

Statistical Learning HW 9 - Unsupervised Learning

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3 points # Extra 67 (3 points)

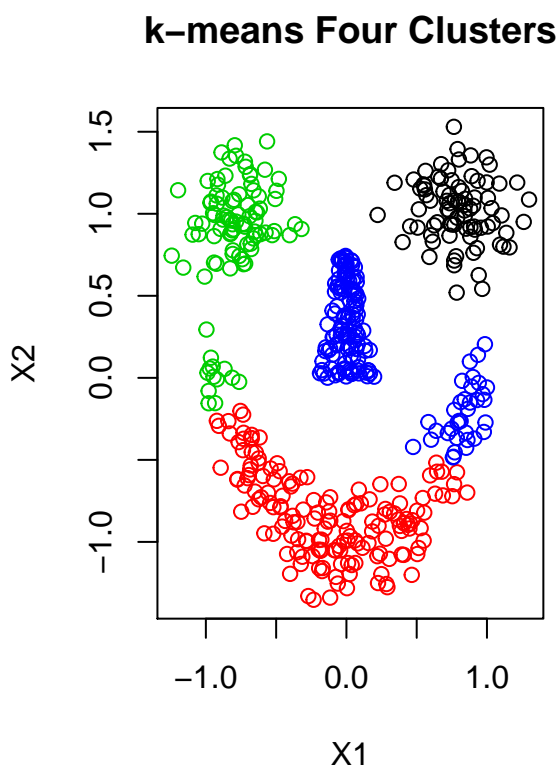
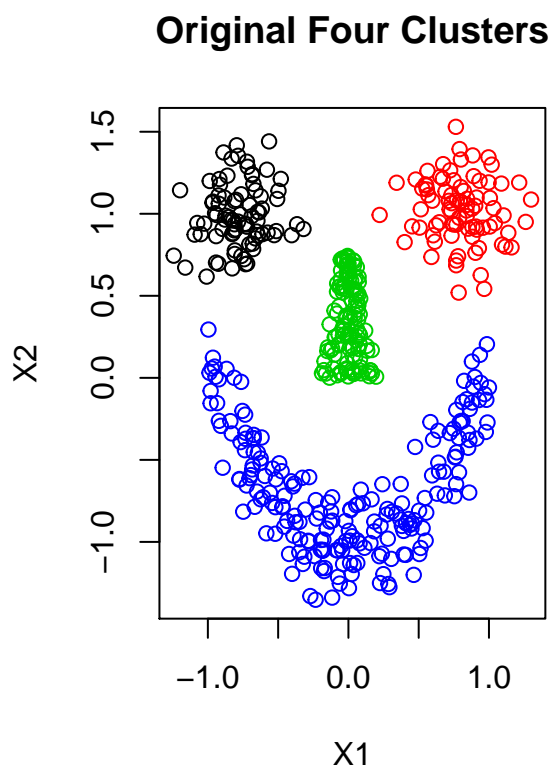
Make 500 smiley data points with $sd1 = sd2 = 0.2$.

```
set.seed(1)
smiley <- mlbench.smiley(n=500, sd1 = 0.2, sd2 = 0.2)
```

- (a) Demonstrate with a colored plot that k-means with four clusters is incapable of recovering the four original clusters exactly. Do another run of k-means and use a confusion matrix to show that the four original clusters are not recovered exactly.

```
# Run K Means
set.seed(1)
km.out <- kmeans(smiley$x,4,nstart=15)

# Set plots on same page
par(mfrow = c(1,2))
# Plot the original clusters
plot(smiley$x[,1],smiley$x[,2], col = smiley$classes, main = "Original Four Clusters", xlab = "X1", ylab = "X2")
# Plot New Clusters
plot(smiley$x[,1],smiley$x[,2], col = km.out$cluster, main = "k-means Four Clusters", xlab = "X1", ylab = "X2")
```

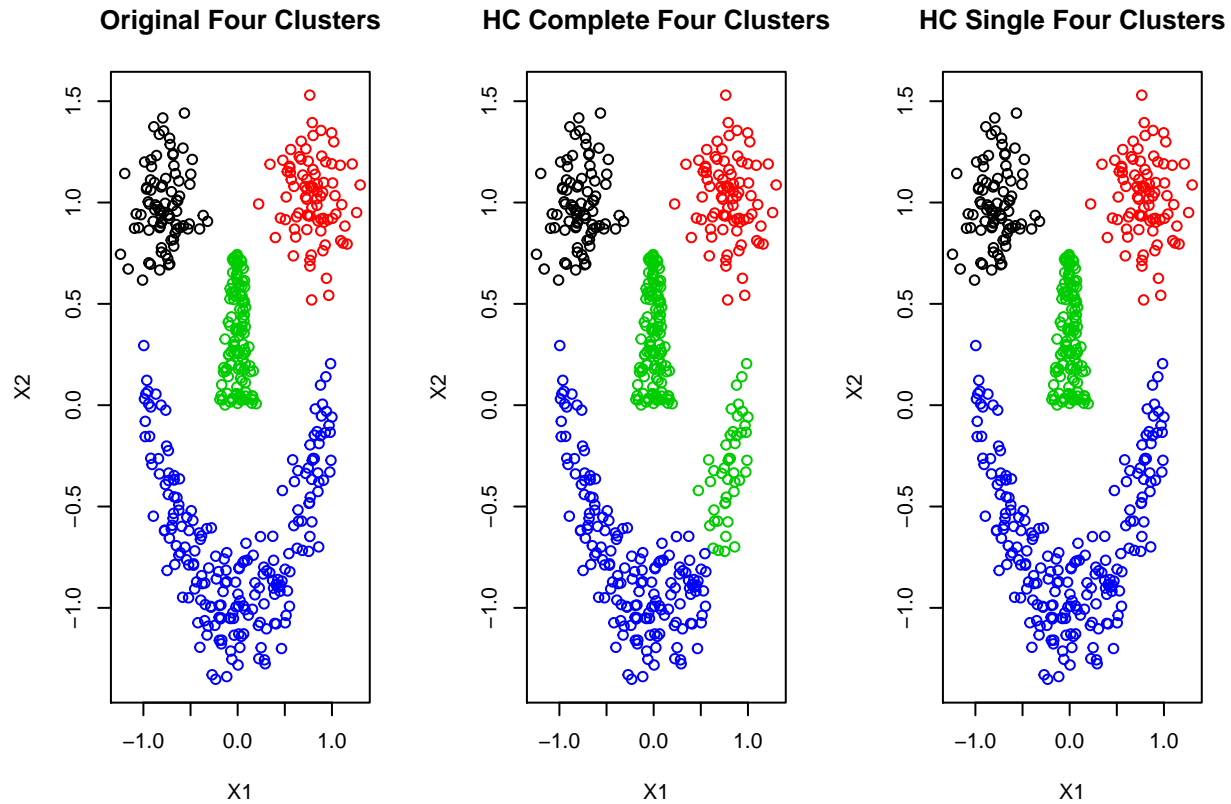


- (b) Try to use hierarchical clustering with a suitable choice of linkage to recover the four clusters. Explain your choice of linkage. Use a confusion matrix to show whether this attempt is successful.

```
# Complete Linkage
clust.complete <- hclust(dist(smiley$x),method="complete")
clust.complete.cut <- cutree(clust.complete,4)

# Complete Linkage
clust.single <- hclust(dist(smiley$x),method="single")
clust.single.cut <- cutree(clust.single,4)

# Set plots on same page
par(mfrow = c(1,3))
# Plot the original clusters
plot(smiley$x[,1],smiley$x[,2], col = smiley$classes, main = "Original Four Clusters", xlab = "X1", ylab = "X2")
# Plot HC with Complete Linkage
plot(smiley$x[,1],smiley$x[,2], col = clust.complete.cut, main = "HC Complete Four Clusters", xlab = "X1", ylab = "X2")
# Plot HC with Single Linkage
plot(smiley$x[,1],smiley$x[,2], col = clust.single.cut, main = "HC Single Four Clusters", xlab = "X1", ylab = "X2")
```



```
# For single linkage
confusionMatrix(smiley$classes, clust.single.cut)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction    1    2    3    4
##           1  83    0    0    0
```

```
##          2    0  83    0    0
##          3    0    0 125    0
##          4    0    0    0 209
##
## Overall Statistics
##
##          Accuracy : 1
##          95% CI : (0.993, 1)
##    No Information Rate : 0.418
##    P-Value [Acc > NIR] : <2e-16
##
##          Kappa : 1
##    McNemar's Test P-Value : NA
##
## Statistics by Class:
##
##          Class: 1 Class: 2 Class: 3 Class: 4
## Sensitivity      1.000    1.000    1.00    1.000
## Specificity      1.000    1.000    1.00    1.000
## Pos Pred Value   1.000    1.000    1.00    1.000
## Neg Pred Value   1.000    1.000    1.00    1.000
## Prevalence       0.166    0.166    0.25    0.418
## Detection Rate   0.166    0.166    0.25    0.418
## Detection Prevalence 0.166    0.166    0.25    0.418
## Balanced Accuracy 1.000    1.000    1.00    1.000
```

```
# For complete linkage
confusionMatrix(smiley$classes, clust.complete.cut)
```

```
## Confusion Matrix and Statistics
##
##          Reference
## Prediction  1    2    3    4
##          1  83    0    0    0
##          2   0   83    0    0
##          3   0    0 125    0
##          4   0    0  45 164
##
## Overall Statistics
##
##          Accuracy : 0.91
##          95% CI : (0.881, 0.934)
##    No Information Rate : 0.34
##    P-Value [Acc > NIR] : <2e-16
##
##          Kappa : 0.875
##    McNemar's Test P-Value : NA
##
## Statistics by Class:
##
##          Class: 1 Class: 2 Class: 3 Class: 4
## Sensitivity      1.000    1.000    0.735    1.000
## Specificity      1.000    1.000    1.000    0.866
## Pos Pred Value   1.000    1.000    1.000    0.785
## Neg Pred Value   1.000    1.000    0.880    1.000
```

## Prevalence	0.166	0.166	0.340	0.328
## Detection Rate	0.166	0.166	0.250	0.328
## Detection Prevalence	0.166	0.166	0.250	0.418
## Balanced Accuracy	1.000	1.000	0.868	0.933

Hierarchical Clustering with single linkage appears to best replicate the original clusters. Because single linkage tends to yield trailing clusters as opposed to complete linkage which yields more balanced attractive, clusters, single linkage here is better able to capture the smile part in the scatter plot.

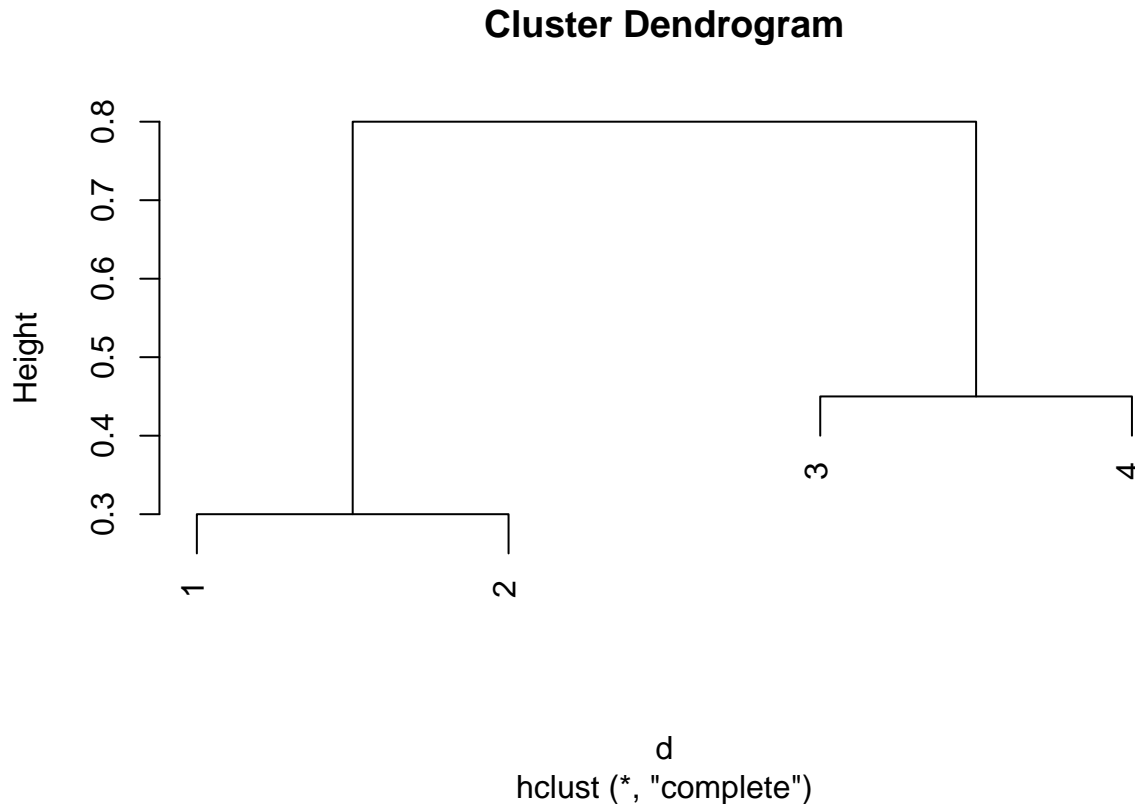
Book 2 (3 points)

Suppose that we have four observations, for which we compute a dissimilarity matrix.

For instance, the dissimilarity between the first and second observations is 0.3, and the dissimilarity between the second and fourth observations is 0.8.

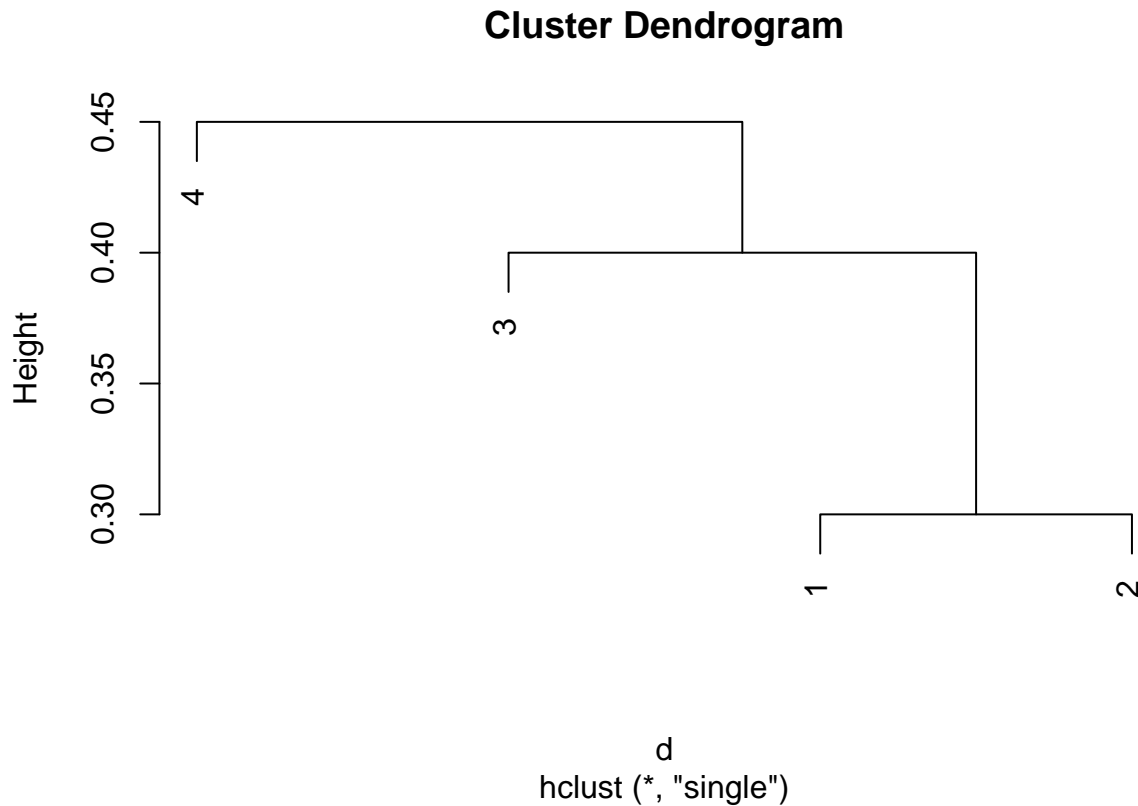
- (a) On the basis of this dissimilarity matrix, sketch the dendrogram that results from hierarchically clustering these four observations using complete linkage. Be sure to indicate on the plot the height at which each fusion occurs, as well as the observations corresponding to each leaf in the dendrogram.

```
d <- as.dist(matrix(c(0, 0.3, 0.4, 0.7,
                     0.3, 0, 0.5, 0.8,
                     0.4, 0.5, 0.0, 0.45,
                     0.7, 0.8, 0.45, 0.0), nrow = 4))
plot(hclust(d, method = "complete"))
```



- (b) Repeat (a), this time using single linkage clustering.

```
plot(hclust(d, method = "single"))
```



(c) Suppose that we cut the dendrogram obtained in (a) such that two clusters result. Which observations are in each cluster?

1 and 2 in cluster 1 and 3 and 4 in cluster 2

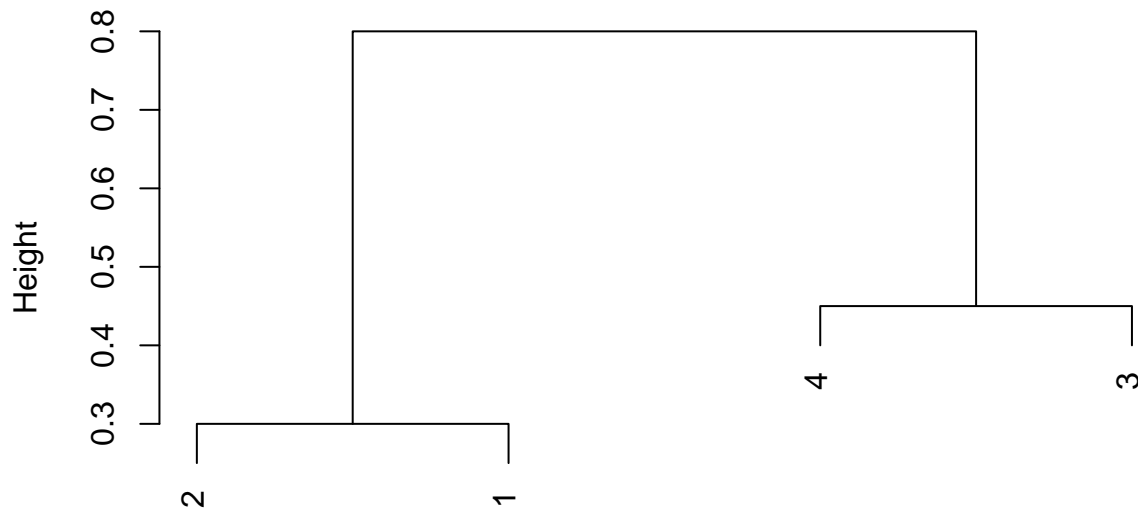
(d) Suppose that we cut the dendrogram obtained in (b) such that two clusters result. Which observations are in each cluster?

1, 2, and 3 in cluster 1 and 4 in cluster 2

(e) It is mentioned in the chapter that at each fusion in the dendrogram, the position of the two clusters being fused can be swapped without changing the meaning of the dendrogram. Draw a dendrogram that is equivalent to the dendrogram in (a), for which two or more of the leaves are repositioned, but for which the meaning of the dendrogram is the same.

```
plot(hclust(d, method = "complete"), labels = c(2,1,4,3))
```

Cluster Dendrogram



d
hclust (*, "complete")

•

Extra 72 (3 points)

Consider the concrete strength data from problem 37. There are eight numerical predictors and one numerical response. Load the data and split them into a training and test set (70% / 30%). We want to predict strength.

```
# Load in Data
concrete <- read_excel("Concrete_Data.xls")
# Clean up names
colnames(concrete) <- c("cementkg", "blustfur", "flyash", "water", "superplas", "courseagg", "fineagg",
# Create Train and Test
train <- sample(nrow(concrete), (nrow(concrete) * .70), replace = FALSE)
concrete_train <- concrete[train,]
concrete_test <- concrete[-train,]
```

- a) Compute the principal components of the matrix of predictors for the training set. Fit a linear model to predict strength from the first principal component (simple regression).

```
# Create Matrix of Predictors
x <- model.matrix(CCS ~ .-1, concrete_train)

# Compute PC
pr.out <- prcomp(x, scale=TRUE)
```

```

# Fit LM from first PC
train.data <- data.frame(CCS = concrete_train$CCS, pr.out$x)
train.data <- train.data[,1:2]
reg <- lm(CCS ~ ., data = train.data)
summary(reg)

##
## Call:
## lm(formula = CCS ~ ., data = train.data)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -31.78 -12.50  -1.38   10.24   45.40
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   36.184      0.625   57.89  <2e-16 ***
## PC1           0.812      0.413    1.97    0.05 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 16.8 on 719 degrees of freedom
## Multiple R-squared:  0.00534,    Adjusted R-squared:  0.00396
## F-statistic: 3.86 on 1 and 719 DF,  p-value: 0.0498

```

- b) Make predictions for the test set, using the same model. You have to use the loading vectors which were found from the principal component analysis of the training data.

```

test.data <- predict(pr.out, newdata = concrete_test)
test.data <- data.frame(CCS = concrete_test$CCS, test.data)
test.data <- test.data[,1:2]

predict(reg, test.data)

```

```

##      1      2      3      4      5      6      7      8      9     10     11     12     13     14     15
## 35.7 32.8 32.4 32.5 33.9 35.4 34.0 33.3 33.2 35.2 33.4 33.0 32.6 33.5 33.4
## 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30
## 32.3 35.7 33.8 35.5 35.5 33.6 33.2 34.0 36.4 36.1 38.9 37.7 37.3 36.4 36.4
## 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45
## 37.0 36.4 36.1 36.2 39.2 37.3 36.4 36.1 36.1 35.2 37.4 37.6 38.8 37.3 36.3
## 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60
## 36.9 36.3 35.1 37.5 37.3 35.2 38.9 37.4 36.0 36.1 36.8 36.5 36.2 37.7 36.2
## 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75
## 36.0 37.6 37.6 36.7 38.2 36.1 36.0 35.9 36.3 36.8 36.6 36.8 37.9 37.7 36.4
## 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90
## 36.2 36.5 37.1 37.1 37.7 37.1 38.3 38.2 38.1 37.8 38.4 38.1 38.1 38.0 37.9
## 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105
## 37.3 37.2 36.9 36.7 37.3 37.7 37.7 37.6 35.0 34.9 34.8 37.1 36.7 34.6 37.5
## 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120
## 36.9 35.6 36.2 35.8 36.3 37.8 37.9 36.4 37.8 37.3 37.9 37.5 36.6 37.5 36.3
## 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135
## 37.2 36.1 37.3 37.2 37.7 36.4 36.4 37.4 37.2 37.0 37.0 37.0 37.0 36.7 37.9
## 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150
## 37.9 37.9 35.5 35.6 35.4 36.9 37.1 36.9 36.1 36.2 36.0 36.9 37.0 36.8 37.8

```

```
## 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165
## 37.8 37.7 35.2 34.9 35.2 36.0 36.3 36.0 36.2 35.7 35.8 35.2 34.7 35.0 34.7
## 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180
## 35.4 35.7 35.6 35.7 35.4 34.9 35.0 35.4 35.4 34.8 34.2 36.0 35.9 34.7 35.8
## 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195
## 35.9 35.2 35.7 36.0 36.0 35.9 35.9 35.8 35.6 35.5 34.4 34.3 35.1 35.4 34.6
## 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210
## 35.7 36.1 35.1 35.7 36.0 35.6 35.2 34.3 35.4 34.6 34.1 35.4 35.4 35.8 35.1
## 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225
## 36.1 33.8 35.4 35.7 35.7 35.6 35.6 35.5 35.4 34.6 35.1 34.9 34.2 35.1 34.7
## 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240
## 35.5 35.1 34.5 35.6 35.6 35.7 35.7 35.4 35.6 35.0 34.3 34.0 35.2 35.6 35.5
## 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255
## 35.4 35.6 35.8 34.7 33.9 35.4 35.4 35.4 35.2 37.3 36.9 36.5 37.0 35.5 36.9
## 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270
## 36.7 36.0 35.5 37.9 36.2 36.3 36.8 35.3 36.2 37.0 36.3 36.2 37.6 36.5 37.3
## 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285
## 36.5 35.7 36.1 36.0 35.9 36.0 36.0 35.7 36.1 34.6 35.4 36.8 35.8 36.4 37.6
## 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300
## 36.8 36.0 35.8 37.4 36.6 38.1 35.7 37.1 36.5 37.2 34.9 36.5 37.7 35.4 37.1
## 301 302 303 304 305 306 307 308 309
## 36.1 36.7 36.1 36.2 37.2 34.8 36.2 36.0 36.8
```

Book 9 (5 points)

Consider the USArrests data. We will now perform hierarchical clustering on the states.

```
data('USArrests')
head(USArrests)
```

```
##           Murder Assault UrbanPop Rape
## Alabama      13.2      236      58 21.2
## Alaska       10.0      263      48 44.5
## Arizona       8.1      294      80 31.0
## Arkansas      8.8      190      50 19.5
## California    9.0      276      91 40.6
## Colorado      7.9      204      78 38.7
```

(a) Using hierarchical clustering with complete linkage and Euclidean distance, cluster the states.

```
x <- dist(USArrests)
clust.complete.euc <- hclust(x, method = "complete")
```

(b) Cut the dendrogram at a height that results in three distinct clusters. Which states belong to which clusters?

```
# Complete Linkage
clust.complete.euc.cut <- cutree(clust.complete.euc,3)
clust.complete.euc.cut
```

```
##           Alabama      Alaska      Arizona      Arkansas      California
##              1              1              1              2              1
##           Colorado Connecticut Delaware      Florida      Georgia
##              2              3              1              1              2
##           Hawaii      Idaho      Illinois      Indiana      Iowa
```


##	3	3	1	3	3
##	Kansas	Kentucky	Louisiana	Maine	Maryland
##	3	3	1	3	1
##	Massachusetts	Michigan	Minnesota	Mississippi	Missouri
##	2	1	3	1	2
##	Montana	Nebraska	Nevada	New Hampshire	New Jersey
##	3	3	1	3	2
##	New Mexico	New York	North Carolina	North Dakota	Ohio
##	1	1	1	3	3
##	Oklahoma	Oregon	Pennsylvania	Rhode Island	South Carolina
##	2	2	3	2	1
##	South Dakota	Tennessee	Texas	Utah	Vermont
##	3	2	2	3	3
##	Virginia	Washington	West Virginia	Wisconsin	Wyoming
##	2	2	3	3	2

- (c) Hierarchically cluster the states using complete linkage and Euclidean distance, after scaling the variables to have standard deviation one.

```
scaleddata <- scale(USArrests)
sx <- dist(scaleddata)
sclust.complete.euc <- hclust(sx, method = "complete")
sclust.complete.euc.cut <- cutree(sclust.complete.euc,3)
sclust.complete.euc.cut
```

##	Alabama	Alaska	Arizona	Arkansas	California
##	1	1	2	3	2
##	Colorado	Connecticut	Delaware	Florida	Georgia
##	2	3	3	2	1
##	Hawaii	Idaho	Illinois	Indiana	Iowa
##	3	3	2	3	3
##	Kansas	Kentucky	Louisiana	Maine	Maryland
##	3	3	1	3	2
##	Massachusetts	Michigan	Minnesota	Mississippi	Missouri
##	3	2	3	1	3
##	Montana	Nebraska	Nevada	New Hampshire	New Jersey
##	3	3	2	3	3
##	New Mexico	New York	North Carolina	North Dakota	Ohio
##	2	2	1	3	3
##	Oklahoma	Oregon	Pennsylvania	Rhode Island	South Carolina
##	3	3	3	3	1
##	South Dakota	Tennessee	Texas	Utah	Vermont
##	3	1	2	3	3
##	Virginia	Washington	West Virginia	Wisconsin	Wyoming
##	3	3	3	3	3

- (d) What effect does scaling the variables have on the hierarchical clustering obtained? In your opinion, should the variables be scaled before the inter-observation dissimilarities are computed? Provide a justification for your answer.

Because statistics for each category of the US Arrests data are reported differently (percent out of an amount of the population versus the number of recorded incidents), the units are different and one variable therefore may have a disproportionate affect on the inter-state dissimilarities, which in turn influences the clustering. Scaling before the dissimilarities are computed is usually best because it gives equal importance to the hierarchical clustering performed. However, this is not always the case as it may give a variable a much greater or smaller effect on the inter-observation dissimilarities obtained. It therefore depends on the application.

Extra 69 (5 points)

In this problem, you will use k-means clustering for the smiley data, for different values of $sd = sd1 = sd2$. Use 500 points and four clusters throughout.

- a) Demonstrate that for small values of sd k-means clustering recovers the four clusters in the data reasonably well. Use confusion matrices to show this.

```
sdops <- c(0.001, 0.01, 0.1, 1)

kmsds <- function(x) {
  # Generate Data
  set.seed(1)
  smiley <- mlbench.smiley(n=500, sd1 = x, sd2 = x)
  # Run K Means
  set.seed(1)
  km.out <- kmeans(smiley$x,4)
  return(confusionMatrix(smiley$classes, km.out$cluster))
}

sdtest <- lapply(sdops, kmsds)

sdtest
```

```
## [[1]]
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   1    2    3    4
##           1    0   83    0    0
##           2   83    0    0    0
##           3    0  119    0    6
##           4    0    1  123   85
##
## Overall Statistics
##
##               Accuracy : 0.17
##               95% CI : (0.138, 0.206)
##       No Information Rate : 0.406
##       P-Value [Acc > NIR] : 1
##
##               Kappa : -0.081
##  McNemar's Test P-Value : NA
##
## Statistics by Class:
##
##               Class: 1 Class: 2 Class: 3 Class: 4
## Sensitivity           0.000    0.000    0.000    0.934
## Specificity           0.801    0.721    0.668    0.697
## Pos Pred Value        0.000    0.000    0.000    0.407
## Neg Pred Value        0.801    0.513    0.672    0.979
## Prevalence            0.166    0.406    0.246    0.182
## Detection Rate        0.000    0.000    0.000    0.170
## Detection Prevalence  0.166    0.166    0.250    0.418
## Balanced Accuracy      0.400    0.360    0.334    0.815
```

```

##
## [[2]]
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  1    2    3    4
##           1    0   83    0    0
##           2   83    0    0    0
##           3    0  119    0    6
##           4    0    2  122   85
##
## Overall Statistics
##
##           Accuracy : 0.17
##           95% CI : (0.138, 0.206)
##           No Information Rate : 0.408
##           P-Value [Acc > NIR] : 1
##
##           Kappa : -0.081
##           McNemar's Test P-Value : NA
##
## Statistics by Class:
##
##           Class: 1 Class: 2 Class: 3 Class: 4
## Sensitivity           0.000    0.000    0.000    0.934
## Specificity           0.801    0.720    0.669    0.697
## Pos Pred Value        0.000    0.000    0.000    0.407
## Neg Pred Value        0.801    0.511    0.675    0.979
## Prevalence            0.166    0.408    0.244    0.182
## Detection Rate        0.000    0.000    0.000    0.170
## Detection Prevalence  0.166    0.166    0.250    0.418
## Balanced Accuracy      0.400    0.360    0.335    0.815
##
## [[3]]
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  1    2    3    4
##           1    0   83    0    0
##           2   83    0    0    0
##           3    0  119    0    6
##           4    0    7  118   84
##
## Overall Statistics
##
##           Accuracy : 0.168
##           95% CI : (0.136, 0.204)
##           No Information Rate : 0.418
##           P-Value [Acc > NIR] : 1
##
##           Kappa : -0.082
##           McNemar's Test P-Value : NA
##
## Statistics by Class:

```

```
##
##               Class: 1 Class: 2 Class: 3 Class: 4
## Sensitivity      0.000    0.000    0.000    0.933
## Specificity      0.801    0.715    0.673    0.695
## Pos Pred Value   0.000    0.000    0.000    0.402
## Neg Pred Value   0.801    0.499    0.685    0.979
## Prevalence       0.166    0.418    0.236    0.180
## Detection Rate   0.000    0.000    0.000    0.168
## Detection Prevalence 0.166    0.166    0.250    0.418
## Balanced Accuracy 0.400    0.357    0.336    0.814
##
## [[4]]
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  1    2    3    4
##           1  35  41    0    7
##           2  18  11    4   50
##           3   0 125    0    0
##           4   5   6 114   24
##
## Overall Statistics
##
##           Accuracy : 0.14
##           95% CI : (0.111, 0.174)
##           No Information Rate : 0.486
##           P-Value [Acc > NIR] : 1
##
##           Kappa : -0.112
##           McNemar's Test P-Value : NA
##
## Statistics by Class:
##
##               Class: 1 Class: 2 Class: 3 Class: 4
## Sensitivity      0.603    0.0453    0.000    0.296
## Specificity      0.891    0.7198    0.673    0.558
## Pos Pred Value   0.422    0.1325    0.000    0.115
## Neg Pred Value   0.945    0.4436    0.685    0.804
## Prevalence       0.116    0.4860    0.236    0.162
## Detection Rate   0.070    0.0220    0.000    0.048
## Detection Prevalence 0.166    0.1660    0.250    0.418
## Balanced Accuracy 0.747    0.3826    0.336    0.427
```

The accuracy as reported by the Confusion Matrices decreases as we increase the value of `sd`, proving that lower values of `sd` are better at recovering the original clusters.

- b) Show that if `sd` becomes larger, the four clusters are no longer recovered well. Find an approximate value of `sd` for which this change occurs (two decimal digits is enough), and explain how k-means clustering behaves for larger values of `sd`, using colored plots and two different examples.

```
sdops <- c(0.01, 0.06, 0.07)
```

```
kmsds <- function(s) {
  # Generate Data
  set.seed(1)
```

```

smiley <- mlbench.smiley(n=500, sd1 = s, sd2 = s)
# Run K Means
set.seed(1)
km.out <- kmeans(smiley$x,4)
return(confusionMatrix(smiley$classes, km.out$cluster))
}

```

```
sdtest <- lapply(sdops, kmsds)
```

```
sdtest
```

```

## [[1]]
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  1    2    3    4
##           1    0   83    0    0
##           2   83    0    0    0
##           3    0  119    0    6
##           4    0    2  122   85
##
## Overall Statistics
##
##               Accuracy : 0.17
##               95% CI : (0.138, 0.206)
##       No Information Rate : 0.408
##       P-Value [Acc > NIR] : 1
##
##               Kappa : -0.081
##  McNemar's Test P-Value : NA
##
## Statistics by Class:
##
##               Class: 1 Class: 2 Class: 3 Class: 4
## Sensitivity           0.000    0.000    0.000    0.934
## Specificity           0.801    0.720    0.669    0.697
## Pos Pred Value        0.000    0.000    0.000    0.407
## Neg Pred Value        0.801    0.511    0.675    0.979
## Prevalence            0.166    0.408    0.244    0.182
## Detection Rate        0.000    0.000    0.000    0.170
## Detection Prevalence  0.166    0.166    0.250    0.418
## Balanced Accuracy      0.400    0.360    0.335    0.815
##
## [[2]]
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  1    2    3    4
##           1    0   83    0    0
##           2   83    0    0    0
##           3    0  119    0    6
##           4    0    4  120   85
##
## Overall Statistics

```

```

##
##          Accuracy : 0.17
##          95% CI : (0.138, 0.206)
##    No Information Rate : 0.412
##    P-Value [Acc > NIR] : 1
##
##          Kappa : -0.081
##    McNemar's Test P-Value : NA
##
## Statistics by Class:
##
##          Class: 1 Class: 2 Class: 3 Class: 4
## Sensitivity      0.000    0.000    0.000    0.934
## Specificity      0.801    0.718    0.671    0.697
## Pos Pred Value   0.000    0.000    0.000    0.407
## Neg Pred Value   0.801    0.506    0.680    0.979
## Prevalence       0.166    0.412    0.240    0.182
## Detection Rate   0.000    0.000    0.000    0.170
## Detection Prevalence 0.166    0.166    0.250    0.418
## Balanced Accuracy 0.400    0.359    0.336    0.815
##
## [[3]]
## Confusion Matrix and Statistics
##
##          Reference
## Prediction  1    2    3    4
##          1    0   83    0    0
##          2   83    0    0    0
##          3    0  119    0    6
##          4    0    6  119   84
##
## Overall Statistics
##
##          Accuracy : 0.168
##          95% CI : (0.136, 0.204)
##    No Information Rate : 0.416
##    P-Value [Acc > NIR] : 1
##
##          Kappa : -0.082
##    McNemar's Test P-Value : NA
##
## Statistics by Class:
##
##          Class: 1 Class: 2 Class: 3 Class: 4
## Sensitivity      0.000    0.000    0.000    0.933
## Specificity      0.801    0.716    0.672    0.695
## Pos Pred Value   0.000    0.000    0.000    0.402
## Neg Pred Value   0.801    0.501    0.683    0.979
## Prevalence       0.166    0.416    0.238    0.180
## Detection Rate   0.000    0.000    0.000    0.168
## Detection Prevalence 0.166    0.166    0.250    0.418
## Balanced Accuracy 0.400    0.358    0.336    0.814

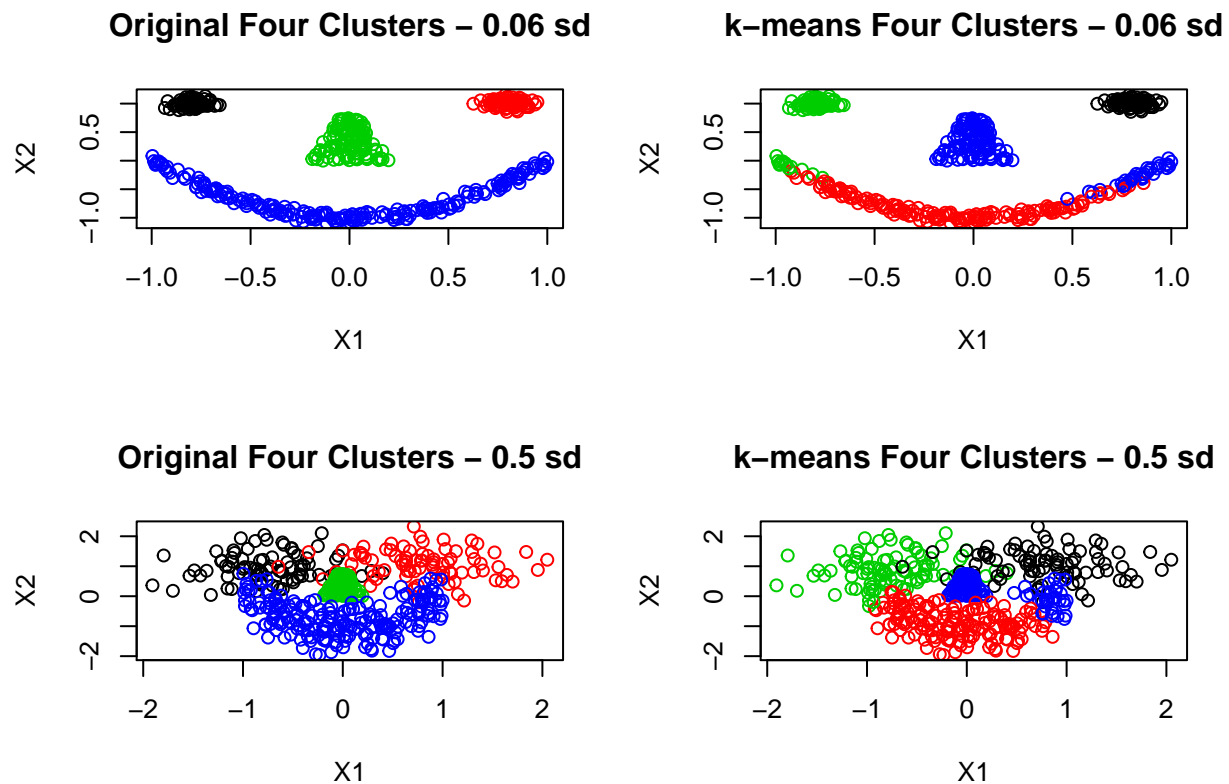
```

```

par(mfrow = c(2,2))
# Generate Data at sd of 0.06
set.seed(1)
smiley <- mlbench.smiley(n=500, sd1 = 0.06, sd2 = 0.06)
# Plot the original clusters at sd of 0.06
plot(smiley$x[,1],smiley$x[,2], col = smiley$classes, main = "Original Four Clusters - 0.06 sd", xlab = "X1", ylab = "X2")
# Plot New Clusters at sd of 0.06
plot(smiley$x[,1],smiley$x[,2], col = km.out$cluster, main = "k-means Four Clusters - 0.06 sd", xlab = "X1", ylab = "X2")

# Generate Data at sd of 0.07
set.seed(1)
smiley <- mlbench.smiley(n=500, sd1 = 0.5, sd2 = 0.5)
# Plot the original clusters at sd of 0.07
plot(smiley$x[,1],smiley$x[,2], col = smiley$classes, main = "Original Four Clusters - 0.5 sd", xlab = "X1", ylab = "X2")
# Plot New Clusters at sd of 0.07
plot(smiley$x[,1],smiley$x[,2], col = km.out$cluster, main = "k-means Four Clusters - 0.5 sd", xlab = "X1", ylab = "X2")

```



We start to see the accuracy decline in moving from an sd of 0.06 to an sd of 0.07. To make the point that the accuracy declines for larger sds, we use plots to exaggerate this trend.

Extra 71 (5 points)

This problem uses the MNIST image classification data, available as `mnist_all.RData` that were used earlier. We use the training data only for all digits. Extract the training data and place them in suitable data frames.

```
mnist <- load('mnist_all.RData')
```

```
mnist_train <- data.frame(train$x, train$y)
```

a) Apply k-means clustering with two clusters. Can you tell which digits tend to be clustered together?

```
km.out <- kmeans(mnist_train$train.y, 2, nstart=25)
```

```
mnist_train$cluster <- km.out$cluster
```

```
clustertabs <- mnist_train %>%
```

```
  group_by(train.y) %>%
```

```
  dplyr::summarize(Cluster = mean(cluster))
```

```
clustertabs
```

```
## # A tibble: 10 x 2
```

```
##   train.y Cluster
```

```
##   <int>   <dbl>
```

```
## 1      0      1
```

```
## 2      1      1
```

```
## 3      2      1
```

```
## 4      3      1
```

```
## 5      4      1
```

```
## 6      5      2
```

```
## 7      6      2
```

```
## 8      7      2
```

```
## 9      8      2
```

```
## 10     9      2
```

The first 5 digits chronologically were put in cluster 1 and the next 5 in cluster 2.

b) Apply k-means clustering with 10 clusters. How well do the cluster labels agree with the actual digits labels? Use a confusion matrix to answer this question.

```
km.out <- kmeans(mnist_train$train.y, 10, nstart=25)
```

```
mnist_train$cluster <- km.out$cluster
```

```
# Mismatch due to the existence of the digit 0 and cluster 10 - Eliminate those two levels and compare
mnist_train2 <- mnist_train[mnist_train$train.y != 0 | mnist_train$cluster != 10,]
```

```
# Confusion Matrix - Done manually because there is at least one number that is not predicted
table(factor(mnist_train2$cluster, levels=min(mnist_train2$train.y):max(mnist_train2$train.y)),
      factor(mnist_train2$train.y, levels=min(mnist_train2$train.y):max(mnist_train2$train.y)))
```

```
##
```

```
##      0      1      2      3      4      5      6      7      8      9
```

```
## 0      0      0      0      0      0      0      0      0      0
```

```
## 1      0      0      0      0      0      0      0 6265      0      0
```

```
## 2      0      0      0      0      0      0      0      0 5949      0
```

```
## 3 5923      0      0      0      0      0      0      0      0      0
```

```
## 4      0      0      0      0      0 5421      0      0      0      0
```

```
## 5      0      0      0 6131      0      0      0      0      0      0
```

```
## 6      0      0 5958      0      0      0      0      0      0      0
```

```
## 7      0      0      0      0      0      0      0      0 5851      0
```

```
## 8      0      0      0      0 5842      0      0      0      0      0
```

```
## 9      0 6742      0      0      0      0      0      0      0      0
```



```
# Accuracy
sum(mnist_train2$cluster == mnist_train2$train.y) / nrow(mnist_train2)
```

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

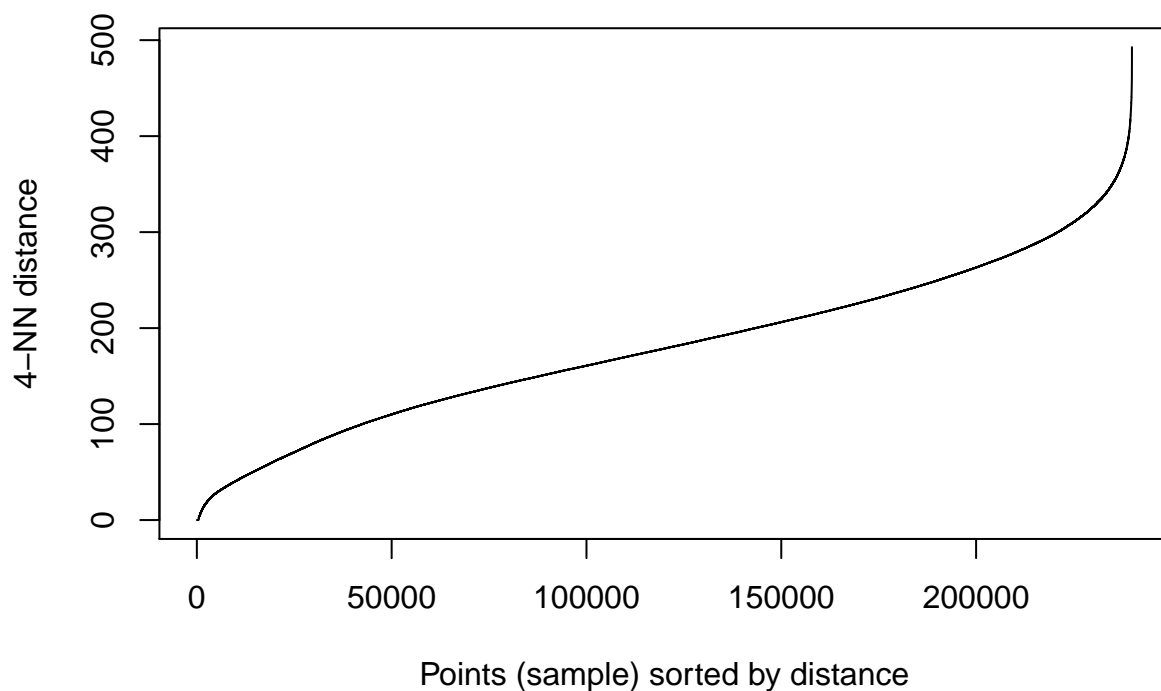
Accuracy is 0.0992, which is not great.

- c) Apply dbSCAN clustering, with suitable choices of ϵ and \minPts obtained from a k-nearest neighbor plot. Justify your choices. Then determine how well the cluster labels agree with the actual digit labels, using a confusion matrix.

```
# Downsample to decrease kNNdistplot runtime
downsamp <- seq(1, ncol(mnist_train), 16)
train2 <- mnist_train[ downsamp]
names(train2)
```

```
## [1] "X1"      "X17"     "X33"     "X49"     "X65"     "X81"     "X97"
## [8] "X113"    "X129"    "X145"    "X161"    "X177"    "X193"    "X209"
## [15] "X225"    "X241"    "X257"    "X273"    "X289"    "X305"    "X321"
## [22] "X337"    "X353"    "X369"    "X385"    "X401"    "X417"    "X433"
## [29] "X449"    "X465"    "X481"    "X497"    "X513"    "X529"    "X545"
## [36] "X561"    "X577"    "X593"    "X609"    "X625"    "X641"    "X657"
## [43] "X673"    "X689"    "X705"    "X721"    "X737"    "X753"    "X769"
## [50] "train.y"
```

```
kNNdistplot(as.matrix(train2[, -50]), k=4)
```



```
dbSCAN_clust <- dbSCAN(as.matrix(train2[, -50]), eps=300)
```

```
# Mismatch due to the existence of the digit 0 and cluster 10 - Eliminate those two levels and compare
#mnist_train2 <- mnist_train[mnist_train$train.y != 0 | mnist_train$cluster != 10,]
```

```
# Confusion Matrix - Done manually because there is at least one number that is not predicted
table(factor(dbscan_clust$cluster, levels=min(train2$train.y):max(train2$train.y)),
      factor(train2$train.y, levels=min(train2$train.y):max(train2$train.y)))
```

```
##
##      0      1      2      3      4      5      6      7      8      9
## 0  372    11   829   488   206   399   200    98   539   149
## 1 5548  6731  5119  5640  5636  5016  5718  6162  5312  5800
## 2     0     0     0     0     0     0     0     5     0     0
## 3     0     0     5     0     0     0     0     0     0     0
## 4     3     0     0     0     0     1     0     0     0     0
## 5     0     0     0     0     0     4     0     0     0     0
## 6     0     0     0     3     0     1     0     0     0     0
## 7     0     0     5     0     0     0     0     0     0     0
## 8     0     0     0     0     0     0     0     0     0     0
## 9     0     0     0     0     0     0     0     0     0     0
```

```
# Accuracy
sum(dbscan_clust$cluster == train2$train.y) / nrow(train2)
```

```
## [1] 0.118
```

The kink in the 4-NN distance plot appears to be located approximately at 300, so we use this for eps. We find an accuracy of 0.118.