Class08

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Background

This source provides materials for a class mini-project focused on unsupervised learning analysis of human breast cancer cell data. Students will conduct principal component analysis (PCA) for dimensionality reduction and then apply hierarchical and k-means clustering techniques. The project involves exploratory data analysis, interpreting PCA results, evaluating clustering performance by comparing cluster assignments to actual diagnoses, and optionally combining PCA with clustering. The goal is to identify potential groupings within the cell data based on their characteristics without prior knowledge of malignancy, and the project concludes with an application of the PCA model to classify new patient samples.

Data Import

Our data comes from the U. of Wisconsin Medical Center.

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

Q1. How many patients/samples are in this dataset?

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

```
[1] 569
```

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

```
table(wisc.df$diagnosis)
```

```
  B   M
357 212
```

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

```
[1] 212
```

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

```
colnames(wisc.df)
```

```
 [1] "diagnosis"               "radius_mean"
 [3] "texture_mean"            "perimeter_mean"
 [5] "area_mean"               "smoothness_mean"
 [7] "compactness_mean"        "concavity_mean"
 [9] "concave.points_mean"     "symmetry_mean"
[11] "fractal_dimension_mean"  "radius_se"
[13] "texture_se"              "perimeter_se"
[15] "area_se"                 "smoothness_se"
[17] "compactness_se"          "concavity_se"
[19] "concave.points_se"       "symmetry_se"
[21] "fractal_dimension_se"    "radius_worst"
[23] "texture_worst"           "perimeter_worst"
[25] "area_worst"              "smoothness_worst"
[27] "compactness_worst"       "concavity_worst"
[29] "concave.points_worst"    "symmetry_worst"
[31] "fractal_dimension_worst"
```

```
length(grep("mean", colnames(wisc.df), value = T))
```

```
[1] 10
```

There is a diagnosis column that is the clinician consensus that I want to exclude from any further analysis. We will come back later and compare our results to this diagnosis.

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

```
[1] M M M M M M
Levels: B M
```

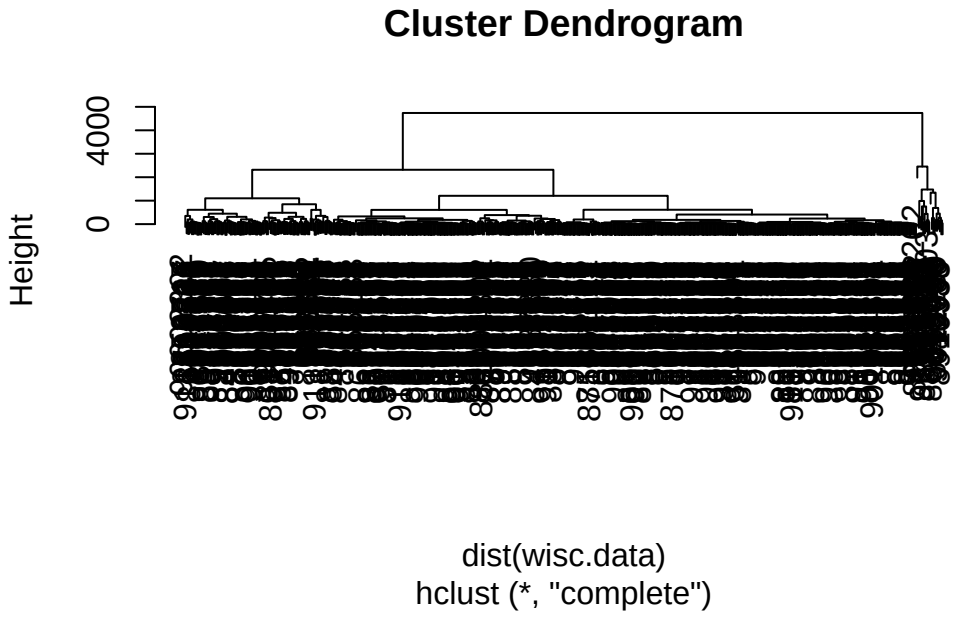
Now we can remove it from the `wisc.df`

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

Clustering

Let's try a `hclust()`

```
hc <- hclust(dist(wisc.data))
plot(hc)
```



We can extract clusters from this rather poor dendrogram/tree with the `cutree()`

```
grps <- cutree(hc, k=2)
```

How many individuals are in each cluster?

```
table(grps)
```

```
grps
  1   2
549  20
```

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

We can generate a cross-table that compares our cluster `grps` vector with our `diagnosis` vector values.

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

```
         grps
diagnosis   1   2
        B 357   0
        M 192  20
```

Principal Component Analysis

The Importance of Data Scaling

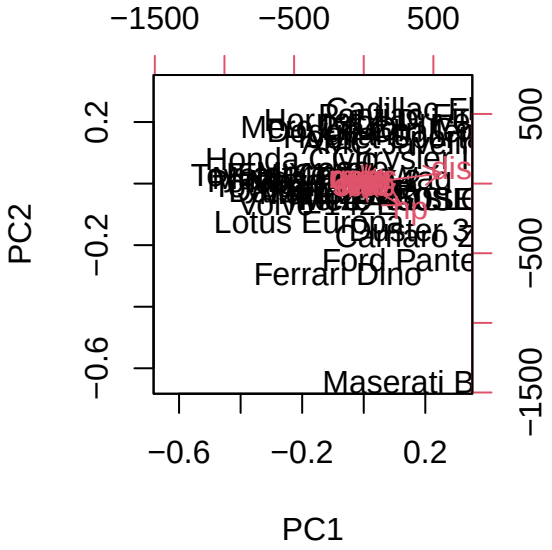
The main function for PCA in base R is `prcomp()`. It has a default input parameter of `scale=FALSE`.

```
#prcomp()
head(mtcars)
```

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Mazda RX4	21.0	6	160	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag	21.0	6	160	110	3.90	2.875	17.02	0	1	4	4
Datsun 710	22.8	4	108	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive	21.4	6	258	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout	18.7	8	360	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225	105	2.76	3.460	20.22	1	0	3	1

We could do a PCA of this data as is and it could be mis-leading...

```
pc <- prcomp(mtcars)
biplot(pc)
```



Let's look at the mean values of each column and their standard deviation.

```
colMeans(mtcars)
```

```
      mpg       cyl      disp        hp      drat        wt      qsec
20.090625  6.187500 230.721875 146.687500  3.596563  3.217250 17.848750
       vs        am      gear      carb
 0.437500  0.406250  3.687500  2.812500
```

```
apply(mtcars, 2, sd)
```

```
       mpg        cyl       disp         hp       drat         wt
 6.0269481  1.7859216 123.9386938 68.5628685  0.5346787  0.9784574
      qsec         vs         am       gear       carb
 1.7869432  0.5040161  0.4989909  0.7378041  1.6152000
```

We can "scale" this data before PCA to get a much better representation and analysis of all the columns.

```
mtscale <- scale(mtcars)
```

```
round(colMeans(mtscale))
```

```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb
   0    0    0    0    0    0    0    0    0    0    0
```

```
apply(mtscale, 2, sd)
```

```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb
   1    1    1    1    1    1    1    1    1    1    1
```

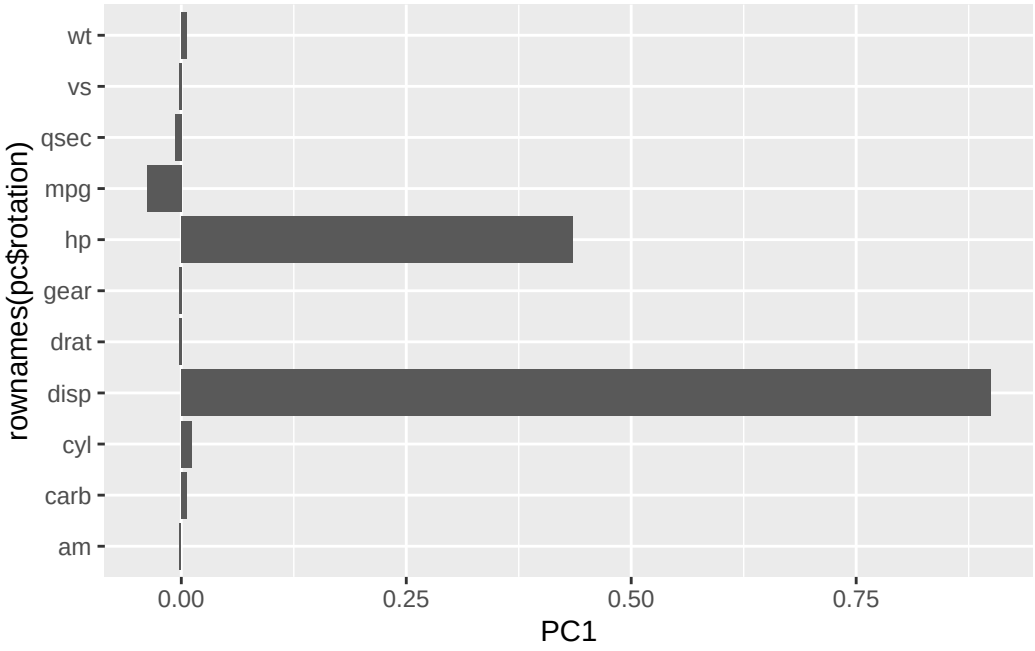
```
pc.scale <- prcomp(mtscale)
```

We can look at the two main results figures from PCA - the "PC plot" (a.k.a score plot, ordienation plot, or PC1 vs PC2 plot). The "loadings plot" shows how the original variables contribute to the new PCs.

A loadings plot of the unscaled PCA results:

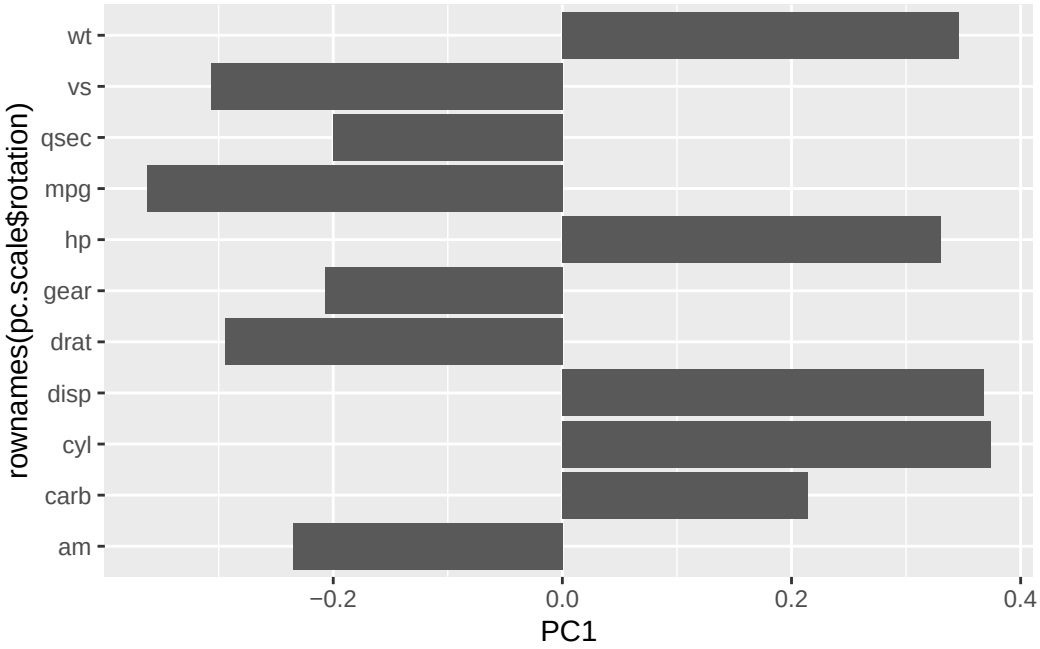
```
library(ggplot2)

ggplot(pc$rotation) +
  aes(PC1, rownames(pc$rotation)) +
  geom_col()
```



Loadings plot of the scaled data.

```
ggplot(pc.scale$rotation) +
  aes(PC1, rownames(pc.scale$rotation)) +
  geom_col()
```

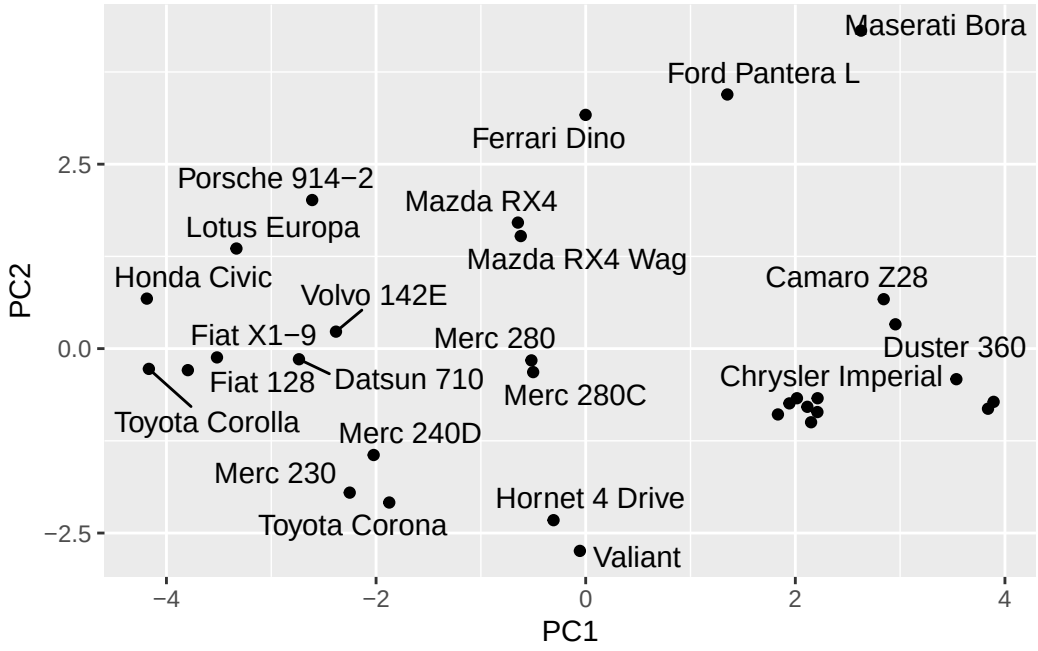


PC plot of scaled PCA results:

```
library(ggrepel)

ggplot(pc.scale$x) +
  aes(PC1, PC2, label=rownames(pc.scale$x)) +
  geom_point() +
  geom_text_repel()
```

```
Warning: ggrepel: 9 unlabeled data points (too many overlaps). Consider
increasing max.overlaps
```



Key point: In general, we will set `scale=TRUE` when we do PCA. This is not the default, but probably should be...

We can check the SD and mean of the different columns in `wisc.data` to see if we need to scale - hint we do!

PCA of wisc.data

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

To see how well PCA is doing here in terms of capturing the variance (or spread) in the data, we can use the `summary()` function.

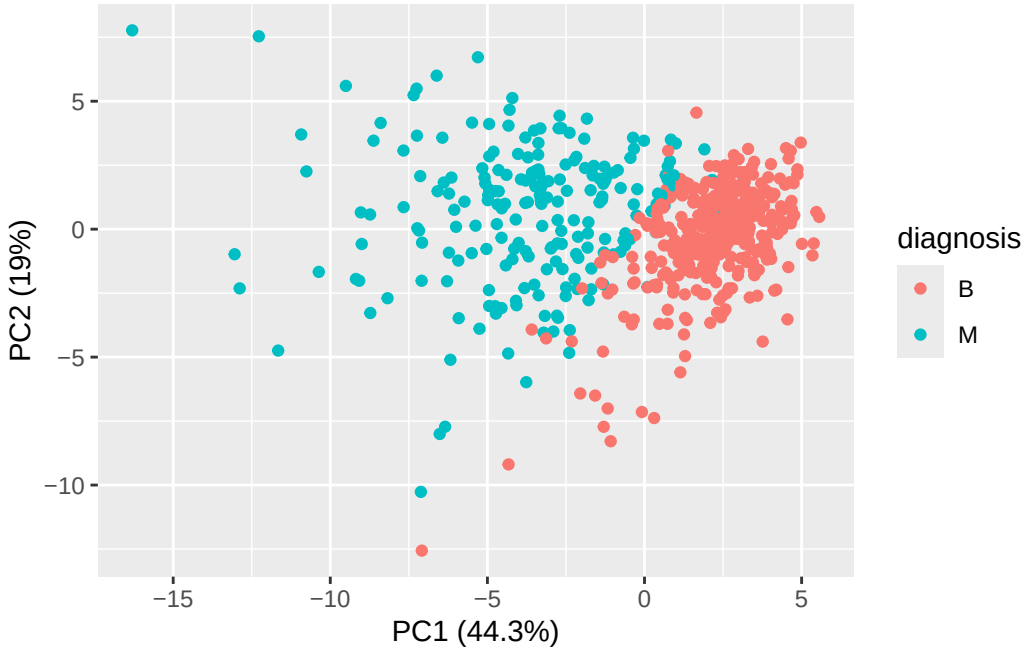
```
summary(wisc.pr)
```

```
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
```

Let's make the main PC1 vs PC2

```
ggplot(wisc.pr$x) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point() +
  xlab("PC1 (44.3%)") +
  ylab("PC2 (19%)")
```



Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)?

44.3% of the original variance is captured by PC1.

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

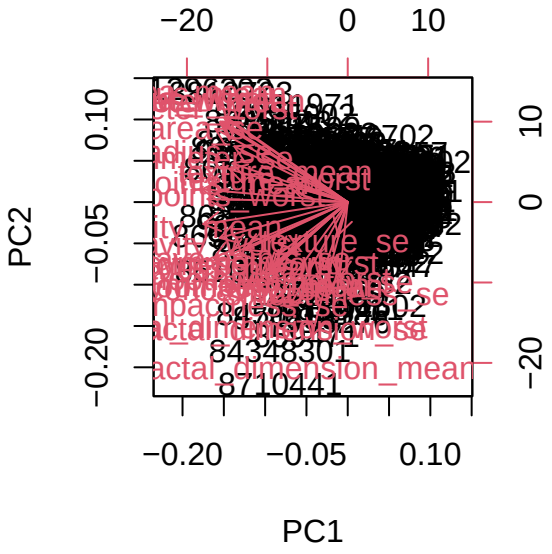
3 PCs are required to capture 70% of the original variance.

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 capture 90% of the original variance.

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

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

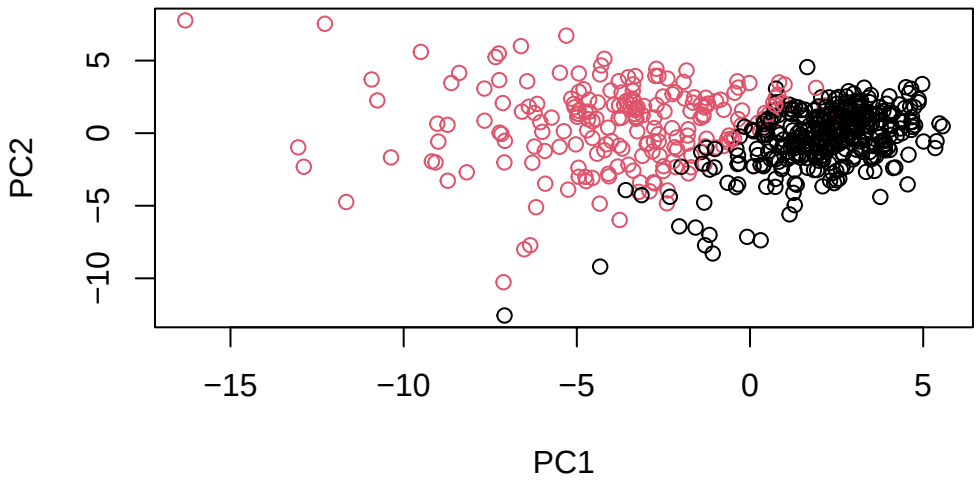


The biplot of the data is not easy to understand because there is too much crowding of the labels, the labels of the points have no significance, and there is no legend describing what the different colors represent.

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

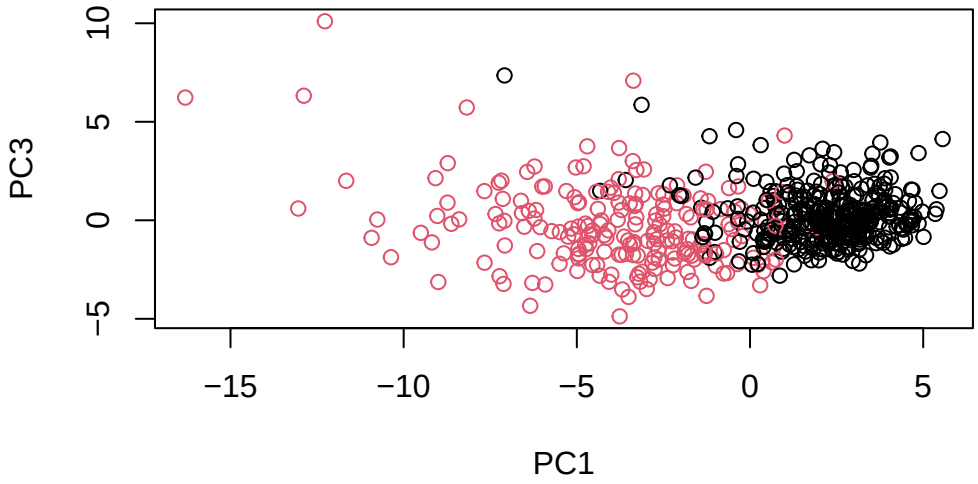
```
#scatter plot for PC1 vs PC2

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




```
#scatter plot for PC1 vs PC3

plot(wisc.pr$x[,c(1,3)], col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```



Both plots have the "B" and "M" groups clustered at similar regions of the plot. But, PC3 has a more positive skew in variation and PC2 has a more negative skew in variation. There are also less overlaps between the two clusters in PC1 vs PC2 than in PC1 vs PC3.

> 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?

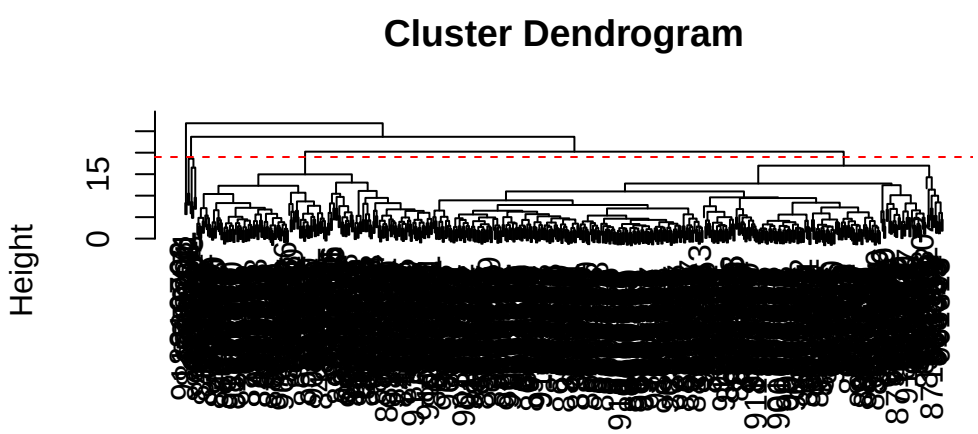
```
wisc.pr$rotation["concave.points_mean",1]
```

```
[1] -0.2608538
```

The PC1 for "concave.points_mean" is -0.2608538.

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

```
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(data.dist, method="complete")
plot(wisc.hclust)
abline(wisc.hclust, h=19, col="red", lty=2)
```



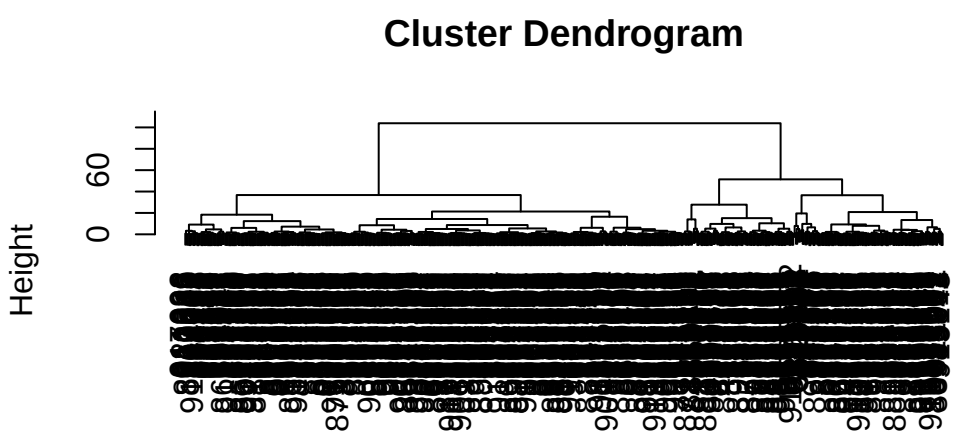
At height 19, the clustering model has 4 clusters.

5. Combining Methods

We can take our PCA results and use them as a basis set for other analysis such as clustering.

Clustering on PCA results

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



We can "cut" this tree to yield our clusters (groups):

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

```
pc.grps
  1   2
195 374
```

How do I cluster grps compare to the expert diagnosis

```
table(diagnosis, pc.grps)
```

```
         pc.grps
diagnosis   1   2
        B  18 339
        M 177  35
```

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

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

"ward.D2" is my favorite method because the clusters are created with most of the diagnosis data points correctly separated and it decreases the variance within the clusters. The other methods result in more skewed clusters where the distribution of the diagnosis data points within each cluster is not as correct as the "ward.D2" method and there is a massive difference in the number of data points in each cluster.

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

The model separates the diagnoses fairly well because most of the "B" and "M" are in separate groups. However, there are still a many false positives for the incorrect diagnosis. For example, there are still 35 "M" that are mixed with the "B" diagnosis and 18 "B" that are mixed with the "M" diagnosis.

> Q14. 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.

They did really badly. We do much better after PCA - the new PCA variables (what we call basis set) gives us much better separation of "M" and "B".

7. Prediction

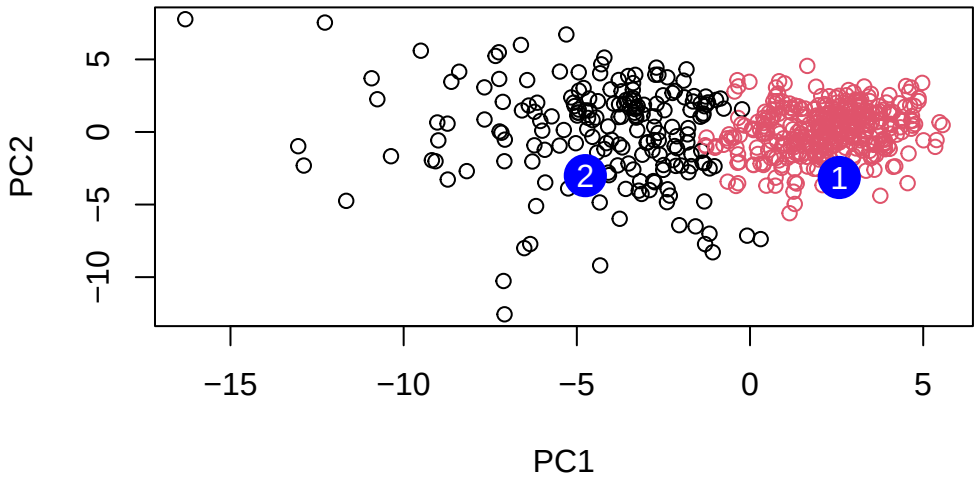
We can use our PCA model for the analysis of new "unseen"data. In this case from U. Mich.

```
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=pc.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?

The patients in cluster 2 because there is more variation among those points than in cluster 1.