Class 8: Mini-Project

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2025-02-06

##1. Exploratory data analysis Data downloaded onto R session

```
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
```

Removing the diagnosis column because it is the "answer"

```
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
```

New vector with diagnosis data

```
diagnosis <- as.factor(wisc.df$diagnosis)
diagnosis
```

```
  [1] M M M M M M M M M M M M M M M M M B B B M M M M M M M M M M M M M M
 [38] B M M M M M M M M B M B B B B B M M B M M B B B B M B M M B B B B M B M M
 [75] B M B M M B B B M M B M M M B B B M B B M M B B B M M B B B M B B M B B
[112] B B B B B B M M M B M M B B B M M B M B M M B M M B B M B B M B B B B M B
[149] B B B B B B B B M B B B B M M B M B B M M B B M M B B B B M B B M M M B M
[186] B M B B B M B B M M B M M M M B M M M B M B M B B M B M M M M B B M M B B
[223] B M B B B B B M M B B M B B M M B M B B B B M B B B B B M B M M M M M M M
[260] M M M M M M M B B B B B B M B M B B M B B M B M M B B B B B B B B B B B B
[297] B M B B M B M B B B B B B B B B B B B B B M B B B M B M B B B B M M M B B
[334] B B M B M B M B B B M B B B B B B B M M M B B B B B B B B B B B M M B M M
[371] M B M M B B B B B M B B B B B M B B B M B B M M B B B B B B M B B B B B B
[408] B M B B B B B M B B M B B B B B B B B B B B B M B M M B M B B B B B M B B
[445] M B M B B M B M B B B B B B B B B M M B B B B B M B B B B B B B B B B M B
[482] B B B B B B M B M B B M B B B B B B M M B M B M B B B B B M B B M B M B M M
[519] B B B M B B B B B B B B B B B B M B M M B B B B B B B B B B B B B B B B B
[556] B B B B B B B M M M M M M B
Levels: B M
```

Q1. How many observations are in this dataset?

```
nrow(wisc.df)
```

```
[1] 569
```

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

```
sum(wisc.df$diagnosis == "M")
```

```
[1] 212
```

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

```
mean_feature <- grep("_mean$", colnames(wisc.data), value = T)
length(mean_feature)
```

```
[1] 10
```

##Performing PCA

Checking standard deviation and mean to see if data should be scaled

```
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
```

```
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 components (PC1)?

PC1 captures 0.4427 of variance

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

3 principal components are required to explain at least 70% of the total variance. (This was found using visualization of Cumulative Proportion).

Also found

```
cumulative_pca <-
#summary(wisc.pr)$importance[2, ] finds the proportion of variance explained for each pc
  #cumsum() finds the cumulative variance with more pc added
  cumsum(summary(wisc.pr)$importance[2, ])
#which evaluates logical vectors that are TRUE
which(cumulative_pca >= 0.70)[1]
```

```
PC3
  3
```

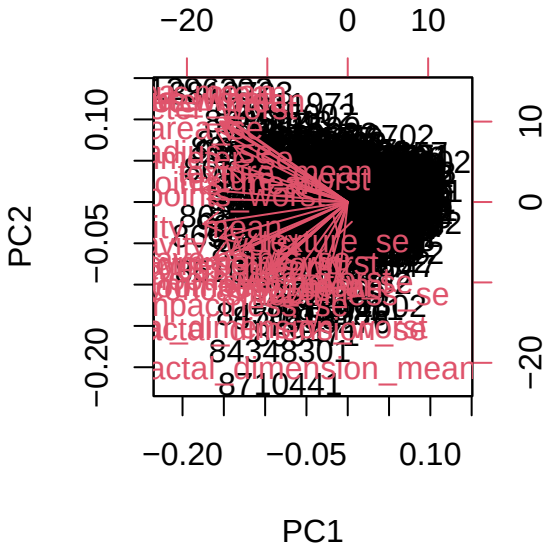
> Q6. Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

```
which(cumulative_pca >= 0.90)[1]
```

```
PC7
  7
```

Interpreting PCA results

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



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

This data is hard to read because the data points are crowded with names in a small plot. It is difficult to understand what the data is conveying.

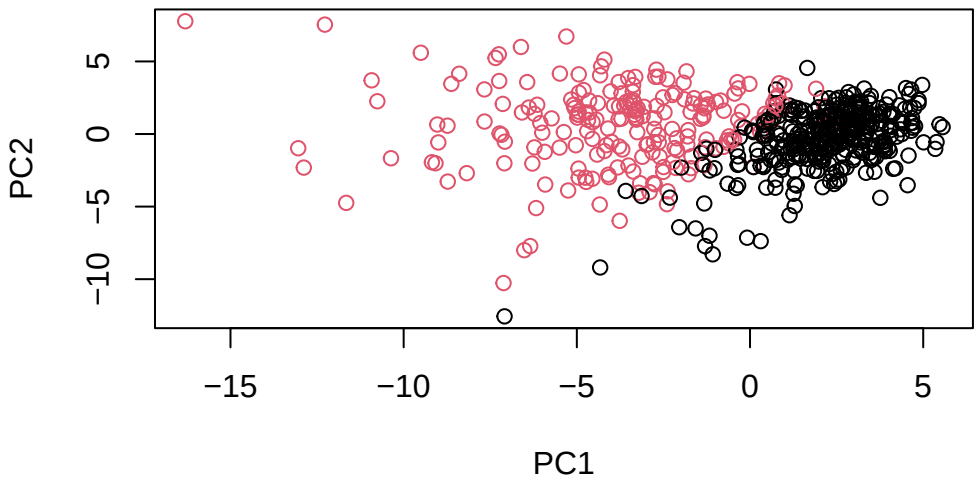
Generating a plot of pc 1 vs. pc 2

```
names(wisc.pr)
```

```
[1] "sdev"     "rotation" "center"   "scale"    "x"
```

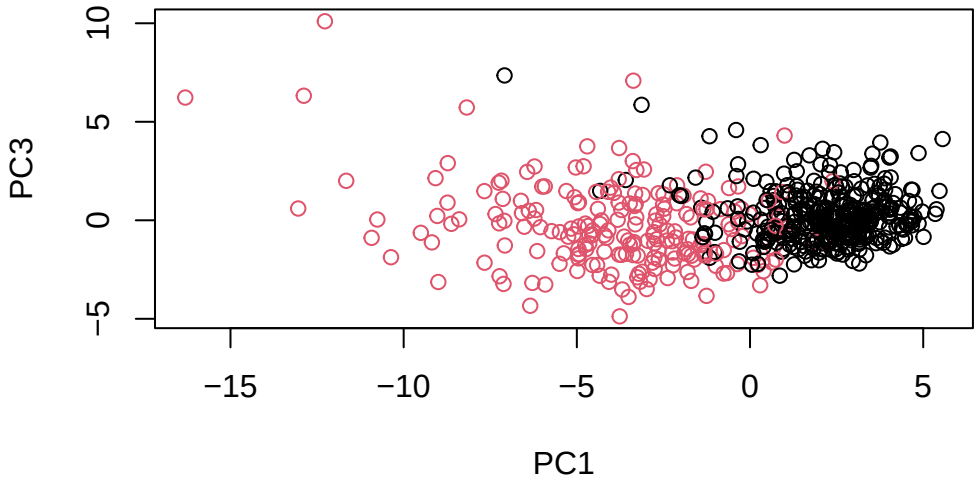
```
# x is used to transform data into new space
```

```
plot(wisc.pr$x[,1], wisc.pr$x[,2], col = diagnosis,
     xlab = "PC1", ylab = "PC2")
```



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,
     xlab = "PC1", ylab = "PC3")
```



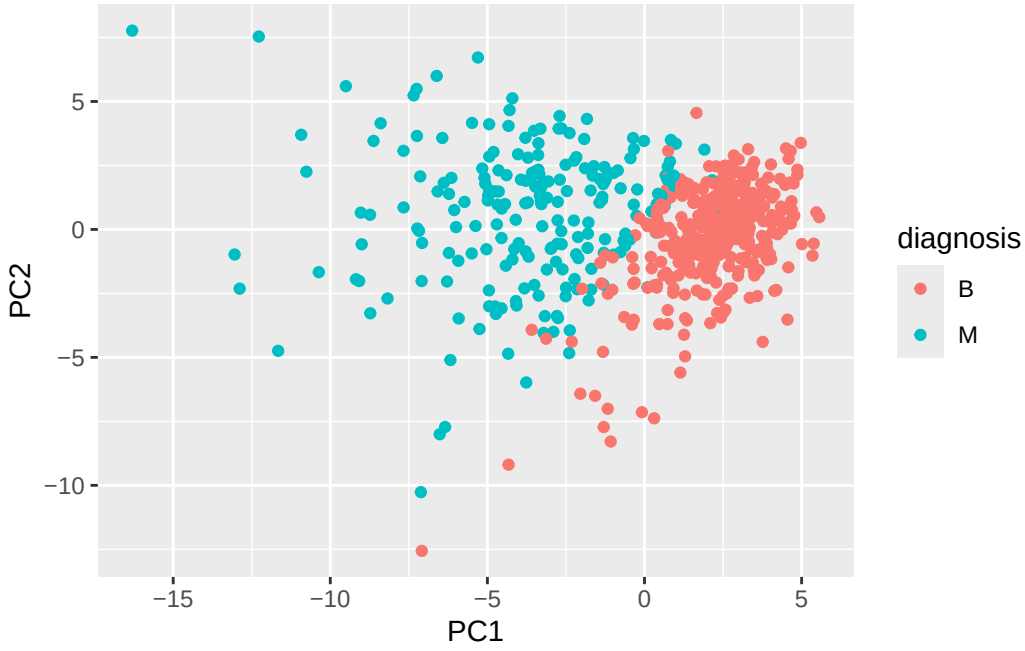
The scatterplot of PC1 vs. PC2 captures most of the variation with PC1 clearly distinguishing between the data points divergence. While PC1 vs. PC3 is unclear with values overlapping malignant points and benign points. PC3's contribution leads to less differentiation between the two groups.

Using ggplot to make a fancy figures of results. First principal component scores must be converted into a data frame format in order for it to be used in ggplot

```
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis
```

```
library(ggplot2)
```

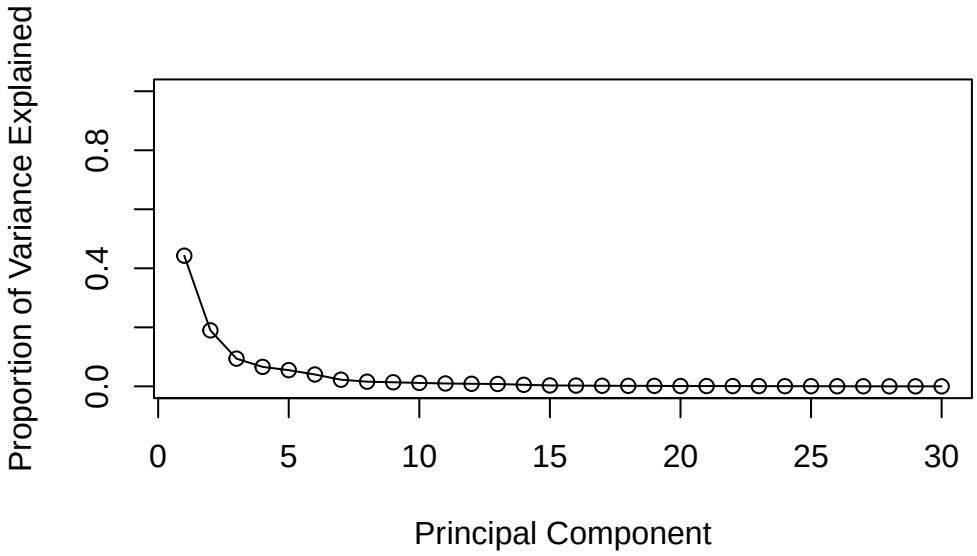
```
ggplot(df) +
    aes(PC1, PC2, col=diagnosis) +
      geom_point()
```




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



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?

Loading tells us how each original variable contributes to a pc

```
#wisc.pr$rotation contains loading values higher absolute value indicates more importance to
wisc.pr$rotation["concave.points_mean",1]
```

```
[1] -0.2608538
```

concave.points_mean seems to have a low contribution to PC1. The negative value indicates it contributes to information of malignant tumor

```
tapply(wisc.pr$x[,1], diagnosis, mean)
```

```
       B         M
2.204035 -3.711511
```

M being negative corresponds to negative loading value

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

```
which(cumulative_pca >= 0.80)[1]
```

```
PC5
  5
```

##3. Hierarchical clustering

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

Calculating Euclidean distance

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

```
[1] 10.309426  6.771675 10.463467  8.663413  8.402233  9.843286
```

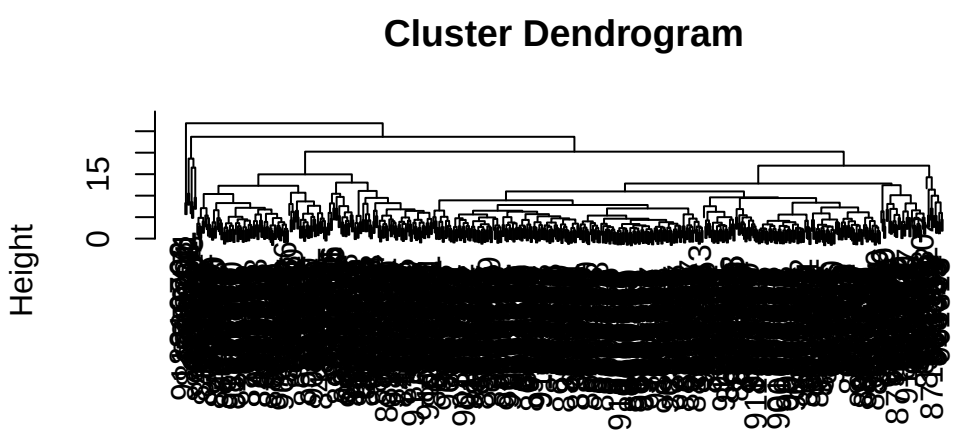
hierarchical clustering model

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

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

18.63658

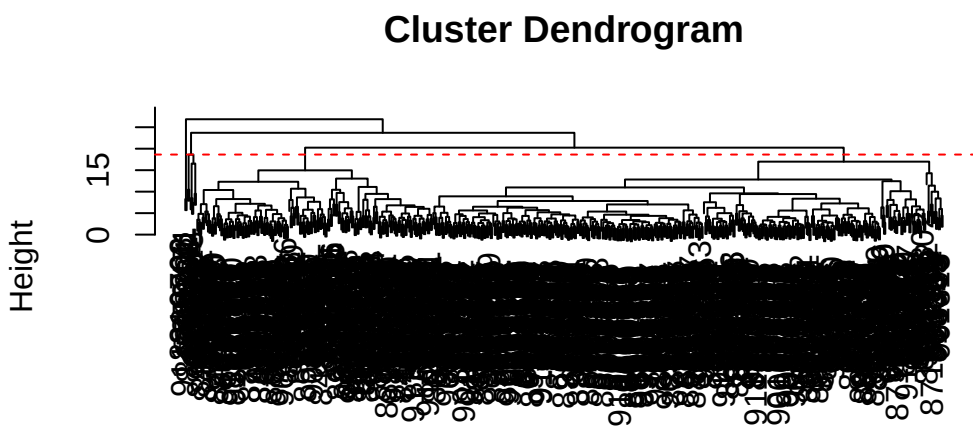
```
plot(wisc.hclust)
```




```
#wisc.hclust$height has the heights at which clusters are merged
#Hierarchical clustering has n-1 merges using the value three picks the 4th last merge on the
cut_height <- wisc.hclust$height[length(wisc.hclust$height)-3]
cut_height
```

```
[1] 18.63658
```

```
plot(wisc.hclust)
abline(h = 18.63658, col="red", lty=2)
```




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

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

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

Choosing the k value where separation between M and B is best. Clusters should be mostly either M or B. k = 8 best represents this distinction between the two.

```
clusters <- cutree(wisc.hclust, k=8)
table(clusters, diagnosis)
```

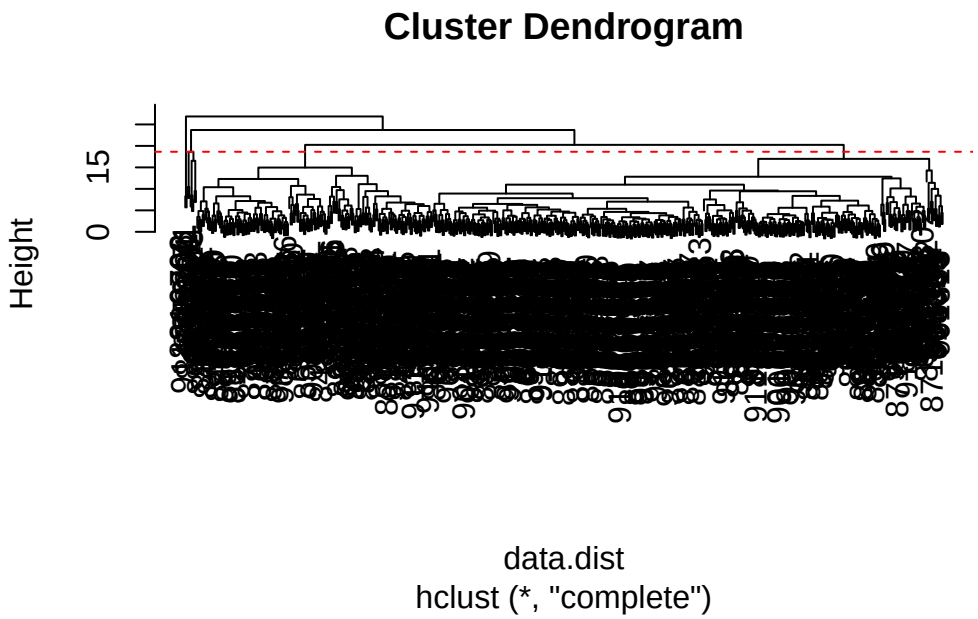
```
        diagnosis
clusters   B   M
       1  12  86
```

```
2   0  79
3   0   3
4 331  39
5   2   0
6  12   1
7   0   2
8   0   2
```

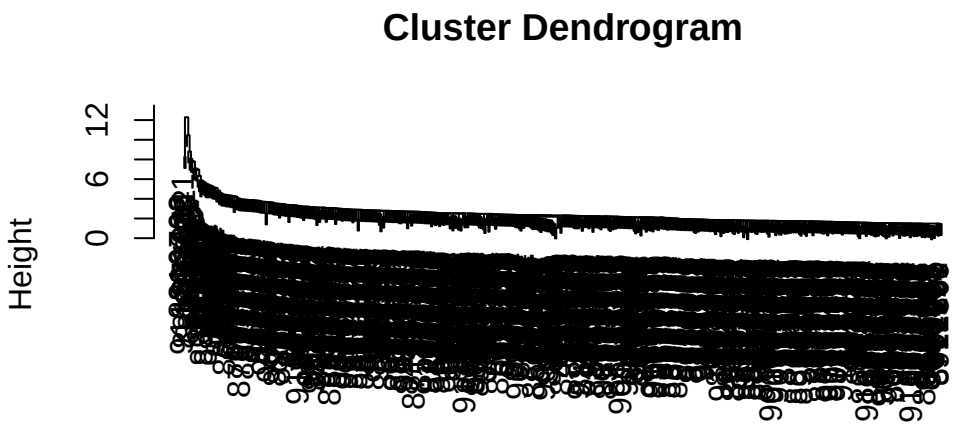
Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

The Ward's method gives the best result, it shows more balanced and distinct clusters. It separates the B and M diagnoses more and its clear that there are two different groups.

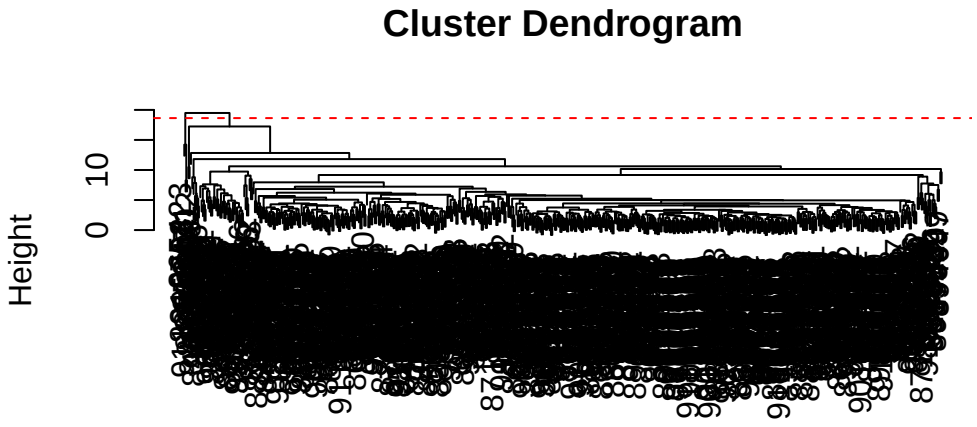
```
wisc.hclust.complete <- hclust(data.dist, method= "complete")
plot(wisc.hclust.complete)
abline(h = 18.63658, col="red", lty=2)
```



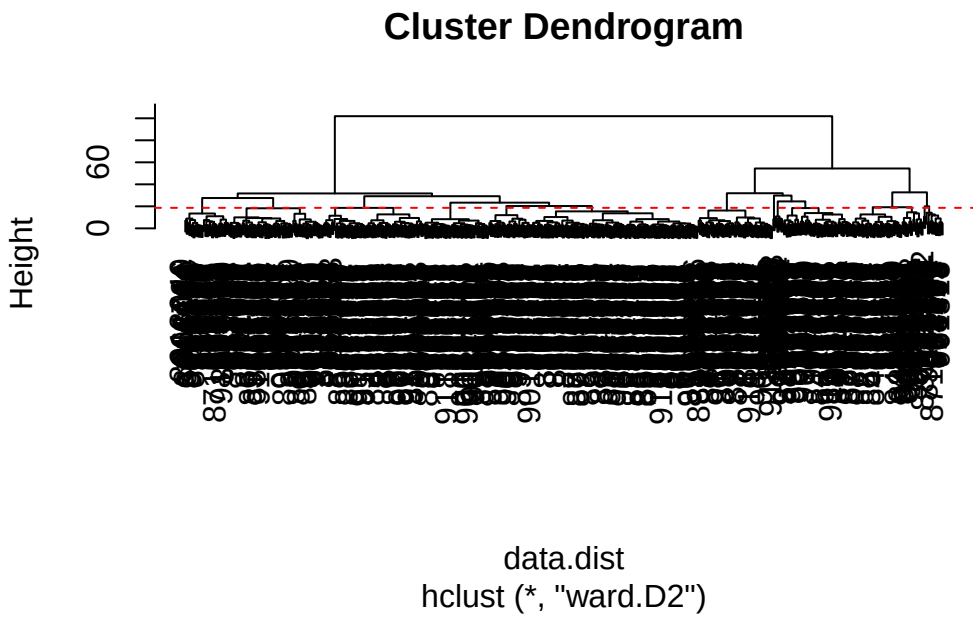

```
wisc.hclust.single <- hclust(data.dist, method= "single")
plot(wisc.hclust.single)
abline(h = 18.63658, col="red", lty=2)
```




```
wisc.hclust.average <- hclust(data.dist, method= "average")
plot(wisc.hclust.average)
abline(h = 18.63658, col="red", lty=2)
```



```
wisc.pr.hclust <- hclust(data.dist, method= "ward.D2")
plot(wisc.pr.hclust)
abline(h = 18.63658, col="red", lty=2)
```



##5. Combining methods

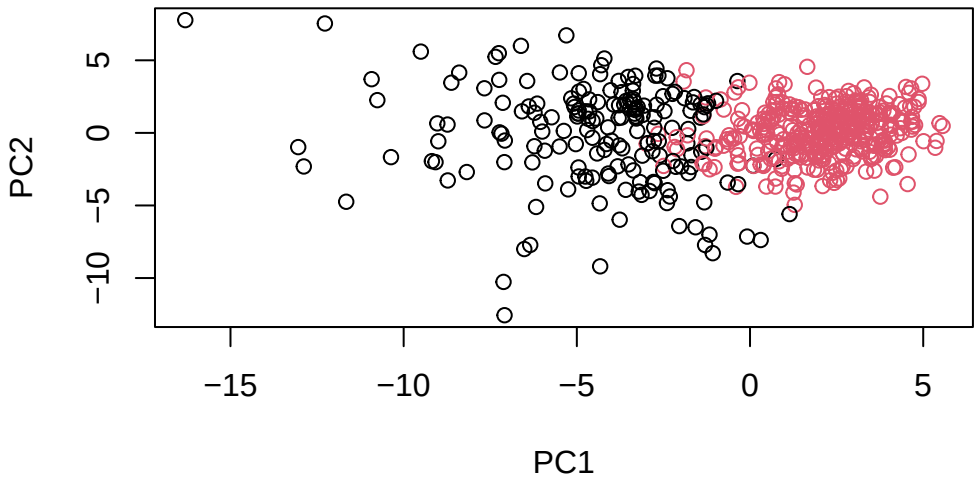
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
184 385
```

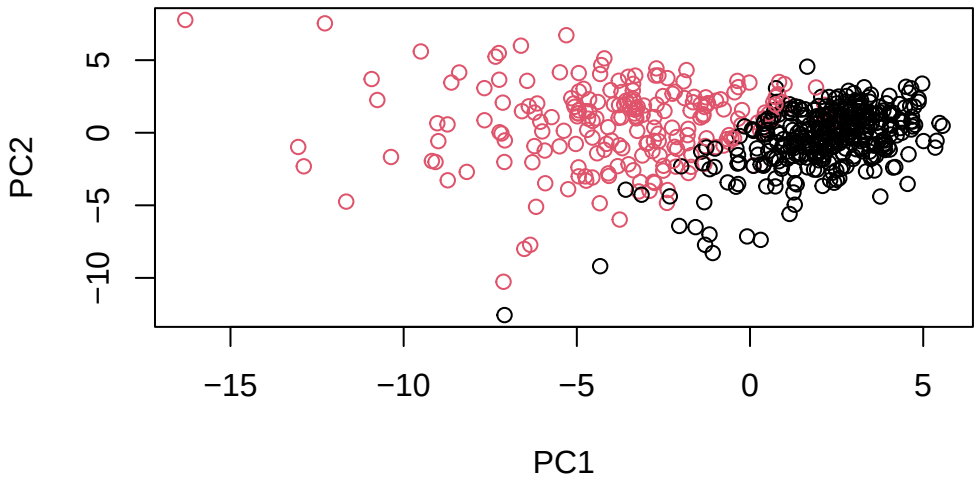
```
table(grps, diagnosis)
```

```
    diagnosis
grps   B   M
   1  20 164
   2 337  48
```

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




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



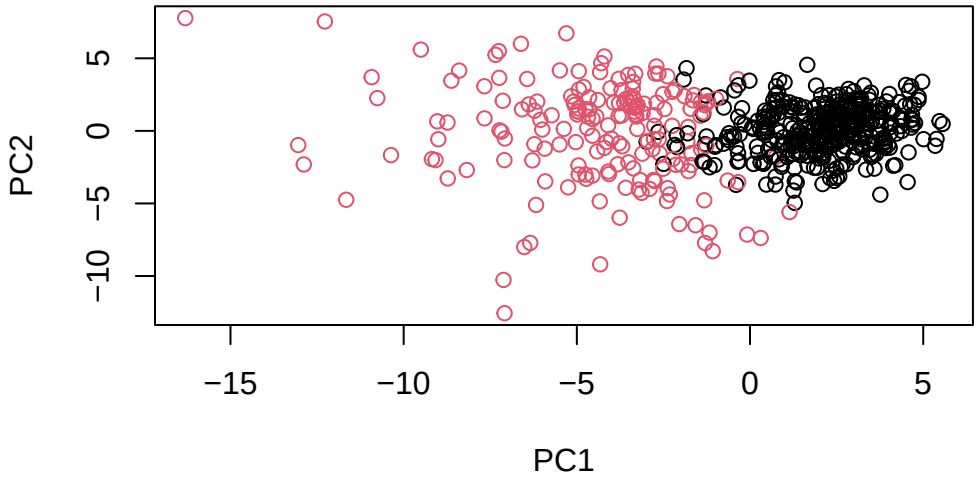
```
g <- as.factor(grps)
levels(g)
```

```
[1] "1" "2"
```

```
g <- relevel(g,2)
levels(g)
```

```
[1] "2" "1"
```

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




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

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

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

The 4 clusters shows improvement compared to the 2-cluster model. The separation is not perfect with some clusters still containing both B and M.

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

```
                    diagnosis
wisc.pr.hclust.clusters   B   M
                      1   0  45
                      2   2  77
                      3  26  66
                      4 329  24
```

> 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 clustering has done a relatively good job of separating benign and malignant diagnoses, with fer misclassifications compared to hierarchical clustering. Hierarchical clustering, with the four clusters was more granular but still has misclassifications.

##6. Sensitivity/Specificity

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

THE PCA-based hierarchical model was better at detecting cancerous tumors, witht he non-pca hierarchical model excelled at identifying health tumors

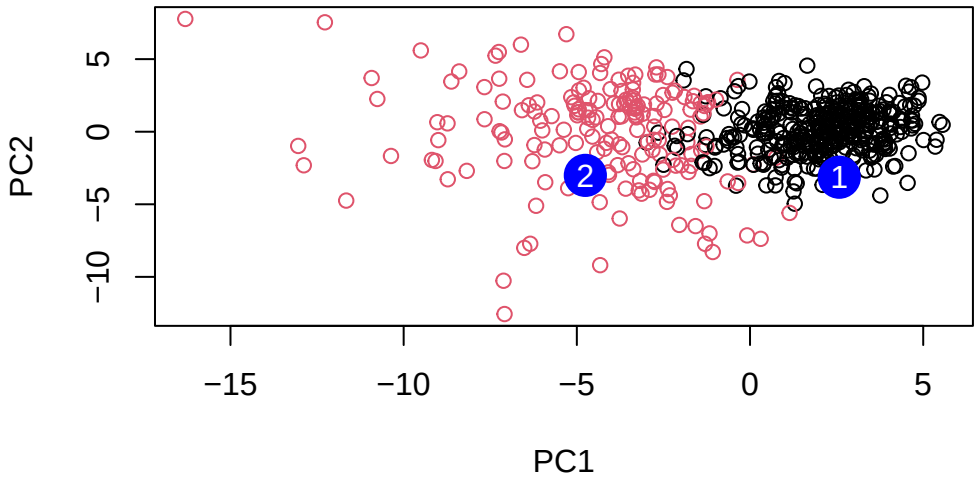
##7. Prediction

```
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
```

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



Q18. Which of these new patients should we prioritize for follow up based on your results?

It would best to prioritize patients who have a M tumor. It seems as the patient number two corresponds to a M tumor and should be followed up on.