# Class 8: Breast cancer mini project

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## Table of contents

### Background

This mini-project explores unsupervised learning techniques applied to the Wisconsin Breast Cancer Diagnostic Data Set, which contains measurements of human breast mass cell nuclei. The project guides the user through exploratory data analysis, performing and interpreting Principal Component Analysis (PCA) to reduce the dimensionality of the data while retaining variance, and applying hierarchical clustering with different linkage methods. The ultimate goal is to combine PCA and clustering to better separate benign and malignant cell samples, evaluate the result using metrics like sensitivity and specificity, and finally demonstrate how to predict the classification of new samples using the developed PCA model.

### Data import

Our data come from the U. of Wiscosin Medical Center.

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

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

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

```
[1] 569
```

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

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

```

  B   M 
357 212 
```

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

```
[1] 212
```

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

```r
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"
```

```r
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.

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

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

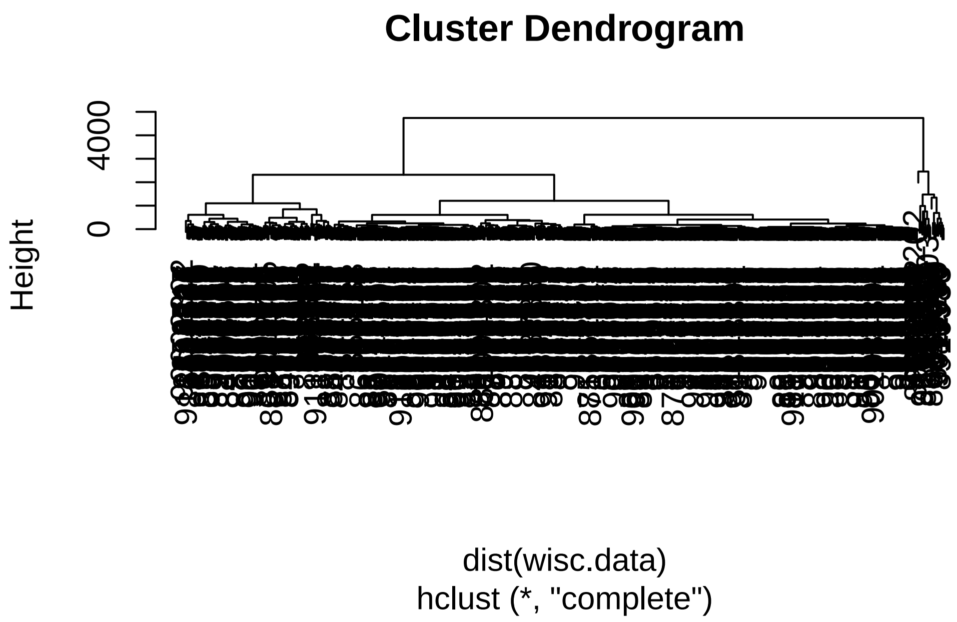
Now we can remove it from the `wisc.df`

```
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 in each cluster?

```
table(grps)
```

```
grps
  1   2 
549  20 
```

```
table(diagnose)
```

```
diagnose
  B   M 
357 212 
```

We can generate a cross-table that compares our cluster `grps` vector without `diagnosis` vector values **(in my case, it's `diagnose`)**

```
table(diagnose, grps)
```

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

## Principal Component Analysis

### The importance of data scaling

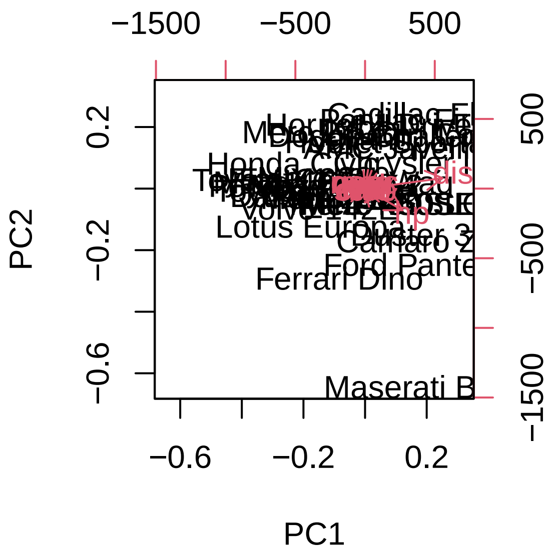
The main function for PCA in "base" R is `prcomp()` it has a dafault input parameter of `scale=FALSE`.

```
#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...

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



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

```r
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 
```

```r
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 represention and analysus of all the columns.

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

```r
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 
```

```r
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 
```

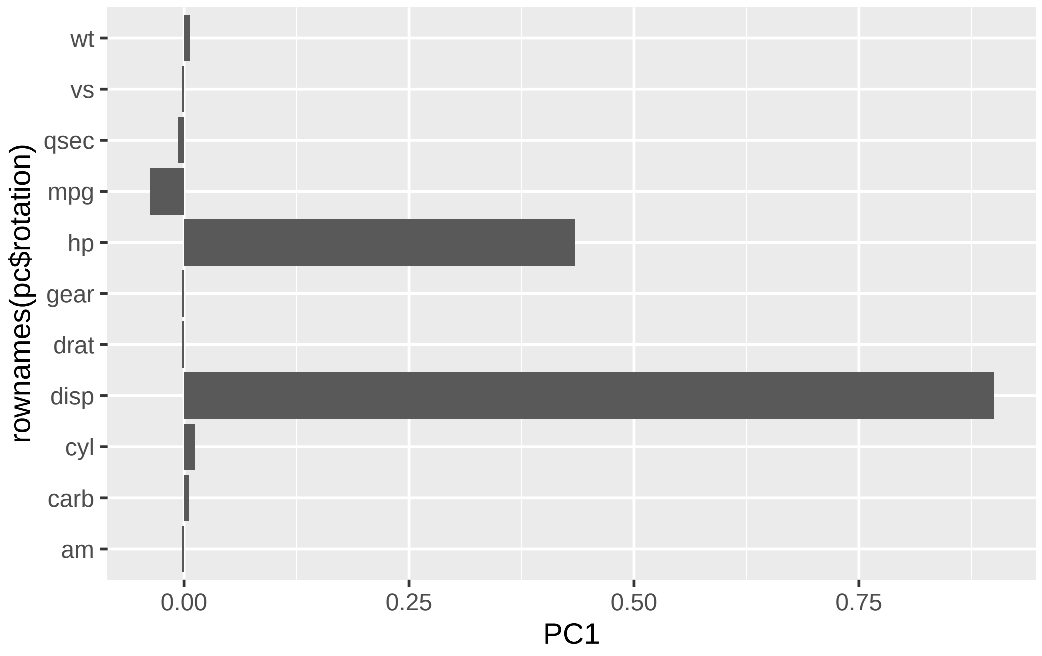
```r
pc.scale <- prcomp(mtscale)
```

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" - how the origional variables contribute to the new PCs.

A loadings plot of the unscaled PCA results

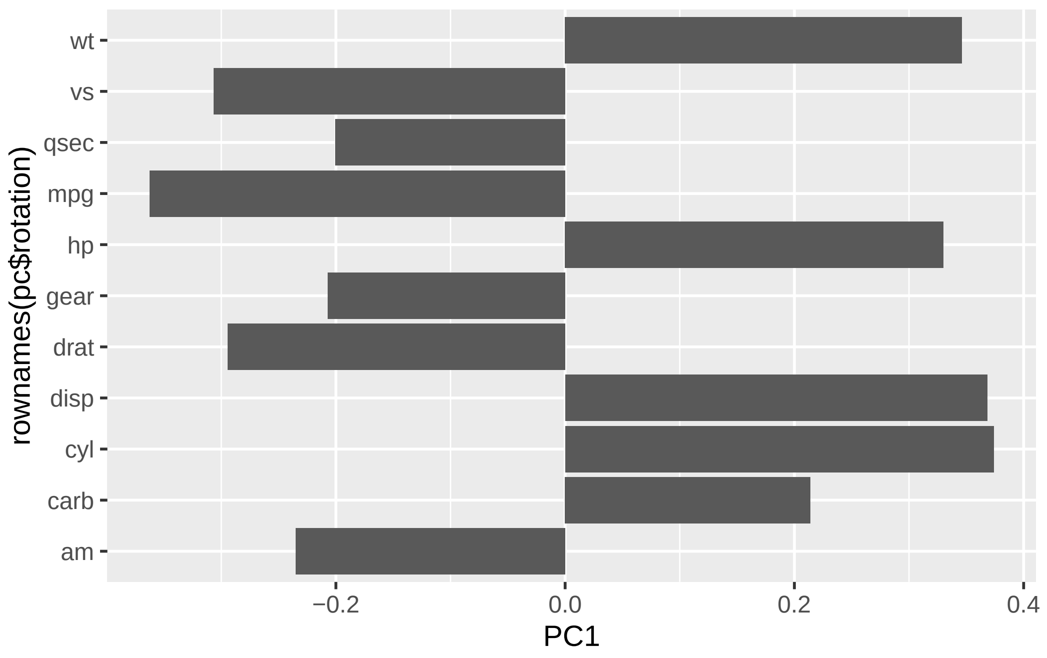
```r
library(ggplot2)

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



Loadings plot of the scaled data

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

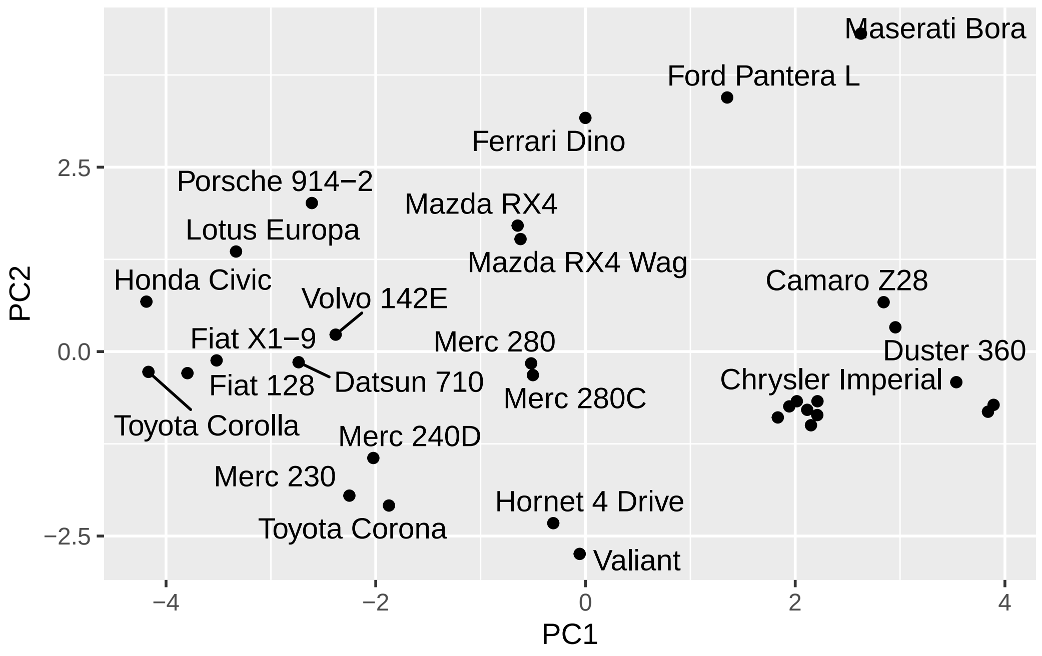


PC plot of scaled PCA results

```
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
```



```
pc$rotation
```

```
              PC1          PC2          PC3          PC4         PC5
mpg  -0.038118199  0.009184847  0.982070847  0.047634784 -0.08832843
cyl   0.012035150 -0.003372487 -0.063483942 -0.227991962  0.23872590
disp  0.899568146  0.435372320  0.031442656 -0.005086826 -0.01073597
hp    0.434784387 -0.899307303  0.025093049  0.035715638  0.01655194
drat -0.002660077 -0.003900205  0.039724928 -0.057129357 -0.13332765
wt    0.006239405  0.004861023 -0.084910258  0.127962867 -0.24354296
qsec -0.006671270  0.025011743 -0.071670457  0.886472188 -0.21416101
vs   -0.002729474  0.002198425  0.004203328  0.177123945 -0.01688851
am   -0.001962644 -0.005793760  0.054806391 -0.135658793 -0.06270200
gear -0.002604768 -0.011272462  0.048524372 -0.129913811 -0.27616440
carb  0.005766010 -0.027779208 -0.102897231 -0.268931427 -0.85520810
              PC6          PC7           PC8          PC9         PC10
mpg  -0.143790084 -0.039239174 -2.271040e-02 -0.002790139  0.030630361
cyl  -0.793818050  0.425011021  1.890403e-01  0.042677206  0.131718534
disp  0.007424138  0.000582398  5.841464e-04  0.003532713 -0.005399132
hp    0.001653685 -0.002212538 -4.748087e-06 -0.003734085  0.001862554
drat  0.227229260  0.034847411  9.385817e-01 -0.014131110  0.184102094
wt   -0.127142296 -0.186558915 -1.561907e-01 -0.390600261  0.829886844
qsec -0.189564973  0.254844548  1.028515e-01 -0.095914479 -0.204240658
```

```
vs    0.102619063 -0.080788938  2.132903e-03  0.684043835  0.303060724
am    0.205217266  0.200858874  2.273255e-02 -0.572372433 -0.162808201
gear  0.334971103  0.801625551 -2.174878e-01  0.156118559  0.203540645
carb -0.283788381 -0.165474186 -3.972219e-03  0.127583043 -0.239954748
             PC11
mpg   0.0158569365
cyl  -0.1454453628
disp -0.0009420262
hp    0.0021526102
drat  0.0973818815
wt    0.0198581635
qsec -0.0110677880
vs   -0.6256900918
am   -0.7331658036
gear  0.1909325849
carb -0.0557957968
```

> **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 capturing the variance (or spread) in the data we can use the `summary()` function.

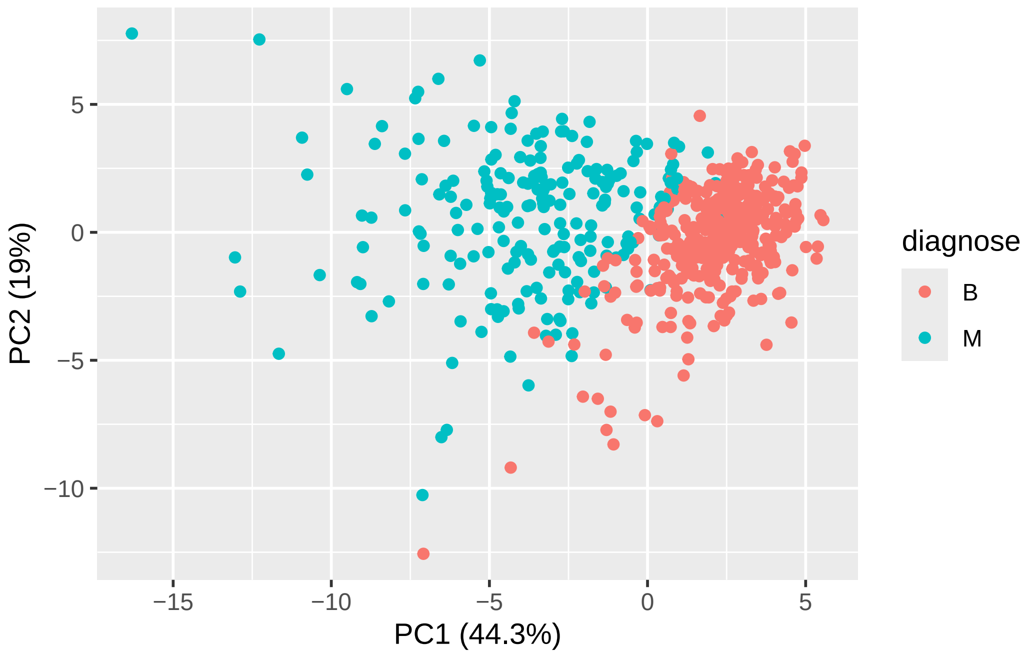
```
summary(wisc.pr)
```

```
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

```r
ggplot(wisc.pr$x) +
  aes(PC1, PC2, col=diagnose) +
  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)?

```r
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
```

44.27% is captured by PC1.

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

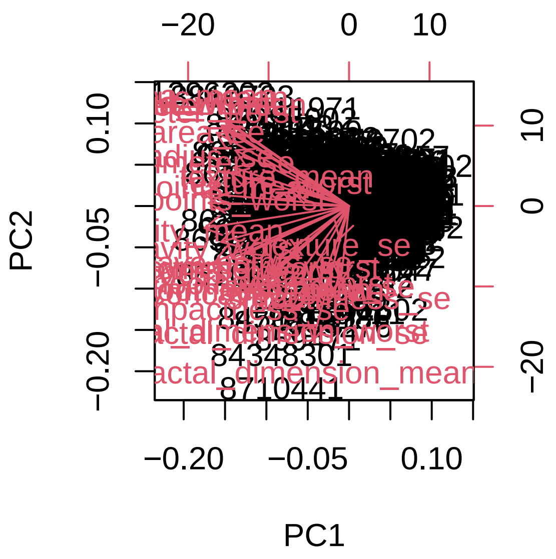
3 PCs

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

7 PCs

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

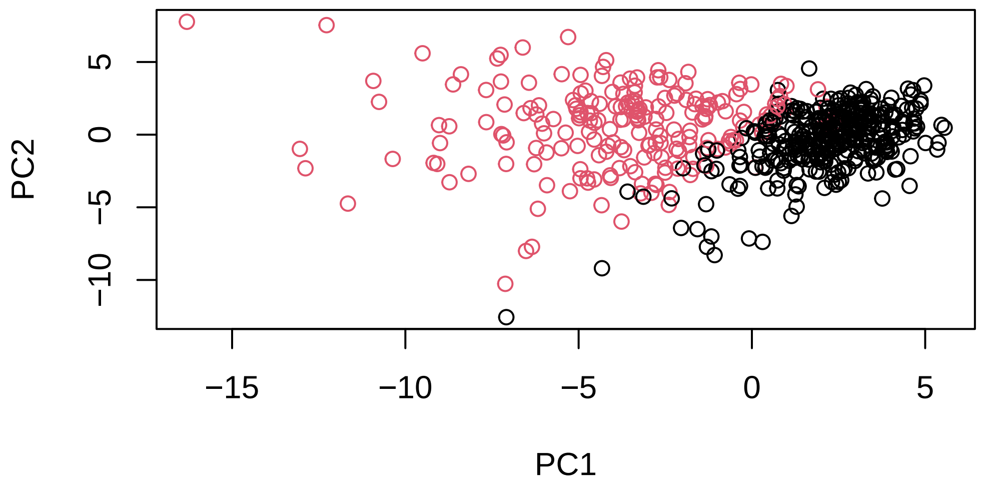
```r
biplot(wisc.pr)
```



This biplot is very hard to understand, because it's too much going on and hard to read, and we're unable to see the trends.

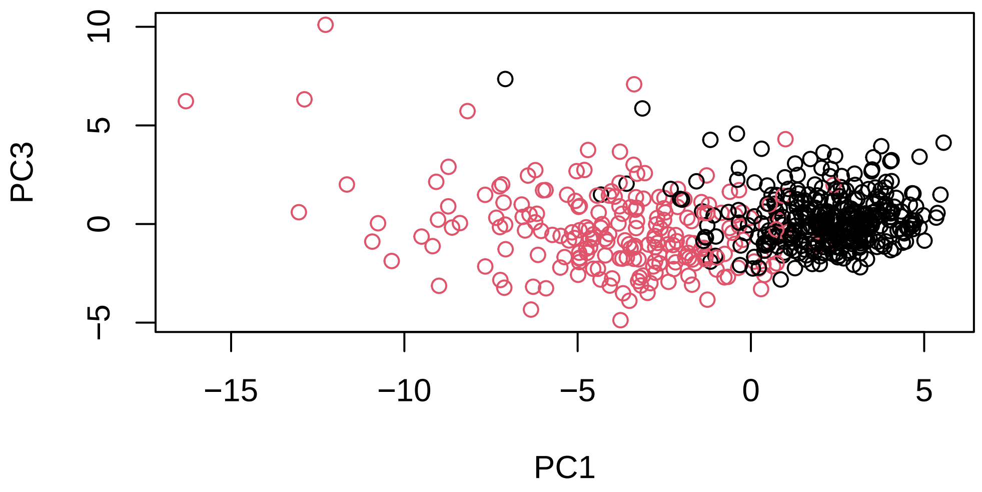
Generate a standard scatter plot for PC1 and PC2:

```r
# Scatter plot observations by components 1 and 2
plot(wisc.pr$x, col = diagnose ,
     xlab = "PC1", ylab = "PC2")
```



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

```r
# Repeat for components 1 and 3
plot(wisc.pr$x[, c(1,3) ], col = diagnose,
     xlab = "PC1", ylab = "PC3")
```



The first plot (PC1 vs PC2) may better distinguish the malignant samples (red dots) from the benign samples (black dots), with the second plot (PC1 vs PC3) showing more overlapping.

> 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`?

```
PC1 <- wisc.pr$rotation[,1]
concave_point <- PC1["concave.points_mean"]
print(concave_point)
```

```
concave.points_mean
         -0.2608538
```

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

```
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

```r
var <- cumsum(wisc.pr$sdev^2) / sum(wisc.pr$sdev^2)
var >= 0.80
```

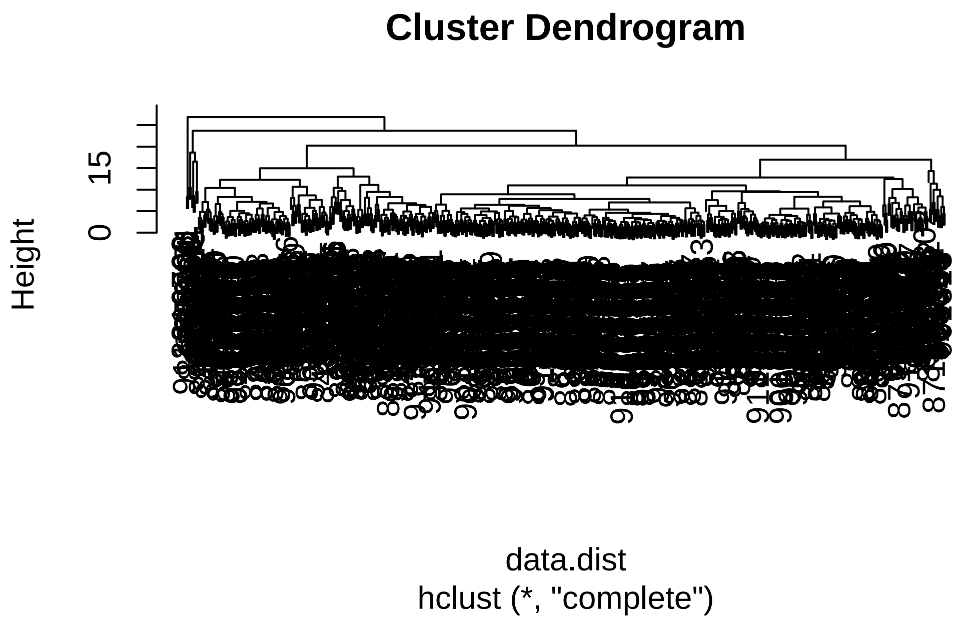
```
 [1] FALSE FALSE FALSE FALSE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
[13]  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
[25]  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
```

Q11. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

```r
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
```

```r
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(data.dist, method = "complete")
```

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



Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

```r
wisc.hclust.clusters <- cutree(wisc.hclust, k = 4)
table(wisc.hclust.clusters, diagnose)
```

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

```r
wisc.hclust.clusters <- cutree(wisc.hclust, k = 2)
table(wisc.hclust.clusters, diagnose)
```

```
                    diagnose
wisc.hclust.clusters   B   M
                   1 357 210
                   2   0   2
```

```r
wisc.hclust.clusters <- cutree(wisc.hclust, k = 10)
table(wisc.hclust.clusters, diagnose)
```

```
                    diagnose
wisc.hclust.clusters   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
```

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

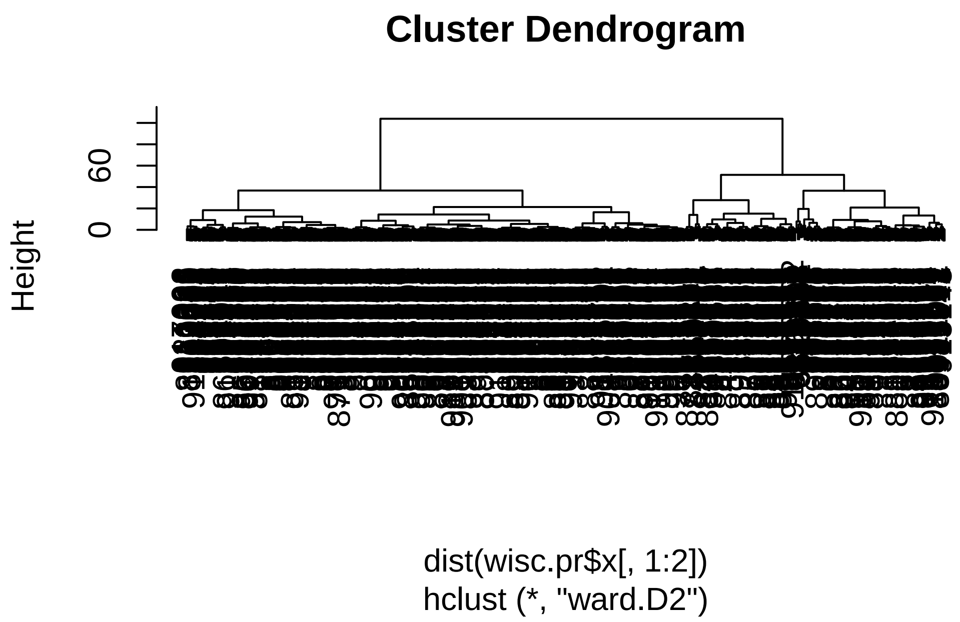
I think the `cutree ()` function will probably give better data that's slightly easier to read. I'm still able to read the number of malignant samples and benign samples in the table above. Overall, I prefer plots over tables, which I think will be much easier to read and analyze.

## 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

```r
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):

```r
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?

```r
table(diagnose, pc.grps)
```

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

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

It's still not really clear on understanding the numbers of malignant samples and benign samples.

```r
table(diagnose)
```

```
diagnose
  B   M 
357 212 
```

> 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.

```r
wisc.km <- kmeans(wisc.data, centers = 2)
table(wisc.km$cluster, diagnose)
```

```
   diagnose
      B   M
  1   1 130
  2 356  82
```

```r
wisc.hclust <- hclust(dist(wisc.data))
wisc.hclust.clusters <- cutree(wisc.hclust, k=4)
table(wisc.hclust.clusters, diagnose)
```

```
                    diagnose
wisc.hclust.clusters   B   M
                   1   1 110
                   2 356  82
                   3   0  19
                   4   0   1
```

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

## 7. Prediction

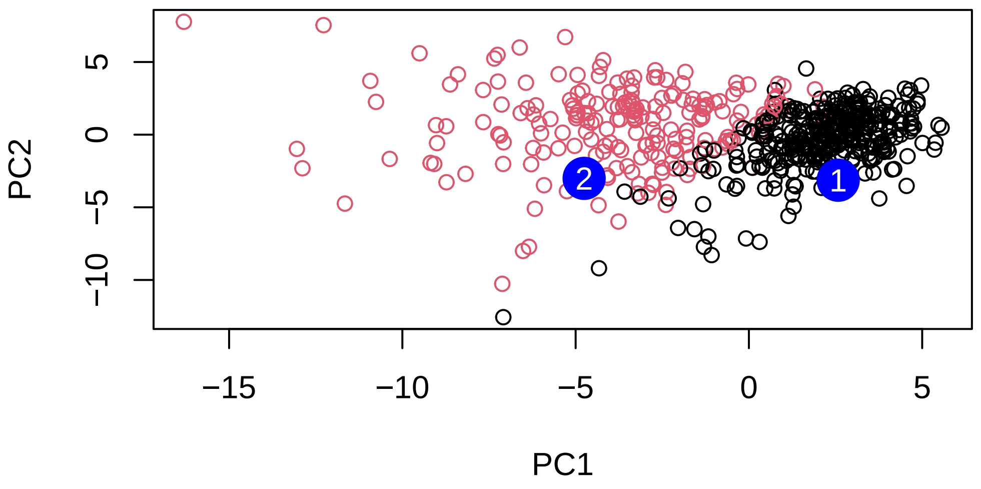
We can use our PCA model for the analysis of new “unseen” data. In this case from U. Mich.

```
#url <- "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
```

> Q18. Which of these new patients should we prioritize for follow up based on your results?

```
plot(wisc.pr$x[,1:2], col = diagnose)
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



Based on this plot, (1) benign samples (black dots) are more clustered and stable, and (2) the malignant samples (red dots) are more spread out, so they are more variable/different. Therefore, (2) should be prioritized for follow-up based on the result.