

Class 08 Breast Cancer Mini Project BIMM 143

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Class 08 Breast Cancer Mini Project

We are going to be using data from a study from the state of Wisconsin about Breast Cancer.

First we downloaded the data from the lab and put it into the file. We still need to extract the data from the files.

```
# Save your 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)
# Let's look at just the first 6 rows!
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				

Next, we want to remove the “diagnosis” column because it will give us all of the answers. We

want to use data to answer the questions instead. So let's remove it.

```
#this code removes it
wisc.data <- wisc.df[,-1]
#we are also going to create a vector for it incase we need it for later
diagnosis <- wisc.df$diagnosis
colors <- rep("black", length(wisc.df$diagnosis))
colors[wisc.df$diagnosis == "M"] <- "red"
#let's look at the first 6 again with the new data set
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			

```
#look at how it changed!
```

Q1. How many observations are in this dataset?

569 observations.

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

```
malignant_diagnosis <- diagnosis == "M"
sum(malignant_diagnosis)
```

```
[1] 212
```

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

10

2. Principal Component Analysis (PCA)

We are going to check the columns and the standard deviations. It's good that we already removed the `wisc.df$diagnosis` because those are not numbers.

```
# 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

Now we are going to the PCA

```
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp(wisc.data, scale=TRUE)
#Let's check the summary too!
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)?

44.27%

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

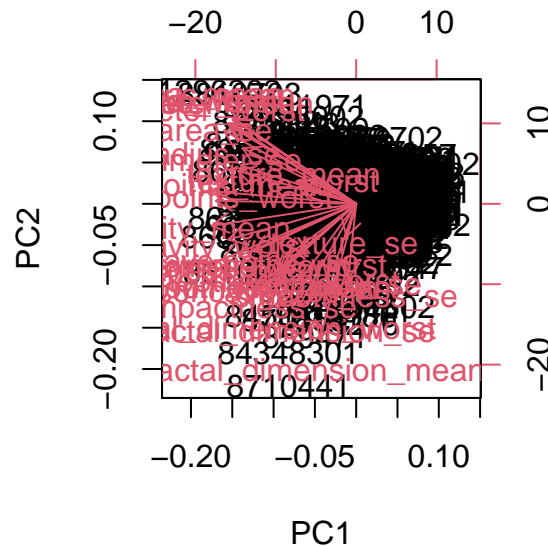
3 PCs (we reach 72.636% in PC3)

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

7 PCs (we reach 91.010% in PC7)

We are going to create a biplot using the `biplot()` function.

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

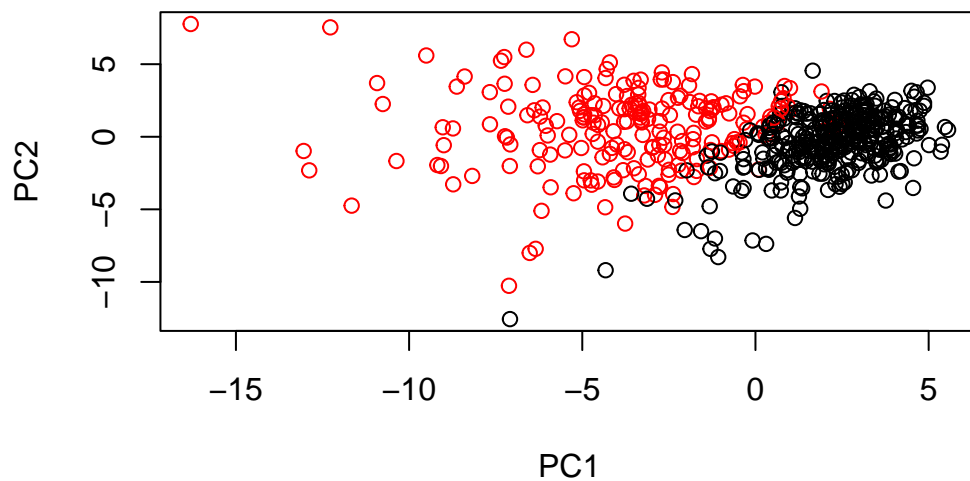


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

This is terrible. It is a jumbled mess of labels and plot points. We need to just to PC1 and PC2 in order to condense the data!

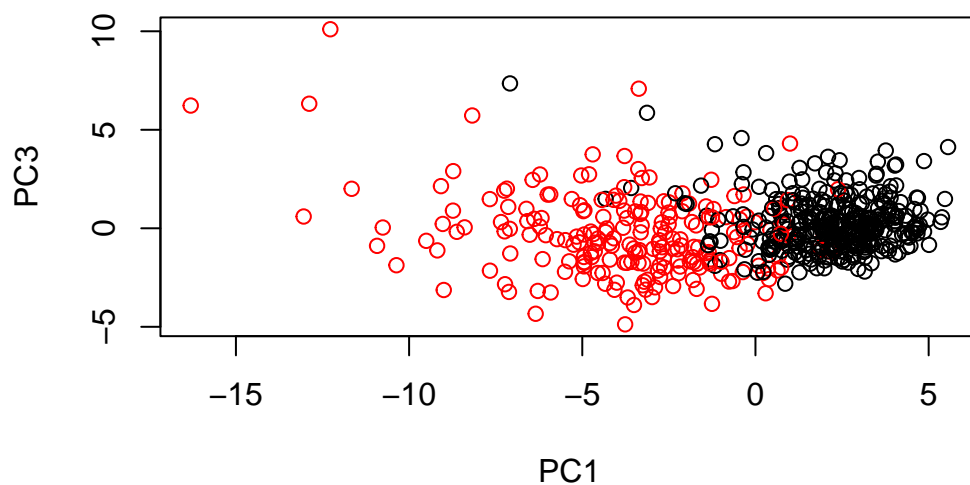
We are going to fix this by only using PC1 and PC2.

```
# Scatter plot observations by components 1 and 2
plot(wisc.pr$x, col=colors, 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[,c(1,3)], col = colors,
     xlab = "PC1", ylab = "PC3")
```

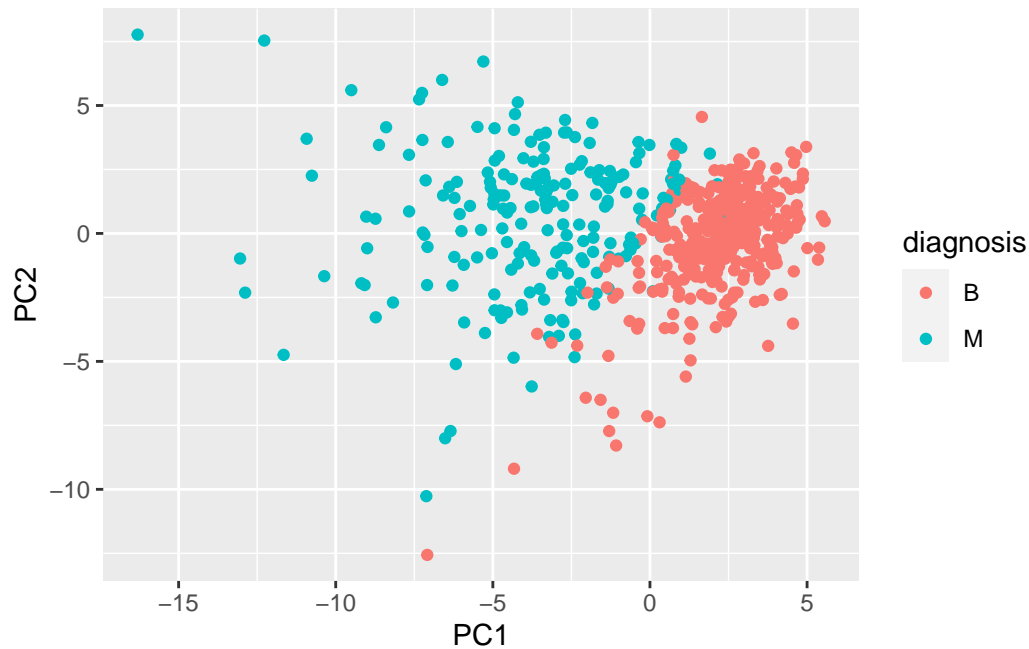
I noticed that the plots are similar but the first plot is a lot cleaner. But both the plots are capturing a separation in the data between the benign (black) and malignant (red).

Now we are going to visualize using `ggplot()`!

```
# 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()
```



Next we are going to calculate the variance!

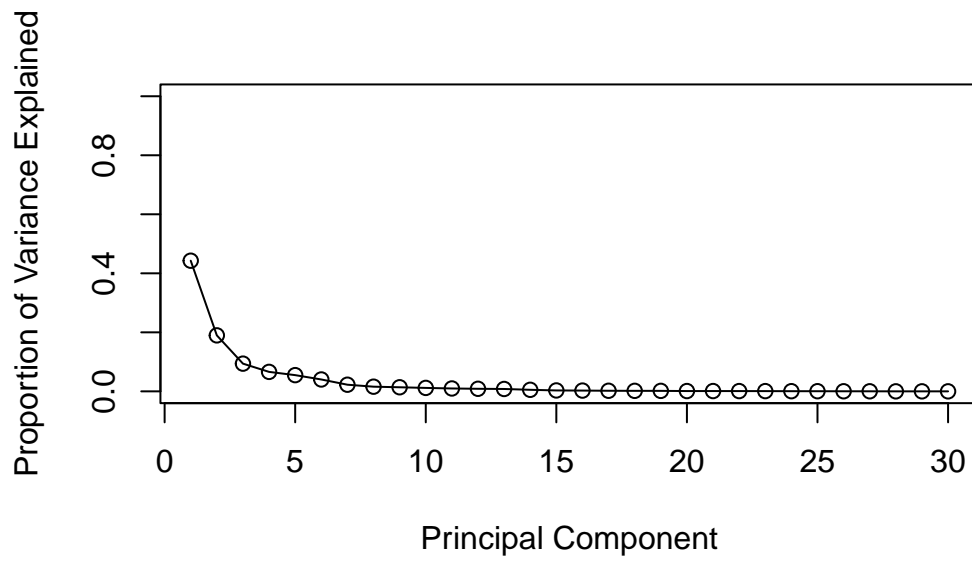
```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

Next we are going to calculate the variance explained by each principal component. Then we are going to plot it!

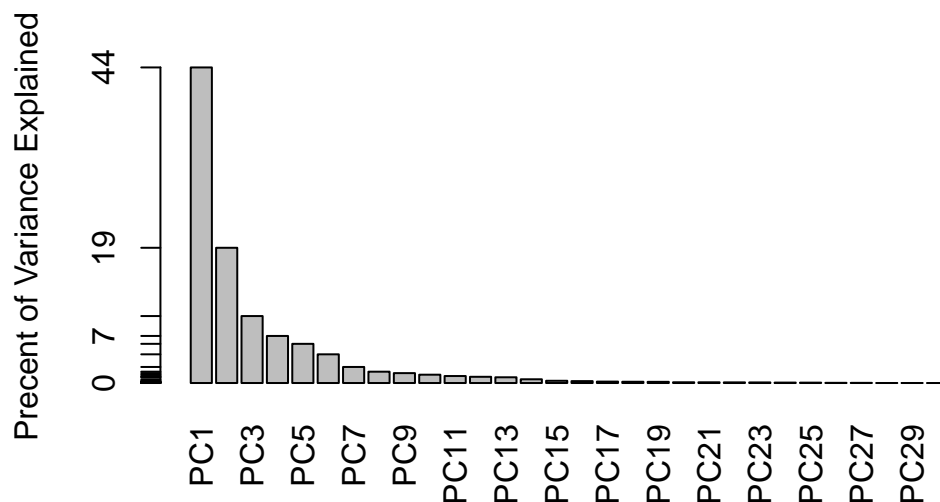
```
# Variance explained by each principal component: pve
pve <- pr.var / sum(pr.var)

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



Here is an alternative to visualize the same data.

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



I am going to skip the optional part of exploring extra graphs.

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`?

We need to find the loading vector for the feature `concave.points_mean`

```
loading_vector_pc1 <- wisc.pr$rotation[, 1]
loading_value_concave_points_mean <- loading_vector_pc1['concave.points_mean']
loading_value_concave_points_mean
```

```
concave.points_mean
-0.2608538
```

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

at PC5 or you need 5 PC's to explain 80% of the data

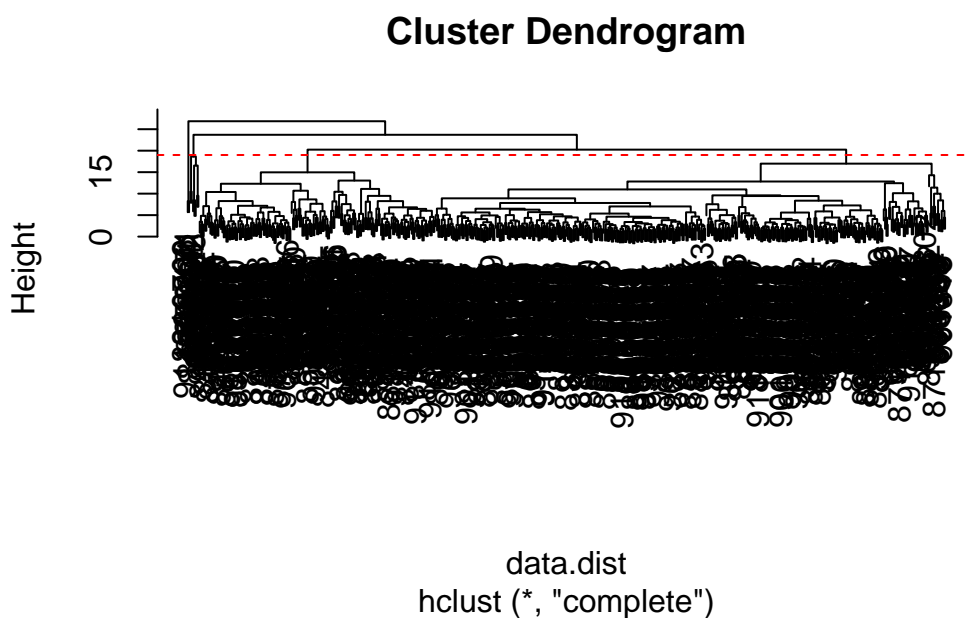
Hierarchical Clustering

We are going to be using hierarchical clustering!

```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
#now calculate the distances
data.dist <- dist(data.scaled)
#now put them into clusters
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?

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



The height would have to be 19!

We are going to cut up the clusters so there are 4!

```
wisc.hclust.clusters <- cutree(wisc.hclust, h=19)
#let's table it!
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?

```
wisc.hclust.clusters2 <- cutree(wisc.hclust, h=13)
#let's table it!
table(wisc.hclust.clusters2, diagnosis)
```

	diagnosis		
wisc.hclust.clusters2	B	M	
1	12	86	
2	0	59	
3	0	3	
4	331	39	
5	0	20	
6	2	0	
7	12	0	
8	0	2	
9	0	2	
10	0	1	

If you cut at 13 you will get 10 clusters and if you cut at 24, you will get 2 clusters. Looking more at these you could explore how different clusters could effect the data.

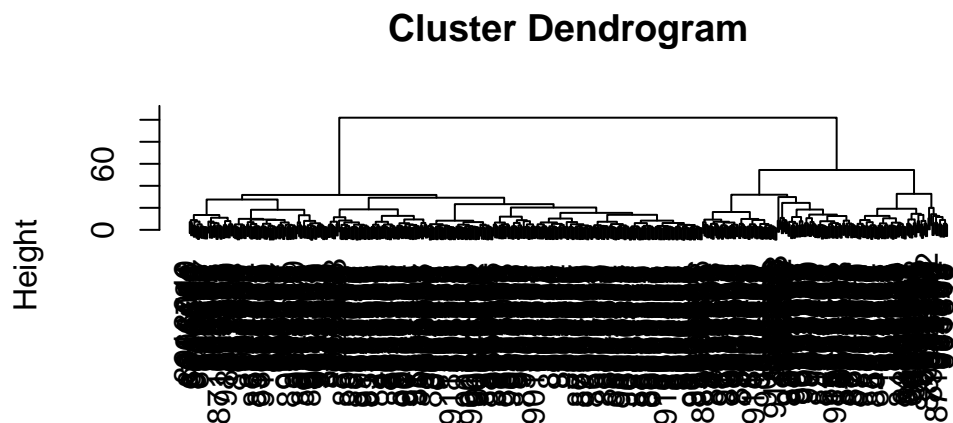
Q13. Which method gives your favorite results for the same data.dist dataset?
Explain your reasoning!

I like ward.D2 the best because it provides tends to produce compact, well-separated clusters, which is preferable.

Combining Methods

We are going to redo the plot. Instead of using the complete method, we are going to use ward.D2

```
wisc.hclust.ward <- hclust(data.dist, method="ward.D2")
plot(wisc.hclust.ward)
```



```
data.dist
hclust (*, "ward.D2")
```

This is a lot more promising. Next we are going to figure if those two main branches are malignant or benign!

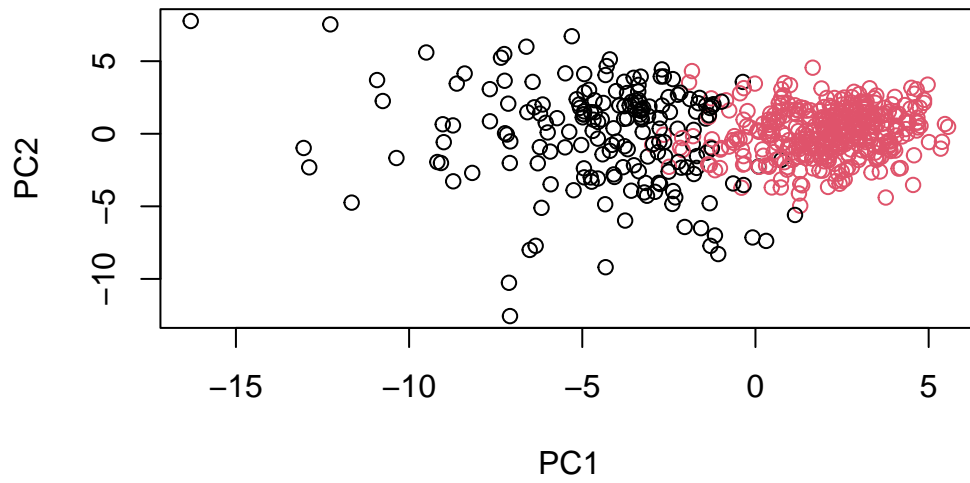
```
grps <- cutree(wisc.hclust.ward, k=2)
table(grps)
```

```
grps
 1  2
184 385
```

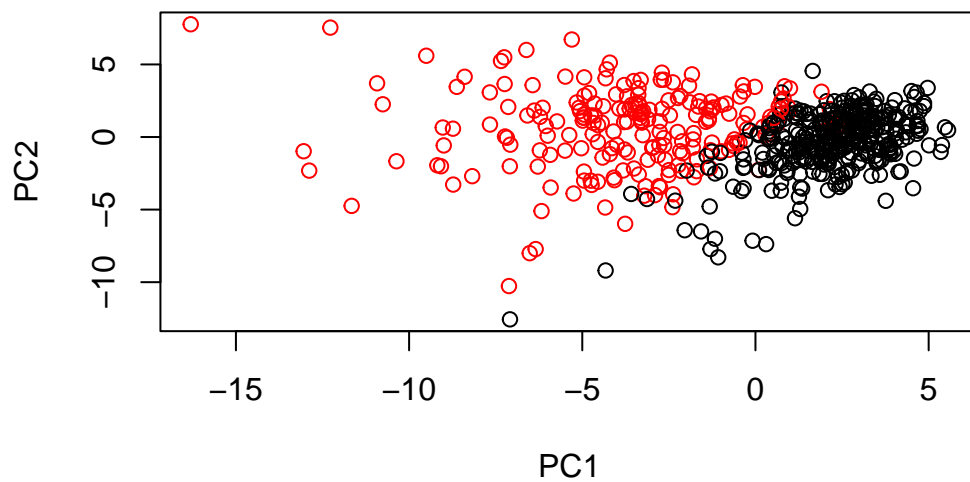
```
table(grps, diagnosis)
```

```
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=colors)
```

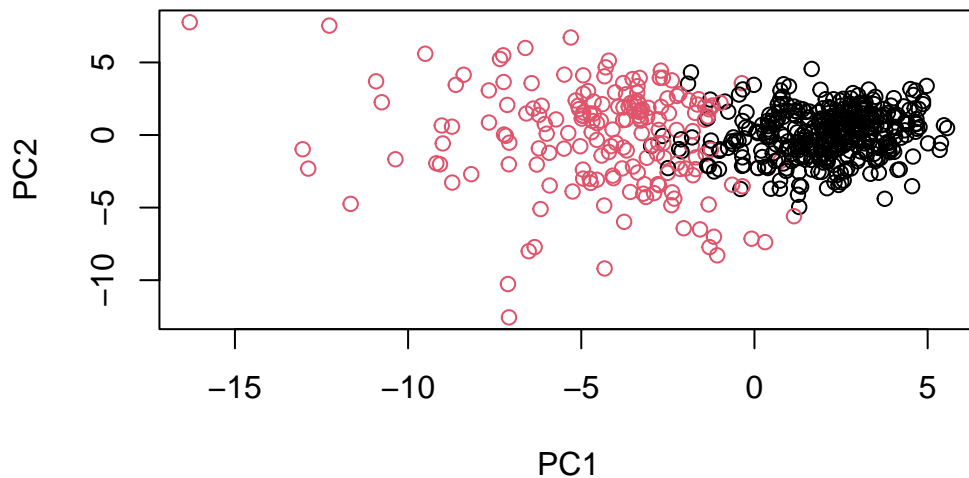
```
g <- as.factor(grps)
levels(g)
```

```
[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)
```



```
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]
wisc.pr.hclust <- hclust(data.dist, method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
# Compare to actual diagnoses
table(wisc.pr.hclust.clusters, diagnosis)
```

	diagnosis	
wisc.pr.hclust.clusters	B	M
1	20	164
2	337	48

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

They are split up in the same exact way!

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.

I don't have the `wisc.km$cluster` because I skipped the optional section. But looking at the table of `wisc.hclust.clusters`, we can see that they are cut up and split more.

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

```

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

```

Sensitivity/Specificity

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

The best sensitivity would be the flipped data set because you can more easily detect the unhealthy patients. The best for specificity would be the regular data set.

Prediction

```

#url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
npc

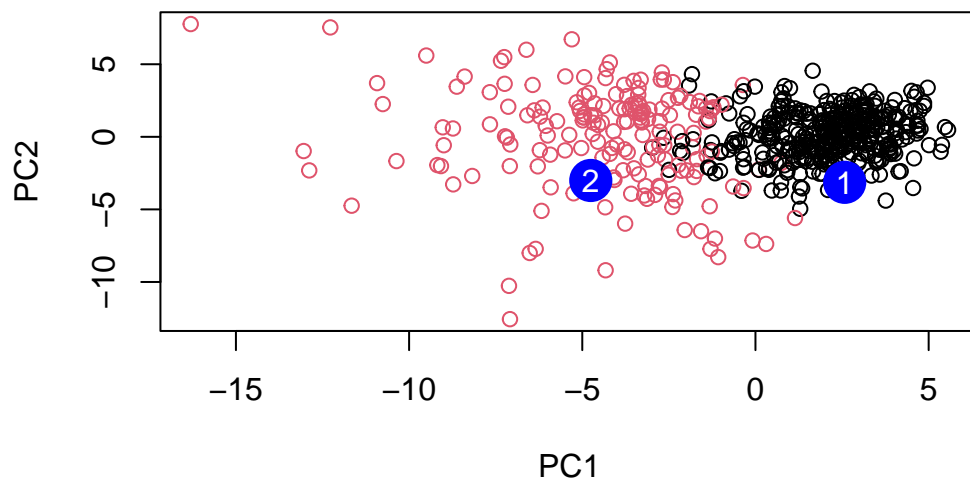
```

```

      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=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?

We should look at patient number 2 because they most like have a lump that is actually cancerous!