Class 8 Mini-Project

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Background

In today's class, we will be employing all the R techniques for data analysis that we have learned thus far — including the machine learning methods of clustering and PCA — to analyze real breast cancer biopsy data.

```
new <- read.csv("new_samples.csv")
wisc.df <- read.csv("WisconsinCancer.csv", row.names = 1)
```

We need to remove the `diagnosis` column before we do any further analysis of this dataset — we don't want to pass this to PCA etc. We will save it as a separate wee vector that we can use later to compare our findings to those of experts.

```
diagnosis <- wisc.df$diagnosis
wisc.data <- wisc.df[,-1]
```

Q1. How many observations are in this dataset?

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

```
[1] 569
```

569 observations

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

```
length(diagnosis[diagnosis == "M"])
```

```
[1] 212
```

212 malignant diagnoses

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

```
length(grep("_mean$", colnames(wisc.df)))
```

```
[1] 10
```

10 variables have `_mean` at the end.

Principal Component Analysis (PCA)

The main function in "base R" is called `prcomp()`. We will use the optional argument `scale = T` here as the data columns/features/dimensions are on very different scales in the original data set.

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

```
attributes(wisc.pr)
```

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

$class
[1] "prcomp"
```

```
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)?

44.27%

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

3

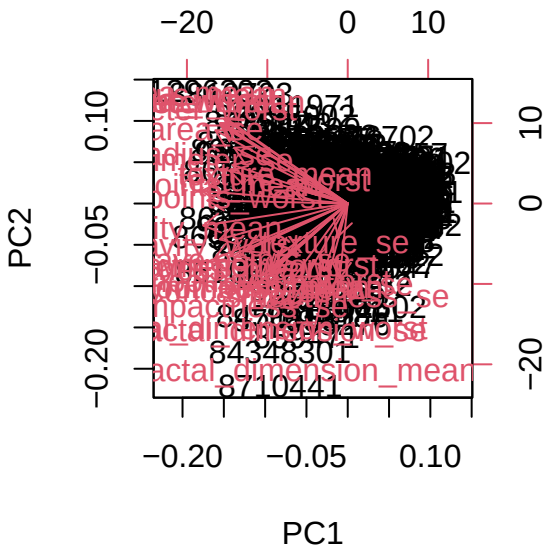
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

7

Interpreting PCA Results

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

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



You can't see very much because it's too crowded from overplotting.

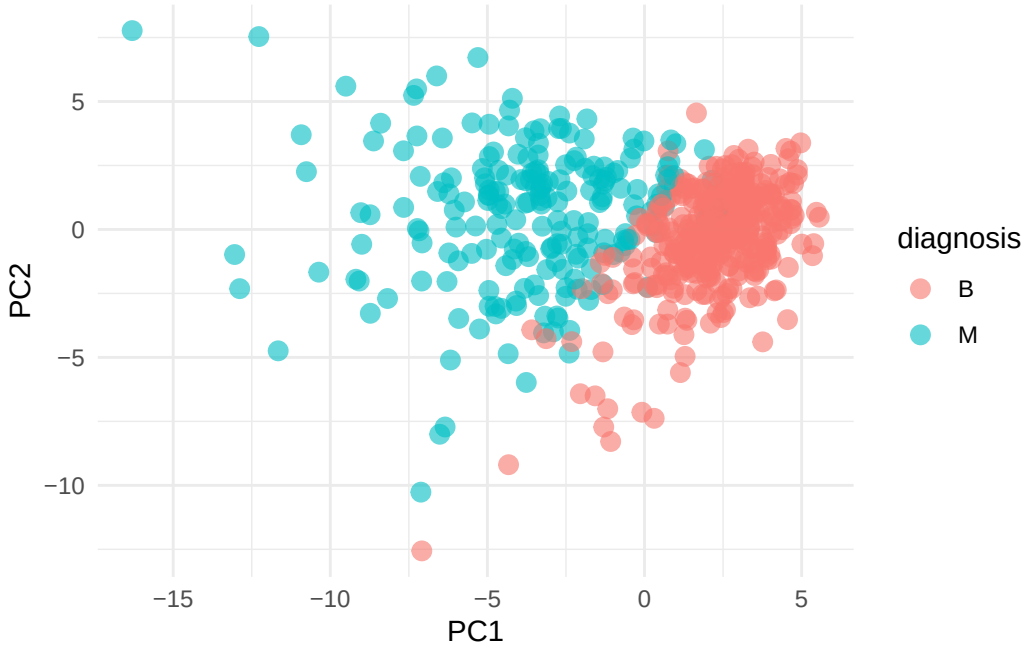
```
library(ggplot2)
```

```
Warning: package 'ggplot2' was built under R version 4.4.3
```

Using `ggplot2`, we can more easily represent our PCA results:

PC1 vs PC2

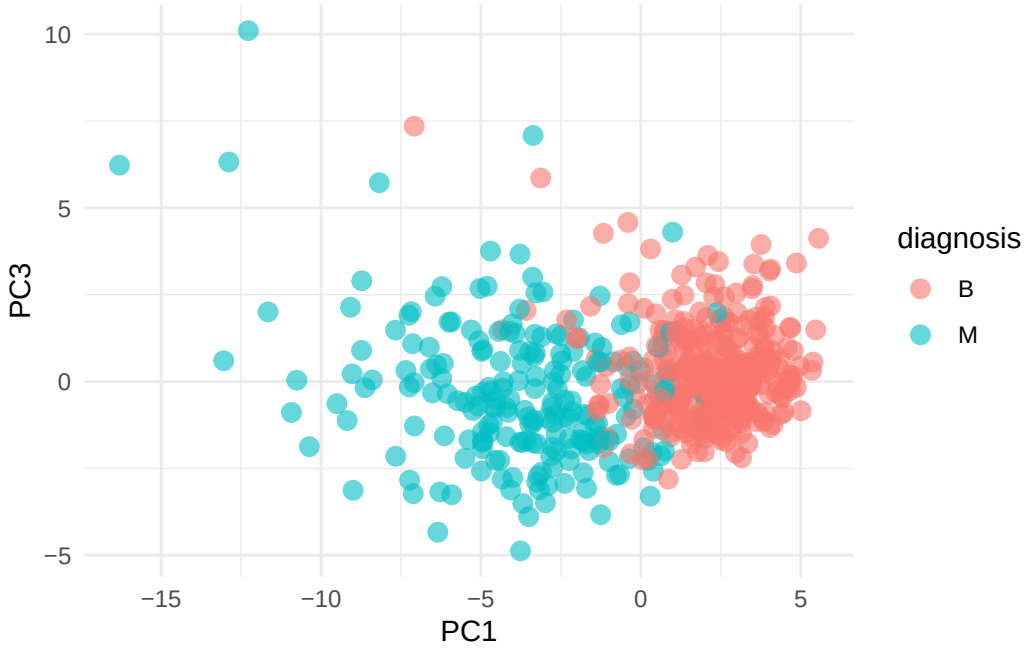
```
ggplot(wisc.pr$x) +
  aes(x = PC1, y = PC2, col = diagnosis) +
  geom_point(size = 3, alpha = 0.6) +
  xlab("PC1") +
  ylab("PC2") +
  theme_minimal()
```



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

PC1 vs PC3

```
ggplot(wisc.pr$x) +
  aes(x = PC1, y = PC3, col = diagnosis) +
  geom_point(size = 3, alpha = 0.6) +
  xlab("PC1") +
  ylab("PC3") +
  theme_minimal()
```



Both of these graphs are actually pretty similar. It does, however, seem like there is more overlap of malignant and benign biopsies in the PC3 graph.

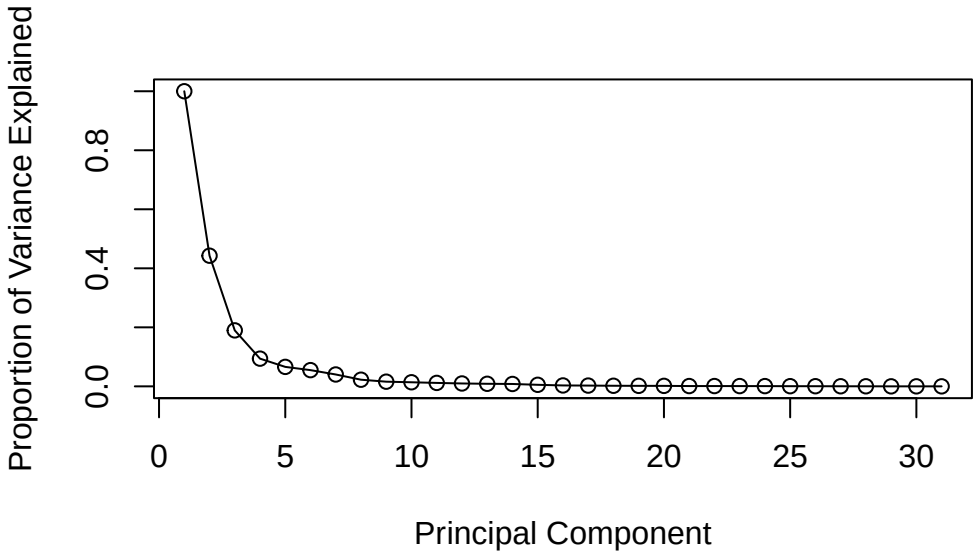
Variance

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

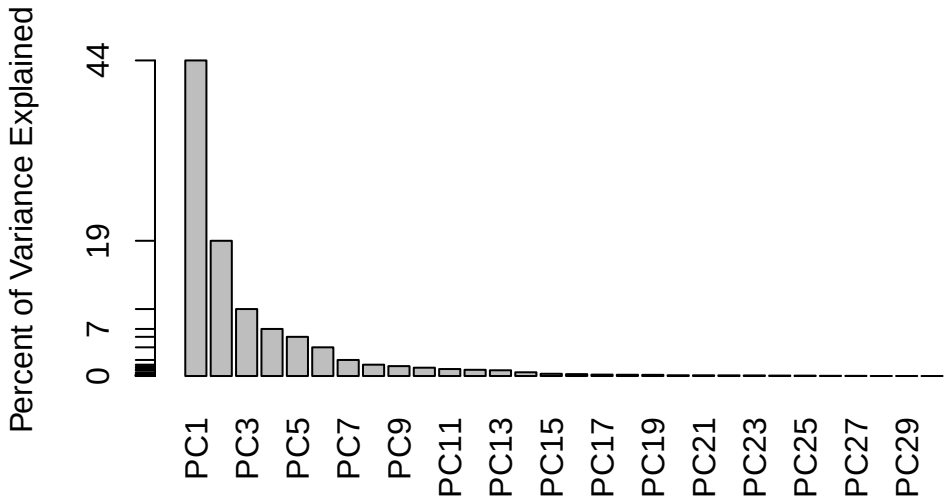
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

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

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




```
# Alternative screen 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 = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```



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. Are there any features with larger contributions than this one?

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

```
[1] -0.2608538
```

```
which.max(abs(wisc.pr$rotation[,1]))
```

```
concave.points_mean
                  8
```

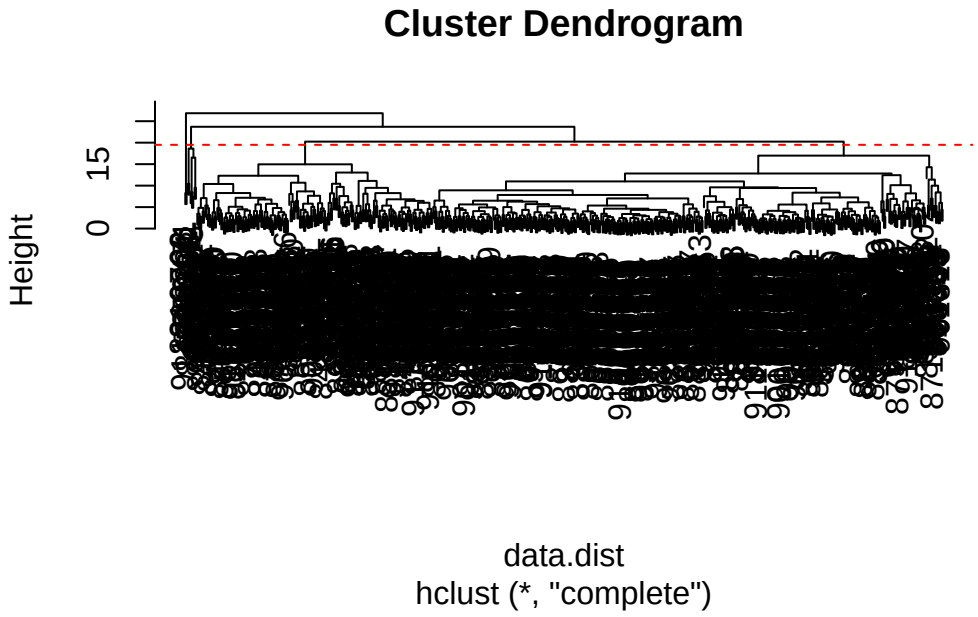
The component is -0.2608538. This feature/dimension/variable has the largest contribution.

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 which the clustering model has 4 clusters?

```
plot(wisc.hclust)
abline(h = 19.5, col="red", lty=2)
```



The height is 19

Selecting number of clusters is difficult, so let's examine

```
for (i in 2:6) {
  wisc.hclust.clusters.groups <- cutree(wisc.hclust, k = i)
  print(table(wisc.hclust.clusters.groups, diagnosis))
}
```

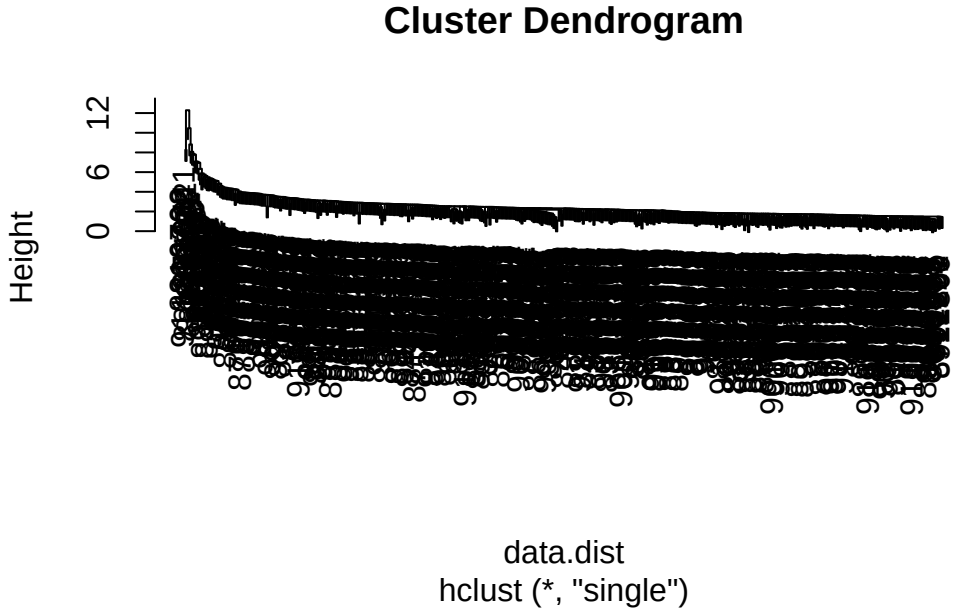
```
                           diagnosis
wisc.hclust.clusters.groups   B   M
                          1 357 210
                          2   0   2
                           diagnosis
wisc.hclust.clusters.groups   B   M
                          1 355 205
                          2   2   5
                          3   0   2
                           diagnosis
wisc.hclust.clusters.groups   B   M
                          1  12 165
                          2   2   5
                          3 343  40
                          4   0   2
                           diagnosis
wisc.hclust.clusters.groups   B   M
                          1  12 165
                          2   0   5
                          3 343  40
                          4   2   0
                          5   0   2
                           diagnosis
wisc.hclust.clusters.groups   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?

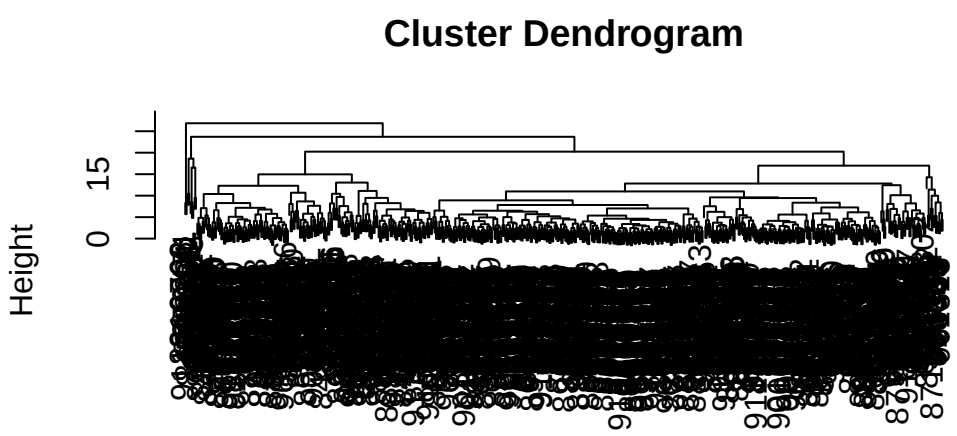
It looks like 4 groups because it's the lowest number of groups that clearly separates the two different diagnoses in the dataset. In terms of quality, I'm not sure how I could do this without having data on the pathologist diagnosis. Because we have the pathologist's diagnoses, we can compare true vs false results.

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

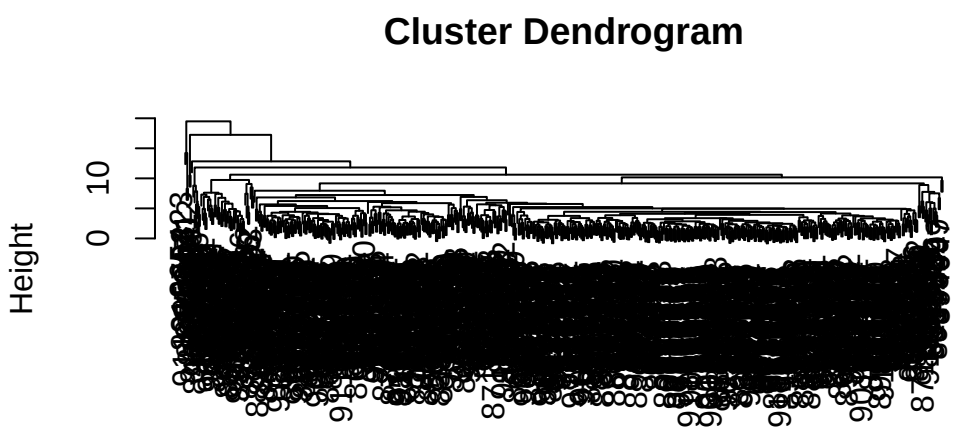
```
for (i in 1:4) {
  method <- c("single", "complete", "average", "ward.D2")
  wisc.hclust.methods <- hclust(data.dist, method = method[i])
  print(plot(wisc.hclust.methods))
}
```



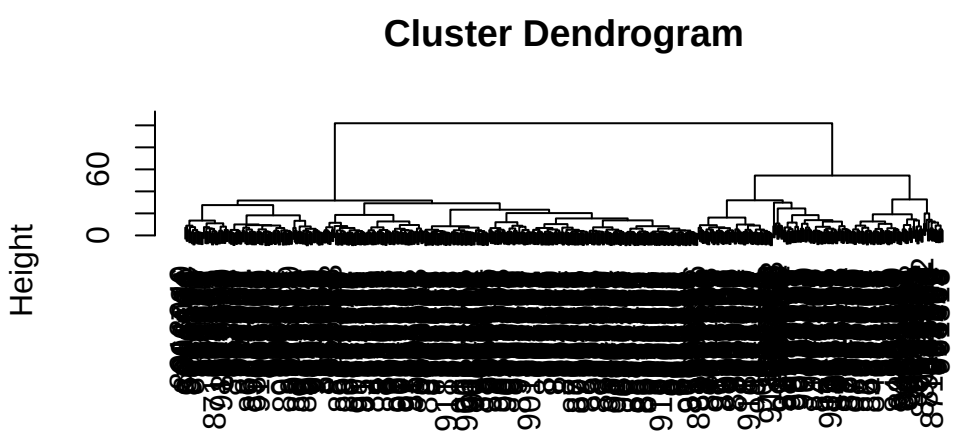

```
NULL
```


Cluster Dendrogram
Height
0
15
data.dist
hclust (*, "complete")

```
NULL
```


Cluster Dendrogram
Height
0
10
data.dist
hclust (*, "average")

```
NULL
```



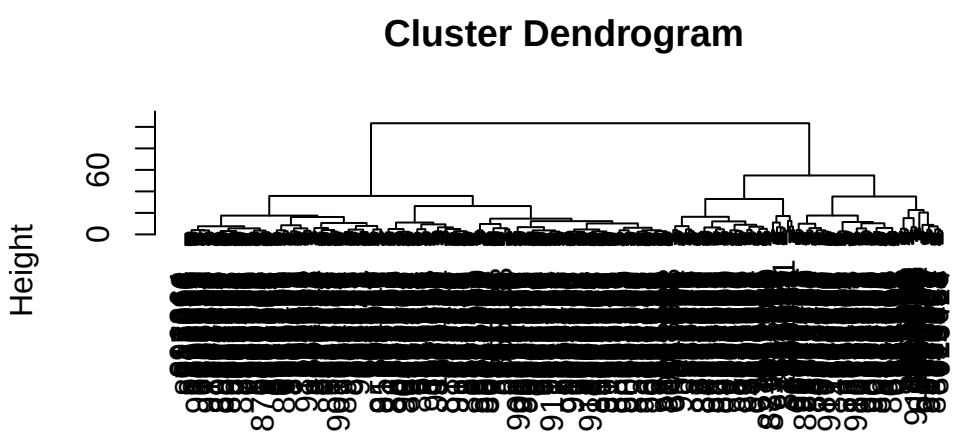

```
NULL
```

I like the `"ward.D2"` the most here. It makes a tree that shows the clearest difference in heights, even towards the bottom of the tree. It can do this because the maximum height of this method is significantly higher than the other methods. This graph also best affirms our prior knowledge of pathologist diagnoses.

Combining Methods

The idea here is that I can take my new variables (i.e. the scores on the PCs `wisc.pr$x`) that are better descriptors of the data set than the original features and use these for the basis of clustering instead.

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




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

```
grps
  1   2
203 366
```

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

I can now run `table()` with both my clustering `grps` and the expert `diagnosis`

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

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

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

It does pretty well. The groups are mostly separated by diagnosis, though there are still many false positives and false negatives.

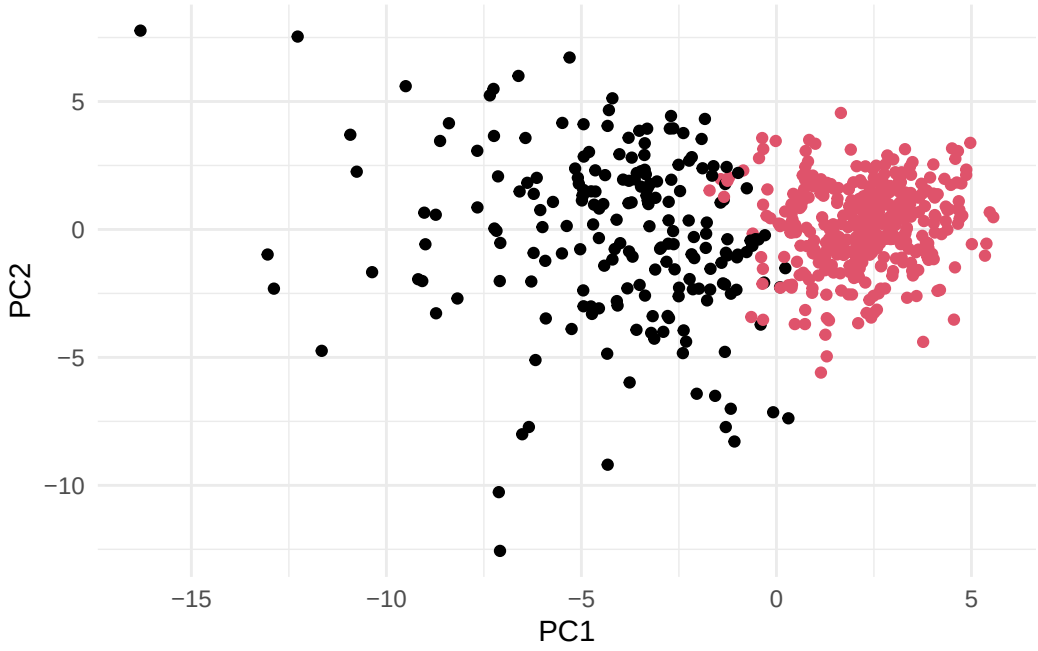
> Q14. How well do the hierarchical clustering models you created in the previous sections (i.e. without first doing PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.hclust.clusters and wisc.pr.hclust.clusters) with the vector containing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

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

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

The earlier hierarchical clustering model with four groups performed similarly to the new combined method. It has more unevenly distributed false positives and negatives though, and there are a new groups that are too small to tell whether they are meaningful at all. Overall, this model is skewed towards having false positives with more "M" diagnoses in the group containing primarily "B" diagnoses.

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



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

Our cluster "1" has 179 "M" diagnoses Our cluster "2" has 333 "B" diagnoses

179 TP 24 FP 333 TN 33 FN

Sensitivity: TP/(TP+FN)

```
179/(179+33)
```

```
[1] 0.8443396
```

Specificity: TN/(TN+FP)

```
333/(333+24)
```

```
[1] 0.9327731
```

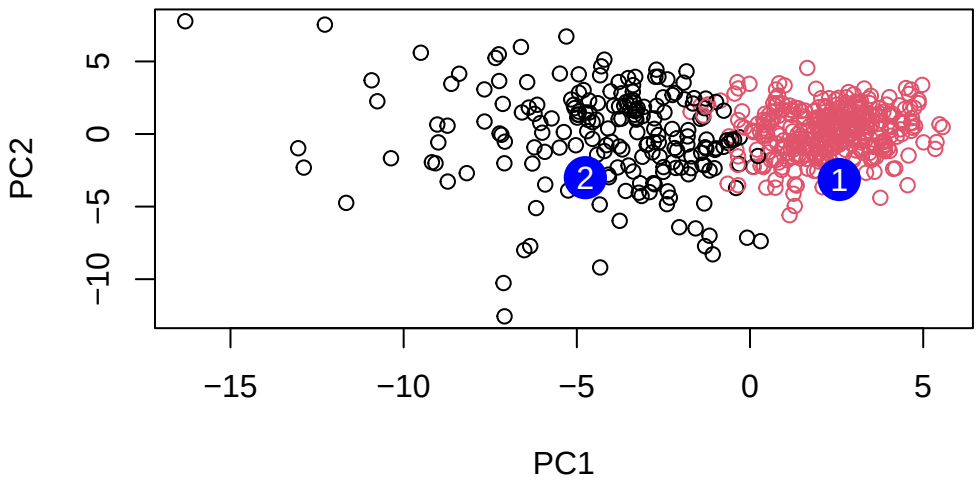
Prediction

We will use the `predict()` function to

```
file <- "new_samples.csv"
new <- read.csv(file)
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?

We should probably follow up with patient 2