\beta|| = \sum \beta^2 = 1$, then the product of the hyperplane and response variables are positive perpendicular distances from the hyperplane, the smallest of which may be termed the hyperplane *margin*, M,

$$y_i(x_i^{'} \beta + \beta_0) \geq M.$$

The maximal margin classifier is the hyperplane with the maximum margin. That is, $\max\{M\}$ subject to $||\beta|| = 1$. A separating hyperplane rarely exists. In fact, even if a separating hyperplane does exist, its resulting margin is probably undesirably narrow.

10.2 Support Vector Classifier

The maximal margin classifier can be generalized to non-separable cases using a so-called "soft margin". The generalization is called the *support vector classifier*. The soft margin allows some misclassification in the interest of greater robustness to individual observations. The support vector classifier optimizes

$$y_i(x_i^{'}\beta + \beta_0) \geq M(1 - \xi_i)$$

where the ξ_i are positive *slack variables* whose sum is bounded by some constant tuning parameter $\sum \xi_i \leq constant$. The slack variable values indicate where the observation lies: $\xi_i = 0$ observations lie on the correct side of the margin; $\xi_i > 0$ observation lie on the wrong side of the margin; $\xi_i > 1$ observations lie on the wrong side of the hyperplane. The constant sets the tolerance for margin violation. If $constant = 0$, then all observations must reside on the correct side of the margin, as in the maximal margin classifier. The *constant* controls the bias-variance trade-off. As the *constant* increases, the margin widens and allows more violations. The classifier bias increases but its variance decreases.

The support vector classifier is usually defined by dropping the $||\beta|| = 1$ constraint, and defining $M = 1/||\beta||$. The optimization problem then becomes

$$\min ||\beta|| \ \ s.t. \ \begin{cases} y_i(x_i^T\beta + \beta_0) \geq 1 - \xi_i, & \forall i \\ \xi_i \geq 0, \ \ \sum \xi_i \leq constant. \end{cases}$$

This is a quadratic equation with linear inequality constraints, so it is a convex optimization problem which can be solved using Lagrange multipliers. Re-express the optimization problem as

$$\min_{\beta_0,\beta} \frac{1}{2}||\beta||^2 = C \sum_{i=1}^{N} \xi_i s.t. \xi_i \geq 0, \ \ y_i(x_i^T\beta + \beta_0) \geq 1 - \xi_i, \ \ \forall i$$

where the "cost" parameter C replaces the constant and penalizes large residuals. This optimization problem is equivalent to *another* optimization problem, the familiar *loss + penalty* formulation:

$$\min_{\beta_0,\beta} \sum_{i=1}^{N} [1 - y_i f(x_i)]_+ + \frac{\lambda}{2}||\beta||^2$$

where $\lambda = 1/C$ and $[1 - y_i f(x_i)]_+$ is a "hinge" loss function with $f(x_i) = sign[Pr(Y = +1|x) - 1/2]$.
The parameter estimates can be written as functions of a set of unknown parameters (α_i) and data points. The solution to the optimization problem requires only the inner products of the observations, represented as $\langle x_i, x_j \rangle$,

$$f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle x, x_i \rangle$$

The solution has the interesting property that only observations on or within the margin affect the hyperplane. These observations are known as support vectors. As the constant increases, the number of violating observations increase, and thus the number of support vectors increases. This property makes the algorithm robust to the extreme observations far away from the hyperplane.

The parameter estimators for α_i are nonzero only for the support vectors in the solution—that is, if a training observation is not a support vector, then its α_i equals zero.

The only shortcoming with the algorithm is that it presumes a linear decision boundary.

10.3 Support Vector Machines

Enlarging the feature space of the support vector classifier accommodates nonlinar relationships. Support vector machines do this in a specific way, using *kernals*. The kernal is a generalization of the inner product with form $K(x_i, x_i^{'})$. So the linear kernal is simply

$$K(x_i, x_i^{'}) = \langle x, x_i \rangle$$

and the solution is

$$f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i K(x_i, x_i^{'})$$

K can take onother form instead, such as polynomial

$$K(x, x') = (\gamma \langle x, x' \rangle + c_0)^d$$

or radial

$$K(x, x') = \exp\{-\gamma ||x - x'||^2\}.$$

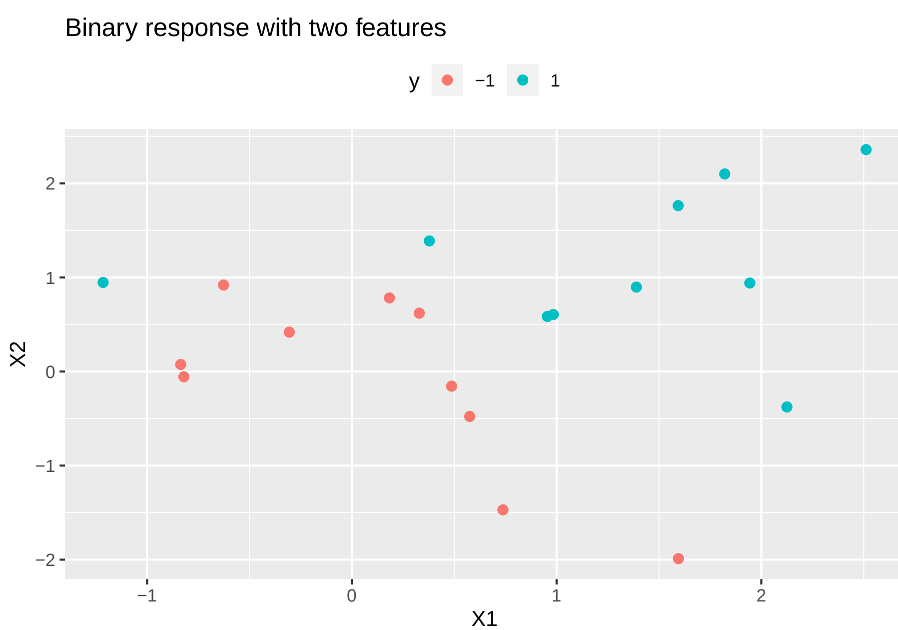
10.4 Example

Here is a data set of two classes $y \in [-1, 1]$ described by two features $X1$ and $X2$.

```
library(tidyverse)
set.seed(1)
x <- matrix(rnorm (20*2), ncol=2)
y <- c(rep(-1, 10), rep(1, 10))
x[y==1, ] <- x[y==1, ] + 1
train_data <- data.frame(x, y)
train_data$y <- as.factor(y)
```

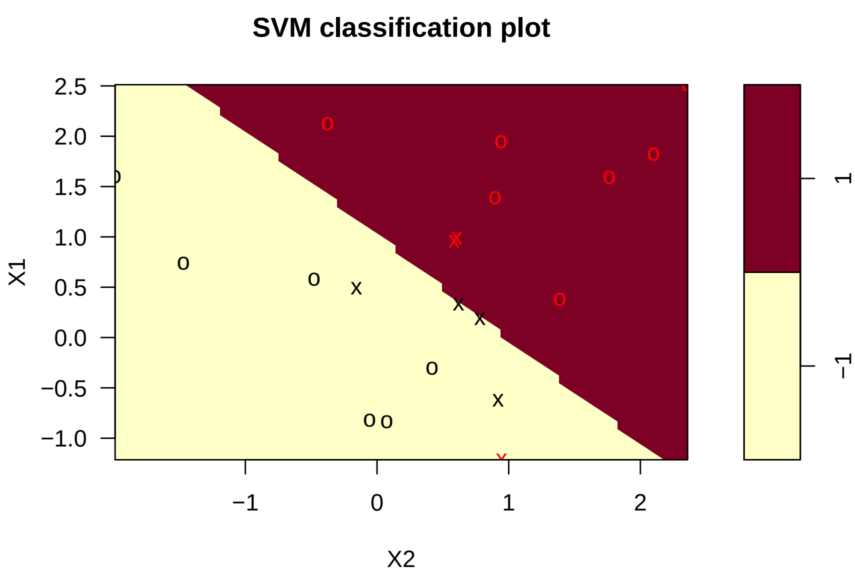
A scatter plot reveals whether the classes are linearly separable.

```
ggplot(train_data, aes(x = X1, y = X2, color = y)) +
  geom_point(size = 2) +
  labs(title = "Binary response with two features") +
  theme(legend.position = "top")
```



No, they are not linearly separable. Now fit a support vector machine. The **e1071** library implements the SVM algorithm. `svm(..., kernel="linear")` fits a support vector classifier. Change the kernal to `c("polynomial", "radial")` for SVM. Try a cost of 10.

```r
library(e1071)
m <- svm(
  y ~ .,
  data = train_data,
  kernel = "linear",
  type = "C-classification",  # (default) for classification
  cost = 10,  # default is 1
  scale = FALSE  # do not standardize features
)
plot(m, train_data)
```



The support vectors are plotted as “x’s”. There are seven of them.

```r
m$index
```

```
## [1]  1  2  5  7 14 16 17
```

The summary shows adds additional information, including the distribution of the support vector classes.

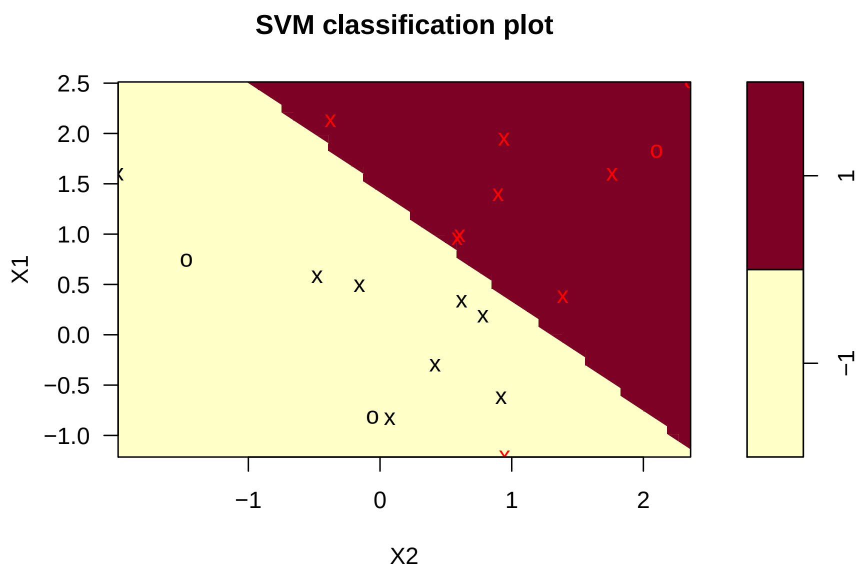
```r
summary(m)
```

```
##
```

```
## Call:
## svm(formula = y ~ ., data = train_data, kernel = "linear", type = "C-classification"
##     cost = 10, scale = FALSE)
##
##
## Parameters:
##    SVM-Type:  C-classification
##  SVM-Kernel:  linear
##        cost:  10
##
## Number of Support Vectors:  7
##
##  ( 4 3 )
##
##
## Number of Classes:  2
##
## Levels:
##  -1 1
```

The seven support vectors are comprised of four in one class, three in the other. What if we lower the cost of margin violations? This will increase bias and lower variance.

```
m <- svm(
  y ~ .,
  data = train_data,
  kernel = "linear",
  type = "C-classification",
  cost = 0.1,
  scale = FALSE
)
plot(m, train_data)
```



There are many more support vectors now. *(In case you hoped to see the linear decision boundary formulation, or at least a graphical representation of the margins, keep hoping. The model is generalized beyond two features, so it evidently does not worry too much about supporting sanitized two-feature demos.)*

Which cost level yields the *best* predictive performance on holdout data? Use cross validation to find out. SVM defaults to 10-fold CV. I'll try seven candidate values for `cost`.

```
set.seed(1)
m_tune <- tune(
  svm,
  y ~ .,
  data = train_data,
  kernel ="linear",
  ranges = list(cost = c(0.001, 0.01, 0.1, 1, 5, 10, 100))
)
summary(m_tune)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
```

```
##  cost
##   0.1
##
## - best performance: 0.05
##
## - Detailed performance results:
##    cost error dispersion
## 1 1e-03  0.55  0.4377975
## 2 1e-02  0.55  0.4377975
## 3 1e-01  0.05  0.1581139
## 4 1e+00  0.15  0.2415229
## 5 5e+00  0.15  0.2415229
## 6 1e+01  0.15  0.2415229
## 7 1e+02  0.15  0.2415229
```

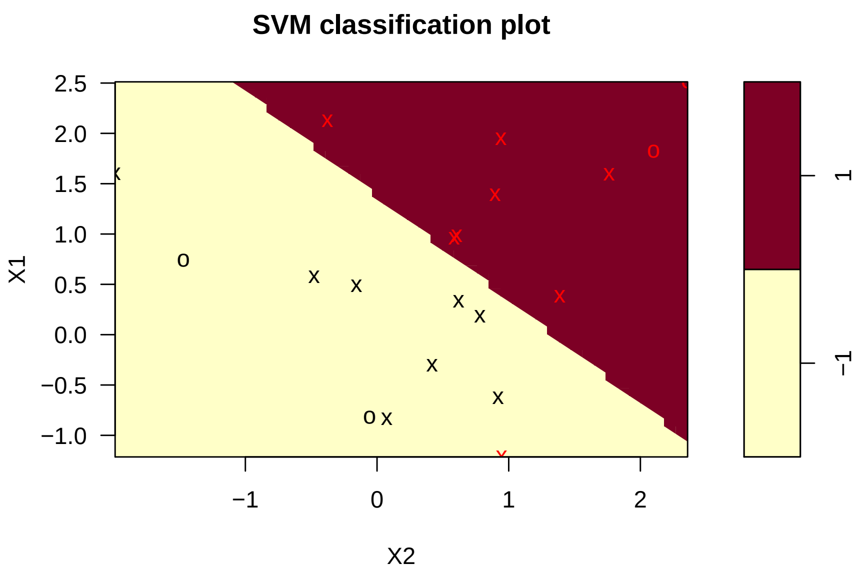
The lowest cross-validation error rate is 0.10 with cost = 0.1. `tune()` saves the best tuning parameter value.

```
m_best <- m_tune$best.model
summary(m_best)
```

```
##
## Call:
## best.tune(method = svm, train.x = y ~ ., data = train_data, ranges = list(cost = c(0
##     0.01, 0.1, 1, 5, 10, 100)), kernel = "linear")
##
##
## Parameters:
##    SVM-Type:  C-classification
##  SVM-Kernel:  linear
##        cost:  0.1
##
## Number of Support Vectors:  16
##
##  ( 8 8 )
##
##
## Number of Classes:  2
##
## Levels:
##  -1 1
```

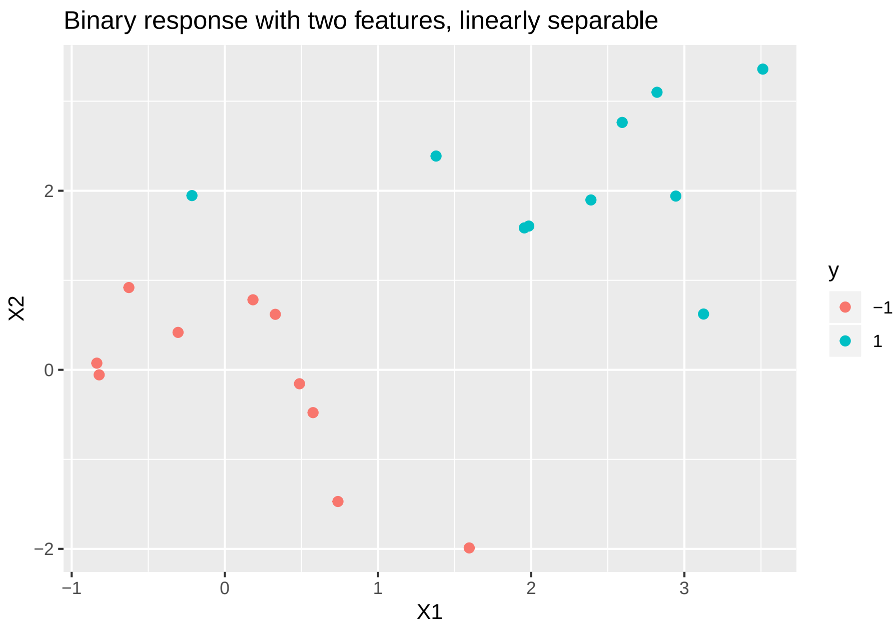
There are 16 support vectors, 8 in each class. This is a pretty wide margin.

```
plot(m_best, train_data)
```



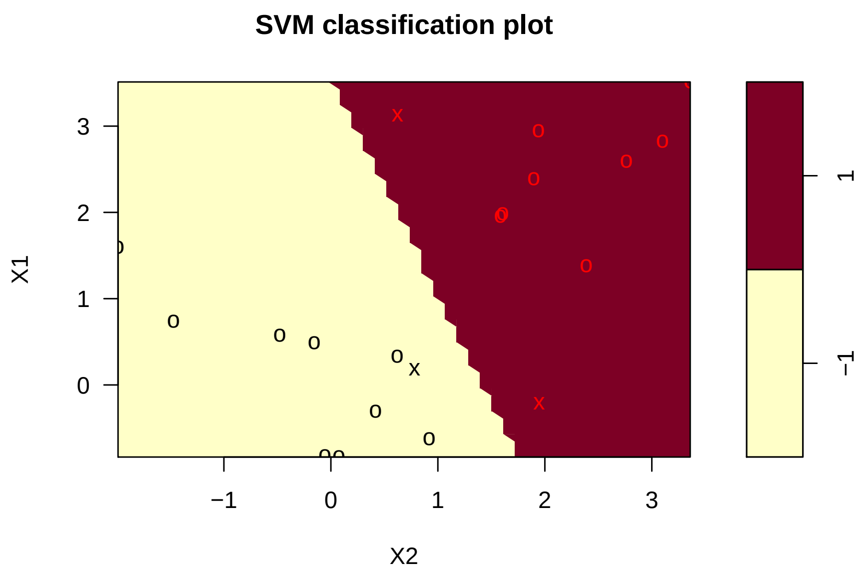
What if the classes had been linearly separable? Then we could create a maximal margin classifier.

```
train_data_2 <- train_data %>%
  mutate(
    X1 = X1 + ifelse(y==1, 1.0, 0),
    X2 = X2 + ifelse(y==1, 1.0, 0)
  )
ggplot(train_data_2, aes(x = X1, y = X2, color = y)) +
  geom_point(size = 2) +
  labs(title = "Binary response with two features, linearly separable")
```



Specify a huge cost = 1e5 so that no support vectors violate the margin.

```
m2 <- svm(
  y ~ .,
  data = train_data_2,
  kernel = "linear",
  cost = 1e5,
  scale = FALSE  # do not standardize features
)
plot(m2, train_data_2)
```




```r
summary(m2)
```

```
##
## Call:
## svm(formula = y ~ ., data = train_data_2, kernel = "linear", cost = 1e+05,
##     scale = FALSE)
##
##
## Parameters:
##    SVM-Type:  C-classification
##  SVM-Kernel:  linear
##        cost:  1e+05
##
## Number of Support Vectors:  3
##
##  ( 1 2 )
##
##
## Number of Classes:  2
##
## Levels:
##  -1 1
```

This model will have very low bias, but very high variance. To fit an SVM, use a different kernel. You can use `kernal = c("polynomial", "radial",` "sigmoid"). For a polynomial model, also specify the polynomial degree. For a radial model, include the gamma value.

```r
set.seed(1)
m3_tune <- tune(
  svm,
  y ~ .,
  data = train_data,
  kernel ="polynomial",
  ranges = list(
    cost = c(0.001, 0.01, 0.1, 1, 5, 10, 100),
    degree = c(1, 2, 3)
  )
)
summary(m3_tune)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
##  cost degree
##     1      1
##
## - best performance: 0.1
##
## - Detailed performance results:
##     cost degree error dispersion
## 1  1e-03      1  0.55  0.4377975
## 2  1e-02      1  0.55  0.4377975
## 3  1e-01      1  0.30  0.2581989
## 4  1e+00      1  0.10  0.2108185
## 5  5e+00      1  0.10  0.2108185
## 6  1e+01      1  0.15  0.2415229
## 7  1e+02      1  0.15  0.2415229
## 8  1e-03      2  0.70  0.4216370
## 9  1e-02      2  0.70  0.4216370
## 10 1e-01      2  0.70  0.4216370
## 11 1e+00      2  0.65  0.2415229
## 12 5e+00      2  0.50  0.3333333
## 13 1e+01      2  0.50  0.3333333
## 14 1e+02      2  0.50  0.3333333
## 15 1e-03      3  0.65  0.3374743
## 16 1e-02      3  0.65  0.3374743
```

```
## 17 1e-01      3  0.50  0.3333333
## 18 1e+00      3  0.40  0.3162278
## 19 5e+00      3  0.35  0.3374743
## 20 1e+01      3  0.35  0.3374743
## 21 1e+02      3  0.35  0.3374743
```

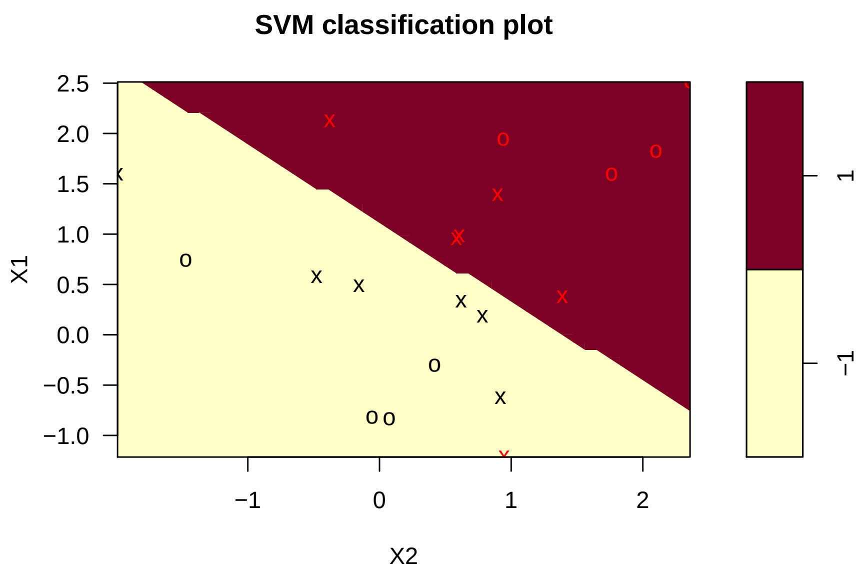
The lowest cross-validation error rate is 0.10 with cost = 1, polynomial degree 1.

```
m3_best <- m3_tune$best.model
summary(m3_best)
```

```
##
## Call:
## best.tune(method = svm, train.x = y ~ ., data = train_data, ranges = list(cost = c(0.001,
##     0.01, 0.1, 1, 5, 10, 100), degree = c(1, 2, 3)), kernel = "polynomial")
##
##
## Parameters:
##    SVM-Type:  C-classification
##  SVM-Kernel:  polynomial
##        cost:  1
##      degree:  1
##      coef.0:  0
##
## Number of Support Vectors:  12
##
##  ( 6 6 )
##
##
## Number of Classes:  2
##
## Levels:
##  -1 1
```

There are 12 support vectors, 6 in each class. This is a pretty wide margin.

```
plot(m3_best, train_data)
```



10.5 Using Caret

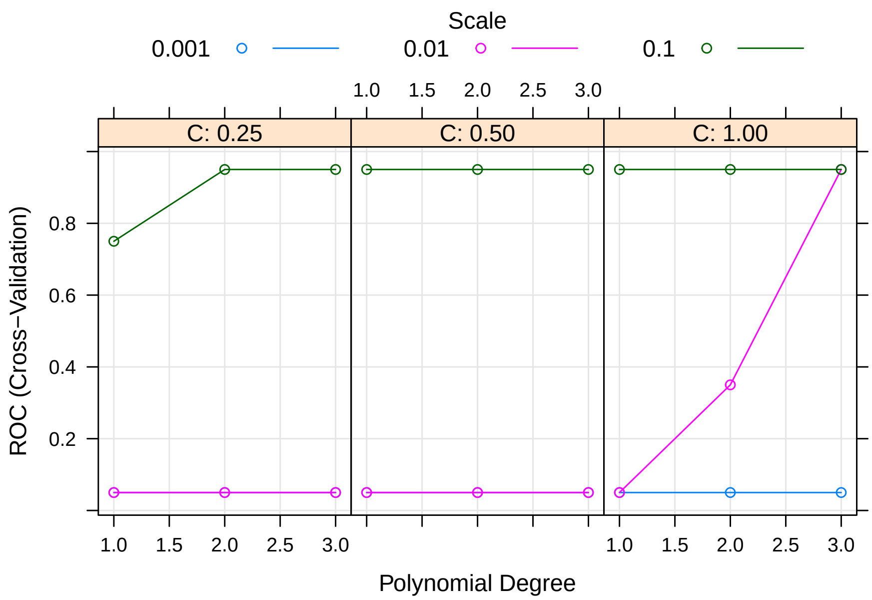
The model can also be fit using **caret**. I'll used LOOCV since the data set is so small. Normalize the variables to make their scale comparable.

```
library(caret)
library(kernlab)

train_data_3 <- train_data %>%
  mutate(y = factor(y, labels = c("A", "B")))

m4 <- train(
  y ~ .,
  data = train_data_3,
  method = "svmPoly",
  preProcess = c("center", "scale"),
  trControl = trainControl(
    method = "cv",
    number = 5,
    summaryFunction = twoClassSummary,  # Use AUC to pick the best model
    classProbs=TRUE
  )
)
```

```
m4$bestTune
```

```
##   degree scale   C
## 8      1   0.1 0.5
```

```
plot(m4)
```



Chapter 11

Principal Components Analysis

Chapter 12

Clustering

Chapter 13

Text Mining

Appendix

Here are miscellaneous skills, knowledge, and technologies I should know.

Publishing to BookDown

The **bookdown** package, written by Yihui Xie, is built on top of R Markdown and the **knitr** package. Use it to publish a book or long manuscript where each chapter is a separate file. There are instructions for how to author a book in his bookdown book (Xie, 2019). The main advantage of **bookdown** over R Markdown is that you can produce multi-page HTML output with numbered headers, equations, figures, etc., just like in a book. I'm using **bookdown** to create a compendium of all my data science notes.

The first step to using **bookdown** is installing the **bookdown* package with `install.packages("bookdown")`.

Next, create an account at bookdown.org, and connect the account to RStudio. Follow the instructions at https://bookdown.org/home/about/.

Finally, create a project in R Studio by creating a new project of type *Book Project using Bookdown*.

After creating all of your Markdown pages, knit the book or click the **Build Book** button in the Build panel.

Shiny Apps

Packages

R Packages (Wickham, 2015) by Hadley Wickham is a good manual on packages, but it does not include a full tutorial. The Developing R Packages Data Camp course is also helpful. I will set up my own exercise and present it here.

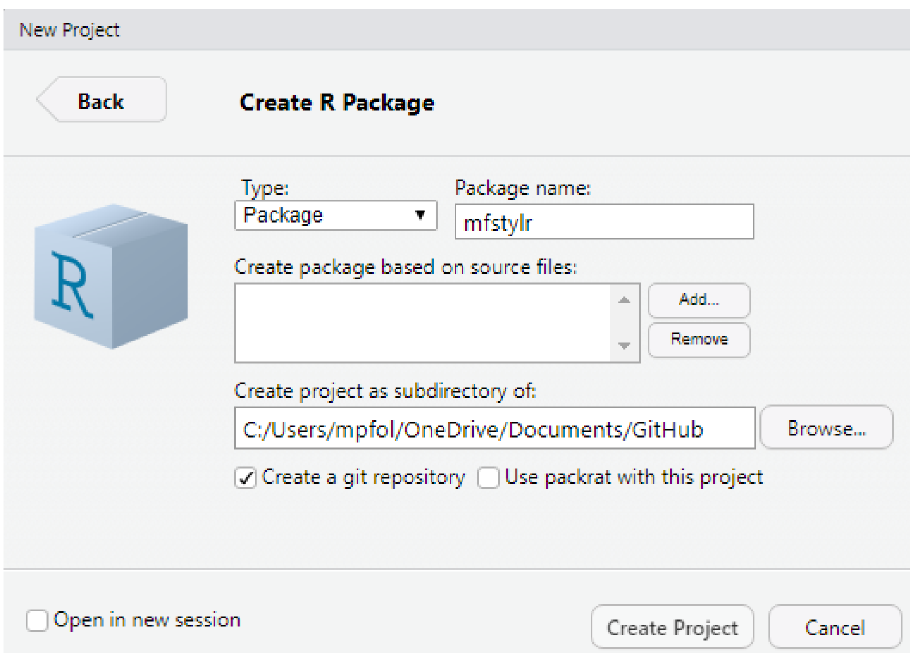
I will create a package for my pretend organization, "MF". The package will include the following:

- R Markdown template. My template will integrate code, output, and commentary in a single R Markdown. The template will produce a familiar work product containing standard content (summary, data management, exploratory analysis, methods, results, conclusions), and a standard style (colors, typeface, size, logo).
- Functions. Common I/O functions for database retrieval, writing to Excel. Common graphing functions for ggplot styling.

I am mostly copying the logic and code from the ggthemes economist.R script.

Create a package

1. In the RStudio IDE, click File > New Project. Select "New Directory". Select "R Package". You can also use `devtools::create("mfstylr")`. This will create the minimum items for an R package.




```
+ R directory: R scripts with function definitions.
+ man directory: documentation
+ NAMESPACE file: information about imported functions and functions made available (ma
+ DESCRIPTION file: metadata about the package
```

2. Write functions in R scripts in R directory. Document with tags readable by *roxygen2* package.

3. Select XYZ > Install and Restart.

13.0.1 Document Functions with roxygen

Add roxygen documentation with `#'` characters. The first three lines are always the title, Description, and Details. They don't need any tags, but you need to separate them with blank lines.

Create Data

Add an RData file to your package with `use_data()`

Create Vignette

Add a directory and template vignette with `use_vignette(name, title)`.

```
use_vignette("Creating-Plots-with-mfstylr", "Creating Plots with mfstylr")
```

Step 2: Create an R Markdown template

I relied on this blog at *free range statistics* for a lot what follows. There is also good information about R Markdown and templates in Yihui Xie's **R Markdown: The Definitive Guide** (Xie et al., 2019).

Use `usethis::use_rmarkdown_template()` to create an Rmd template. I will create a "Kaggle Report" template. In the Console (or a script), enter

```
usethis::use_rmarkdown_template(
  template_name = "Kaggle Report",
  template_dir = "kaggle_report",
  template_description = "Template for creating Kaggle reports in RMarkdown.",
  template_create_dir = FALSE
)
```

Since my project directory is `C:\Users\mpfol\OneDrive\Documents\GitHub\mfstylr`, `use_rmarkdown_template()` creates subdirectories `.\inst\rmarkdown\templates\kaggle_report\skeleton` with three files

- `.\inst\rmarkdown\templates\kaggle_report\template.yaml`

- `.\inst\rmarkdown\templates\kaggle_report\skeleton\skeleton.Rmd`

My kaggle report template will include a logo. Looks like there are two ways to embed an image in your document. One is a direct image loading reference `!()`, but I don't think you can control the attributes this way. A second way is adding html tags.

```
![](logo.png)

# or for more control
<img src="logo.png" style="position:absolute;top:0px;right:0px;" />
```

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