Class 08

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Table of contents

Background

In today's class we will apply the methods and techniques clustering and PCA to help make sense of a real world breast cancer fine needle aspiration (FNA) biopsy data set.

```
fna.data <- read.csv("WisconsinCancer.csv", row.names = 1)
```

Removing the first 'diagnosis' column - I do not want to use this for my machine learning models. We will use it later to compare our results to the expert diagnosis.

```
head(fna.data)
```

```
         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
```

```r
wisc.data <- fna.data[,-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
```

```
dim(wisc.data)
```

```
[1] 569  30
```

Q1. How many observations are in this dataset?

There are 568 observations in this dataset.

Q2. How many observations have a malingnant diagnosis?

212 are malignant and 357 are benign.

```
table(fna.data$diagnosis)
```

```
  B   M
357 212
```

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

10 variables/features are suffixed with "_mean".

```
length(grep("mean", names(wisc.data)))
```

```
[1] 10
```

Performing PCA:

```
#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
```

```
diagnosis <- fna.data$diagnosis
```

```
#Executing PCA
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)?

Around 44% of variance is captured by the first PC.

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

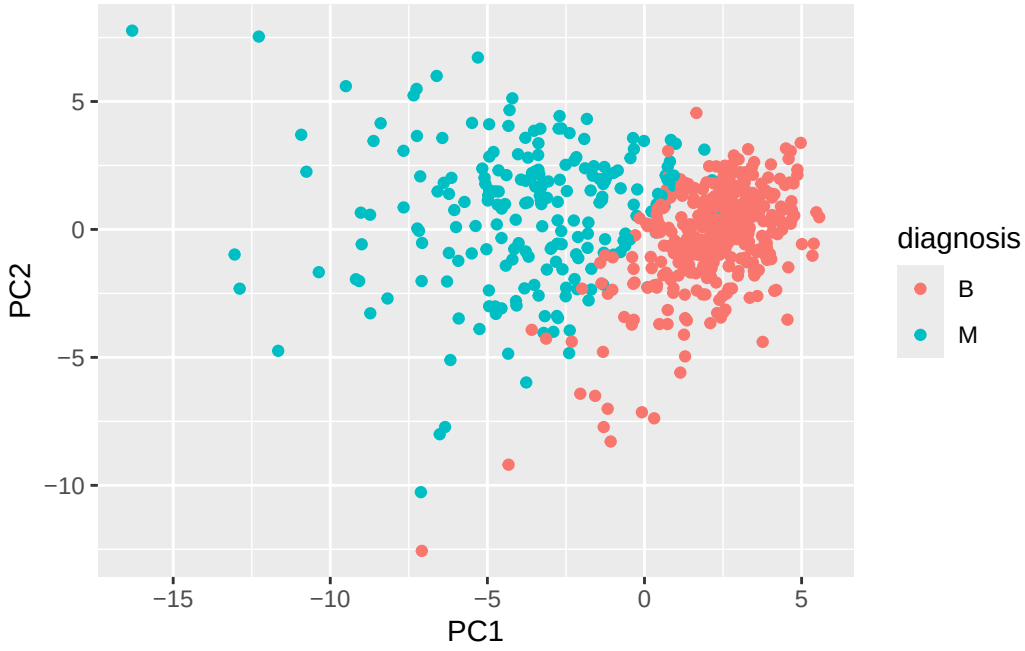
3 PCs are required to describe at least 70% of variance.

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

7 PCs are required to describe at least 90% of variance.

Interperting PCA results:

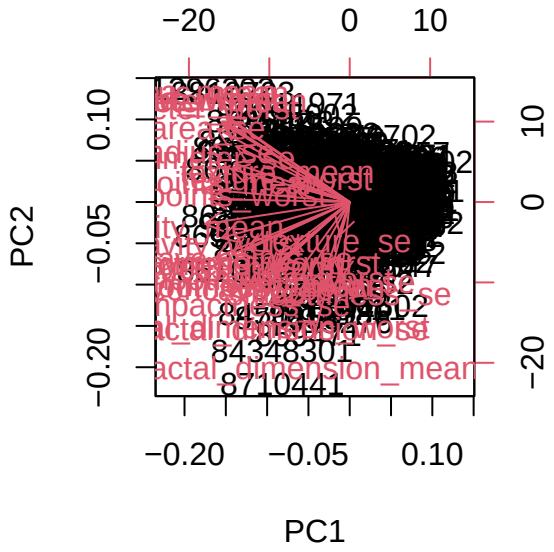
```
library(ggplot2)
ggplot(wisc.pr$x) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point()
```



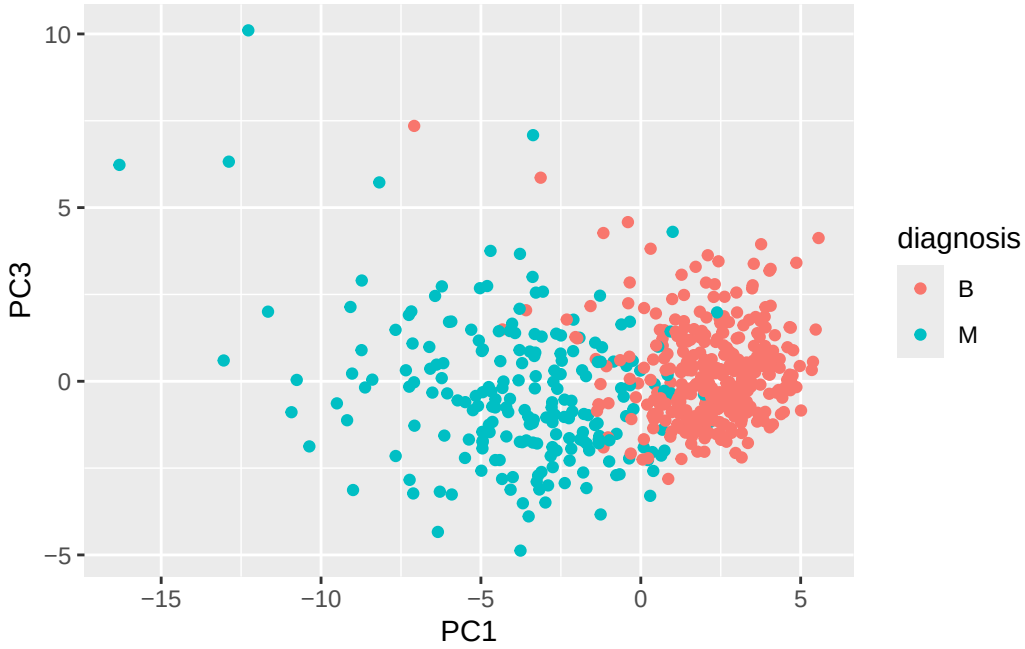
Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

This plot is very difficult to understand, it is plutting individual intergers which end up melding into a black blob on the plot.

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




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



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

Both of these plots have clear 'lines' of separation of where malignant and benign diagnoses are plotted.

Variance Explained:

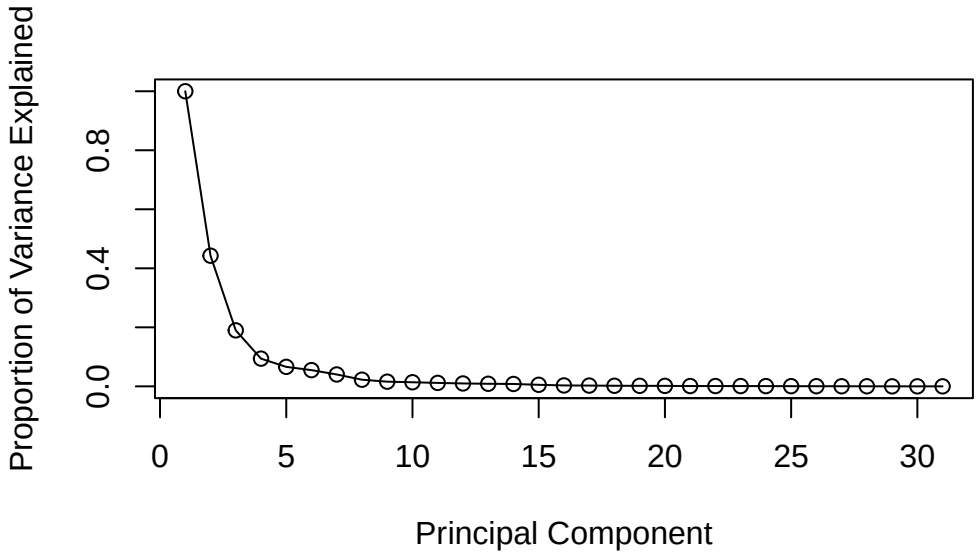
Calculating variance of each principal component by squaring the `sdev` component of wisc.pr.

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

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

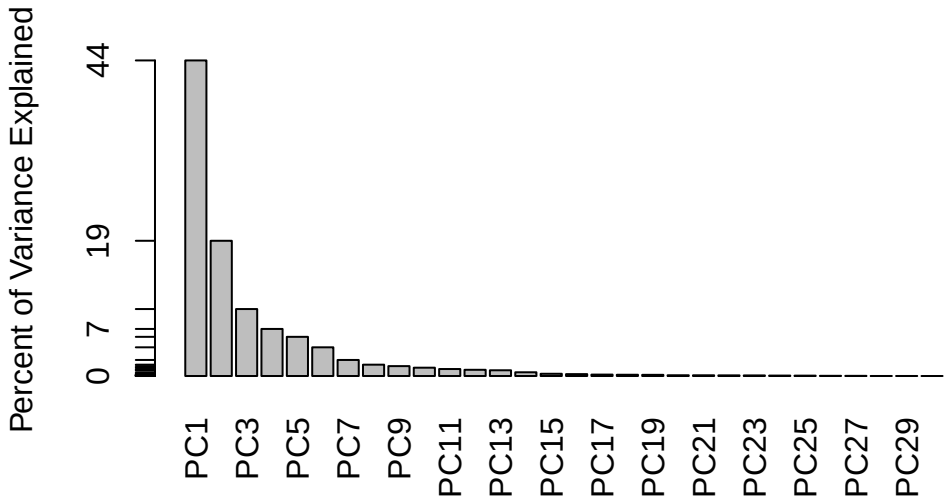
Calculating the variance explained by each principal component by dividing by the total variance explained of all principal components.

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

#Plot variance expained for each principal component
plot(c(1,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-axis:

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



Communicating PCA results:

Collectively these two plots ("score plot" and "loadings plot") tell us that if a cell's nucleus are deeply indented ("concave")

> 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?

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

```
[1] -0.2608538
```

```
sort(abs(wisc.pr$rotation[,1]), decreasing = TRUE)[1:10]
```

```
 concave.points_mean       concavity_mean concave.points_worst
           0.2608538            0.2584005            0.2508860
     compactness_mean      perimeter_worst      concavity_worst
           0.2392854            0.2366397            0.2287675
        radius_worst       perimeter_mean           area_worst
```

```
0.2279966           0.2275373           0.2248705
area_mean
0.2209950
```

The loading vector for `concave.points_mean` feature is -0.2608538. There is not a feature that contributes more than the `concave.points_mean`.

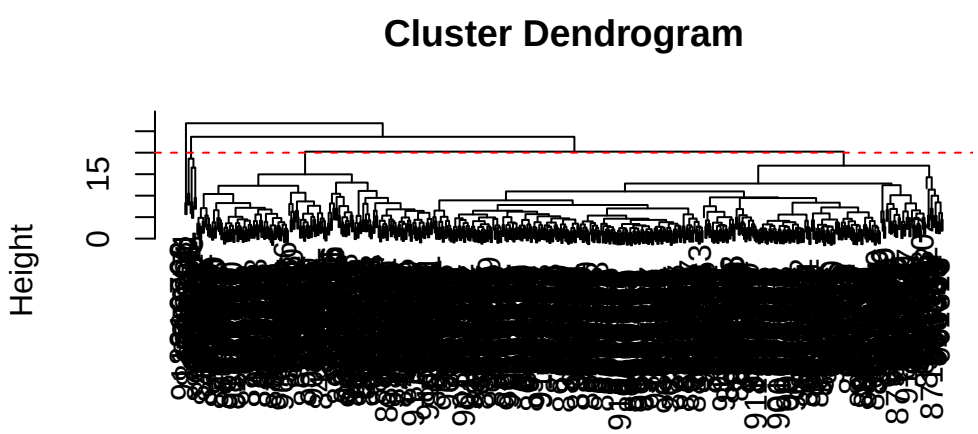
Hierarchical Clustering:

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

#Calculating Euclidean distances between pairs of all observations.
data.dist <-  dist(data.scaled)

#Creating hieracrchical clustering model using complete linkage.
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?

Height = 20, is the height at which the clustering model has 4 clusters.

```
plot(wisc.hclust)
abline(h=20, col="red", lty=2)
```




```
wisc.hclust.clusters <- cutree(wisc.hclust, h=20)
table(wisc.hclust.clusters, diagnosis)
```

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

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

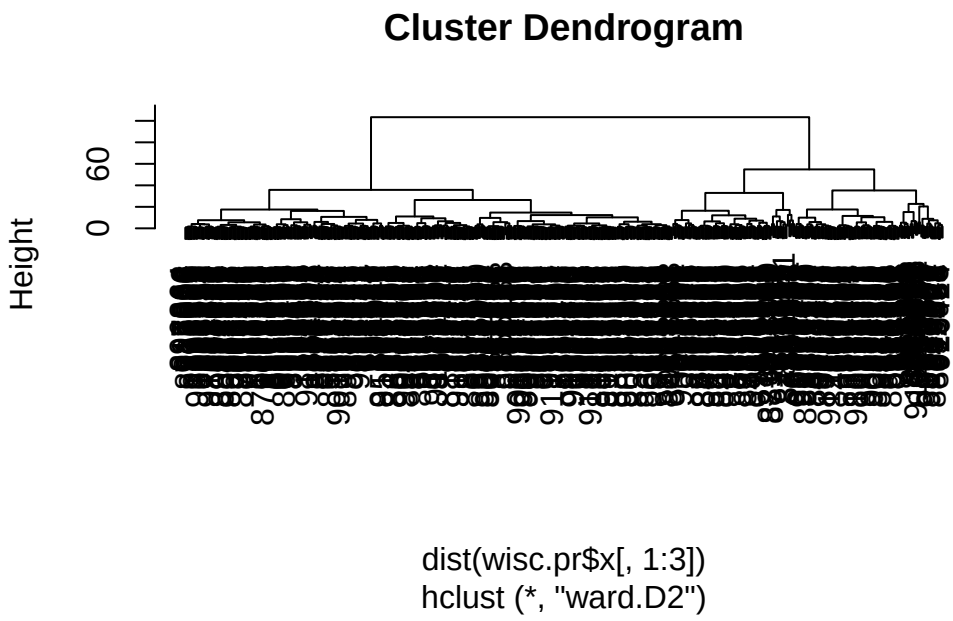
The best method is `ward.D2` since it gives the clearest separation that matches the actual diagnoses. This method also minimized the variance within each cluster.

Combining Methods

Here we will take our PCA results and use those as input for clustering, in other words our "wisc.pr$x" scores that we plotted above (the main output from PCA - how the data lie on our new principal component axis/variables) and use a subset of the PCs as input for `hclust()`.

I want to know how the clustering in **grps** with values of 1 or 2 to correspond with the diagnosis.

```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:3]), method="ward.D2")
grps <- cutree(wisc.pr.hclust, k=2)
plot(wisc.pr.hclust)
```




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

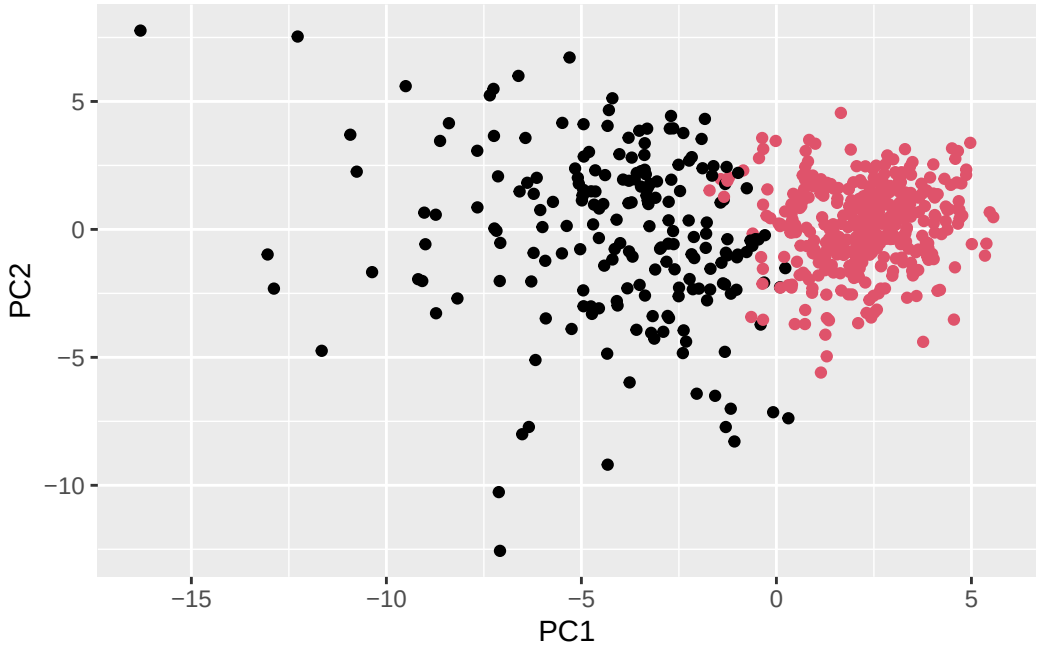
```
    diagnosis
grps   B   M
   1  24 179
   2 333  33
```

My clustering group 1 is mostly 'M' diagnoses (188) , and my clustering group 2 is mostly 'B' (329).

24 FP 179 TP 333 TN 33 FN

Results of new hierarchical clustering model wth the actual diagnoses.

```
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?

The model is fairly accurate at clustering out the two "M" and "B" diagnoses with few false negatives/positives compared to accurate diagnoses.

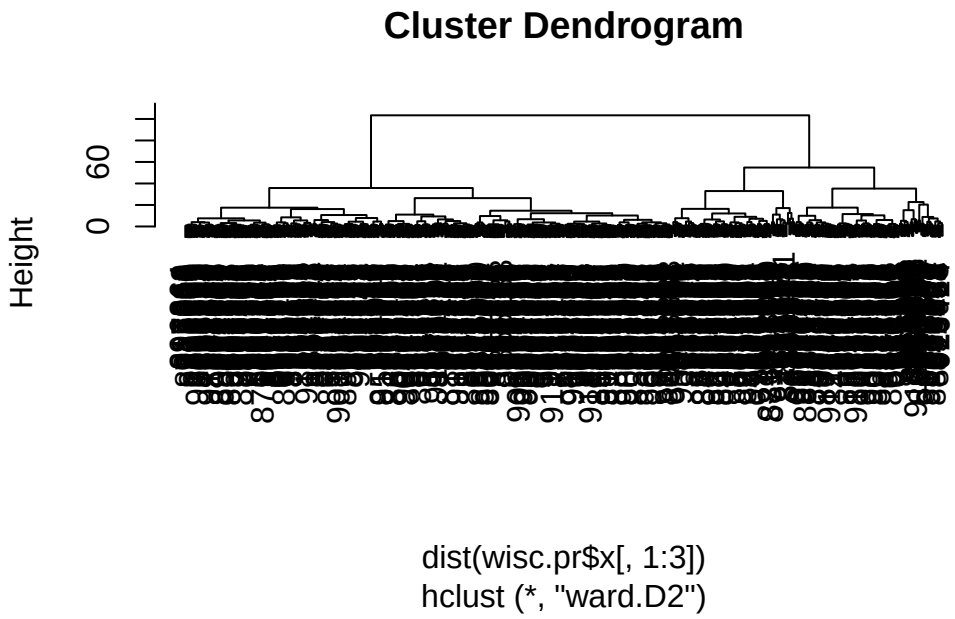
```
table(grps, diagnosis)
```

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

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.

As we begin combining clustering models the model becomes much more accurate at outputting accurate diagnoses compared to the actual diagnoses from the data. With `hclust()` and `prcomp()` being the far less accurate than our combined method.

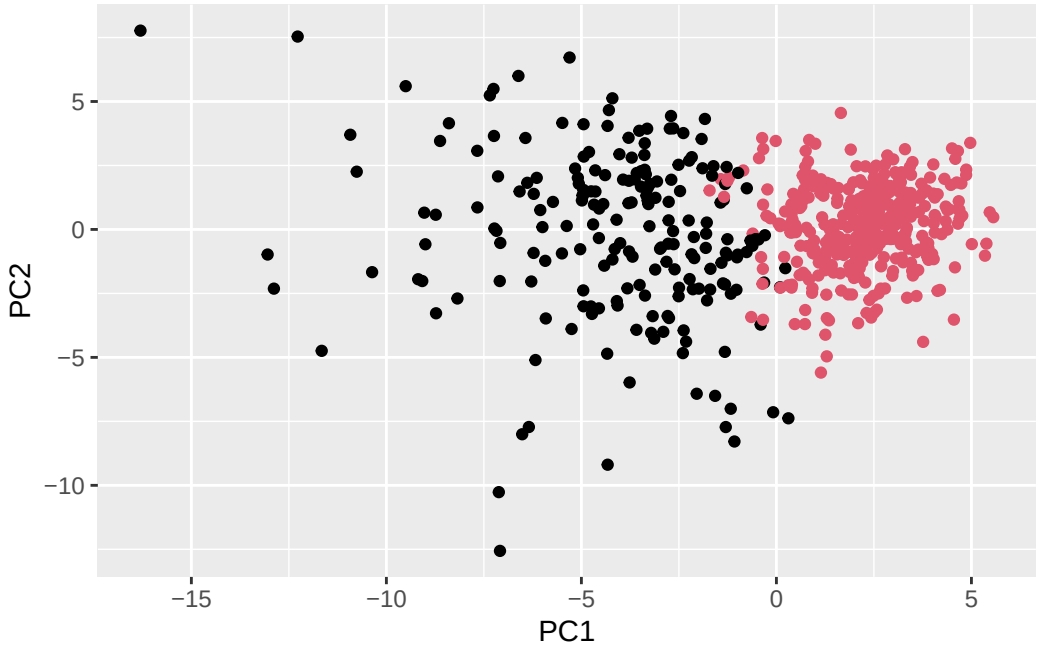
```
wisc.pr.hclust2 <- hclust(dist(wisc.pr$x[,1:3]), method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust2, k=2)
plot(wisc.pr.hclust2)
```




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

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

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



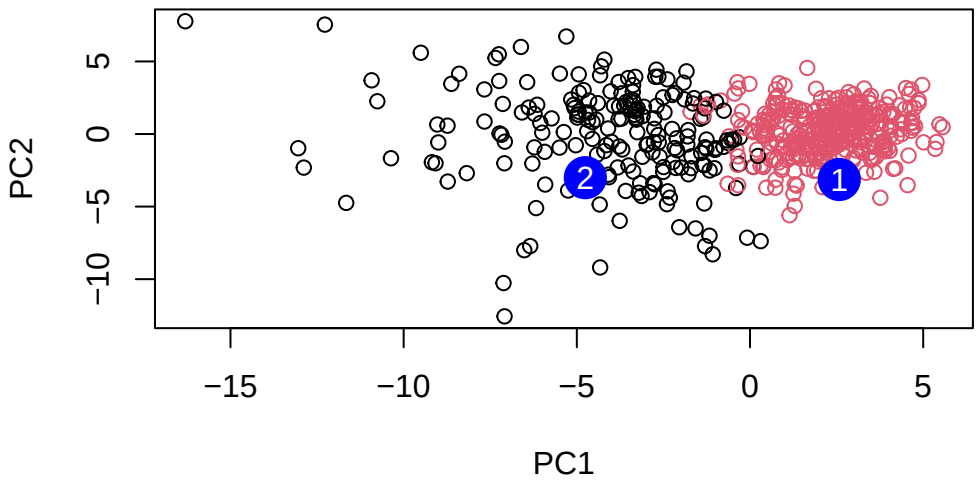
Sensitivity/Specificity:

Q15. OPTIONAL: Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

Prediction

We will use the `predict()` function that will take our PCA model from before and new cancer cell data and project that data onto our PCA space.

```
new <- read.csv("new_samples.csv")
npc <- predict(wisc.pr, newdata=new)
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?

We should focus on patient 2 as it this patients falls within our "malignant" diagnosis cluster while patient 2 falls within our "benign" cluster. Since our model is largely accurate we can somewhat rely on it to decide which patient to prioritize.