class08

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Our data come from U. of Wisconsin Medical Center

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

Q1. How many observations 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"
```

```
sum(grepl("_mean",colnames(wisc.df)))
```

```
[1] 10
```

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

```
[1] 10
```

There is a diagnosis column that is the clinician consenus 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)
```

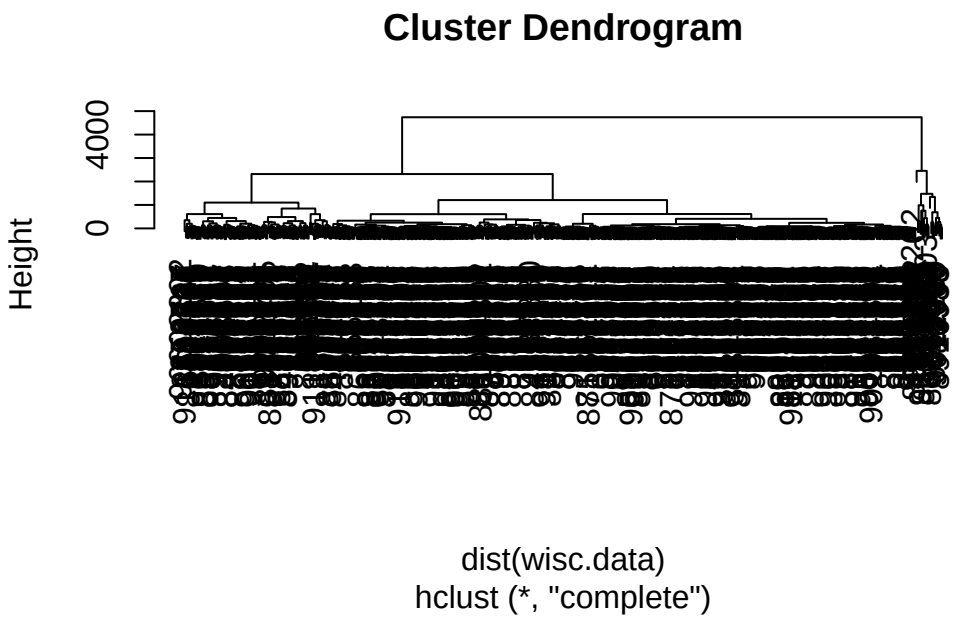
```
[1] M M M M M M
Levels: B M
```

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

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

Clustering

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

plot(hc)
```



we can extract cluster from this rather poor dendrogram/tree with the 'cutree()'

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

Hom many individuals 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 out 'diagnosis' vector values

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

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

Principal Component Analysis

The importance of data scaling

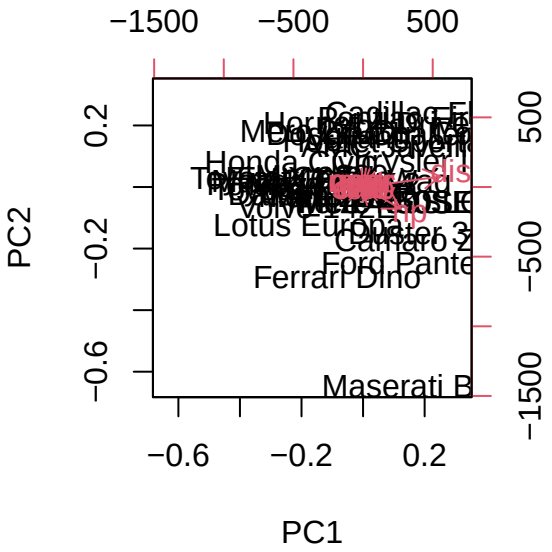
The main function for PCA in base R is 'prcomp()' it has a default input parameter of 'scale = FALSE'.

```
#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 represetation 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)
```

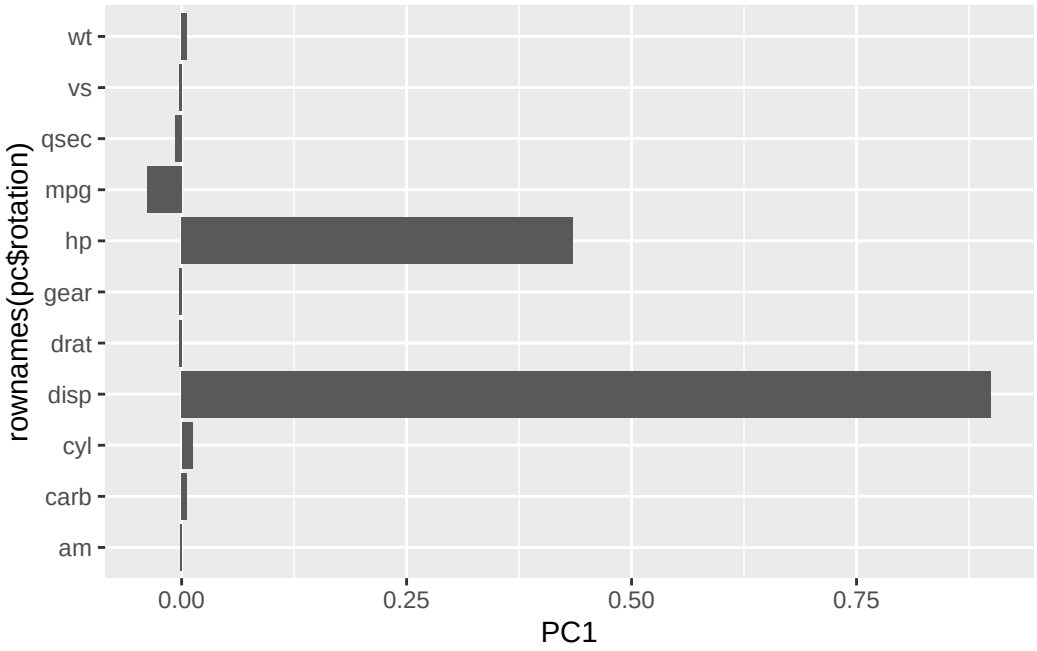
```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb
   1    1    1    1    1    1    1    1    1    1    1
```

```
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 "loading plot" how the original variables contribute to the new PCs

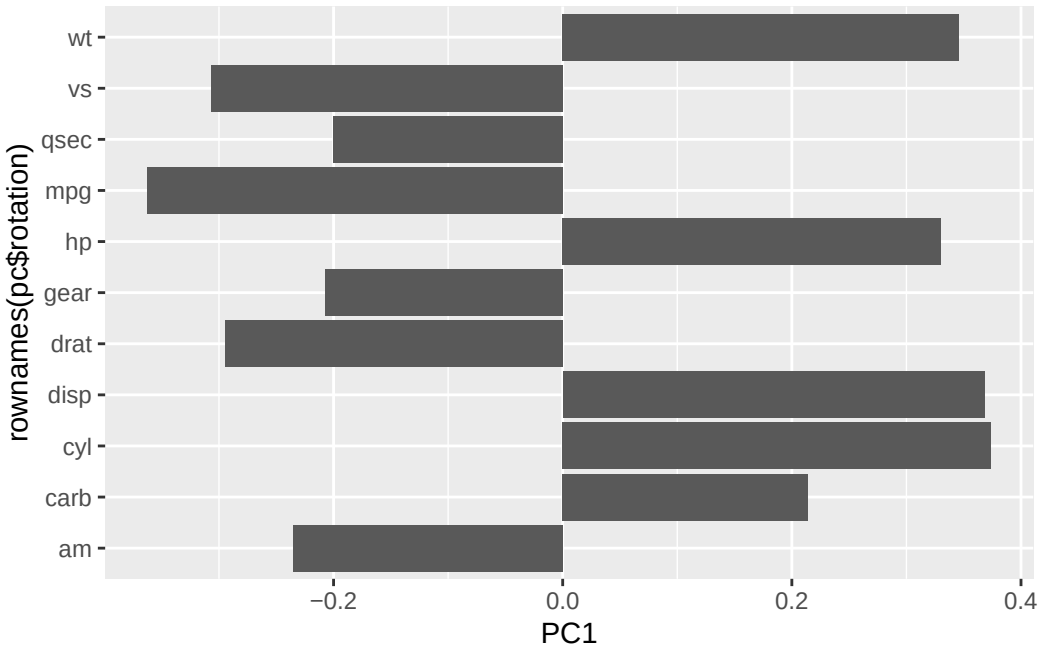
A loadings plot of the unscalled PCA results

```
library(ggplot2)

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



Loading plots of the scalled data.

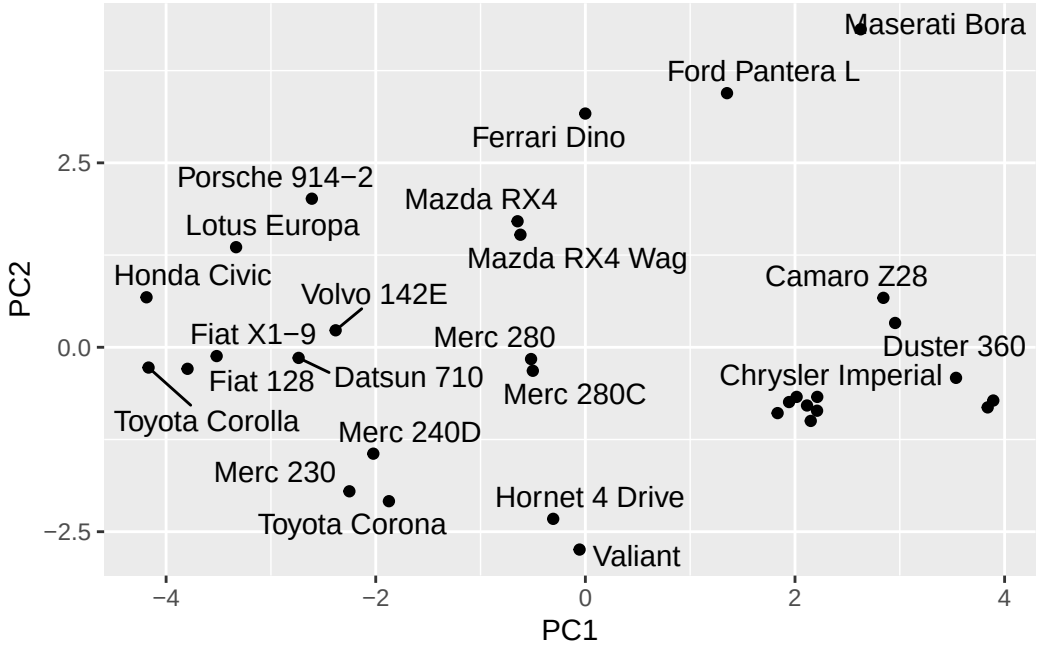
```
library(ggplot2)

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
```



Keypoint: 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!

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

To see how wll PCA is doing here in terms capturing the variance (or spread) in the data we can use the 'summary()' function.

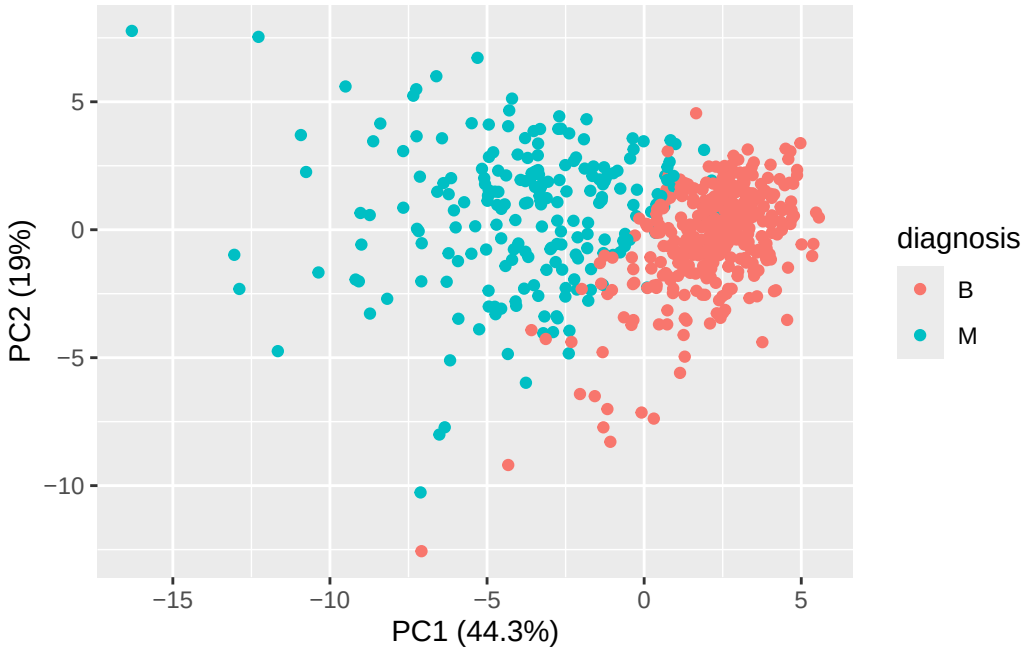
```
summary(wisc.pr)
```

```
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 orignal variance is captured by the first principle components (PC1) ?

From my result only 44% of the original variance is captured by the first principle components (PC1).

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

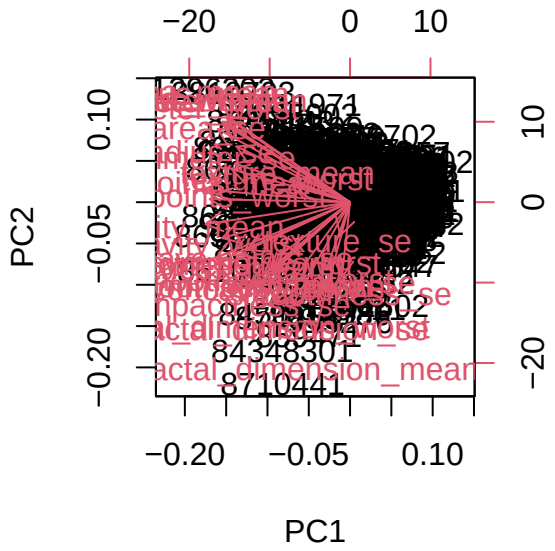
3 principal components (PC1 , PC2 and PC3) are required to describe atleast 70% of the original variance in the data.

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

7 principal components (PC1-7) are required to describe atleast 90% of the orignal variance data.

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

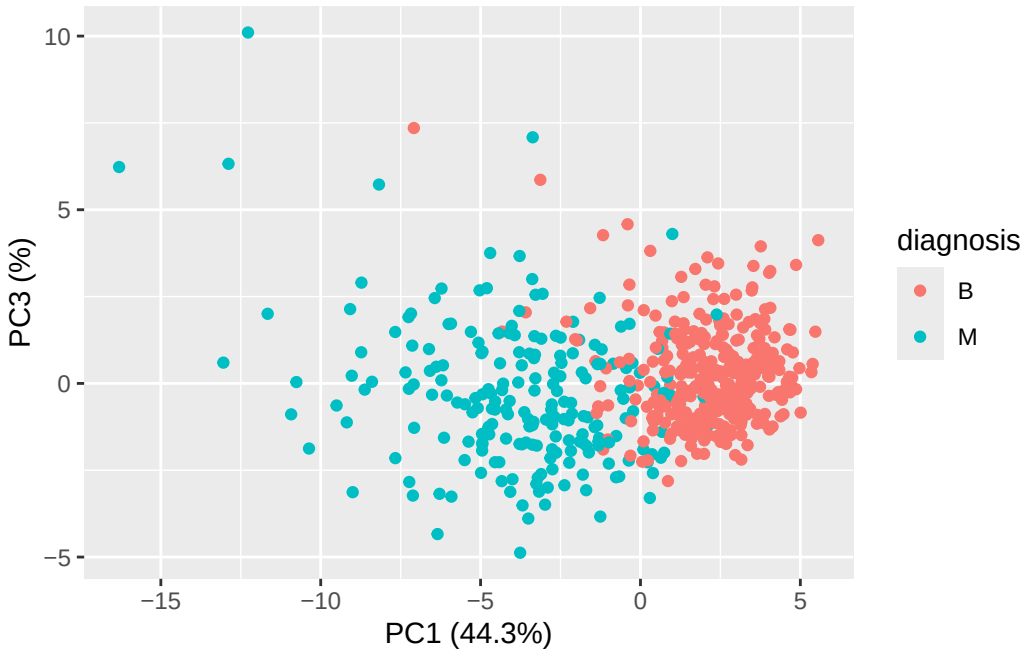
```
biplot(wisc.pr, scale = TRUE )
```



There was nothing stands out about this plot. It was really difficult to understand the result. Everythiong just clump up together.

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

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



In this plot the diagnosis are clearly separate in two sides of benign and malignant. You can clearly see the data in the left of the plot are mostly maglinant and the data on the right of the plot are mostly benign.

> Q9. For the first principal component, what is the component of the loading vector (i.e. wisc.pr$rotationp[,1]) for the feature concave.points_mean ?

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

```
[1] -0.2608538
```

> Q10. Please answer up to this Q10...

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

```
summary(wisc.pr)$importance["Cumulative Proportion", ]
```

```
    PC1     PC2     PC3     PC4     PC5     PC6     PC7     PC8     PC9     PC10
0.44272 0.63243 0.72636 0.79239 0.84734 0.88759 0.91010 0.92598 0.93988 0.95157
   PC11    PC12    PC13    PC14    PC15    PC16    PC17    PC18    PC19    PC20
0.96137 0.97007 0.97812 0.98335 0.98649 0.98915 0.99113 0.99288 0.99453 0.99557
   PC21    PC22    PC23    PC24    PC25    PC26    PC27    PC28    PC29    PC30
0.99657 0.99749 0.99830 0.99890 0.99942 0.99969 0.99992 0.99997 1.00000 1.00000
```

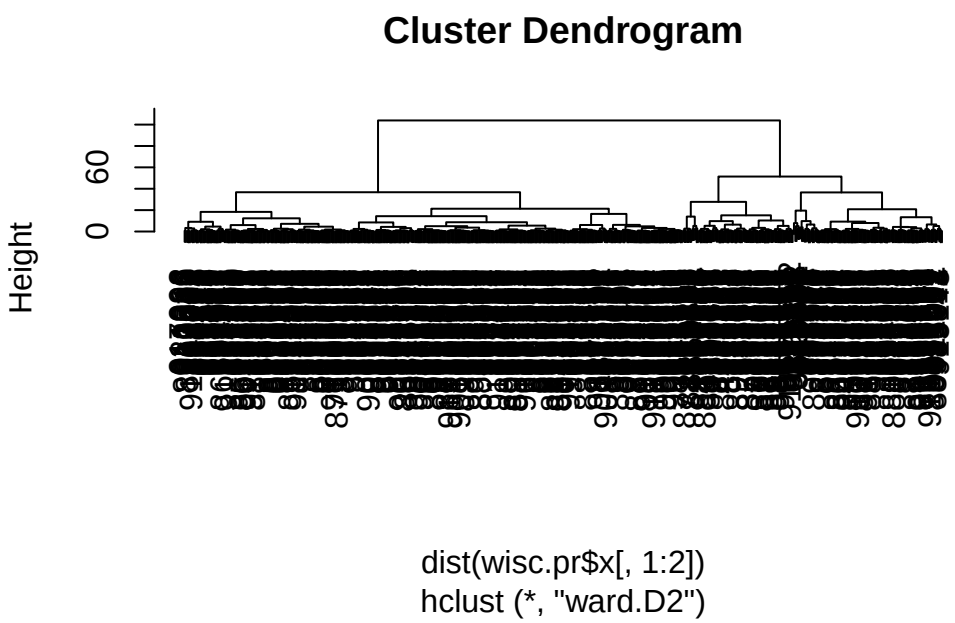
Minimum 5 components required to explain 80% of the variance in the data.

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 resutls.

```
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 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
```

ROC plot - comparing true possitive and false possitive.

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

The newly created model uising PCA followed by hierarchical clustering separtes the two diagnoses fairly well. Cluster 1 is primiarly composed of maglinant cases (177 out of 195), while cluster 2 contains mostly benign cases (339 out of 374). Although not perfect, this approach results in a much clearer sperataion compared to cluistering onthe original unscaled data.

> Q16. How well do the hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separting 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 diagnosses.

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

7. Prediction

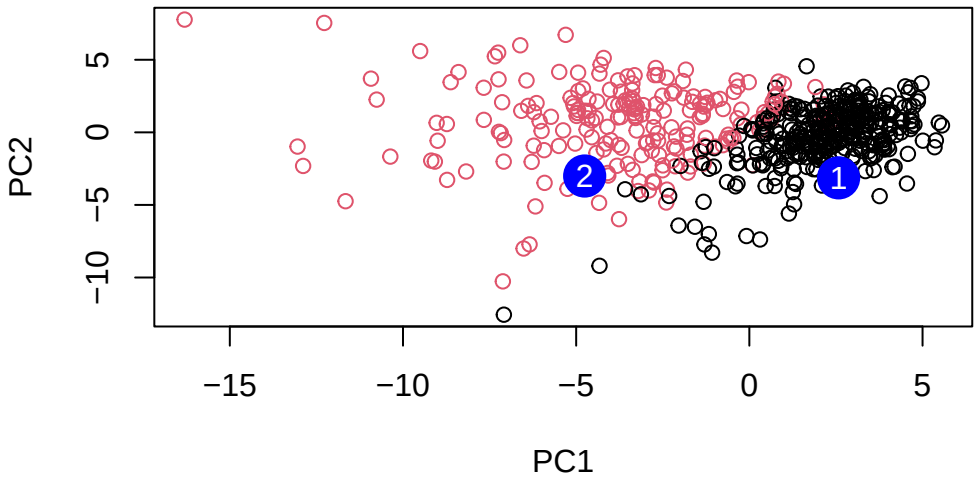
We can use our PCA model for the analysis of new "unseen" data. In this case from U. Mich.

```
g <- ifelse(diagnosis == "M", "red", "black")

g <- as.numeric(diagnosis)
```

```
#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")
```



Q.18 Which of these new patients should we prioritze for following up tbased on your results?

Based on this we should prioritize patient 2 because the patient is in the red region (maglinant) and patient 1 is in the black region (benign) so the patient 1 is not in the immediate danger but patient 2 is.