BIMM 143 Class 08: Mini Project

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Background

In today's class, we will apply the methods of clustering techniques and PCA to make sense of a real-world breast cancer FNA biopsy data.

Setting up the data frame with `read.csv()` to read the csv file. Don't forget set the FIRST column as the name with `row.name=T` because we don't want the first column to be read as numeric.

```
fna.data <- "WisconsinCancer.csv"
wisc.df <- read.csv(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
```

We want to omit the `diagnosis` column because that gives away the answer. To do this, use the code ‘df[,-1]. Name this new data frame.

```
wisc.data <- wisc.df[,-1]
head(wisc.data)
```

```
         radius_mean texture_mean perimeter_mean area_mean smoothness_mean
842302         17.99        10.38         122.80    1001.0         0.11840
842517         20.57        17.77         132.90    1326.0         0.08474
84300903       19.69        21.25         130.00    1203.0         0.10960
84348301       11.42        20.38          77.58     386.1         0.14250
84358402       20.29        14.34         135.10    1297.0         0.10030
843786         12.45        15.70          82.57     477.1         0.12780
         compactness_mean concavity_mean concave.points_mean symmetry_mean
842302            0.27760         0.3001             0.14710        0.2419
842517            0.07864         0.0869             0.07017        0.1812
84300903          0.15990         0.1974             0.12790        0.2069
84348301          0.28390         0.2414             0.10520        0.2597
84358402          0.13280         0.1980             0.10430        0.1809
843786            0.17000         0.1578             0.08089        0.2087
         fractal_dimension_mean radius_se texture_se perimeter_se area_se
842302                  0.07871    1.0950     0.9053        8.589  153.40
842517                  0.05667    0.5435     0.7339        3.398   74.08
84300903                0.05999    0.7456     0.7869        4.585   94.03
84348301                0.09744    0.4956     1.1560        3.445   27.23
84358402                0.05883    0.7572     0.7813        5.438   94.44
843786                  0.07613    0.3345     0.8902        2.217   27.19
         smoothness_se compactness_se concavity_se concave.points_se
842302        0.006399        0.04904      0.05373           0.01587
842517        0.005225        0.01308      0.01860           0.01340
84300903      0.006150        0.04006      0.03832           0.02058
84348301      0.009110        0.07458      0.05661           0.01867
84358402      0.011490        0.02461      0.05688           0.01885
843786        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
```

Let's set up a new vector called `diagnosis` that has the diagnosis data.

```
diagnosis <- wisc.df$diagnosis
```

Exploring the Data Structure

Q1. How many observations are in this dataset?

There are 569 observations.

```
nrow(wisc.data)
```

```
[1] 569
```

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

The number of "M" malignant diganosis is 212.

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

Q3. How many variables/features in the data are suffixed with _mean?

There are ten variables in the data with the "_mean" suffix. We use the `colname()` to list out all the column names, we then use `grep(pattern, data)` to count the number of the pattern "_mean", and finally we use length to sum the number of patterns

```
colnames(wisc.data)
```

```
 [1] "radius_mean"             "texture_mean"
 [3] "perimeter_mean"          "area_mean"
 [5] "smoothness_mean"         "compactness_mean"
 [7] "concavity_mean"          "concave.points_mean"
 [9] "symmetry_mean"           "fractal_dimension_mean"
[11] "radius_se"               "texture_se"
[13] "perimeter_se"            "area_se"
[15] "smoothness_se"           "compactness_se"
[17] "concavity_se"            "concave.points_se"
[19] "symmetry_se"             "fractal_dimension_se"
[21] "radius_worst"            "texture_worst"
[23] "perimeter_worst"         "area_worst"
[25] "smoothness_worst"        "compactness_worst"
[27] "concavity_worst"         "concave.points_worst"
[29] "symmetry_worst"          "fractal_dimension_worst"
```

```
length(grep("_mean",colnames(wisc.data)))
```

```
[1] 10
```

Principal Component Analysis

We want to make sure the data is scaled to the right unit of measurements and make sure the variables have significantly different variances because these could potentially violate our assumptions in statistical testing.

Check the means and SDs for ALL the columns with the function ‘

```
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
```

Execute PCA with `scale = T` to make sure the variance are not wildly different between each column

```
wisc.pr <- prcomp(wisc.data, scale = T)
summary(wisc.pr)
```

```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
                           PC8    PC9    PC10   PC11    PC12    PC13    PC14
Standard deviation     0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 0.39624
Proportion of Variance 0.01589 0.0139 0.01169 0.0098 0.00871 0.00805 0.00523
Cumulative Proportion  0.92598 0.9399 0.95157 0.9614 0.97007 0.97812 0.98335
                          PC15    PC16    PC17    PC18    PC19    PC20   PC21
Standard deviation     0.30681 0.28260 0.24372 0.22939 0.22244 0.17652 0.1731
Proportion of Variance 0.00314 0.00266 0.00198 0.00175 0.00165 0.00104 0.0010
Cumulative Proportion  0.98649 0.98915 0.99113 0.99288 0.99453 0.99557 0.9966
                          PC22    PC23   PC24    PC25    PC26    PC27    PC28
Standard deviation     0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 0.03987
Proportion of Variance 0.00091 0.00081 0.0006 0.00052 0.00027 0.00023 0.00005
Cumulative Proportion  0.99749 0.99830 0.9989 0.99942 0.99969 0.99992 0.99997
                          PC29    PC30
Standard deviation     0.02736 0.01153
Proportion of Variance 0.00002 0.00000
Cumulative Proportion  1.00000 1.00000
```

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

PC1 captures 44.27% of the variance.

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

PC1 and PC2 is enough to explain at least 70% of the variance.

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

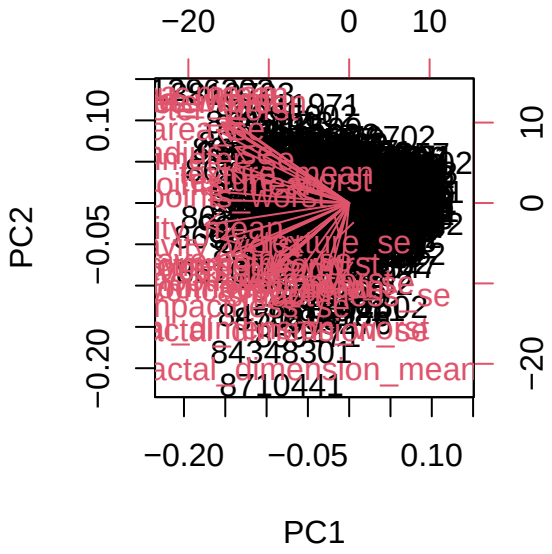
Up to PC7 is enough to explain at least 90% of the variance.

Interpreting PCA Results

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

This plot is a mess because I only see letters and numbers on the plot.

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



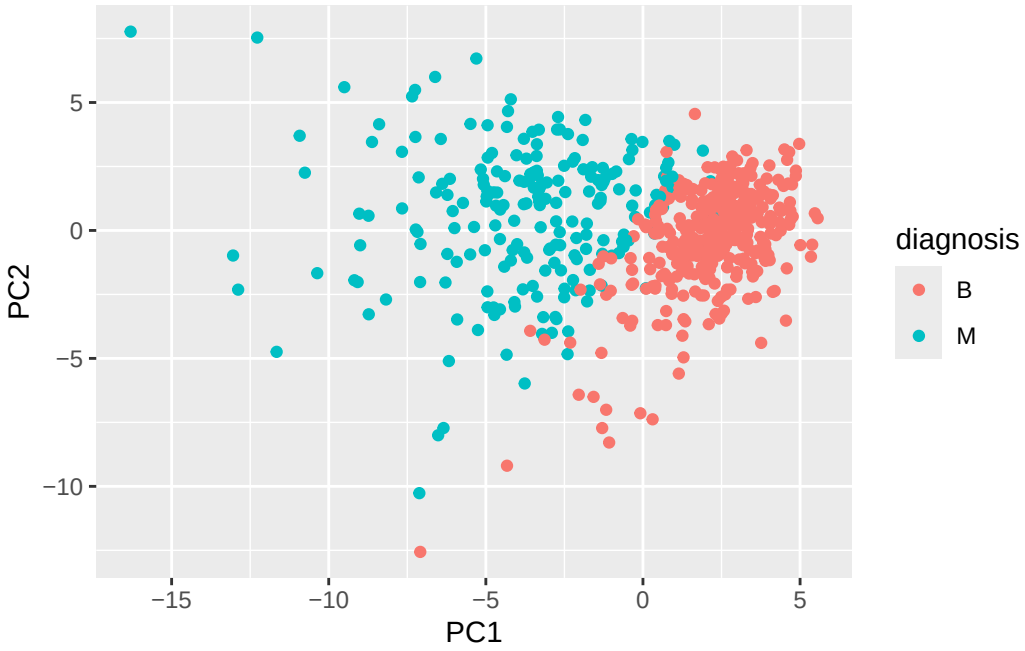
Let's use ggplot instead

```
library(ggplot2)
```

```
Warning: package 'ggplot2' was built under R version 4.3.3
```

PC1 VS PC2

```
ggplot(wisc.pr$x) +
  aes(PC1, PC2, col= diagnosis) +
  geom_point()
```

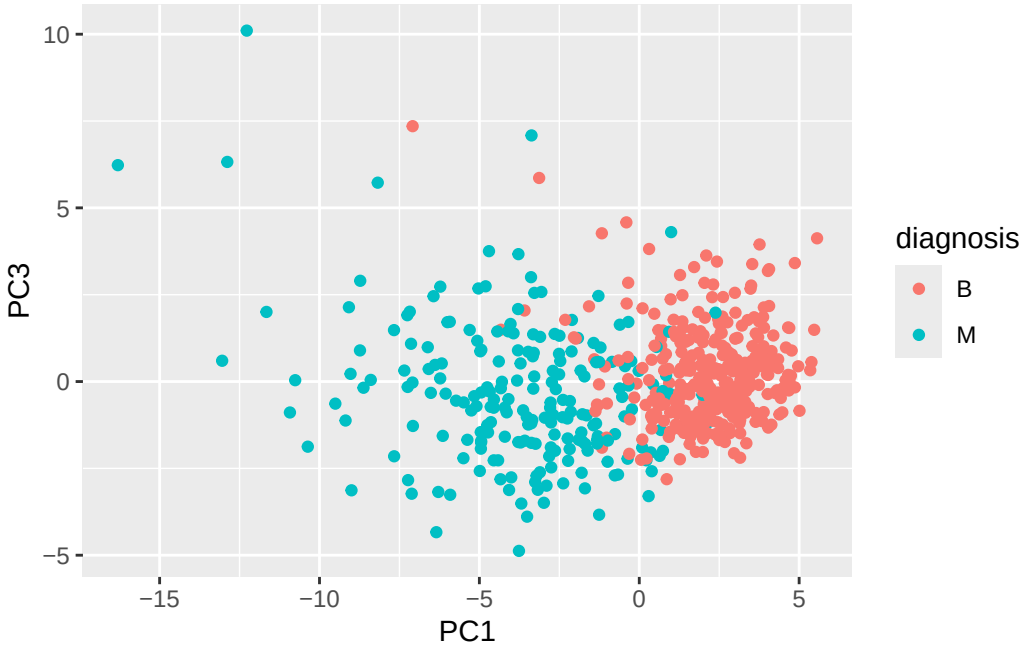


Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

Nothing much changed, but I noticed that the outliers tend to shift up. Overall, the PC1 can discern the differences between benign and malignant. PC2 VS PC3 does not show a separation (not shown).

PC1 VS PC3

```
ggplot(wisc.pr$x) +
  aes(PC1, PC3, col= diagnosis) +
  geom_point()
```



Variance Explained

Use a scree plot to show the amount of variance each PC captures. Look for the "elbow" to show diminishing returns (usually with threshold 70% or 90%).

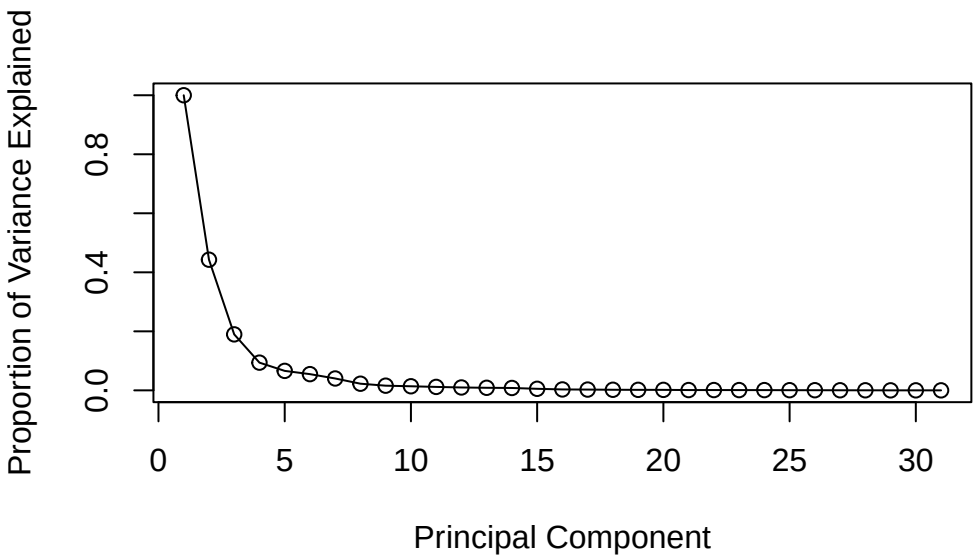
Recall variance is the square of SD.

```
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

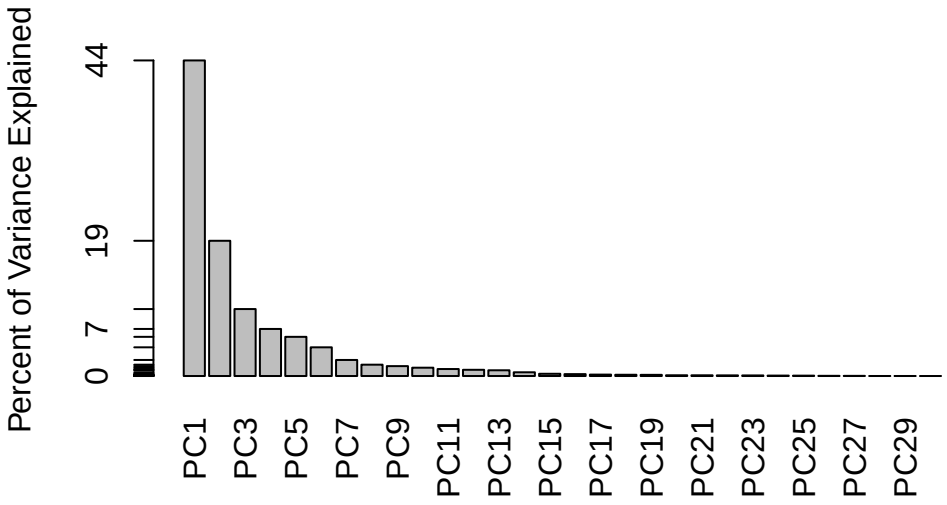
```
pve <- pr.var/sum(pr.var)

plot(c(1,pve), xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



An alternative scree plot

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



Communicating PCA Results

Let's analyze the `loading` instead of the `variance explained`

> 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? This tells us how much this original feature contributes to the first PC. Are there any features with larger contributions than this one?

The concave points mean for PC1 is -0.26. All the other measurements have a smaller negative (more positive) value than the concave point mean. Thus, nothing has more contribution than the concave points (in the negative direction).

```
wisc.pr$rotation["concave.points_mean",1]
```

```
[1] -0.2608538
```

Hierarchical Clustering

Recall `hclust()` and its methods of clustering: `single`, `complete`, and `average`. Remember to scale `wisc.data` with `scale()`, and name this new data frame.

```
data.scaled <- scale(wisc.data)
```

Now, calculate the Euclidean distances with `dist()`

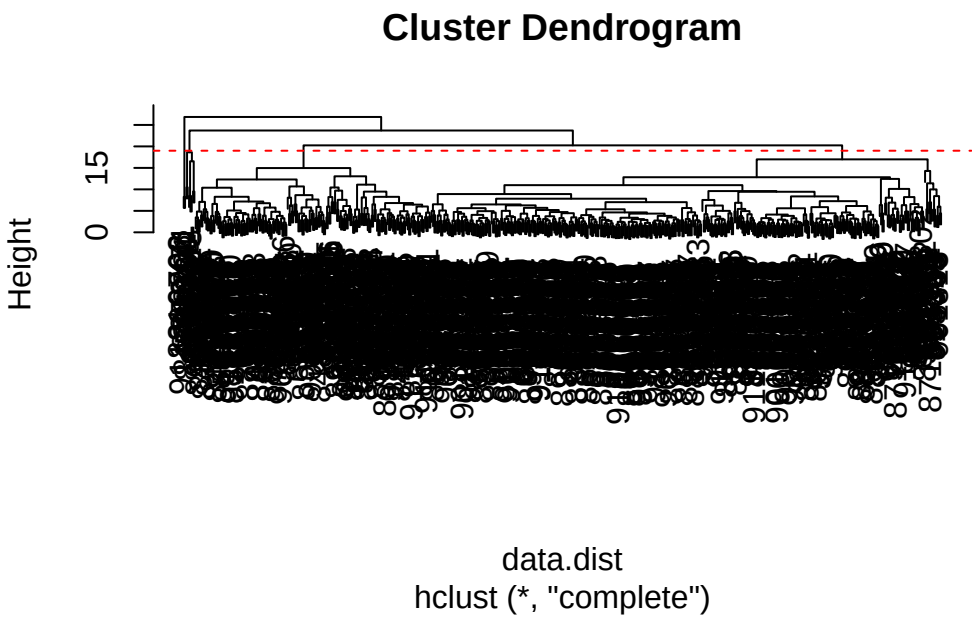
```
data.dist <- dist(data.scaled)
```

Use `hclust()` with the `complete` method

```
wisc.hclust <- hclust(data.dist, method = "complete")
```

Q10. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

```
plot.hclust <- plot(wisc.hclust) +
  abline(h = 19, col = "red", lty = 2)
```



Selecting the Number of Clusters

Cut the tree where the `abline` is using `cutree()`. Set the number of clusters `k` to 4

```
wisc.hclust.clusters.4 <- cutree(wisc.hclust, k = 4)
table(wisc.hclust.clusters.4, diagnosis)
```

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

Clust into 6 groups

```
wisc.hclust.clusters.6 <- cutree(wisc.hclust, k = 6)
table(wisc.hclust.clusters.6, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters.6   B   M
                     1  12 165
                     2   0   5
                     3 331  39
                     4   2   0
                     5  12   1
                     6   0   2
```

> Q11. OPTIONAL: Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 6? How do you judge the quality of your result in each case?

Besides four clusters, none of the clusters between 2 to 6 better clusters the data.

Using Different Methods

> Q12. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

Here is a function that specifies the number of clusters and the method for the wisc.hclust data.

```
wisc.hclust.method <- function(x, y) {
  wisc.hclust.a <- hclust(data.dist, method = y)
```

```
  wisc.hclust.b <- cutree(wisc.hclust.a, k = x)
  table(wisc.hclust.b, diagnosis)
  }
```

Ward D2 is also my favorite method because it shows the separation with the least number of clusters.

```
  wisc.hclust.method(2,"complete")
```

```
             diagnosis
wisc.hclust.b   B   M
            1 357 210
            2   0   2
```

```
  wisc.hclust.method(2,"single")
```

```
             diagnosis
wisc.hclust.b   B   M
            1 357 210
            2   0   2
```

```
  wisc.hclust.method(2,"average")
```

```
             diagnosis
wisc.hclust.b   B   M
            1 357 209
            2   0   3
```

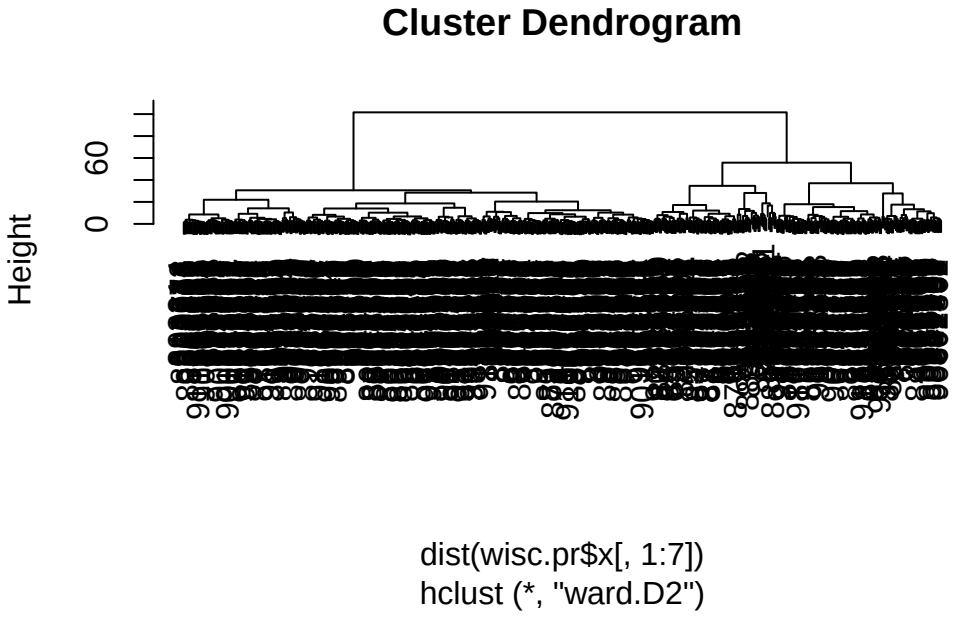
```
  wisc.hclust.method(2,"ward.D2")
```

```
             diagnosis
wisc.hclust.b   B   M
            1  20 164
            2 337  48
```

Combining Methods

Using the minimum number of PCs to describe 90% of the variablity (PC1 through PC7), create a hierarchical clustering model with the method `ward.D2`. Instead of `hclust(dist(x))`, we use `hclust(dist(pr$x[,PCs]))`. In other words, we are combining both PCA and hierarchical clustering for this data analysis.

```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]), method = "ward.D2")
plot(wisc.pr.hclust)
```



Let's cut this new tree. Cluster 1 mostly have `M` diagnosis and Cluster 2 has `B` diagnosis.

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

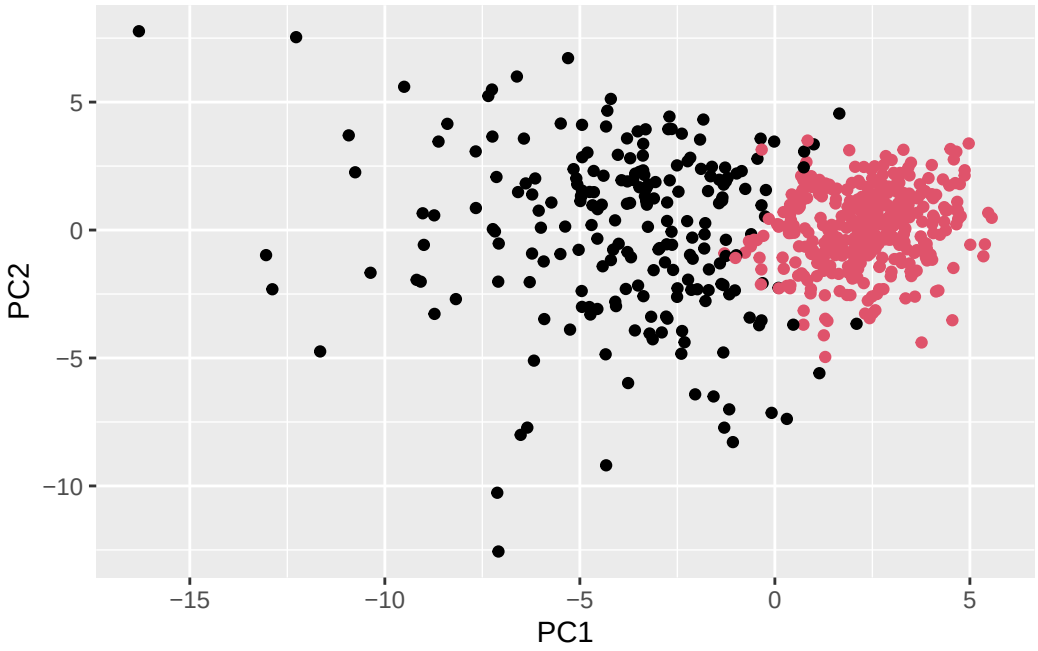
```
grps
  1   2
216 353
```

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

```
    diagnosis
grps   B   M
   1  28 188
   2 329  24
```

Let's make a ggplot.

```
ggplot(wisc.pr$x) +
  aes(PC1, PC2) +
  geom_point(col = grps)
```



Q13. How well does the newly created hclust model with two clusters separate out the two "M" and "B" diagnoses?

Without calculating the specificity or the selectivity, I do not see a noticeable difference between the hclust method and the PC + hclust method.

```
# v.name <- c("FP", "TP", "TN", "FN")
# sp.ward <- merge(wisc.hclust.method(2,"ward.D2"), v.name)
# sp.pr.ward <- merge(table(grps, diagnosis), v.name)
# sp.ward
```

Q14. How well do the hierarchical clustering models you created in the previous sections (i.e. without first doing PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.hclust.clusters and wisc.pr.hclust.clusters) with the vector containing the actual diagnoses.

```
wisc.hclust.method(2,"complete")
```

```
             diagnosis
wisc.hclust.b   B   M
            1 357 210
            2   0   2
```

```
wisc.hclust.method(2,"single")
```

```
             diagnosis
wisc.hclust.b   B   M
            1 357 210
            2   0   2
```

```
wisc.hclust.method(2,"average")
```

```
             diagnosis
wisc.hclust.b   B   M
            1 357 209
            2   0   3
```

```
wisc.hclust.method(2,"ward.D2")
```

```
             diagnosis
wisc.hclust.b   B   M
            1  20 164
            2 337  48
```

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

```
    diagnosis
grps   B   M
   1  28 188
   2 329  24
```

Every hierarchical clustering method besides `ward.D2` did not cluster properly. The `complete` method also worked, but it needed four clusters to separate out the diagnosis.

Sensitivity and Specificity

Sensitivity = True Positive / (True Positive + False Negative)

Specificity = True Negative / (True Negative + False Positive)

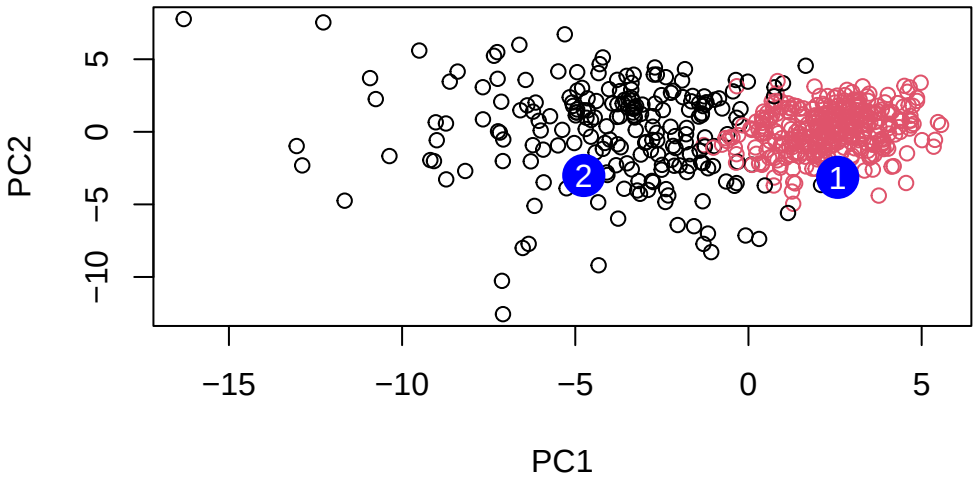
Prediction

Use `predict()` to predice the old data `wisc.pr` and the new data `new`.

```
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=grps)
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



Q16. Which of these new patients should we prioritize for follow up based on your results?

Patient one likely has a malignant diagnosis because they are in the malignant cluster according to PCA prediction.