Class 8: Mini Project

Emily Chen (PID: A16925878)

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 come from the U. of Wisconsin mecial Center

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

Q1. How many people are in the dataset?

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

```
[1] 569
```

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

```
  B   M
357 212
```

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

```
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"
```

The grep function has two required arguments: pattern and x. In this case since we are trying to find how many of the variable have the suffix mean so our pattern is "mean" and then for x we are looking at the colnames(wisc.df). to find the total number of number we will use the function `length()`

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

```
[1] 10
```

There is a diagnosis column that is the clinician's consensus, which I want to exclude from any feature analysis. We will come back to it later and compare our results to this diagnosis.

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

```
  [1] M M M M M M M M M M M M M M M M M B B B M M M M M M M M M M M M M M
 [38] B M M M M M M M M B M B B B B B M M B M M B B B B M B M M B B B B M B M M
 [75] B M B M M B B B M M B M M M B B B M B B M M B B B M M B B B B M B B M B B
[112] B B B B B B M M M B M M B B B M M B M B M M B M M B B M B B M B B B B M B
[149] B B B B B B B B M B B B B M M B M B B M M B B M M B B B B M B B M M M B M
[186] B M B B B M B B M M B M M M M B M M M B M B M B B M B M M M M B B M M B B
[223] B M B B B B B M M B B M B B M M B M B B B B M B B B B B M B M M M M M M M
[260] M M M M M M M B B B B B B M B M B B M B B M B M M B B B B B B B B B B B B
[297] B M B B M B M B B B B B B B B B B B B B B B M B B B M B M B B B B M M M B B
[334] B B M B M B M B B B M B B B B B B B M M M B B B B B B B B B B B M M B M M
[371] M B M M B B B B B M B B B B B M B B B M B B M M B B B B B B M B B B B B B
[408] B M B B B B B M B B M B B B B B B B B B B B B M B M M B M B B B B B M B B
[445] M B M B B M B M B B B B B B B B M M B B B B B B M B B B B B B B B B B M B
[482] B B B B B B M B M B B M B B B B B B M M B M B M B B B B B M B B M B M B M M
[519] B B B M B B B B B B B B B B B B M B M M B B B B B B B B B B B B B B B B B
[556] B B B B B B B M M M M M M B
Levels: B M
```

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

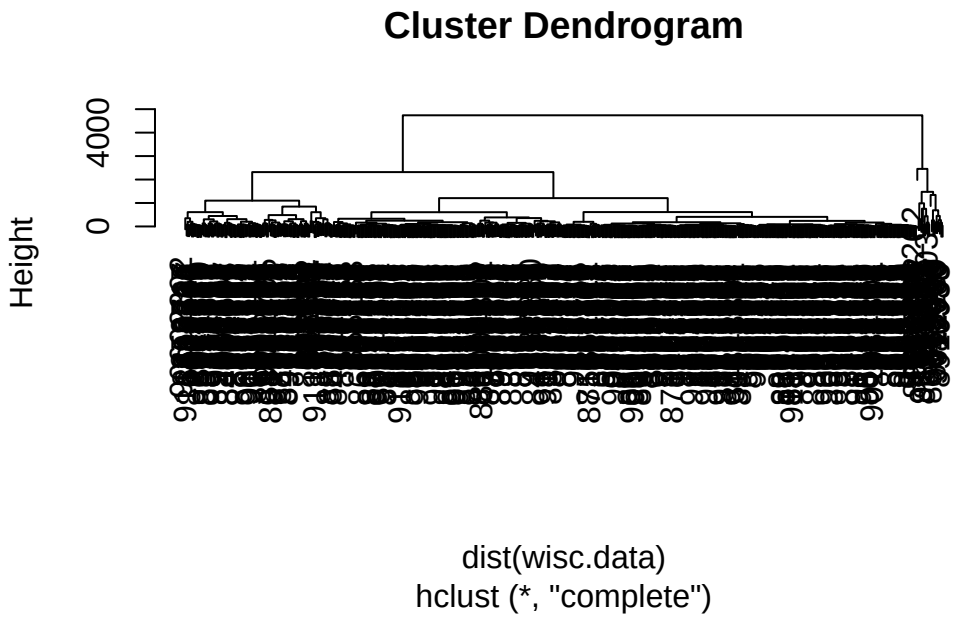
```
wisc.data<- wisc.df[,-1]
```

Clustering

We can use k-means or hierarchical clustering aka hclust. In k-means, we have to give it the data and then the number of clusters so `kmeans(wisc.data, ccenter=2)`. In `hclsut(dist(wisc.data))`

Let's try a hclust()

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



We can extract clusters from this rather than the poor dendrogram/tree with the code `cutree()` make sur you give it a height

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

How many individual 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
```

From the table, we can see that in group 1, there are 357 that are benign, and then 192 are malignant. For group 2, there are 0 benign and 20 malignant.

Principle Component Analysis

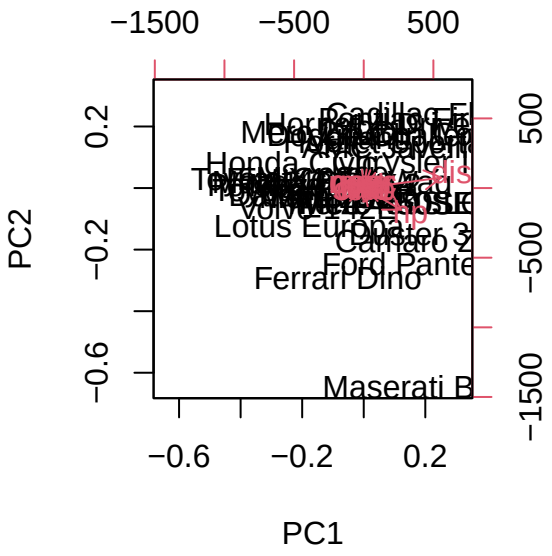
In the function prcomp there are three arguments x, scale=F, center=F. Only the x argument is required. The main function for PCA in base R is `prcomp()` it has a default input parameter of `scale=false`

```
#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 coudl be mis-leading....

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




```
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
```

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
```

Our means as seen above was 20,... but not they are zero

```
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
```

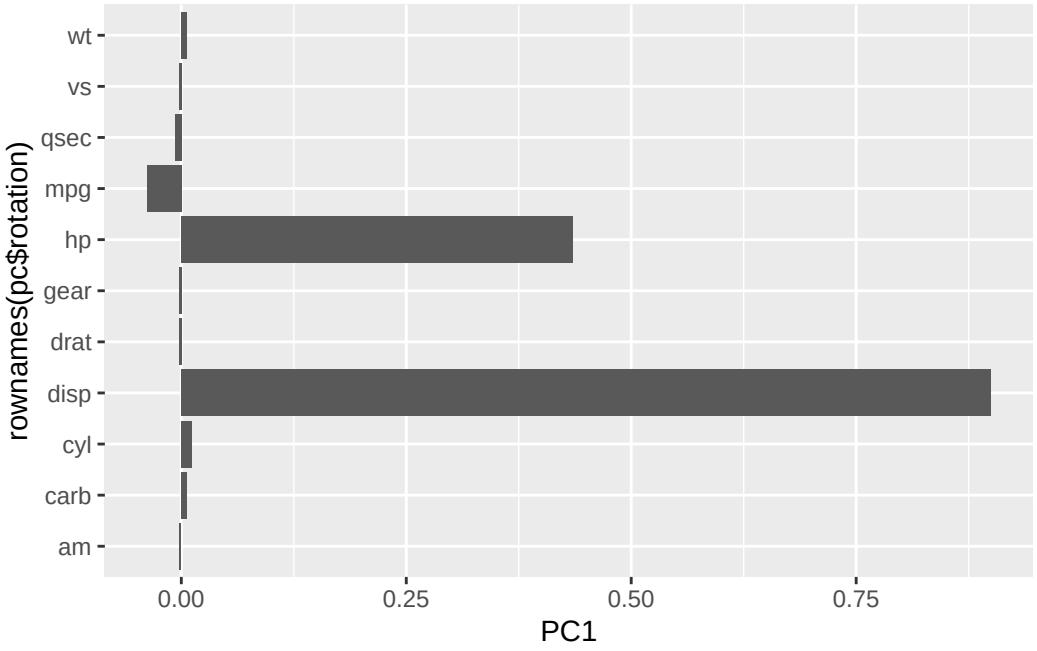
```
pc.scale<- prcomp(mtscale)
```

We can look at the two main figures from PCA- the "PC plot" (aka score plot, ordienation plot, or PC1 vs PC2 plot). The "loading plot" how the orientation variables contributing to the new PCs

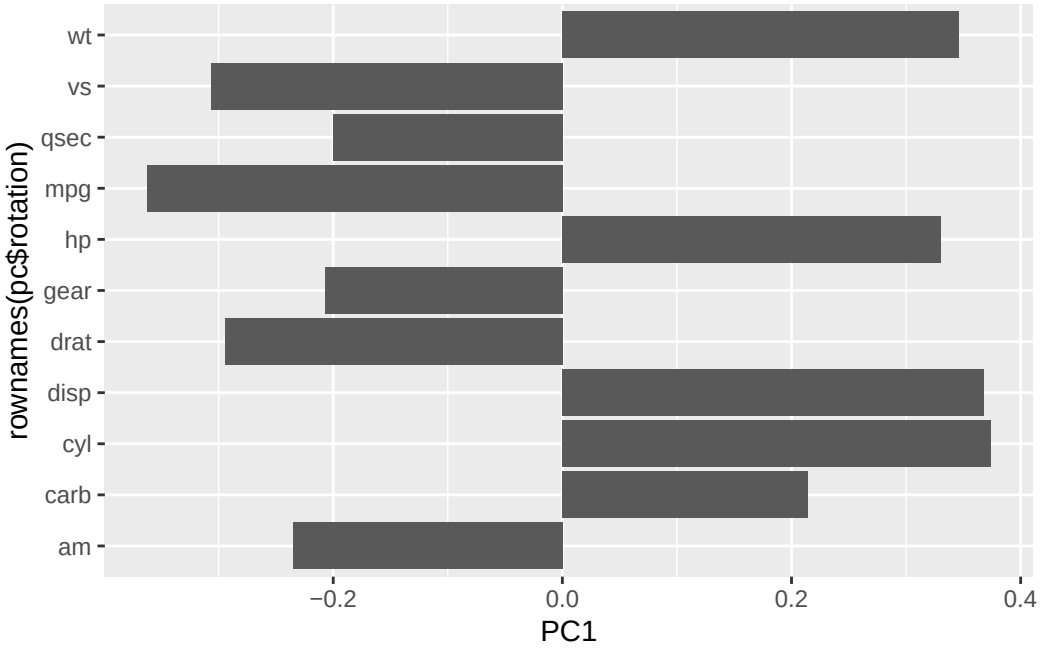
A loadings plots of the unscaled PCA results

```
library(ggplot2)

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



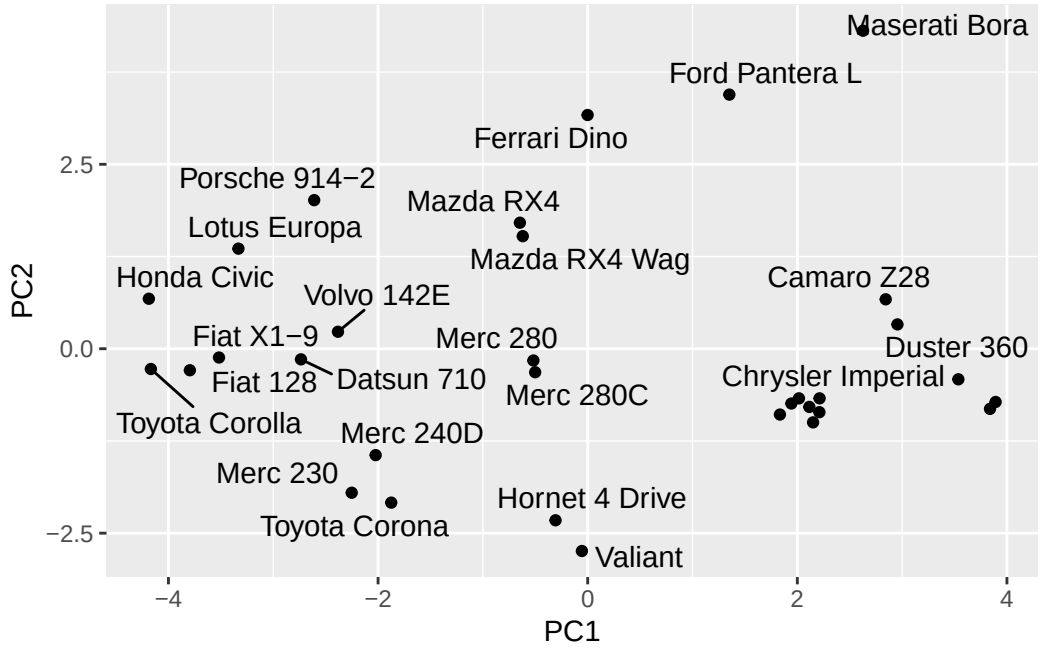

```
ggplot(pc.scale$rotation)+
  aes(PC1, rownames(pc$rotation))+
  geom_col()
```



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 propaly should be.

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

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

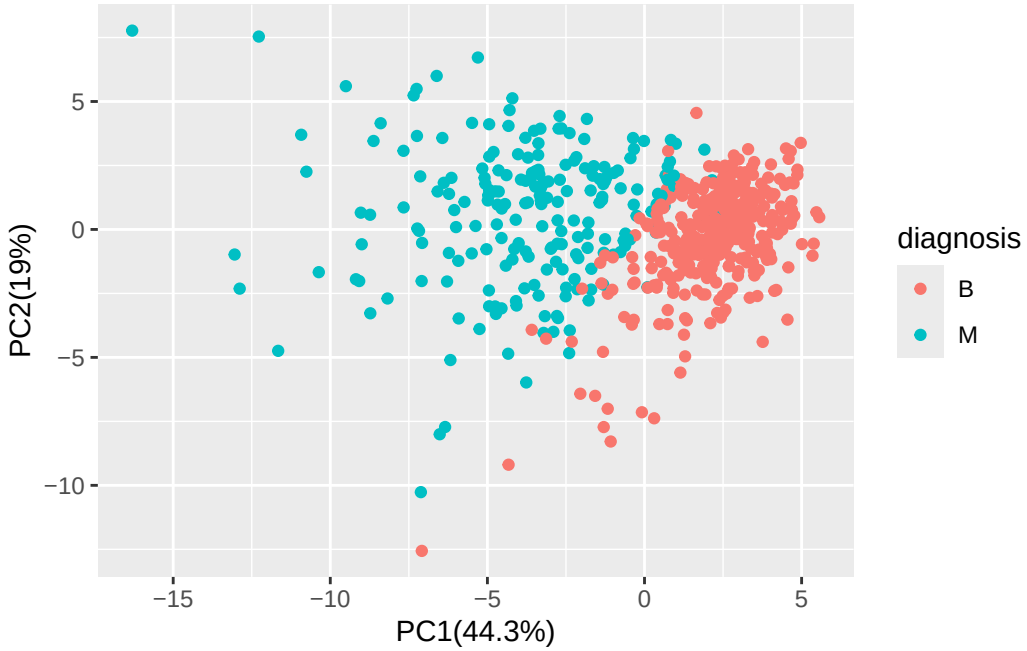
To se how well PCA is doing here in terms of capturing the spread we use `sumamry` to help

```
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
```

Lets make the main PC1 vs PC2

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



This plot shows a separation of malignant and benign samples. Each point represents a sample and it measured cell characteristic in the data set.PCA takes a data set with a lot if dimensions. PC stands for principle component.

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

44% of the original variance is captured by the first principle component.

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

Three principle components are required to describe at least 70% of the original variance in the data

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

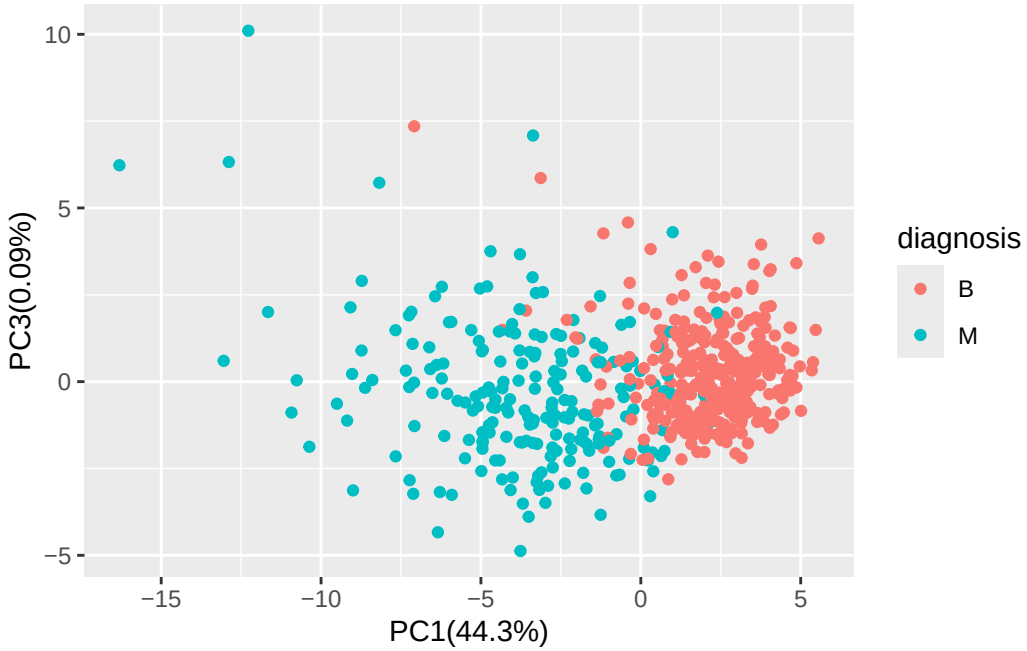
Seven principle components are required to describe at least 70% of the original variance in the data

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

What stands out to me about the plot is that the we see that the samples that are considered benign are on one side of the plot and then the samples that are malignant are on the other side of the plot.

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

```
ggplot(wisc.pr$x)+
  aes(PC1,PC3, col=diagnosis)+
  geom_point()+
  xlab("PC1(44.3%)") +
  ylab("PC3(0.09%)")
```



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 <- prcomp(wisc.data, scale = TRUE)
wisc.pr$rotation["concave.points_mean", 1]
```

```
[1] -0.2608538
```

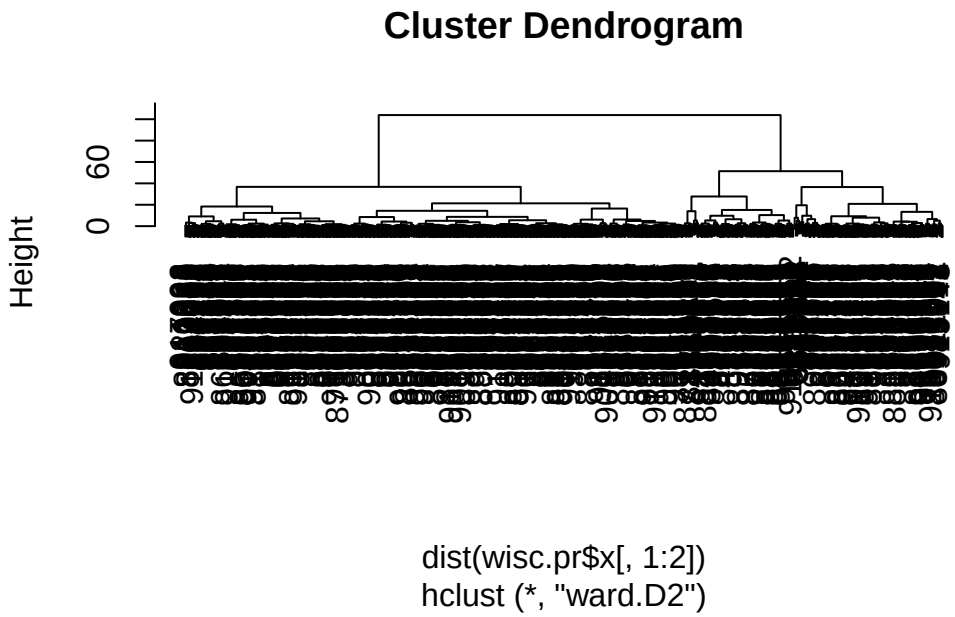
Q10. What is the minimum number of principal components required to explain 80% of the variance of the data?

The minimum number of principal components required to explain 80% of the variance of the data is five

5. Combining methods

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

```
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 my cluster groups 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
```

Clustering on the PCA results

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

It is better because now we can see see which one were mismatched. Such as in the the table we can see that in group one 18 were mismacthed to benign

> 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.

They did really bad. We do much better after PCA.The new PCA variables(what we call a baseis set) gives us much better separation of M and B

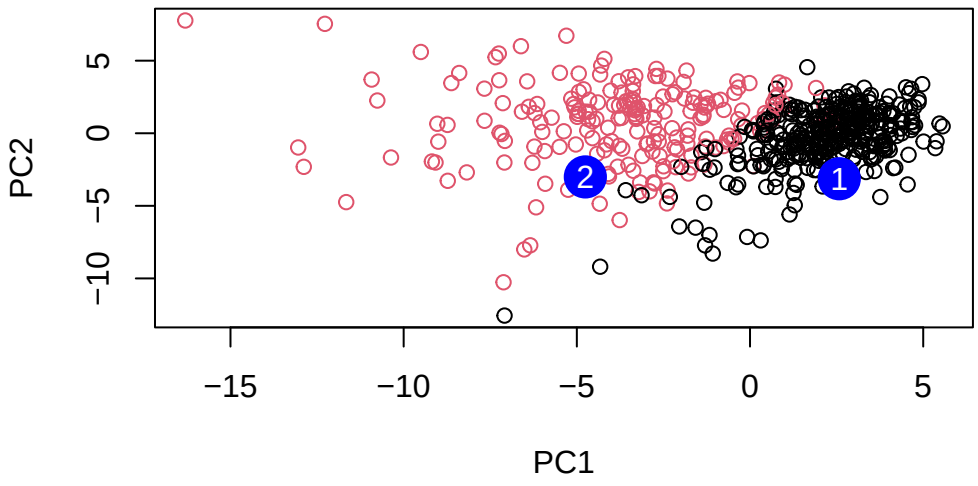
7. Prediction

We can use our PCA model for the analysis of new "unseen" data. In this case from the 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=diagnosis)
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?

Patient 2 should prioritize for follow up based on your results