

MSSC 6250 Machine Learning Homework 4

Support Vector Machines, Tree Methods, Unsupervised Learning

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- Deadline: **Friday, April 28 11:59 PM**
- Homework presentation date: **Tuesday, May 2**
- Please submit your work in **one PDF** file to **D2L > Assessments > Dropbox**. *Multiple files or a file that is not in pdf format are not allowed.*
- Any relevant code should be attached.
- Read **ISL** Chapter 8, 9, and 12.

Exercises required for all students

1. **ISL** Sec. 8.4: 12 (Don't do BART)

Solution:

The chosen data set is Boston, since it is of easy access, and we have worked on it previously.

```
set.seed(1)
library(ISLR2)
```

Warning: package 'ISLR2' was built under R version 4.2.2

```
summary(Boston)
```

crim	zn	indus	chas
Min. : 0.00632	Min. : 0.00	Min. : 0.46	Min. : 0.00000
1st Qu.: 0.08205	1st Qu.: 0.00	1st Qu.: 5.19	1st Qu.: 0.00000
Median : 0.25651	Median : 0.00	Median : 9.69	Median : 0.00000
Mean : 3.61352	Mean : 11.36	Mean : 11.14	Mean : 0.06917
3rd Qu.: 3.67708	3rd Qu.: 12.50	3rd Qu.: 18.10	3rd Qu.: 0.00000

nox	rm	age	dis
Max. :88.97620	Max. :100.00	Max. :27.74	Max. :1.00000
Min. :0.3850	Min. :3.561	Min. : 2.90	Min. : 1.130
1st Qu.:0.4490	1st Qu.:5.886	1st Qu.: 45.02	1st Qu.: 2.100
Median :0.5380	Median :6.208	Median : 77.50	Median : 3.207
Mean :0.5547	Mean :6.285	Mean : 68.57	Mean : 3.795
3rd Qu.:0.6240	3rd Qu.:6.623	3rd Qu.: 94.08	3rd Qu.: 5.188
Max. :0.8710	Max. :8.780	Max. :100.00	Max. :12.127

rad	tax	ptratio	lstat
Min. : 1.000	Min. :187.0	Min. :12.60	Min. : 1.73
1st Qu.: 4.000	1st Qu.:279.0	1st Qu.:17.40	1st Qu.: 6.95
Median : 5.000	Median :330.0	Median :19.05	Median :11.36
Mean : 9.549	Mean :408.2	Mean :18.46	Mean :12.65
3rd Qu.:24.000	3rd Qu.:666.0	3rd Qu.:20.20	3rd Qu.:16.95
Max. :24.000	Max. :711.0	Max. :22.00	Max. :37.97

medv
Min. : 5.00
1st Qu.:17.02
Median :21.20
Mean :22.53
3rd Qu.:25.00
Max. :50.00

Let's try to predict - the per capita crime rate by town. And use MSE as the metric to measure our performance.

```
train <- sample(nrow(Boston), 0.8 * nrow(Boston))
test <- -train
```

Linear regression:

```
lm.fit <- lm(crim ~ zn + nox + dis + rad + ptratio + medv,
             data = Boston[train,])

lm.prediction <- predict(lm.fit, newdata = Boston[test,])
(mse <- mean((Boston[test,1]-lm.prediction)^2))
```

```
[1] 64.77735
```

Linear regression gave a MSE of 64.77735.

Boosting:

```
library(gbm)
```

Warning: package 'gbm' was built under R version 4.2.3

Loaded gbm 2.1.8.1

```
gbm.fit <- gbm::gbm(crim ~ zn + nox + dis + rad + ptratio + medv,  
  data = Boston[train,],  
  distribution = "gaussian", n.trees = 300,  
  shrinkage = 0.5, bag.fraction = 0.8,  
  cv.folds = 10)  
  
gbm.prediction <- predict(gbm.fit, newdata = Boston[test,])
```

Using 18 trees...

```
(mse <- mean((Boston[test,1]-gbm.prediction)^2))
```

```
[1] 53.76935
```

Boosting gave a MSE around 54. Which was better than the linear regression model.

Bagging:

```
library(randomForest)
```

Warning: package 'randomForest' was built under R version 4.2.3

randomForest 4.7-1.1

Type rfNews() to see new features/changes/bug fixes.

```
bag.fit <- randomForest(crim ~ zn + nox + dis + rad + ptratio + medv,  
  data = Boston[train,],  
  mtry = 5)  
bag.prediction <- predict(bag.fit, newdata = Boston[test,])  
(mse <- mean((Boston[test,1]-bag.prediction)^2))
```

```
[1] 53.84921
```

Bagging gave a MSE around 52. Which was better than both previous models.

Random forests:

```
rngF.fit <- randomForest(crim ~ zn + nox + dis + rad + ptratio + medv,
                        data = Boston[train,],
                        mtry = 2)
rngF.prediction <- predict(rngF.fit, newdata = Boston[test,])
(mse <- mean((Boston[test,1]-rngF.prediction)^2))
```

[1] 52.41303

Random forests also gave a MSE around 52.

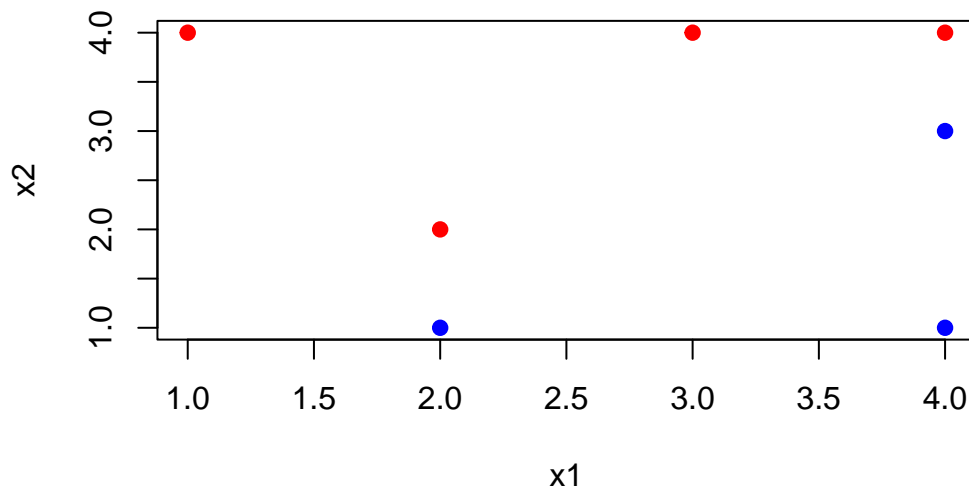
Therefore, both Random forests and Bagging were the models that resulted in the best performance in this data set.

2. ISL Sec. 9.7: 3

Solution:

a-)

```
x1 = c(3,2,4,1,2,4,4)
x2 = c(4,2,4,4,1,3,1)
colors = c("red", "red", "red", "red", "blue", "blue", "blue")
plot(x1,x2,col=colors,pch=19)
```



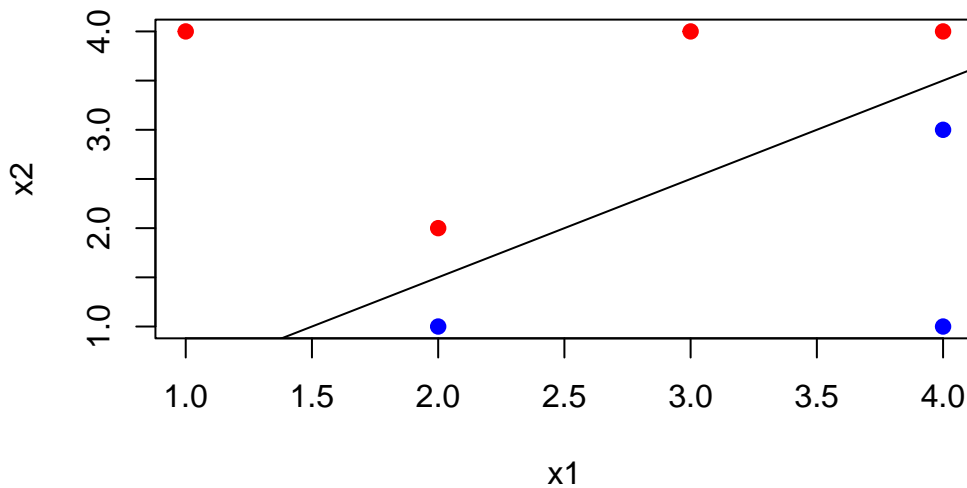
b-) Since we are using margin my_classifier. Then we need to look at observations #2, #3 and #5, #6. Since they are the closest to the boundary.

$(2, 2), (4, 4)(2, 1), (4, 3)$

Then just use the equation of the line and rewrite it.

$$\Rightarrow (2, 1.5), (4, 3.5) b = (3.5 - 1.5)/(4 - 2) = 1 a = X_2 - X_1 = 1.5 - 2 = -0.5$$

```
plot(x1,x2,col=colors,pch=19)
abline(-0.5, 1)
```



c-)

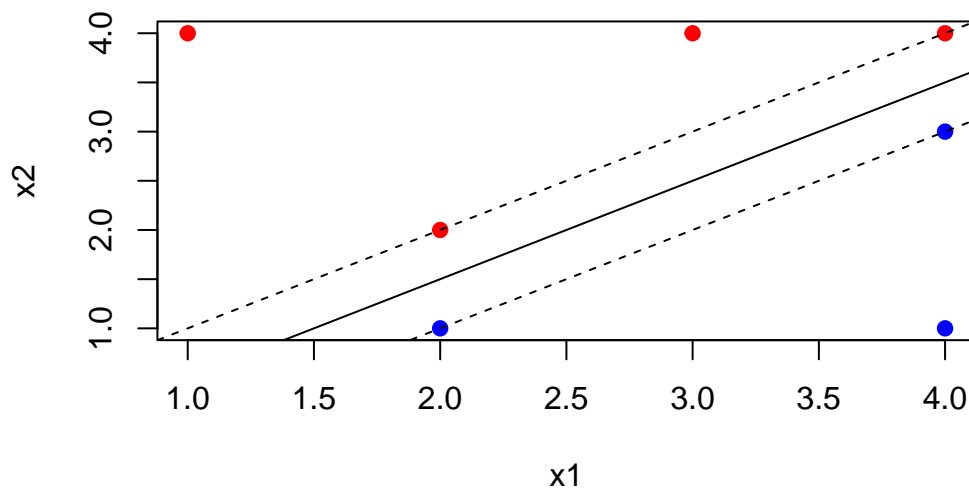
The values for β s: $\beta_0 = 0.5$, $\beta_1 = 1$, and $\beta_0 = -1$

So the rules are:

$$0.5 - X_1 + X_2 > 0 \Rightarrow \text{Blue and } 0.5 - X_1 + X_2 \leq 0 \Rightarrow \text{Red}$$

d-)

```
plot(x1,x2,col=colors,pch=19)
abline(-0.5, 1)
abline(-1, 1, lty=2)
abline(0, 1, lty=2)
```



e-) There are four support vector for the maximal margin my_classifier.

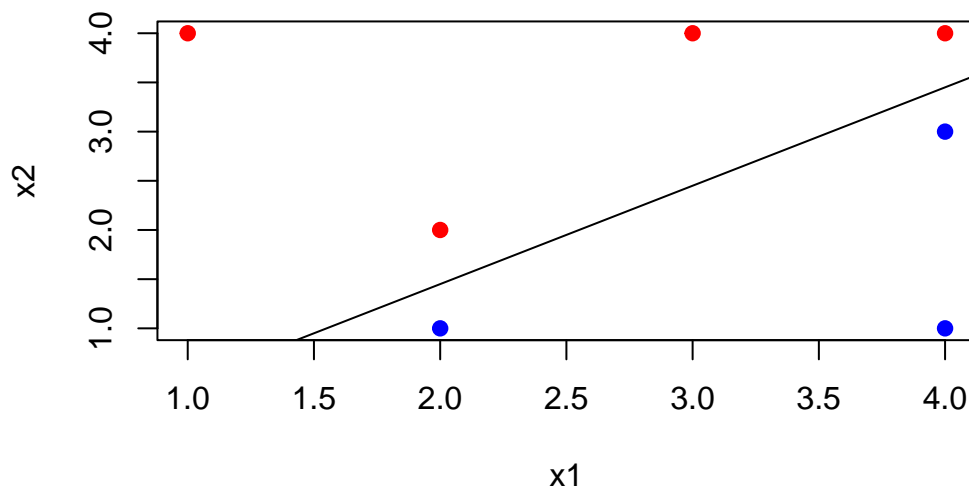
The observations 2,3,5 and 6.

f-)

Since the seventh observation is not a support vector, any small change to that observation would not affect the hyperplane.

g-)

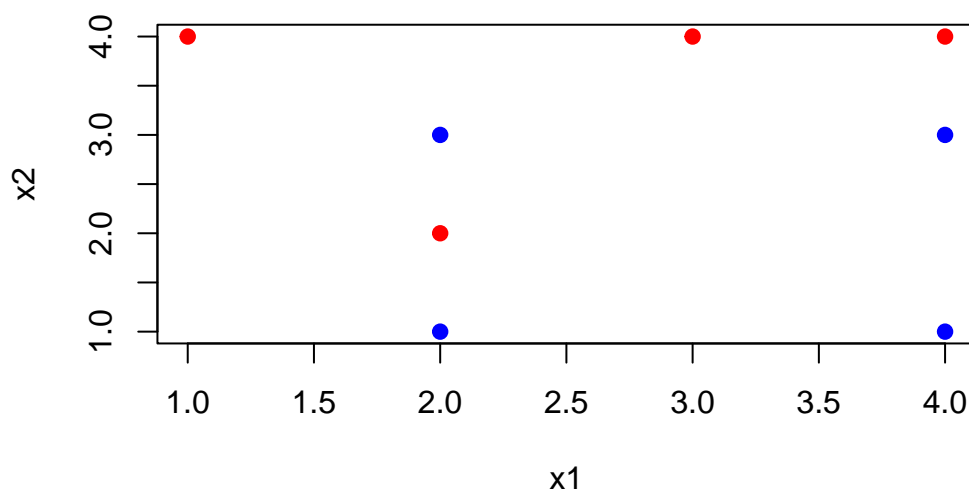
```
plot(x1,x2,col=colors,pch=19)
abline(-0.55, 1)
```



$$-0.55 - X_1 + X_2 > 0$$

h -)

```
plot(x1,x2,col=colors,pch=19)
points(c(2), c(3), col=c("blue"),pch=19)
```



3. ISL Sec. 9.7: 5

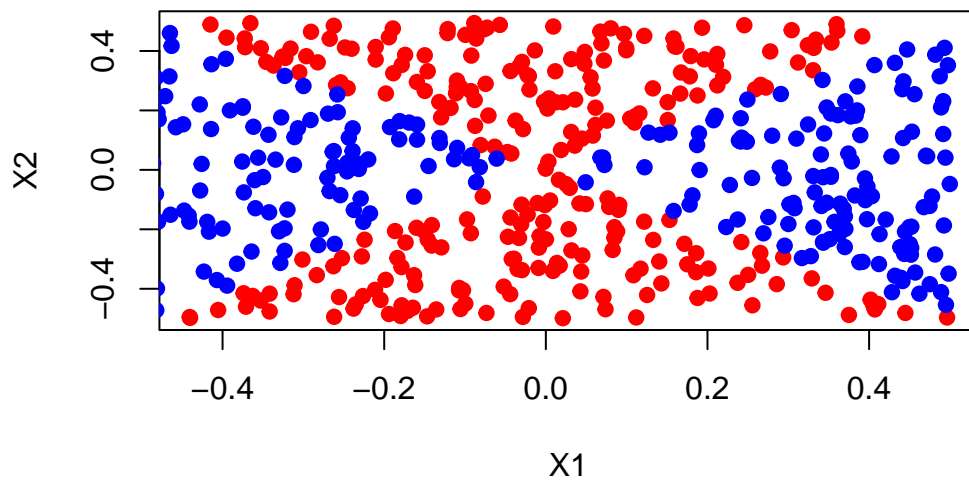
Solution:

a-)

```
x1 <- runif(500) - 0.5
x2 <- runif(500) - 0.5
y <- 1*(x1**2-x2**2>0)
```

b-)

```
plot(x1[y==0], x2[y==0], col="red", xlab="X1", ylab="X2", pch=19)
points(x1[y==1], x2[y==1], col="blue", pch=19)
```



c-)

```
glm.fit=glm(y~. ,family='binomial', data=data.frame(x1,x2,y))
glm.fit
```

Call: glm(formula = y ~ ., family = "binomial", data = data.frame(x1, x2, y))

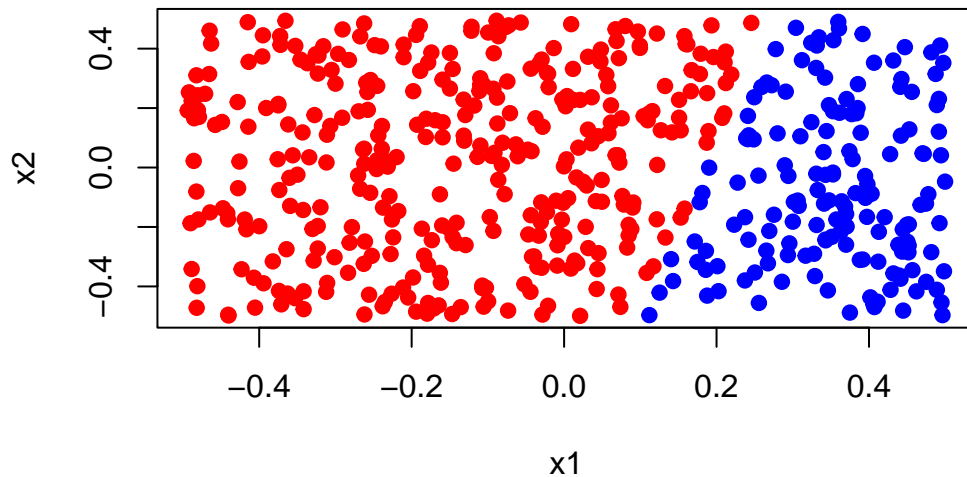
Coefficients:

(Intercept)	x1	x2
-0.1487	0.7817	-0.1381

Degrees of Freedom: 499 Total (i.e. Null); 497 Residual
Null Deviance: 690.8
Residual Deviance: 684.4 AIC: 690.4

d-)

```
glm.pred=predict(glm.fit,data.frame(x1,x2))  
plot(x1,x2,col=ifelse(glm.pred>0,'blue','red'),pch=19)
```



As expected, by comparing the graphs we can see this model does not do a good job.

e-) Let's try a polynomial of degree 2.

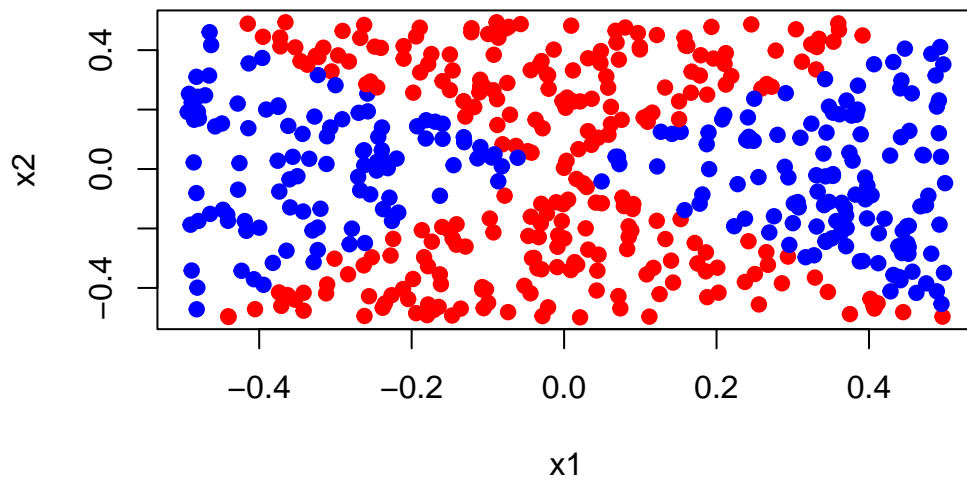
```
glm.fit2=glm(y~poly(x1,2)+poly(x2,2) ,family='binomial', data=data.frame(x1,x2,y))
```

Warning: glm.fit: algorithm did not converge

Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

f-)

```
glm.pred=predict(glm.fit2,data.frame(x1,x2))  
plot(x1,x2,col=ifelse(glm.pred>0,'blue','red'),pch=19)
```

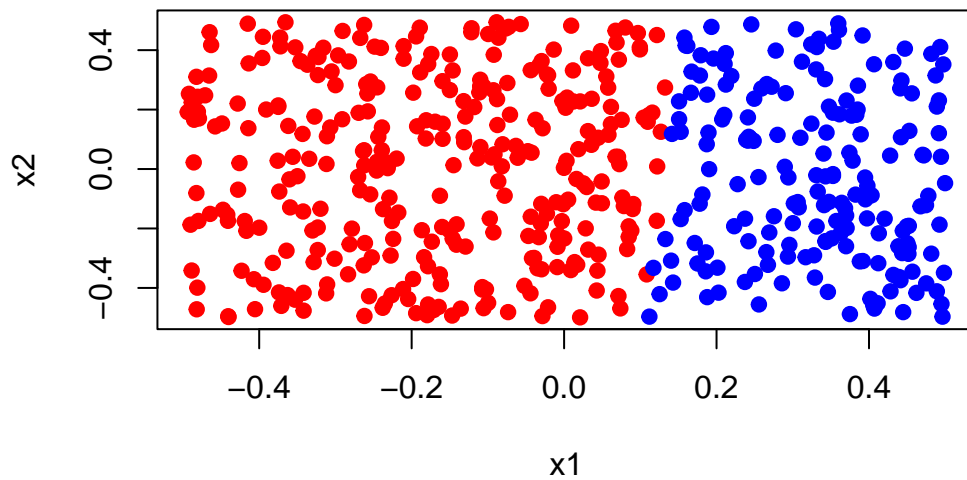


g-)

```
library(e1071)
```

Warning: package 'e1071' was built under R version 4.2.3

```
svm.fit=svm(y~.,data=data.frame(x1,x2,y=as.factor(y)),kernel='linear')
svm.pred=predict(svm.fit,data.frame(x1,x2),type='response')
plot(x1,x2,col=ifelse(svm.pred!=0,'blue','red'),pch=19)
```

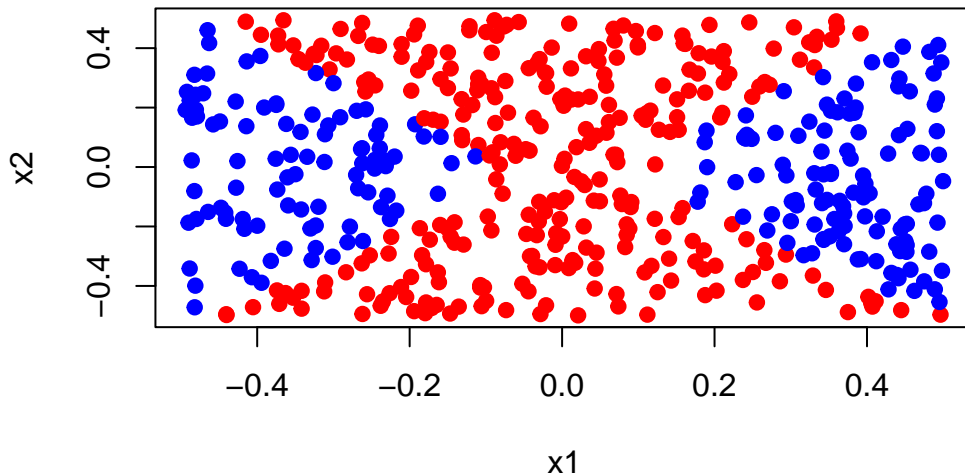


As expected, by comparing the graphs we can see this model does not do a good job, since the relation is not linear.

h-)

Let's try a polynomial of degree 2.

```
svm.fit=svm(y~.,data=data.frame(x1,x2,y=as.factor(y))
           ,kernel='polynomial',degree=2)
svm.pred=predict(svm.fit,data.frame(x1,x2),type='response')
plot(x1,x2,col=ifelse(svm.pred!=0,'blue','red'),pch=19)
```



As expected, by comparing the graphs we can see this model does not do a good job, since the relation is not linear. And we know the relationship is quadratic.

i-)

This experiment demonstrates the effectiveness of SVMs with non-linear kernels for locating non-linear boundaries. SVMs using linear kernels and logistic regression with no interactions both fall short in locating the decision boundary. Logistic regression appears to have the same power as radial-basis kernels when interaction factors are included. However, choosing the proper interaction terms requires some manual work and fine adjustment.

4. ISL Sec. 12.6: 10

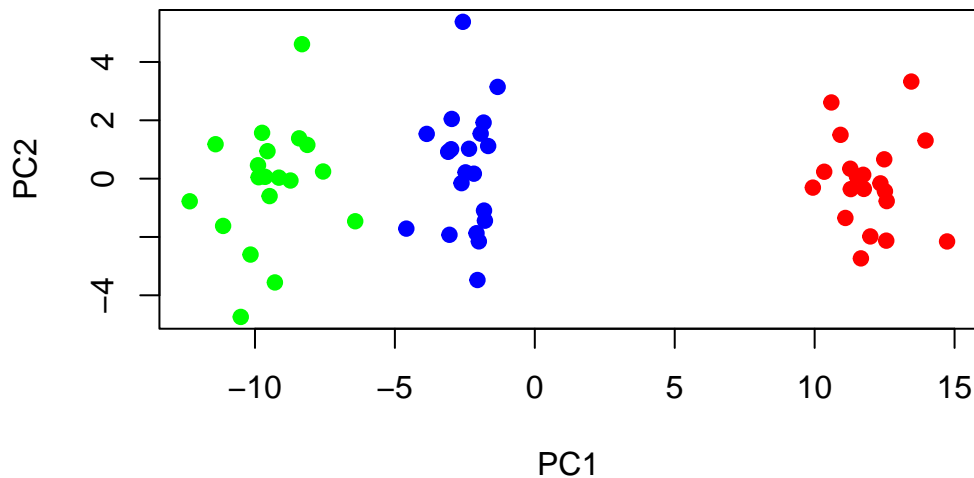
Solution:

a-)

```
data = matrix(c(rnorm(20 * 50, mean = 4),
                rnorm(20 * 50, mean = 2),
                rnorm(20 * 50, mean = 5)), ncol = 50, byrow = TRUE)
my_class <- rep(0, 60)
my_class[1:20] <- "blue"
my_class[21:40] <- "red"
my_class[41:60] <- "green"
```

b-)

```
pcs = prcomp(data)
plot(pcs$x[,1:2], col=my_class, pch=19)
```



c-)

```
kmeans.result = kmeans(data, centers=3, nstart = 100)
table(my_class, kmeans.result$cluster)
```

```
my_class  1  2  3
blue      0  0 20
green     0 20  0
red       20  0  0
```

As we can see all observations are correctly my_classified. This is expected as the observations in the three my_classes are well separated, and we happen to know that there are 3 my_classes.

d-)

```
kmeans.result = kmeans(data, centers=2, nstart = 100)
table(my_class, kmeans.result$cluster)
```

```
my_class  1  2
blue     20  0
green    20  0
red       0 20
```

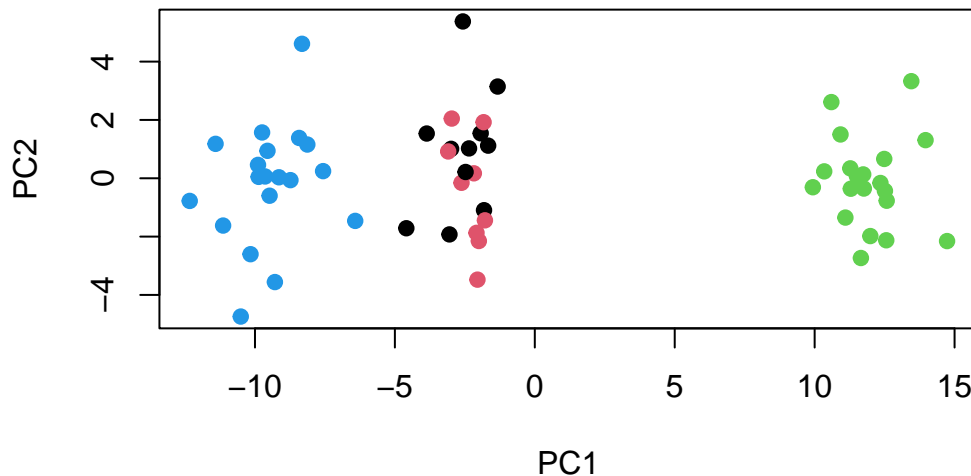
From looking at the plot of the `my_classes`, it makes sense that all the green and blue are `my_classified` together, since the distance from the red is much larger.

e-)

```
kmeans.result = kmeans(data, centers=4, nstart = 100)
table(my_class, kmeans.result$cluster)
```

```
my_class  1  2  3  4
blue    11  9  0  0
green    0  0  0 20
red      0  0 20  0
```

```
plot(pcs$x[,1:2], col=kmeans.result$cluster, pch=19)
```



Since we already knew that we had 3 `my_classes`, using 4 clusters would have divided into more clusters than necessary. And we can see that it happened. The “middle” cluster got separated into two.

f-)

```
kmeans.res2 = kmeans(pcs$x[,1:2], centers=3, nstart = 100)
table(kmeans.res2$cluster, my_class)
```

```
my_class
blue green red
```

1	20	0	0
2	0	20	0
3	0	0	20

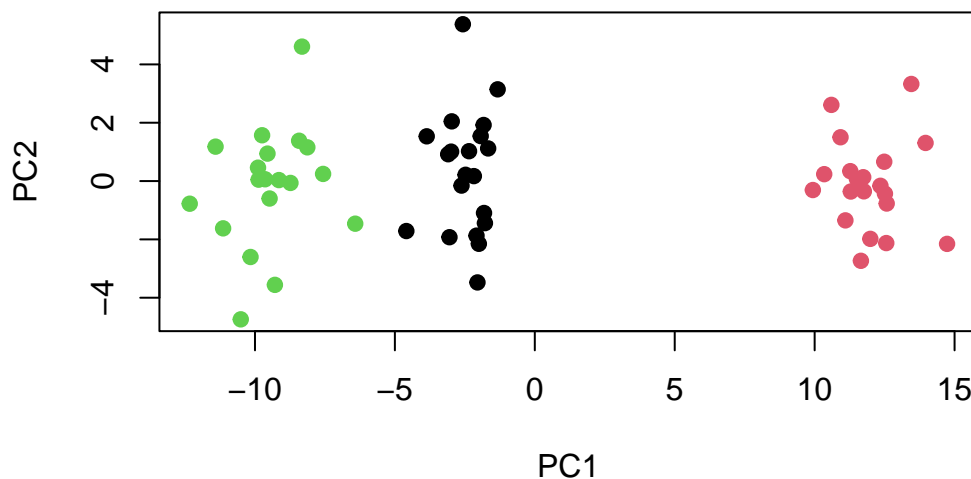
The results show that it perfectly separated the clusters.

g-)

```
kmeans.result = kmeans(scale(data), centers=3, nstart = 100)
table(my_class, kmeans.result$cluster)
```

```
my_class  1  2  3
blue    20  0  0
green    0  0 20
red      0 20  0
```

```
plot(pcs$x[,1:2], col=kmeans.result$cluster, pch=19)
```



The outcomes are the same as part (b), where the assigned clusters are flawlessly mapped to the original my_classes. Since there was no overlapping in the simulated data. However, results from data sets with overlapping observations would probably differ.

Exercises required for MSSC PhD students

None.

Optional Exercises

None.