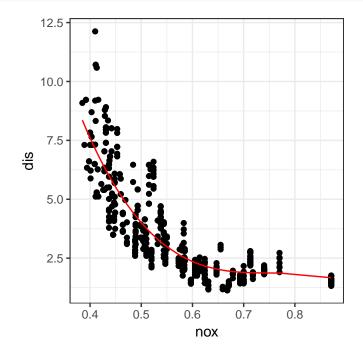
Assigment 4

- 1. For the Boston data available in package MASS we wish to relate dis (weighted mean of distances to five Boston employment centres) to nox (nitrogen oxides concentration in parts per 10 million).
- (a) Fit a cubic polynomial to the data. Plot the data and the fit. Comment on the fit. Calculate the MSE.

```
library(tidyverse)
library(MASS)

f1 <- lm(dis ~ poly(nox,3), data = Boston)

ggplot(data=Boston, aes(x=nox, y=dis)) +
  geom_point() +
  geom_line(aes(y = fitted(f1)), color ="red") +
  theme_bw()</pre>
```



mean(residuals(f1)^2)

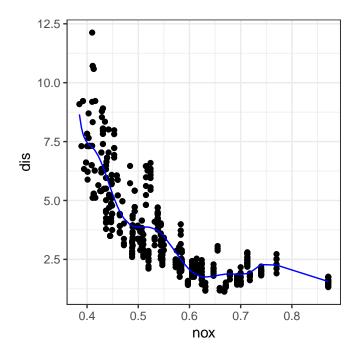
[1] 1.094805

A reasonable fit. Residual plots show increasing variance. Very mild curvature.

(b) Repeat (a), this time using a 10th degree polynomial. Compare the fits and the MSE. Use anova to compare the two fits and comment on your findings.

```
f2 <- lm(dis ~ poly(nox, 10), data = Boston)

ggplot(data=Boston, aes(x=nox, y=dis)) +
  geom_point() +
  geom_line(aes(y = fitted(f2)), color = "blue") +
  theme_bw()</pre>
```



mean(residuals(f2)^2)

[1] 1.011485

Some of the terms in f2 are significant (not all = 0). From the graph it overfits the data, but picks up the increase in dis with increasing nox past 0.65.

(c) Describe how you might use cross-validation to select the optimal degree (say between 1 and 10).

Split the data into 5 groups of approximately equal size. for each degree (j) between 1 and 10, - for each hold out sample, fit the model on the rest and calculate the average test error on the hold out sample, this gives mse1... mse5. the cv error for degree j is the (weighted) average of the mse1... mse5. Pick the degree with the smallest cv error.

(d) Carry out the cross-validation procedure. What is the optimal degree?

```
library(tidymodels)
set.seed(2019)

set.seed(2018)
cv_splits <- vfold_cv(
    data = Boston,
    v = 5
)

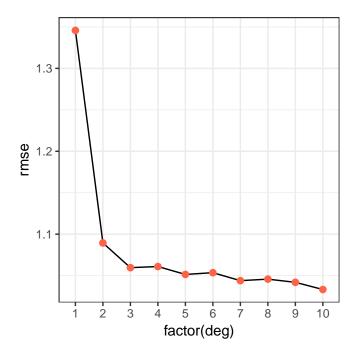
spec_lm <- linear_reg() %>% set_engine("lm")
geo_form <- dis ~ poly(nox, 3)

fit_model <- function(split, spec) {</pre>
```

```
fit(
    object = spec,
    formula = geo_form,
    data = analysis(split)
  )
}
compute_pred <- function(split, model) {</pre>
  # Extract the assessment set
  assess <- assessment(split)</pre>
  # Compute predictions (a df is returned)
  pred <- predict(model, new_data = assess)</pre>
  bind_cols(assess, pred)
compute_perf <- function(pred_df) {</pre>
  numeric_metrics <- metric_set(rmse, rsq)</pre>
  numeric_metrics(
    pred_df,
    truth = dis,
    estimate = .pred
  )
}
mse_cv <- function(degree){</pre>
  geo_form <- dis ~ poly(nox, degree)</pre>
  fit_model <- function(split, spec) {</pre>
    fit(
      object = spec,
      formula = geo_form,
      data = analysis(split)
  }
  cv_splits <- cv_splits %>%
    mutate(models_lm = map(splits, fit_model, spec_lm),
           pred_lm = map2(splits, models_lm, compute_pred),
           perf = map(pred_lm, compute_perf))
  cv_splits %>%
    unnest(perf) %>%
    filter(.metric == 'rmse') %>%
    summarise(m = mean(.estimate)) %>%
    pull(m)
}
mses <- data.frame(rmse = 1:10 %>% map_dbl(mse_cv),
```

```
deg = 1:10)

mses %>%
    ggplot(aes(y = rmse, factor(deg), group = 1)) +
    geom_line() +
    geom_point(colour = "tomato", size = 2) +
    theme_bw()
```



which.min(mses\$rmse)

geom_point() +

theme_bw()

geom_line(aes(y = fitted(f3)), color = "red") +

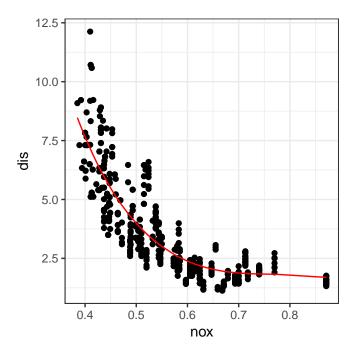
[1] 10

(e) Use bs() to fit a regression spline with 4 degrees of freedom. What are the knots used? Plot the data and the fit. Comment on the fit. Calculate the MSE.

```
library(splines)
f3 <- lm(dis ~ bs(nox, df = 4), data = Boston)
attr(bs(Boston$nox, df = 4), "knots")

## 50%
## 0.538

Boston %>%
ggplot(aes(x = nox, y = dis)) +
```



```
sqrt(mean(residuals(f3)^2))
```

[1] 1.046016

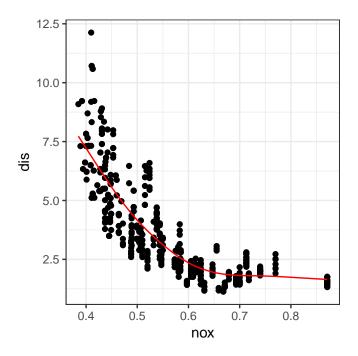
(f) Fit a curve using a smoothing spline with the automatically chosen amount of smoothing. Display the fit. Does the automatic λ give a good result?

```
f4 <- smooth.spline(Boston$nox, Boston$dis, cv = TRUE)
f4

## Call:
## smooth.spline(x = Boston$nox, y = Boston$dis, cv = TRUE)
##

## Smoothing Parameter spar= 1.050661 lambda= 0.07031691 (16 iterations)
## Equivalent Degrees of Freedom (Df): 4.128915
## Penalized Criterion (RSS): 407.277
## PRESS(l.o.o. CV): 1.119355

Boston %>%
ggplot(aes(x = nox, y = dis)) +
    geom_point() +
    geom_line(aes(y = fitted(f4)), color = "red") +
    theme_bw()
```

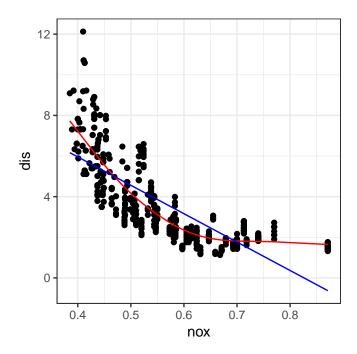


sqrt(mean(residuals(f4)^2))

[1] 1.050964

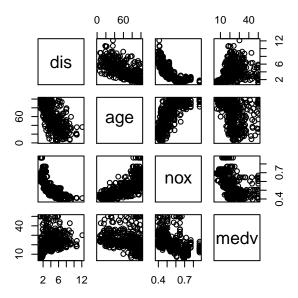
(g) Now use smoothing spline with a larger value of spar. Overlay both smoothing spline fits on the plot. Which looks better?

```
## Call:
## call:
## smooth.spline(x = Boston$nox, y = Boston$dis, spar = 2)
##
## Smoothing Parameter spar= 2 lambda= 508171.7
## Equivalent Degrees of Freedom (Df): 1.999947
## Penalized Criterion (RSS): 762.6087
## GCV: 1.82113
Boston %>%
## ggplot(aes(x = nox, y = dis))+ geom_point() +
geom_line(aes(y = fitted(f4)), color = "red")+
geom_line(aes(y = fitted(f5)), color = "blue") +
theme_bw()
```



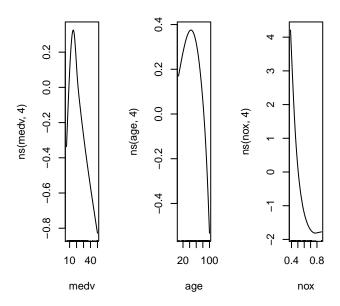
- 2. Using the Boston data, with dis as the response and predictors medv, age and nox.
- (a) Split the data into training 60% and test 40%. Using the training data, fit a generalised additive model (GAM). Use ns with 4 degrees of freedom for each predictor.

```
library(splines)
Boston <- Boston %>%
  mutate(part = ifelse(runif(nrow(.)) > 0.6, "test", "train"))
Boston %>%
  janitor::tabyl(part)
##
                percent
     part
            n
##
     test 189 0.3735178
    train 317 0.6264822
train <- Boston %>% filter(part == "train") %>% dplyr::select(-part)
test <- Boston %>% filter(part == "test") %>% dplyr::select(-part)
gfit1 <- lm(dis \sim ns(medv, 4) + ns(age, 4) + ns(nox, 4), data = train)
pairs(Boston[, c(8, 7, 5, 14)])
```



(b) Use plot.gam to display the results. Does it appear if a linear term is appropriate for any of the predictors?

```
par(mfrow = c(1, 3))
gam::plot.Gam(gfit1)
```



The linear model does not seem appropriate.

(c) Simplify the model fit in part (a). Refit the model. Use anova to compare the two fits and comment on your results.

```
attr(ns(train$age, 4), "knots")
```

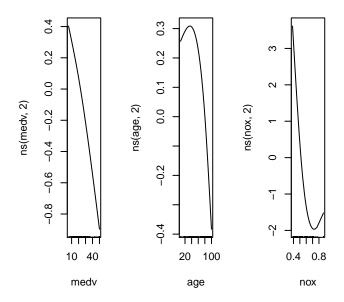
```
## 25% 50% 75%
## 45.4 79.7 94.5
```

```
attr(ns(train$age, 2), "knots")

## 50%
## 79.7

gfit2 <- lm(dis ~ ns(medv, 2) + ns(age, 2) + ns(nox, 2), data = train)

par(mfrow=c(1,3))</pre>
```



anova(gfit1, gfit2)

gam::plot.Gam(gfit2)

```
## Analysis of Variance Table
##
## Model 1: dis ~ ns(medv, 4) + ns(age, 4) + ns(nox, 4)
## Model 2: dis ~ ns(medv, 2) + ns(age, 2) + ns(nox, 2)
## Res.Df RSS Df Sum of Sq F Pr(>F)
## 1 304 260.44
## 2 310 274.64 -6 -14.203 2.7631 0.01248 *
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

the model with fewer df is not appropriate.

4.

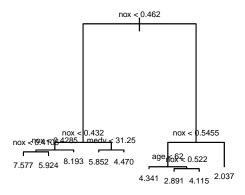
(a) For the training data in question 2, fit a tree model. Use dis as response, and predictors medv, age and nox. Draw the tree. Calculate the training and test MSE.

```
library(tree)
tree <- tree(dis ~ medv + age + nox, data = train)
summary(tree)</pre>
```

```
##
## Regression tree:
## tree(formula = dis ~ medv + age + nox, data = train)
## Number of terminal nodes: 9
## Residual mean deviance: 0.5356 = 165 / 308
## Distribution of residuals:
## Min. 1st Qu. Median Mean 3rd Qu. Max.
## -2.10400 -0.42980 -0.06625 0.00000 0.38060 3.29900
```

The fitted tree has 5 leaf nodes.

```
plot(tree)
text(tree, cex = 0.5, pretty = 0)
```



```
sqrt(mean(residuals(tree)^2))
```

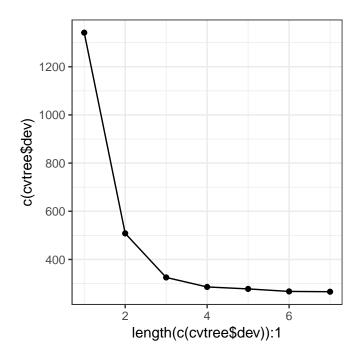
[1] 0.7213952

```
pred <- predict(tree, test)
sqrt(mean((test$dis - pred)^2))</pre>
```

[1] 1.199322

(b) Use cv.tree to select a pruned tree. If pruning is required, fit and draw the pruned tree. Calculate the training and test MSE. Compare the results to those in (a).

```
cvtree <- cv.tree(tree)</pre>
cvtree
## $size
## [1] 9 8 6 4 3 2 1
##
## $dev
## [1]
        266.0019
                  267.2256
                            277.7006 285.8440
                                                 325.2640 508.1814 1341.4652
##
## $k
## [1]
            -Inf 14.31800 16.52661 20.31122 54.70596 175.73910 854.63983
##
## $method
```



(c) Which fit is better, the (optionally pruned) tree or the GAM? Compare their performance on the test data.

```
pred <- predict(tree, test)
sqrt(mean((test$dis - pred)^2))

## [1] 1.199322

pred <- predict(gfit2, test)
sqrt(mean((test$dis - pred)^2))</pre>
```

The GAM has a slightly lower test MSE, but this is seed dependant.

5. For the data generated in question 6, Assignment 3:

[1] 1.169403

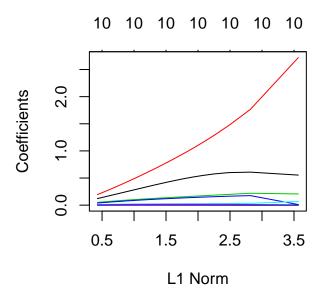
```
set.seed(1)
x <- rnorm(100)
y <- 1 + .2*x+3*x^2+.6*x^3 + rnorm(100)
d <- data.frame(x = x, y = y)</pre>
```

(a) Fit a regression model containing predictors $X, X^2, \dots X^{10}$. Based on the output in summary() which terms are needed in the model?

```
lm(y ~ poly(x, 10, raw = TRUE), data = d) %>% summary()
##
## Call:
## lm(formula = y ~ poly(x, 10, raw = TRUE), data = d)
##
## Residuals:
##
      Min
                10 Median
                                       Max
## -1.9774 -0.5895 -0.1238 0.4923
                                    2.1505
## Coefficients:
##
                             Estimate Std. Error t value Pr(>|t|)
                                                   5.873 7.28e-08 ***
## (Intercept)
                              1.17283
                                         0.19971
## poly(x, 10, raw = TRUE)1
                              0.71409
                                         0.59009
                                                   1.210
                                                            0.229
## poly(x, 10, raw = TRUE)2
                              1.86854
                                         1.29174
                                                   1.447
                                                            0.152
## poly(x, 10, raw = TRUE)3
                            -0.33114
                                         1.68567 -0.196
                                                            0.845
## poly(x, 10, raw = TRUE)4
                             1.90383
                                         2.14977
                                                   0.886
                                                            0.378
## poly(x, 10, raw = TRUE)5
                             0.55110
                                         1.35654
                                                   0.406
                                                            0.686
## poly(x, 10, raw = TRUE)6
                           -1.26499
                                         1.31956 -0.959
                                                            0.340
                                                            0.696
## poly(x, 10, raw = TRUE)7
                                         0.39731 -0.392
                             -0.15569
## poly(x, 10, raw = TRUE)8
                              0.31987
                                         0.32511
                                                   0.984
                                                            0.328
## poly(x, 10, raw = TRUE)9
                              0.01628
                                         0.03817
                                                   0.426
                                                            0.671
## poly(x, 10, raw = TRUE)10 -0.02690
                                         0.02749 -0.979
                                                            0.330
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.9719 on 89 degrees of freedom
## Multiple R-squared: 0.951, Adjusted R-squared: 0.9455
## F-statistic: 172.7 on 10 and 89 DF, p-value: < 2.2e-16
```

(b) Fit a ridge regression model using the glmnet function over a grid of values for λ ranging from 0.001 to 50. Plot coefficients vs penalty using the default plot method. Use the inbuilt function cv.glmnet to choose the tuning parameter λ . How do the coefficients at the optimal value of λ compare to the linear regression ones in (a)?

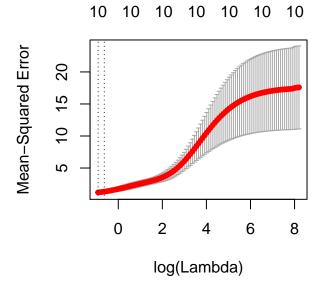
```
library(glmnet)
X <- model.matrix(y ~ poly(x, 10, raw = TRUE), data = d)
grid <- seq(0.001, 50, length = 100)
ridge.fit <- glmnet(X, y, alpha=0, lambda = grid)
plot(ridge.fit)</pre>
```



```
cv.out <- cv.glmnet(X,y,alpha=0)
cv.out$lambda.min</pre>
```

[1] 0.4000507

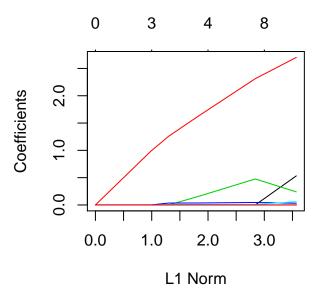
plot(cv.out)



```
## poly(x, 10, raw = TRUE)1
                              6.119103e-01
## poly(x, 10, raw = TRUE)2
                              1.859173e+00
                              2.221955e-01
## poly(x, 10, raw = TRUE)3
## poly(x, 10, raw = TRUE)4
                              1.736758e-01
## poly(x, 10, raw = TRUE)5
                              3.293830e-02
## poly(x, 10, raw = TRUE)6
                              1.120493e-02
## poly(x, 10, raw = TRUE)7
                              3.820191e-03
## poly(x, 10, raw = TRUE)8 -7.804433e-05
## poly(x, 10, raw = TRUE)9
                              2.623561e-04
## poly(x, 10, raw = TRUE)10 -2.576105e-04
```

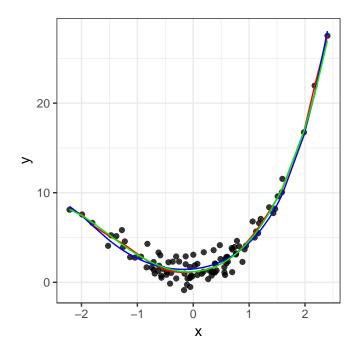
(c) Repeat (b) for lasso regression instead of ridge.

```
lasso.fit <- glmnet(X, y, alpha=1, lambda = grid)
plot(lasso.fit)</pre>
```



```
## poly(x, 10, raw = TRUE)5   0.032879765
## poly(x, 10, raw = TRUE)6   .
## poly(x, 10, raw = TRUE)7   0.002025108
## poly(x, 10, raw = TRUE)8   .
## poly(x, 10, raw = TRUE)9   .
## poly(x, 10, raw = TRUE)10   .
```

(d) Plot the data y vs x and superimpose the fitted models from linear regression, ridge and lasso with optimal values of lambda as chosen by cross-validation.



6. Titanic data from Assignment 3:

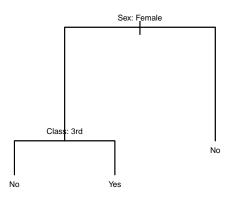
```
ttrain <- read.csv("data/ttrain.csv", header = TRUE, row.names = 1)
ttest <- read.csv("data/ttest.csv", header = TRUE, row.names = 1)</pre>
```

(a) For the training data, fit a tree model using all three predictors. Draw the tree. Interpret the model. For the training and test data what proportion of survivors are missclassified? What proportion of those who died are missclassified? What proportion of the predicted survivors actually survived? What is the overall error rate for the training data?

```
library(tree)
tree <- tree(Survived ~ ., data = ttrain)
summary(tree)

##
## Classification tree:
## tree(formula = Survived ~ ., data = ttrain)
## Variables actually used in tree construction:
## [1] "Sex" "Class"
## Number of terminal nodes: 3
## Residual mean deviance: 0.9852 = 1732 / 1758
## Misclassification error rate: 0.2107 = 371 / 1761

plot(tree)
text(tree, cex = 0.5, pretty = 0)</pre>
```



Fitted model: males have no chance of survival. For females, those in 3rd class have no chance of survival. The rest are predicted as survived. Age is not in the model.

```
prob <- predict(tree, ttrain)[,2]
ttrain$pred <- factor(ifelse(prob < .5, "No", "Yes"))

ttrain %>%
  group_by(Survived, pred) %>%
  count() %>%
  group_by(Survived) %>%
  mutate(perc = scales::percent(n/sum(n)))
```

```
## # A tibble: 4 x 4
## # Groups:
               Survived [2]
     Survived pred
                         n perc
              <fct> <int> <chr>
##
     <fct>
## 1 No
              No
                      1178 98.7%
## 2 No
              Yes
                        15 1.3%
## 3 Yes
              No
                       356 62.7%
## 4 Yes
                       212 37.3%
              Yes
```

```
prob <- predict(tree, ttest)[,2]
ttest$pred <- factor(ifelse(prob < .5, "No", "Yes"))

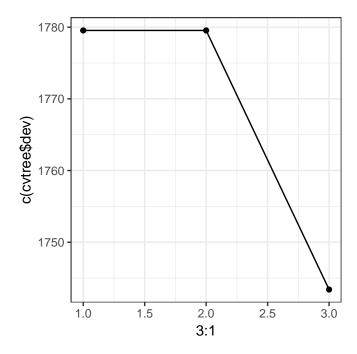
ttest %>%
  group_by(Survived, pred) %>%
  count() %>%
  group_by(Survived) %>%
  mutate(perc = scales::percent(n/sum(n)))
```

```
## # A tibble: 4 x 4
## # Groups:
               Survived [2]
##
     Survived pred
                         n perc
##
     <fct>
              <fct> <int> <chr>
## 1 No
                       292 98.3%
              No
## 2 No
                         5 1.7%
              Yes
## 3 Yes
              No
                       101 70.6%
              Yes
## 4 Yes
                        42 29.4%
```

(b) Use cv.tree to select a pruned tree. If pruning is required, fit and draw the pruned tree.

```
cvtree <- cv.tree(tree)

ggplot() +
  geom_point(aes(x = 3:1, y = c(cvtree$dev))) +
  geom_line(aes(x = 3:1, y = c(cvtree$dev))) +
  theme_bw()</pre>
```

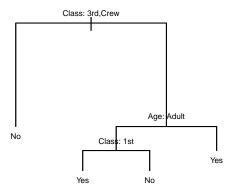


(c) Fit a tree model using only Age and Class as predictors. Draw the tree. Interpret the model. Compare the test set results to (a).

```
tree <- tree(Survived ~ Age + Class, data = ttrain)
summary(tree)

##
## Classification tree:
## tree(formula = Survived ~ Age + Class, data = ttrain)
## Number of terminal nodes: 4
## Residual mean deviance: 1.148 = 2017 / 1757
## Misclassification error rate: 0.2731 = 481 / 1761

plot(tree)
text(tree, cex = 0.5, pretty = 0)</pre>
```



```
prob <- predict(tree, ttrain)[,2]
ttrain$pred <- factor(ifelse(prob < .5, "No", "Yes"))

ttrain %>%
  dplyr::select(1:3, pred) %>%
  group_by_all() %>%
  count() %>%
  arrange(pred, n)
```

```
## # A tibble: 14 x 5
## # Groups: Class, Sex, Age, pred [14]
##
     Class Sex
                  Age pred
      <fct> <fct> <fct> <fct> <fct> <int>
##
## 1 Crew Female Adult No
## 2 3rd
           Female Child No
                                 19
## 3 3rd
           Male
                  Child No
                                 37
## 4 2nd
           Female Adult No
                                 80
## 5 3rd
           Female Adult No
                                130
## 6 2nd
           Male
                 Adult No
                                132
## 7 3rd
           Male
                  Adult No
                                381
## 8 Crew Male
                 Adult No
                                686
## 9 1st
           Female Child Yes
                                 1
           Male
## 10 1st
                 Child Yes
                                  4
## 11 2nd
           Male
                  Child Yes
                                  7
## 12 2nd
           Female Child Yes
                                 13
## 13 1st
          Female Adult Yes
                                116
## 14 1st Male Adult Yes
                                138
```

Fitted model: 3rd class and crew have no chance of survival. For those in 1st and 2nd class children are predicted to have survived. Adults in 1st class are predicted to have survived, but those in the 2nd did not.

```
prob <- predict(tree, ttest)[,2]
ttest$pred <- factor(ifelse(prob < .5, "No", "Yes"))

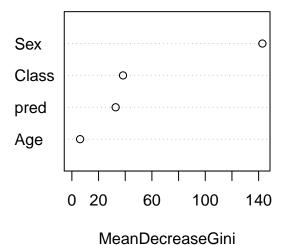
ttest %>%
  group_by(Survived, pred) %>%
  count() %>%
  group_by(Survived) %>%
  mutate(perc = scales::percent(n/sum(n)))
```

```
## # A tibble: 4 x 4
## # Groups:
               Survived [2]
##
     Survived pred
                         n perc
##
     <fct>
              <fct> <int> <chr>
## 1 No
              No
                      271 91.2%
## 2 No
                        26 8.8%
              Yes
## 3 Yes
              No
                        99 69.2%
## 4 Yes
                        44 30.8%
              Yes
```

(d) Fit a random forest model (using randomForest) using all three predictors and compare the test set results to (a) and (c). Which variables are important?

```
library(randomForest)
bag <- randomForest(Survived ~ ., data = ttrain)
varImpPlot(bag)</pre>
```

bag



```
ttest$pred <- predict(bag, newdata = ttest)

ttest %>%
  group_by(Survived, pred) %>%
```

```
count() %>%
group_by(Survived) %>%
mutate(perc = scales::percent(n/sum(n)))
```

```
## # A tibble: 4 x 4
## # Groups:
               Survived [2]
     Survived pred
##
                        n perc
##
     <fct>
              <fct> <int> <chr>
                      292 98.3%
## 1 No
              No
## 2 No
                        5 1.7%
              Yes
## 3 Yes
                       96 67.1%
              No
                       47 32.9%
## 4 Yes
              Yes
```

7. Heart data: binary outcome AHD for 303 patients who presented with chest pain. An outcome value of Yes indicates the presence of heart disease, while No means no heart disease.

There are 13 predictors including Age, Sex, Chol (a cholesterol measurement), and other heart and lung function measurements.

Fit a support vector machine with a radial kernel to this data. Use cross validation to tune the λ and cost parameters (see function tune() in e1071 library). How does your result (test error) compare to the test error in the notes (obtained using trees and random forrests)?

```
set.seed(2019)
heart <- read.csv("data/heart.csv", row.names=1) %>% na.omit()
heart <- heart %>%
  mutate(part = ifelse(runif(nrow(.)) > 0.66, "test", "train"))
  janitor::tabyl(part)
              percent
##
     part
          n
##
     test 92 0.3097643
    train 205 0.6902357
train <- heart %>% filter(part == "train") %>% dplyr::select(-part)
test <- heart %>% filter(part == "test") %>% dplyr::select(-part)
library(e1071)
fit.svm <- svm(AHD ~ ., data = train, kernel = "radial")
summary(fit.svm)
##
## Call:
## svm(formula = AHD ~ ., data = train, kernel = "radial")
##
##
## Parameters:
```

```
##
     SVM-Type: C-classification
##
   SVM-Kernel: radial
##
         cost: 1
##
         gamma: 0.05882353
##
## Number of Support Vectors: 117
   (57 60)
##
##
##
## Number of Classes: 2
##
## Levels:
## No Yes
test$pred <- predict(fit.svm, newdata = test)</pre>
test %>%
  group_by(AHD, pred) %>%
count()
## # A tibble: 4 x 3
## # Groups: AHD, pred [4]
     AHD
          pred
     <fct> <fct> <int>
## 1 No
        No
## 2 No
          Yes
## 3 Yes No
                    12
## 4 Yes
         Yes
tune.out <- tune(svm,AHD~., data = train, kernel = "radial",</pre>
                 ranges = list(cost = 10^seq(-1, 6, by = 1),
                              gamma = 10^seq(-6, 1, by = 1))
tune.out
## Parameter tuning of 'svm':
## - sampling method: 10-fold cross validation
## - best parameters:
##
    cost gamma
## 1e+05 1e-04
## - best performance: 0.1554762
fit.svm <- svm(AHD~., data = train, kernel = "radial",
               cost = 10000, gamma = 0.00001)
summary(fit.svm)
##
## Call:
```

```
## svm(formula = AHD ~ ., data = train, kernel = "radial", cost = 10000,
##
       gamma = 1e-05)
##
##
## Parameters:
##
     SVM-Type: C-classification
   SVM-Kernel: radial
         cost: 10000
##
##
        gamma: 1e-05
##
## Number of Support Vectors: 82
##
## (40 42)
##
##
## Number of Classes: 2
##
## Levels:
## No Yes
test$pred <- predict(fit.svm, newdata = test)</pre>
test %>%
  group_by(AHD, pred) %>%
count()
## # A tibble: 4 x 3
## # Groups: AHD, pred [4]
## AHD
         pred
##
   <fct> <fct> <int>
## 1 No
           No
## 2 No
          Yes
                   3
## 3 Yes
          No
                    11
## 4 Yes
          Yes
                    36
bag <- randomForest(AHD ~ ., data = train)</pre>
test$pred <- predict(bag, test)</pre>
test %>%
  group_by(AHD, pred) %>%
count()
## # A tibble: 4 x 3
## # Groups: AHD, pred [4]
    AHD
           pred
##
     <fct> <fct> <int>
## 1 No
           No
                    5
## 2 No
           Yes
## 3 Yes No
                   11
## 4 Yes Yes
                    36
```