Class 08 Mini-Project

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Class 8 Mini-Project: Unsupervised Learning Analysis of Human Breast Cancer Cells

1. Preparing the Data

```r
# Save you input data file into your Project directory
fna.data <- "WisconsinCancer.csv"

# Complete the following code to input the data and store as wisc.df
wisc.df <- read.csv(fna.data, row.names=1)
```

```r
wisc.data <- wisc.df[,-1]
```

```r
# Create diagnosis vector for later

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

Q1. How many observations are in this dataset?

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

```
[1] 569
```

There are 569 observations in this dataset.

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

```
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

212 of the observations have a malignant diagnosis.

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

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

```
[1] 10
```

10 variable/features are suffixed with _mean.

2. Principal Component Analysis

```
# 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 
```

```r
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 
```

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

```r
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)?

```r
pca_var <- wisc.pr$sdev^2 # extract the eigenvalues
prop_var <- pca_var/sum(pca_var) # calculate the proportion of variance
prop_var[1] # print the proportion of variance captured by PC1
```

```
[1] 0.4427203
```

44% of the original variance is capture by PC1.

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

```r
cum_prop_var <- cumsum(prop_var) # calculate cumulative proportion of variance
which.min(cum_prop_var < 0.7) + 1 # print the number of PCs required to explain at least 7
```

```
[1] 4
```

4 PCs are required.

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

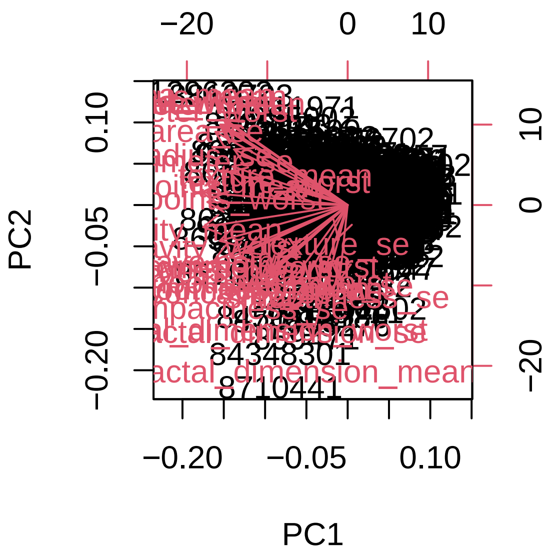
```
which.min(cum_prop_var < 0.9) + 1 # print the number of PCs required to explain at least 9
```

```
[1] 8
```

8 PCs are required.

Interpreting PCA Results

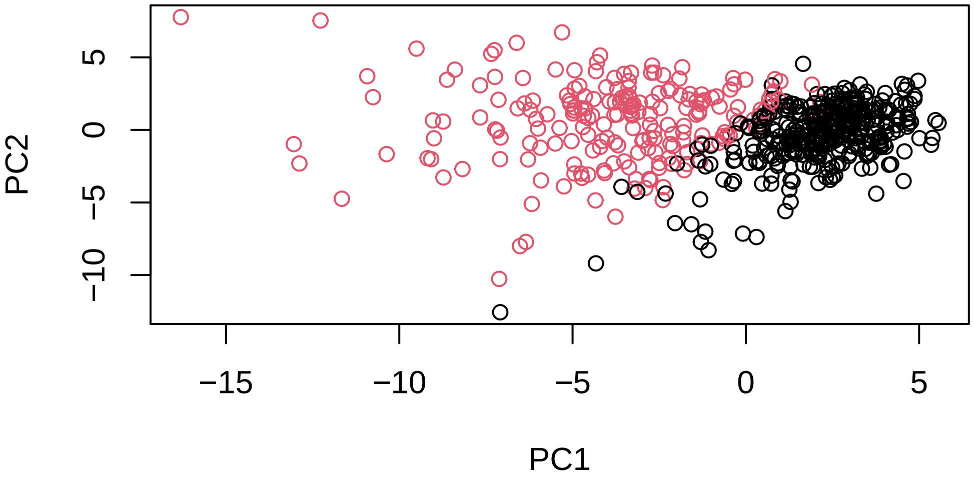
```
biplot(wisc.pr)
```



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

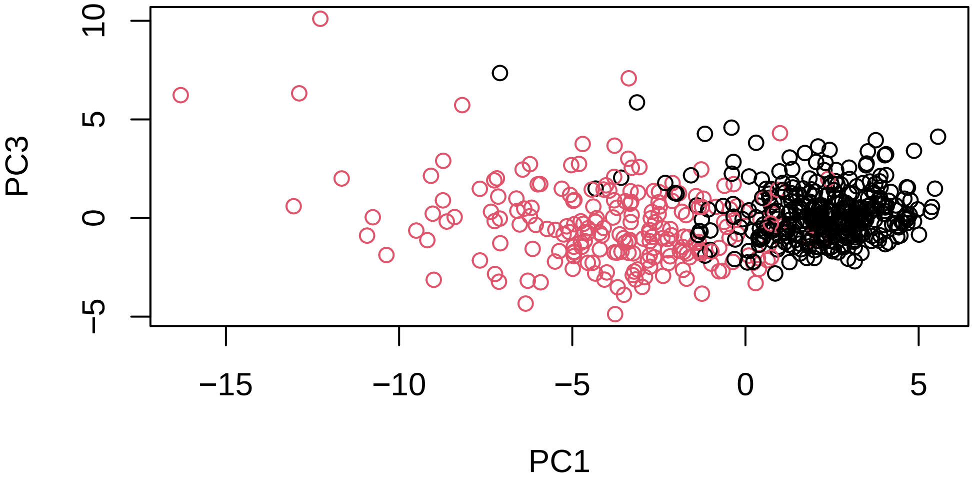
This plot is very messy, making it extremely difficult to understand.

```
# Scatter plot observations by components 1 and 2
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?

```
# Repeat for components 1 and 3
plot(wisc.pr$x[,1], wisc.pr$x[,3], col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```

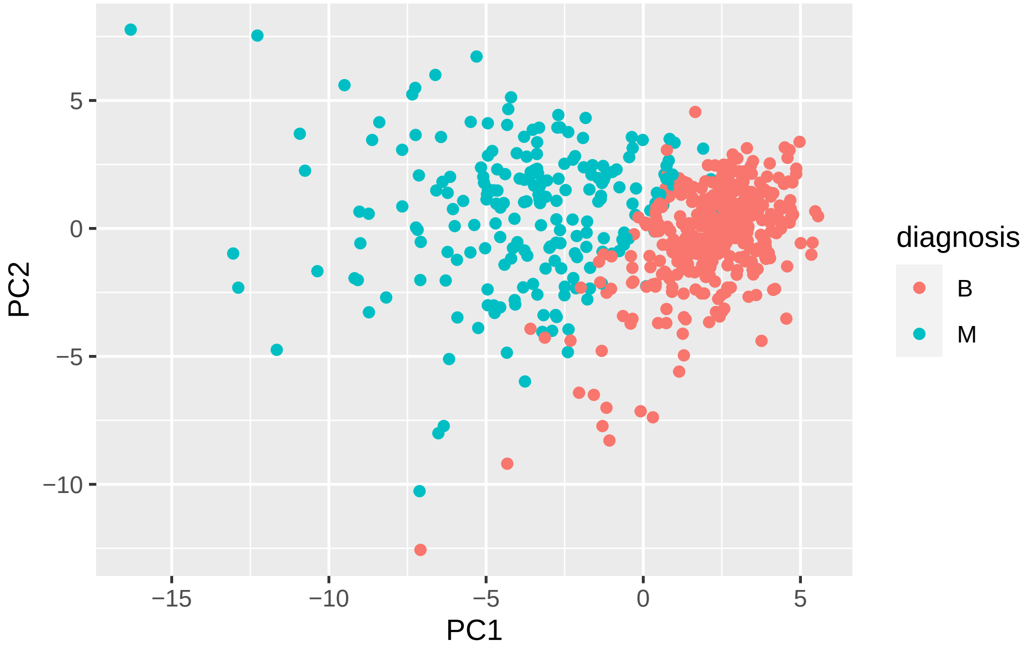


Compared to PC3, PC2 does a much better job at cleanly separating the different subgroups; therefore, the first plot is the preferred plot.

```
# 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()
```

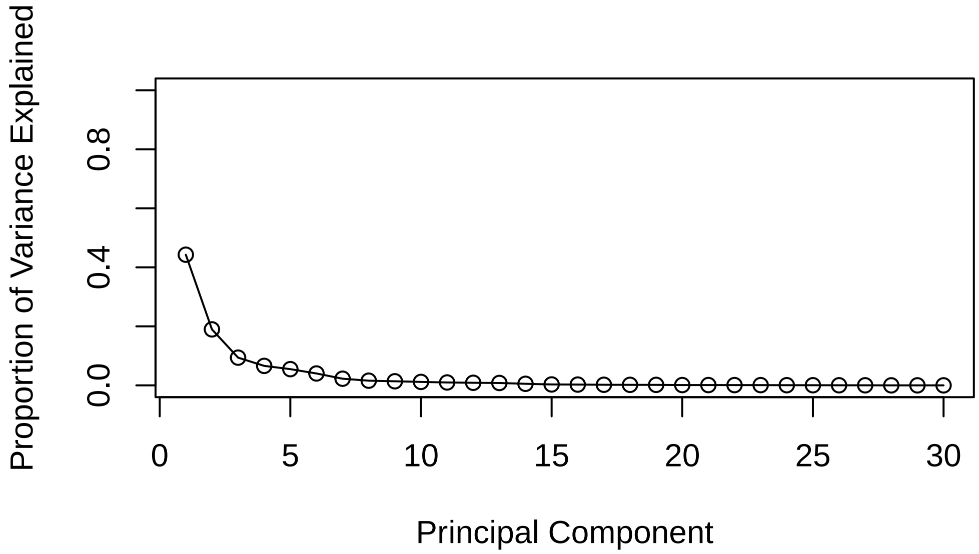


```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

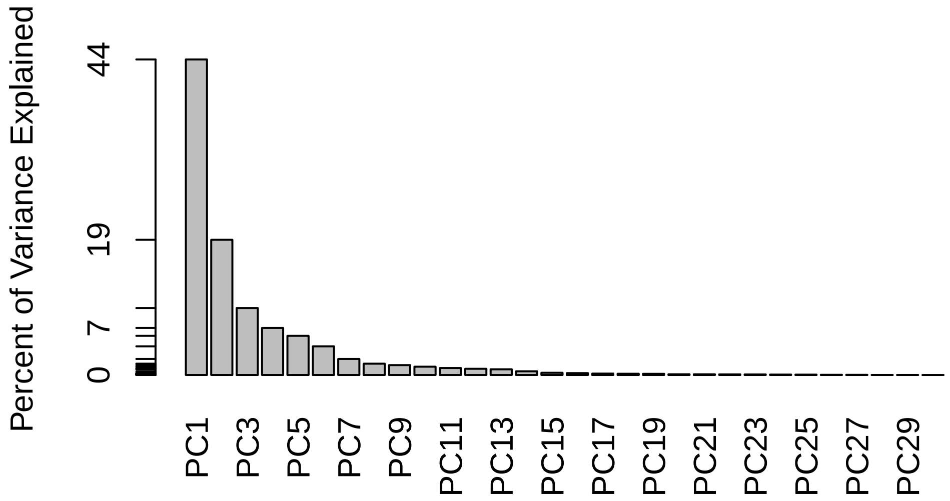
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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")
```



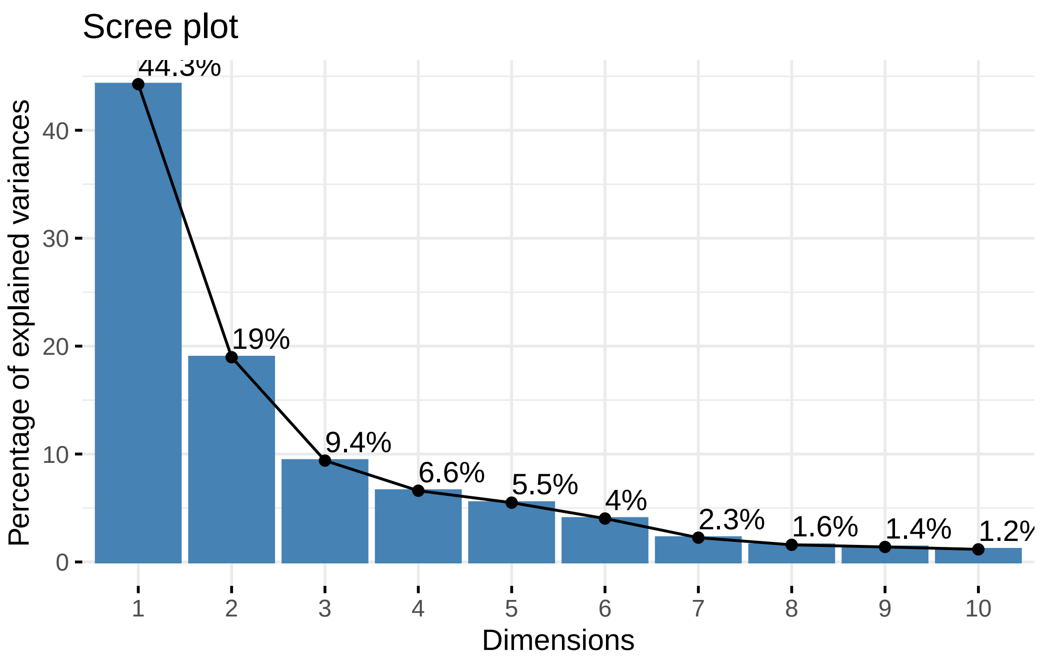
```
# Alternative scree plot of the same data, note dat driven y-axis
barplot(pve, ylab = "Percent of Variance Explained",
        names.arg = paste0("PC", 1:length(pve)), las = 2, axes = FALSE)
axis(2, at = pve, labels = round(pve,2)*100)
```



```
## ggplot based graph
library(factoextra)
```

```
Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
```

```
fviz_eig(wisc.pr, addlabels = TRUE)
```



Communicating PCA Results

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.

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

```
[1] -0.2608538
```

3. Hierarchical Clustering

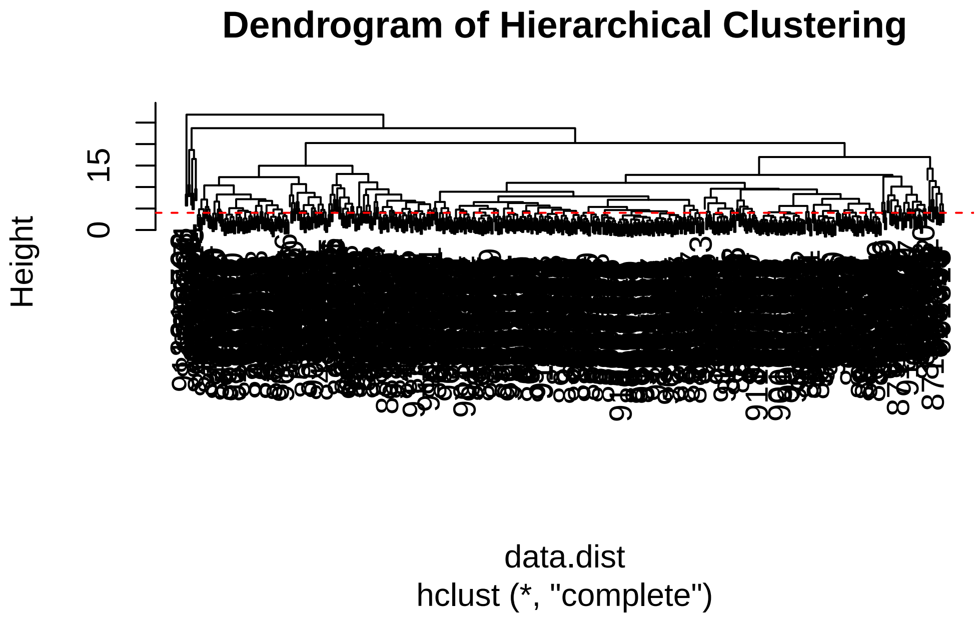
```
data.scaled <- scale(wisc.data)
```

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

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

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

```
plot(wisc.hclust, main="Dendrogram of Hierarchical Clustering")
abline(h=4, col="red", lty=2)
```



Selecting number of clusters

```
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
```

Using different methods

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

I don't think I have favorite method, per se, but I appreciate the results of "average" linkage since it is a compromise of the "single" and "complete" linkages, and is very applicable to many data sets.

4. Combining methods

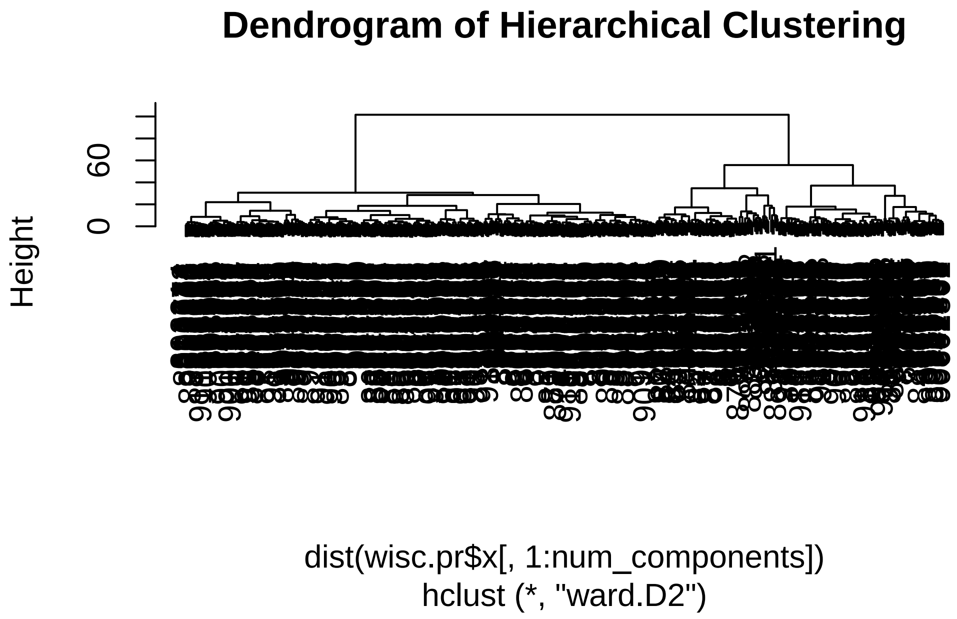
Clustering on PCA results

```r
# Calculate cumulative variance explained by each principal component
cumulative_var <- cumsum(wisc.pr$sdev^2) / sum(wisc.pr$sdev^2)

# Find the minimum number of principal components required to explain 90% of the variabili
num_components <- min(which(cumulative_var >= 0.9))

# Create hierarchical clustering model with linkage method="ward.D2"
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:num_components]), method="ward.D2")
```

```r
plot(wisc.pr.hclust, main="Dendrogram of Hierarchical Clustering")
```



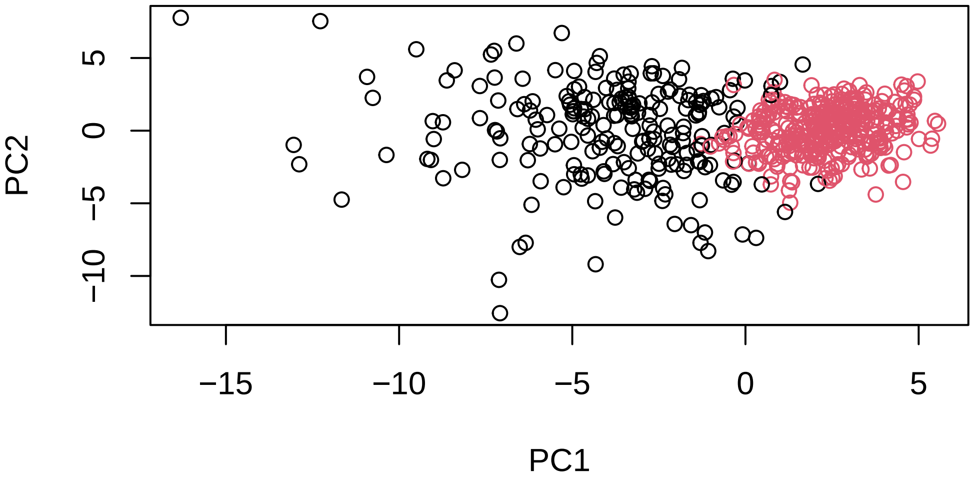
```
grps <- cutree(wisc.pr.hclust, k = 2)
table(grps)
```

```
grps
  1   2
216 353
```

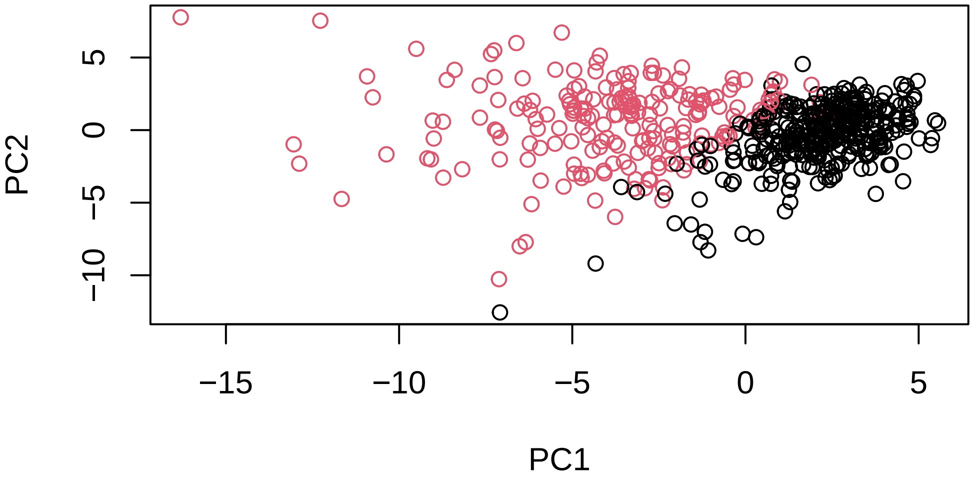
```
table(grps, diagnosis)
```

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

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



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



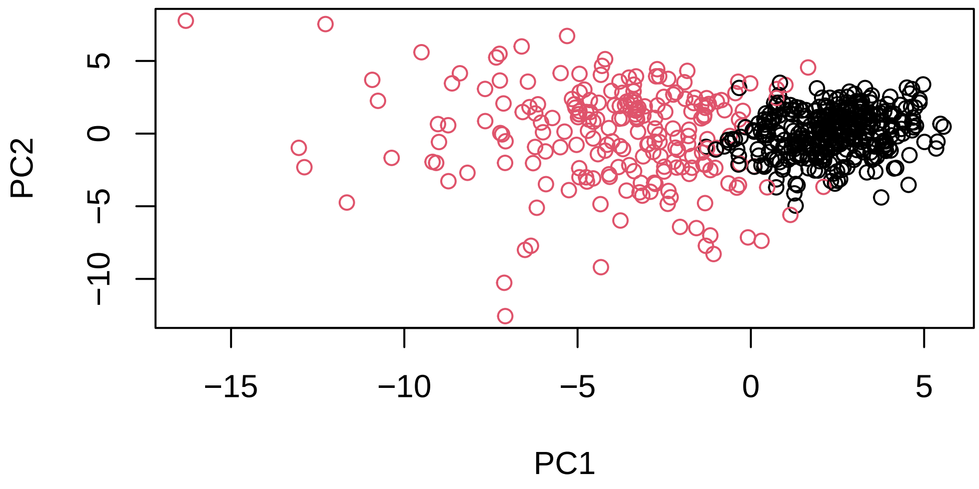
```
g <- as.factor(grps)
levels(g)
```

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

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

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

```
# Plot using our re-ordered factor
plot(wisc.pr$x[,1:2], col = g)
```



```
# Calculate cumulative variance explained by each principal component
cumulative_var <- cumsum(wisc.pr$sdev^2) / sum(wisc.pr$sdev^2)

# Find the minimum number of principal components required to explain 90% of the variabili
min_components <- min(which(cumulative_var >= 0.9))
```

```
# Create hierarchical clustering model with linkage method="ward.D2"
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:min_components]), method="ward.D2")
```

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

Q13. How well does the newly created model with four clusters separate out the two diagnoses?

```
# Compare to actual diagnoses
table(wisc.pr.hclust.clusters, diagnosis)
```

```
                       diagnosis
wisc.pr.hclust.clusters   B   M
                      1  28 188
                      2 329  24
```

The new model works efficiently to separate the two diagnoses from the four clusters.

Q14. How well do the hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses?

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

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

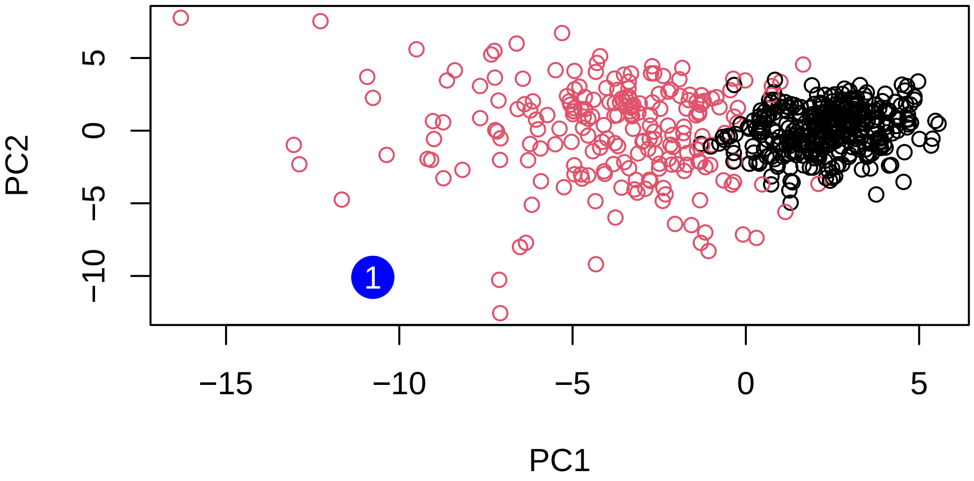
They do fine but they require more work/code/math to be done, while the newer model does not.

6. Prediction

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

```
           PC1        PC2        PC3       PC4      PC5       PC6        PC7
[1,] -10.76452 -10.093978 -0.5897994 -4.164748 10.61922 -1.630738 0.03566861
[2,] -18.09606  -9.967098 -2.1549431 -4.006848  6.69687 -2.034714 1.25088149
           PC8       PC9     PC10       PC11     PC12       PC13      PC14
[1,] 0.7308658 -1.580861 3.166451 -0.7167150 3.850569 -0.8259764 1.0195729
[2,] 0.6308585 -1.155629 3.608207 -0.3405375 2.288732 -0.3976672 0.1347203
         PC15      PC16      PC17      PC18     PC19      PC20      PC21
[1,] 3.735687 -4.068783 1.0877034 0.9985959 1.022760 -2.430215 -1.295749
[2,] 3.543905 -3.749616 0.7613603 1.1763217 1.366702 -2.609643 -1.541050
          PC22       PC23      PC24       PC25      PC26      PC27       PC28
[1,] -1.348026 -0.7388274 -1.083000 -0.4220831 -1.892993 -1.176056 0.05527974
[2,] -1.424290 -0.7591376 -1.439202 -0.6508838 -1.981711 -1.397390 0.18112357
          PC29       PC30
[1,] 0.2658028 0.05162840
[2,] 0.2842191 0.02734355
```

```
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")
```



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

For some reason, this plot does not match the plot shown in the lab. For the purposes of this question, I will base my results on the plot in the lab. Patient 2 (blue dot #2) should be prioritized for follow up. They are an outlier compared to the other patients, which are clustered together near zero on the first principal component. Because of this, patient 2 should be a priority for follow-up as they may have a higher risk of malignancy or require further investigation.