Class 08 Mini Project

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Exploratory Data Analysis

```
#read.csv("https://bioboot.github.io/bimm143_S20/class-material
```

```
fna.data <- read.csv("https://bioboot.github.io/bimm143_S20/ la


#Save input data file into project directory

wisc.df <- data.frame(fna.data, row.names=1)

head(wisc.df)
```

```
         diagnosis radius_mean texture_mean perimeter_mean
area_mean
842302           M       17.99        10.38         122.80
1001.0
842517           M       20.57        17.77         132.90
1326.0
84300903         M       19.69        21.25         130.00
1203.0
84348301         M       11.42        20.38          77.58
386.1
84358402         M       20.29        14.34         135.10
1297.0
843786           M       12.45        15.70          82.57
477.1
         smoothness_mean compactness_mean concavity_mean
concave.points_mean
842302           0.11840          0.27760         0.3001
0.14710
842517           0.08474          0.07864         0.0869
0.07017
84300903         0.10960          0.15990         0.1974
0.12790
84348301         0.14250          0.28390         0.2414
```

```
0.10520
84358402         0.10030          0.13280         0.1980
0.10430
843786           0.12780          0.17000         0.1578
0.08089
         symmetry_mean fractal_dimension_mean radius_se
texture_se perimeter_se
842302           0.2419               0.07871    1.0950
0.9053        8.589
842517           0.1812               0.05667    0.5435
0.7339        3.398
84300903         0.2069               0.05999    0.7456
0.7869        4.585
84348301         0.2597               0.09744    0.4956
1.1560        3.445
84358402         0.1809               0.05883    0.7572
0.7813        5.438
843786           0.2087               0.07613    0.3345
0.8902        2.217
         area_se smoothness_se compactness_se concavity_se
concave.points_se
842302    153.40      0.006399        0.04904      0.05373
0.01587
842517     74.08      0.005225        0.01308      0.01860
0.01340
84300903   94.03      0.006150        0.04006      0.03832
0.02058
84348301   27.23      0.009110        0.07458      0.05661
0.01867
84358402   94.44      0.011490        0.02461      0.05688
0.01885
843786     27.19      0.007510        0.03345      0.03672
0.01137
         symmetry_se fractal_dimension_se radius_worst
texture_worst
842302       0.03003             0.006193        25.38
17.33
842517       0.01389             0.003532        24.99
23.41
84300903     0.02250             0.004571        23.57
25.53
84348301     0.05963             0.009208        14.91
26.50
84358402     0.01756             0.005115        22.54
16.67
```

```
843786       0.02165             0.005082        15.47
23.75
         perimeter_worst area_worst smoothness_worst
compactness_worst
842302            184.60     2019.0           0.1622
0.6656
842517            158.80     1956.0           0.1238
0.1866
84300903          152.50     1709.0           0.1444
0.4245
84348301           98.87      567.7           0.2098
0.8663
84358402          152.20     1575.0           0.1374
0.2050
843786            103.40      741.6           0.1791
0.5249
         concavity_worst concave.points_worst symmetry_worst
842302            0.7119               0.2654         0.4601
842517            0.2416               0.1860         0.2750
84300903          0.4504               0.2430         0.3613
84348301          0.6869               0.2575         0.6638
84358402          0.4000               0.1625         0.2364
843786            0.5355               0.1741         0.3985
         fractal_dimension_worst
842302                   0.11890
842517                   0.08902
84300903                 0.08758
84348301                 0.17300
84358402                 0.07678
843786                   0.12440
```

```
#Remove the 1st column
wisc.data <- wisc.df[,-1]

#Create diagnosis factor for later
diagnosis <- as.factor(wisc.df[,1])
```

> Q1. How many observations are in this dataset?

```
nrow(wisc.data) #number of observations
```

```
[1] 569
```

> Q2. How many of the observations have a malignant diagnosis?

212 observations

```
table(wisc.df$diagnosis) #numbers of benign and malignant dia
        gnoses
```

```
  B   M
357 212
```

> Q.3 How many variables/features in the data are suffixed with _mean?

```
#colnames(wisc.df)
length(
grep("_mean", colnames(wisc.df))) #Number of column names wit
        h "_mean"
```

```
[1] 10
```

Principal Component Analysis

First, we need to consider whether the data needs “scaling” to make our comparison fair.

Yes, we need to scale because the means of the columns are very different.

```
# Check column means and standard deviations
colMeans(wisc.data)
```

```
            radius_mean            texture_mean
perimeter_mean
           1.412729e+01            1.928965e+01
9.196903e+01
              area_mean         smoothness_mean
compactness_mean
           6.548891e+02            9.636028e-02
1.043410e-01
```

```
         concavity_mean     concave.points_mean
symmetry_mean
           8.879932e-02            4.891915e-02
1.811619e-01
 fractal_dimension_mean               radius_se
texture_se
           6.279761e-02            4.051721e-01
1.216853e+00
           perimeter_se                 area_se
smoothness_se
           2.866059e+00            4.033708e+01
7.040979e-03
         compactness_se            concavity_se
concave.points_se
           2.547814e-02            3.189372e-02
1.179614e-02
            symmetry_se    fractal_dimension_se
radius_worst
           2.054230e-02            3.794904e-03
1.626919e+01
          texture_worst         perimeter_worst
area_worst
           2.567722e+01            1.072612e+02
8.805831e+02
       smoothness_worst       compactness_worst
concavity_worst
           1.323686e-01            2.542650e-01
2.721885e-01
   concave.points_worst          symmetry_worst
fractal_dimension_worst
           1.146062e-01            2.900756e-01
8.394582e-02
```

```
apply(wisc.data,2,sd)
```

```
            radius_mean            texture_mean
perimeter_mean
           3.524049e+00            4.301036e+00
2.429898e+01
              area_mean         smoothness_mean
compactness_mean
           3.519141e+02            1.406413e-02
5.281276e-02
         concavity_mean     concave.points_mean
```

```
symmetry_mean
          7.971981e-02            3.880284e-02
2.741428e-02
 fractal_dimension_mean               radius_se
texture_se
          7.060363e-03            2.773127e-01
5.516484e-01
          perimeter_se                 area_se
smoothness_se
          2.021855e+00            4.549101e+01
3.002518e-03
         compactness_se            concavity_se
concave.points_se
          1.790818e-02            3.018606e-02
6.170285e-03
           symmetry_se    fractal_dimension_se
radius_worst
          8.266372e-03            2.646071e-03
4.833242e+00
         texture_worst         perimeter_worst
area_worst
          6.146258e+00            3.360254e+01
5.693570e+02
       smoothness_worst       compactness_worst
concavity_worst
          2.283243e-02            1.573365e-01
2.086243e-01
   concave.points_worst          symmetry_worst
fractal_dimension_worst
          6.573234e-02            6.186747e-02
1.806127e-02
```

```
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp(wisc.data, scale=TRUE)
```

```
# Look at summary of results
y <- summary(wisc.pr)
attributes(y)
```

```
$names
[1] "sdev"       "rotation"   "center"     "scale"      "x"
[6] "importance"
```

```
$class
[1] "summary.prcomp"
```

> Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)?

44.27%

> Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

3 PCs

```
which(y$importance[3,] >= 0.7) [1]
```

```
PC3
  3
```

> Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

7 PCs

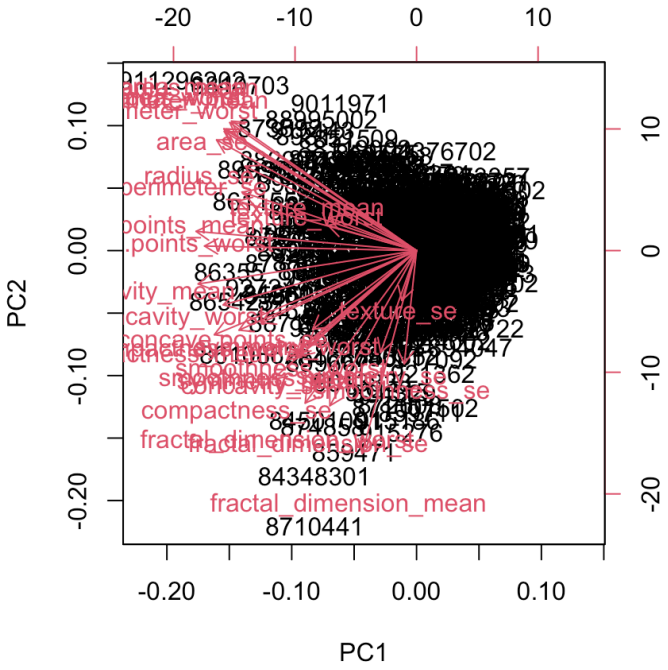
```
which(y$importance[3,] >= 0.90) [1]
```

```
PC7
  7
```

Interpreting PCA results

Making a biplot of the data

```
biplot(wisc.pr)
```

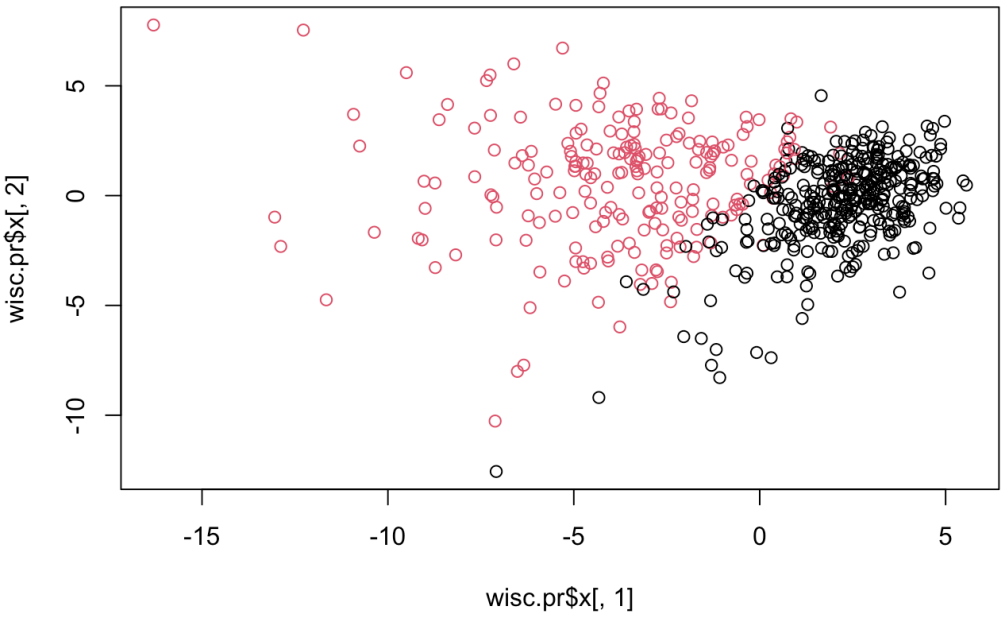


> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

No patterns stand out, because this graph is too messy and difficult to understand.

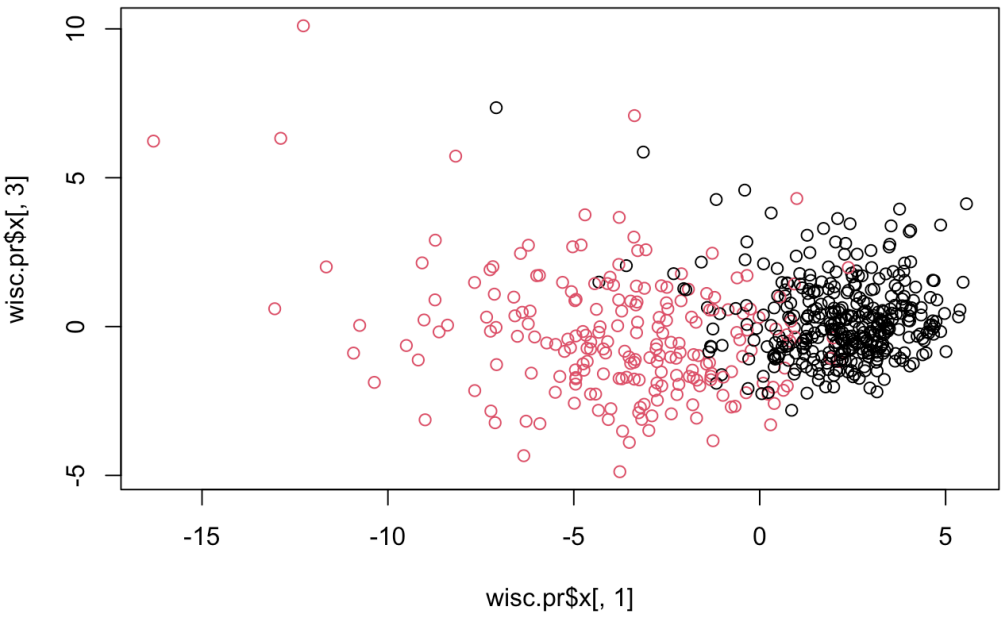
Let's make a PC plot (a.k.a. "score plot" or "PC1 vs PC2" plot)

```
plot(wisc.pr$x[,1], wisc.pr$x[,2], col=diagnosis)
```



> Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

```
plot(wisc.pr$x[,1], wisc.pr$x[,3], col=diagnosis)
```

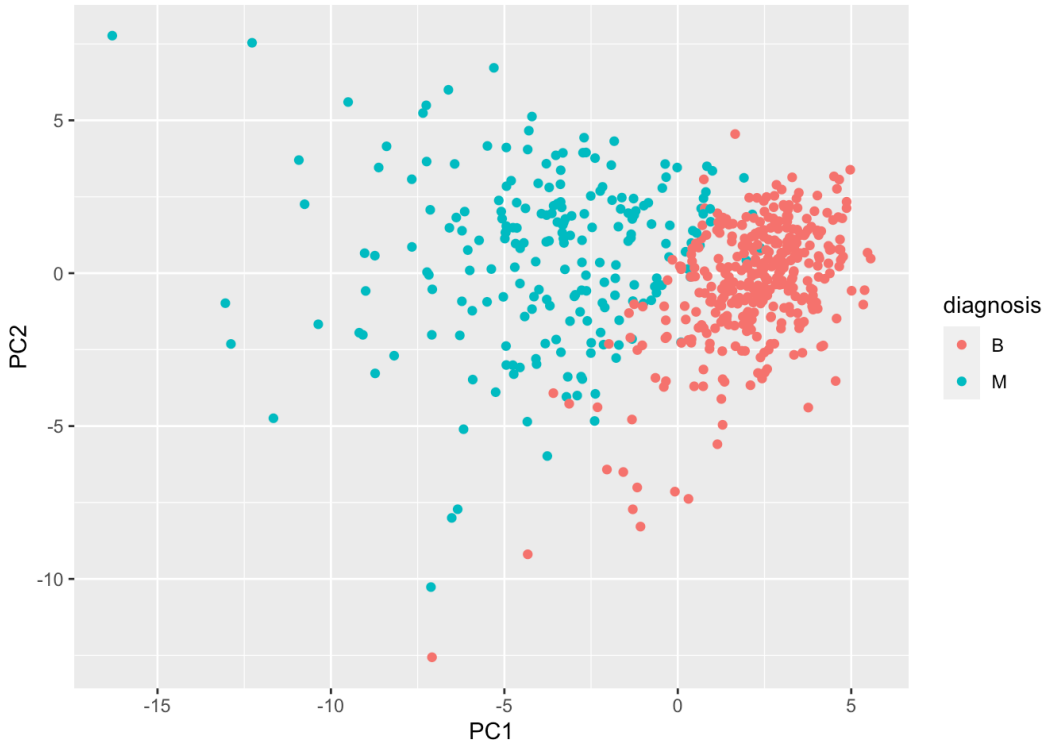


These plots show that there is a clear separation between the sequences for malignant and benign tumors, as shown by the clear division between the areas of red (malignant) and black (benign) data points.

```
# Create a data.frame for ggplot
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis

# Load the ggplot2 package
library(ggplot2)

# Make a scatter plot colored by diagnosis
ggplot(df) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point()
```

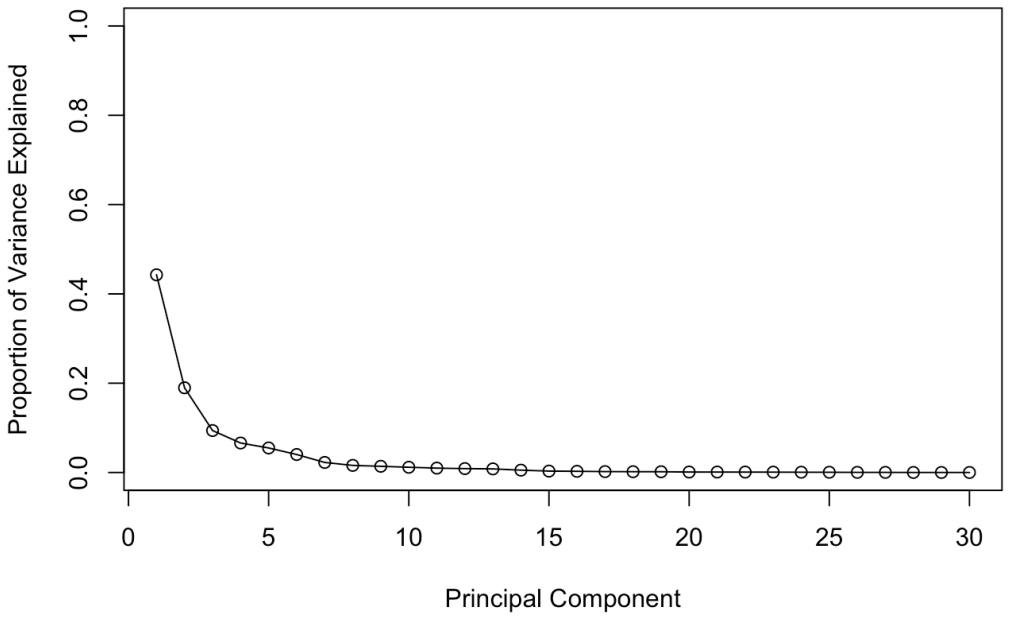



```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731
1.207357
```

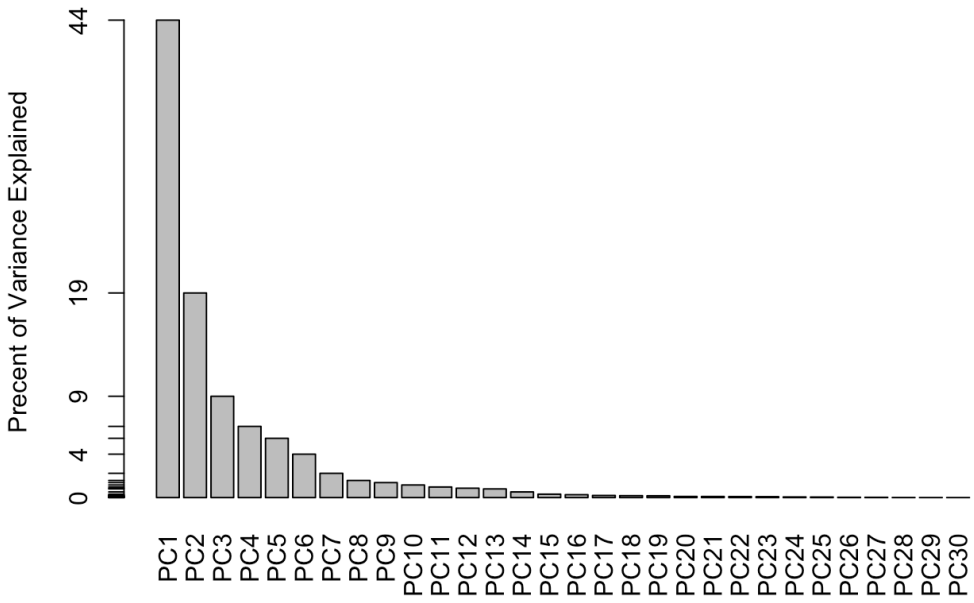
```
# Variance explained by each principal component: pve
pve <- pr.var / sum(pr.var)

# Plot variance explained for each principal component
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```




```
# Alternative scree plot of the same data, note data driven y-a

barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALS
        E)
axis(2, at=pve, labels=round(pve,2)*100 )
```



> Q9. For the first principal component, what is the component of the loading vector (i.e. wisc.pr$rotation[,1]) for the feature concave.points_mean?

-0.26085376

```
#wisc.pr$rotation[,1]
```

> Q10. What is the minimum number of principal components required to explain 80% of the variance of the data?

```
which(y$importance[3,] >= 0.80) [1]
```

```
PC5
  5
```

#Hierarchical Clustering

```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
```

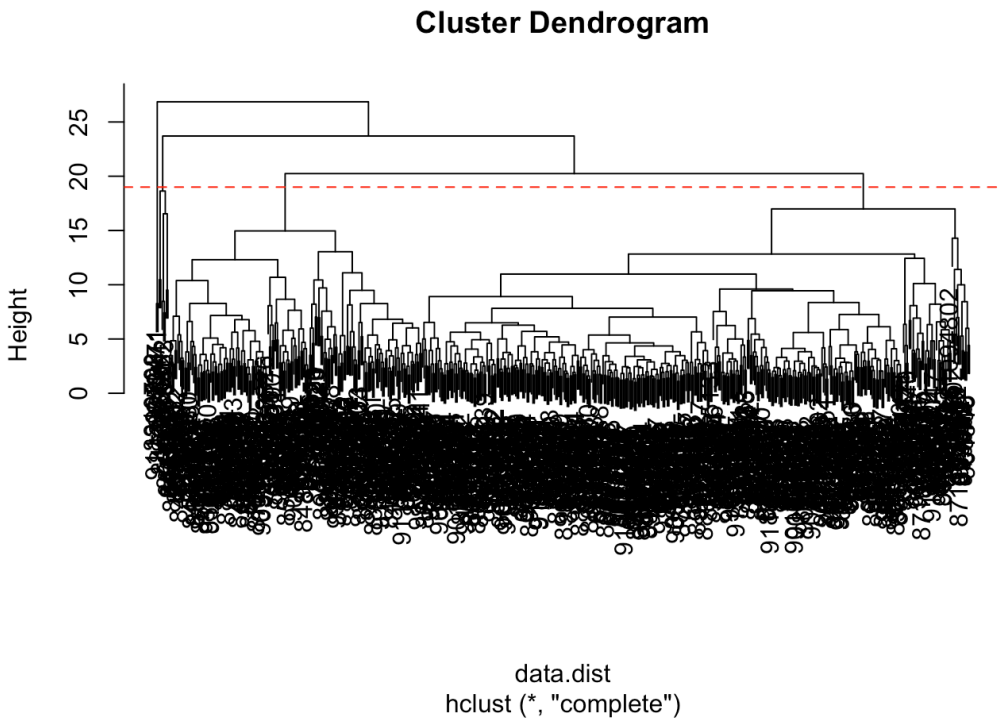
```
data.dist <- dist(data.scaled)
```

```
wisc.hclust <- hclust(data.dist)
```

> Q11. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

The height is 19.

```
plot(wisc.hclust)
abline(a=19, b=0, col="red", lty=2 )
```




```
wisc.hclust.clusters <- cutree(wisc.hclust, k=4) #Cut into the


table(wisc.hclust.clusters, diagnosis)
```

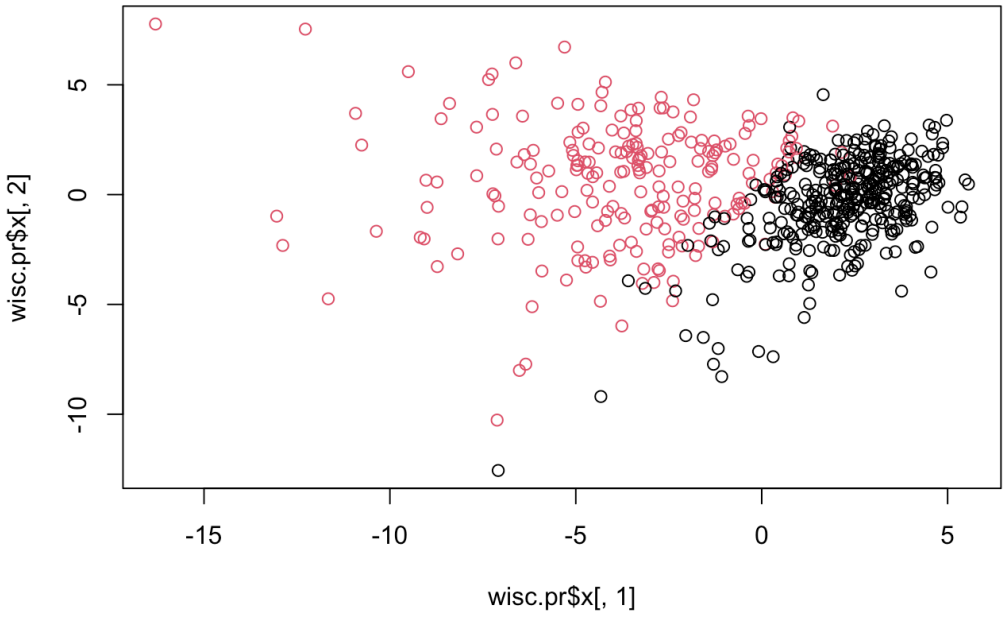
```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   2   5
```

```
  3 343  40
  4   0   2
```

Combine PCA with clustering

I want to cluster in "PC space"

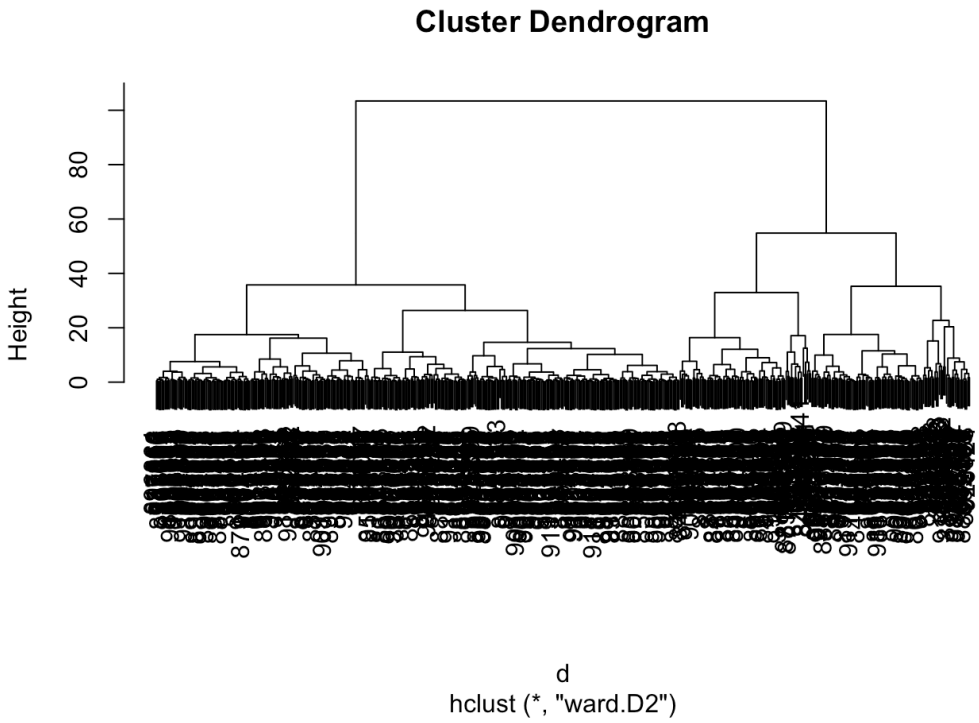
```
plot(wisc.pr$x[,1], wisc.pr$x[,2], col=diagnosis)
```




```
#wisc.pr$x #Patients on each PC
```

The 'hclust()' function wants a distance matrix as input...

```
d <- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <- hclust(d, method = "ward.D2")
plot(wisc.pr.hclust)
```



> Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

Yes, cut into 2 clusters.

Find my patient's membership vector with the 'cutree()' function.

```
grps <- cutree(wisc.pr.hclust, k=2)

table(grps)
```

```
grps
  1   2
203 366
```

```
table(diagnosis, grps)
```

```
         grps
diagnosis   1   2
        B  24 333
        M 179  33
```

Can see potential misdiagnoses and false positives from this table.

> Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

'ward.D2' is my favorite method because it results in the clearest clustering with more distinct groups than the other methods.

> Q14.

```
wisc.km <- kmeans(wisc.data, centers= 2, nstart= 20)
```

> Q15. How well does the newly created model with four clusters separate out the two diagnoses?

The newly created model separates out the two diagnoses better than the kmeans; the majority of the malignant cases are in the 1st cluster while the majority of the benign cases are in the 3rd cluster. However, this sorting is not completely inefficient data was misclassified and sorted into 4 instead of 2 groups.

```
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
table(wisc.pr.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.pr.hclust.clusters   B   M
                      1  24 179
                      2 333  33
```

> Q16. How well do the k-means and hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.km$cluster and wisc.hclust.clusters) with the vector containing the actual diagnoses.

k-means and the hierarchical clusters were not as effective at separating the diagnoses. K-means did not separate the diagnoses efficiently, as there was only 1 benign tumor with 130 malignant ones, while there were

82 malignant tumors with 356 benign ones. These 82 malignant tumors were misclassified as benign. Meanwhile, the pre-PCA hierarchical clustering sorted the data into 4 different groups (not the 2 that we expect). Meanwhile, the PCA clustering sorted the data into 2 clear groups.

```
table(wisc.km$cluster,diagnosis) #kmeans
```

```
   diagnosis
      B   M
  1 356  82
  2   1 130
```

```
table(wisc.hclust.clusters, diagnosis) #hierarchical
```

```
                   diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   2   5
                   3 343  40
                   4   0   2
```

```
table(wisc.pr.hclust.clusters, diagnosis) #pca
```

```
                      diagnosis
wisc.pr.hclust.clusters   B   M
                      1  24 179
                      2 333  33
```

> Q17. Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

The PCA analysis resulted in the most specificity, while the Kmeans analysis resulted in the highest sensitivity.

```
#Sensitivity
kmeans <- 130/(130 + 82)
kmeans
```

```
[1] 0.6132075
```

```
hclust <- 165/(165+5+40+2)
hclust
```

```
[1] 0.7783019
```

```
PCAclust <- 179/(179+33)
PCAclust
```

```
[1] 0.8443396
```

```
#Specificity
kmeanss <- 356/(356+1)
hclusts <- 343/(343+12+2)
PCAclusts <- 333/(333+24)

kmeanss
```

```
[1] 0.9971989
```

```
hclusts
```

```
[1] 0.9607843
```

```
PCAclusts
```

```
[1] 0.9327731
```

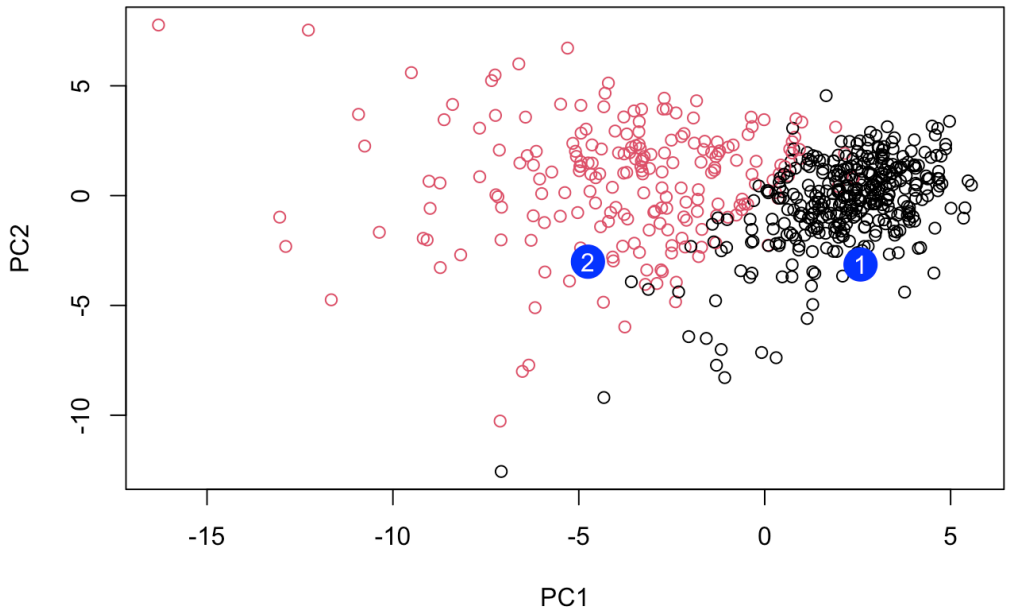
Prediction

```
#url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
npc
```

```
          PC1       PC2        PC3        PC4       PC5
PC6        PC7
[1,]  2.576616 -3.135913  1.3990492 -0.7631950  2.781648
-0.8150185 -0.3959098
[2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698
```

```
-1.2189945  0.8193031
            PC8        PC9        PC10       PC11       PC12
PC13     PC14
[1,] -0.2307350 0.1029569 -0.9272861 0.3411457  0.375921
0.1610764 1.187882
[2,] -0.3307423 0.5281896 -0.4855301 0.7173233 -1.185917
0.5893856 0.303029
          PC15       PC16        PC17        PC18        PC19
PC20
[1,] 0.3216974 -0.1743616 -0.07875393 -0.11207028 -0.08802955
-0.2495216
[2,] 0.1299153  0.1448061 -0.40509706  0.06565549  0.25591230
-0.4289500
           PC21       PC22       PC23       PC24        PC25
PC26
[1,]  0.1228233 0.09358453 0.08347651  0.1223396  0.02124121
0.078884581
[2,] -0.1224776 0.01732146 0.06316631 -0.2338618 -0.20755948
-0.009833238
             PC27        PC28         PC29         PC30
[1,]  0.220199544 -0.02946023 -0.015620933  0.005269029
[2,] -0.001134152  0.09638361  0.002795349 -0.019015820
```

```
plot(wisc.pr$x[,1:2], col=diagnosis)
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



> Q.18 Which of these new patients should we prioritize for follow up based on your results?

Patient 2