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. It also includes an optional section on K-means clustering for comparison. The ultimate goal is to combine PCA and clustering to better separate benign and malignant cell samples, evaluating the results using metrics like sensitivity and specificity, and finally demonstrating how to predict the classification of new samples using the developed PCA model.

Data Import

Our data come from the U. of Wisconsin Medical Center

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

Question 1: How many patients/samples are in this dataset?

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

```
[1] 569
```

Question 2: How many of the observations have a malignant diagnosis?

```
wisc.df$diagnosis
```

```
  [1] "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M"
 [19] "M" "B" "B" "B" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M"
 [37] "M" "B" "M" "M" "M" "M" "M" "M" "M" "M" "B" "M" "B" "B" "B" "B" "B" "M"
 [55] "M" "B" "M" "M" "B" "B" "B" "B" "M" "B" "M" "M" "B" "B" "B" "B" "M" "B"
 [73] "M" "M" "B" "M" "B" "M" "M" "B" "B" "B" "M" "M" "B" "M" "M" "M" "B" "B"
 [91] "B" "M" "B" "B" "M" "M" "B" "B" "B" "M" "M" "B" "B" "B" "B" "M" "B" "B"
[109] "M" "B" "B" "B" "B" "B" "B" "B" "B" "M" "M" "M" "B" "M" "M" "B" "B" "B"
[127] "M" "M" "B" "M" "B" "M" "M" "B" "M" "M" "B" "B" "M" "B" "B" "M" "B" "B"
[145] "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "M"
[163] "M" "B" "M" "B" "B" "M" "M" "B" "B" "M" "M" "B" "B" "B" "B" "M" "B" "B"
[181] "M" "M" "M" "B" "M" "B" "M" "B" "B" "B" "M" "B" "B" "M" "M" "B" "M" "M"
[199] "M" "M" "B" "M" "M" "M" "B" "M" "B" "M" "B" "B" "M" "B" "M" "M" "M" "M"
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[235] "B" "B" "M" "M" "B" "M" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "M" "B"
[253] "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "B" "B" "B" "B"
[271] "B" "B" "M" "B" "M" "B" "B" "M" "B" "B" "M" "B" "M" "M" "B" "B" "B" "B"
[289] "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "B" "B"
[307] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "M" "B" "M"
[325] "B" "B" "B" "B" "M" "M" "M" "B" "B" "B" "B" "M" "B" "M" "B" "M" "B" "B"
[343] "B" "M" "B" "B" "B" "B" "B" "B" "B" "M" "M" "M" "B" "B" "B" "B" "B" "B"
[361] "B" "B" "B" "B" "B" "M" "M" "B" "M" "M" "M" "B" "M" "M" "B" "B" "B" "B"
[379] "B" "M" "B" "B" "B" "B" "B" "M" "B" "B" "B" "M" "B" "B" "M" "M" "B" "B"
[397] "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B"
[415] "M" "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B"
[433] "M" "M" "B" "M" "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "B" "M"
[451] "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "M" "M" "B" "B" "B" "B" "B" "B"
[469] "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "B"
[487] "B" "M" "B" "M" "B" "B" "M" "B" "B" "B" "B" "B" "M" "M" "B" "M" "B" "M"
[505] "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "M" "M" "B" "B" "B" "M"
[523] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "M" "M" "B" "B" "B"
[541] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B"
[559] "B" "B" "B" "B" "M" "M" "M" "M" "M" "M" "B"
```

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

```
  B   M
357 212
```

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

```
[1] 212
```

```
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"
```

Question 3: How many variables/features in the data are suffixed with _mean?

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

```
 [1] "radius_mean"            "texture_mean"           "perimeter_mean"
 [4] "area_mean"              "smoothness_mean"        "compactness_mean"
 [7] "concavity_mean"         "concave.points_mean"    "symmetry_mean"
[10] "fractal_dimension_mean"
```

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
```

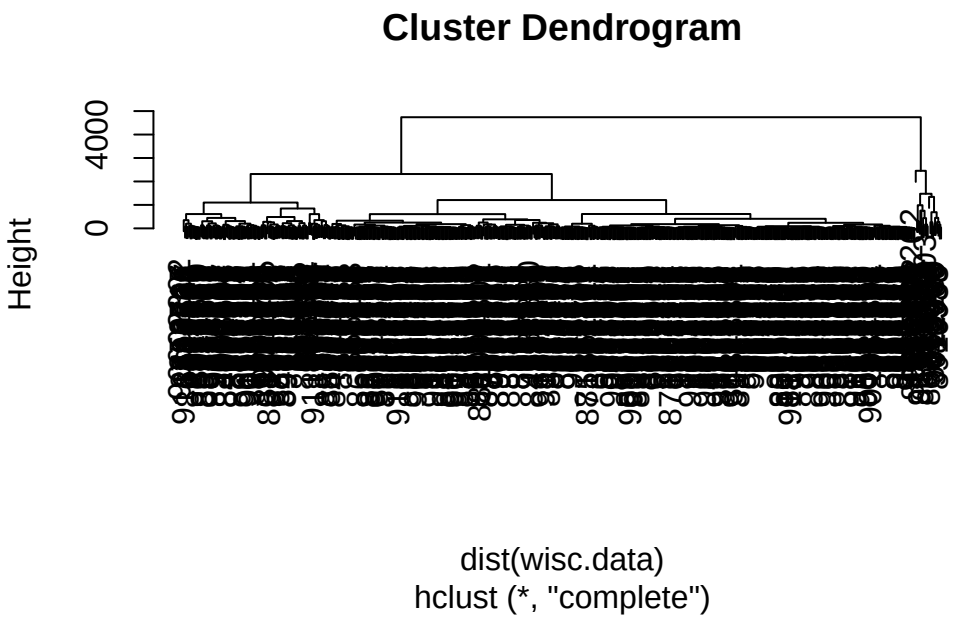
Now we can remove it from the `wisc.df`

```
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 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 scalling

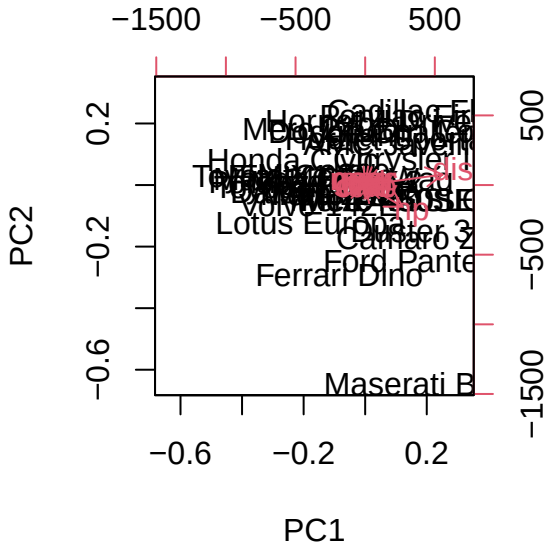
The main function for PCA in base R is `prcomp()` it has a default input parameter of `scale=FALSE`.

```
#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 coudl 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
```

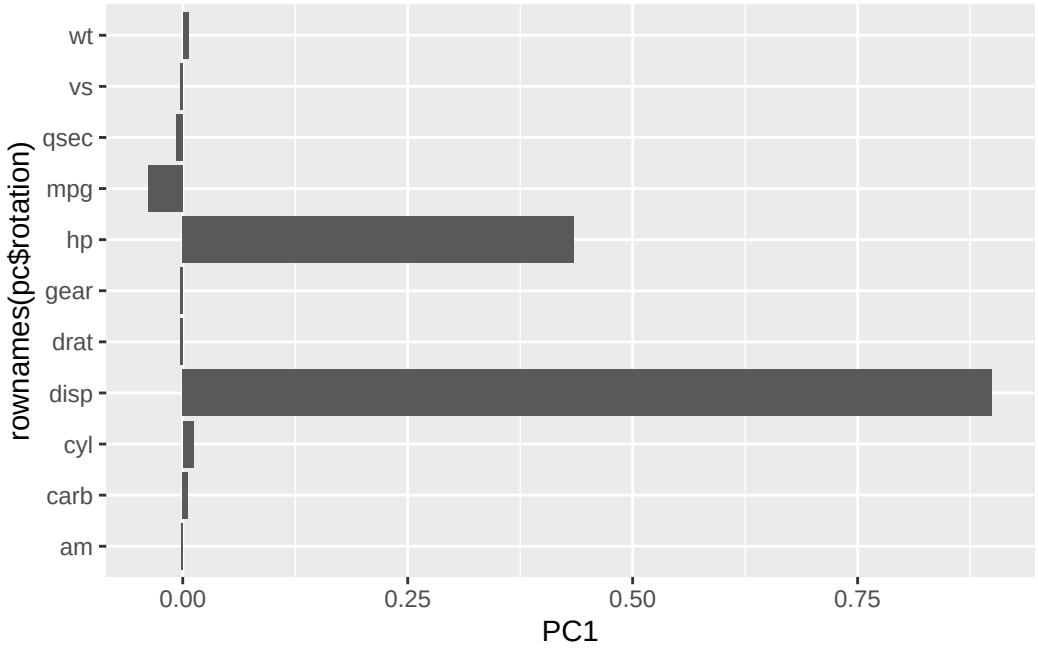
```
pc.scale <- prcomp(mtscale)
```

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" how the original variables contribute to the new PCs

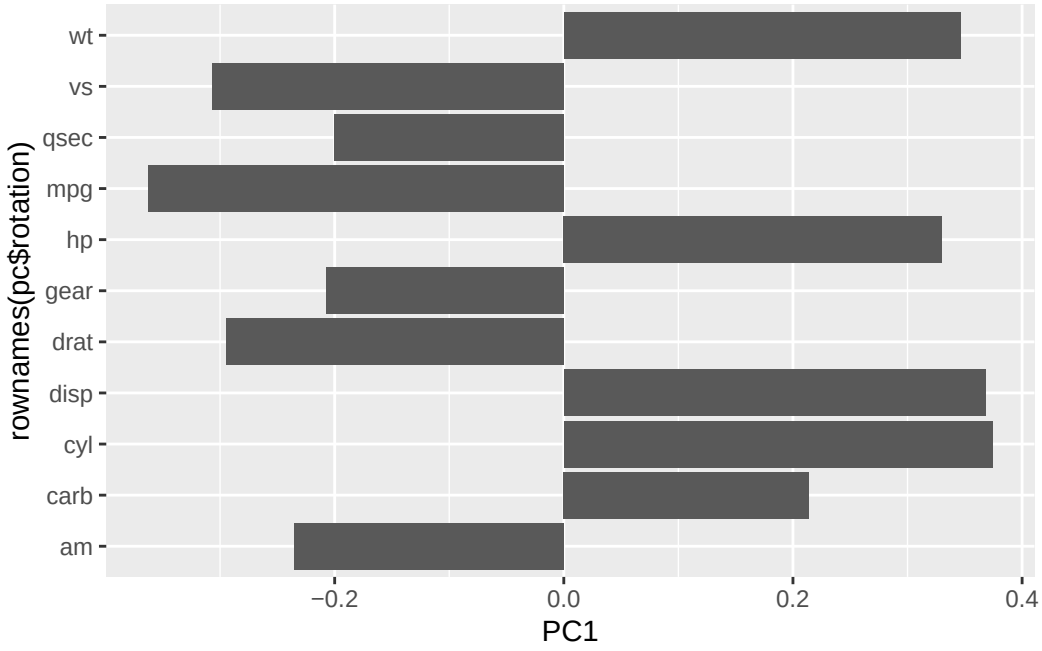
A loadings plot of the unscalled PCA results

```
library(ggplot2)

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




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

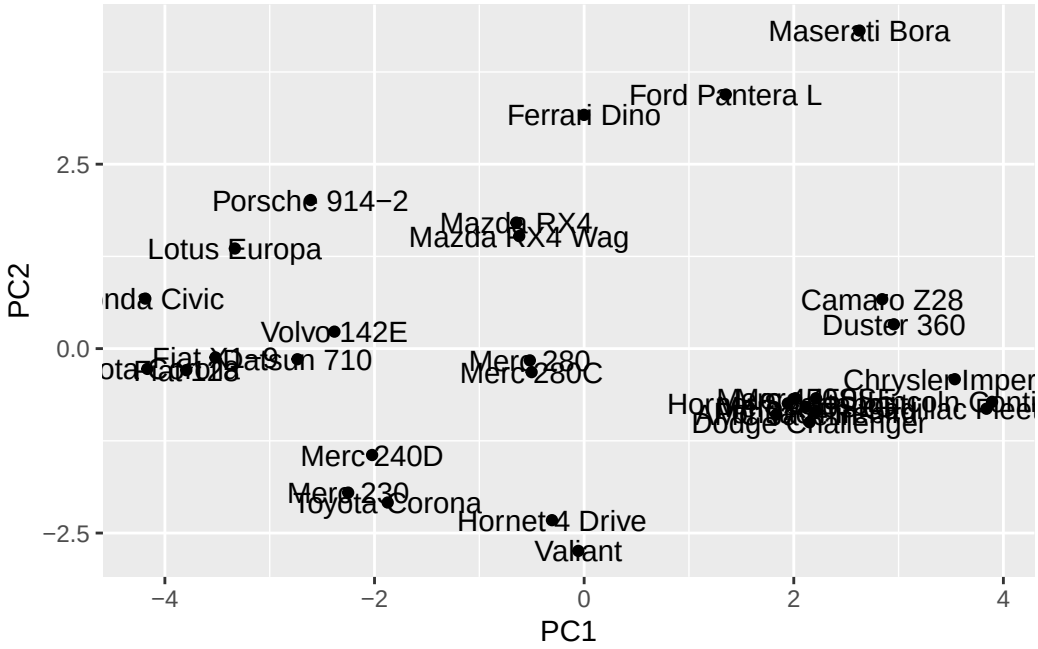


PC plot of scaled PCA results

```
library(ggrepel)
```

```
Warning: package 'ggrepel' was built under R version 4.3.3
```

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



Key point: In general we will set `scale=TRUE` wehn 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=T)
```

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
```

Question 4: From your results, what proportion of the original variance is captured by the first principal components (PC1)

44.27%

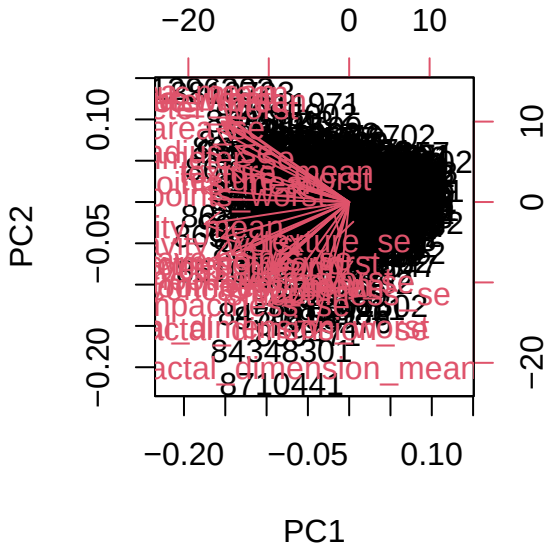
Question 5: How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

3

Question 6:How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

7

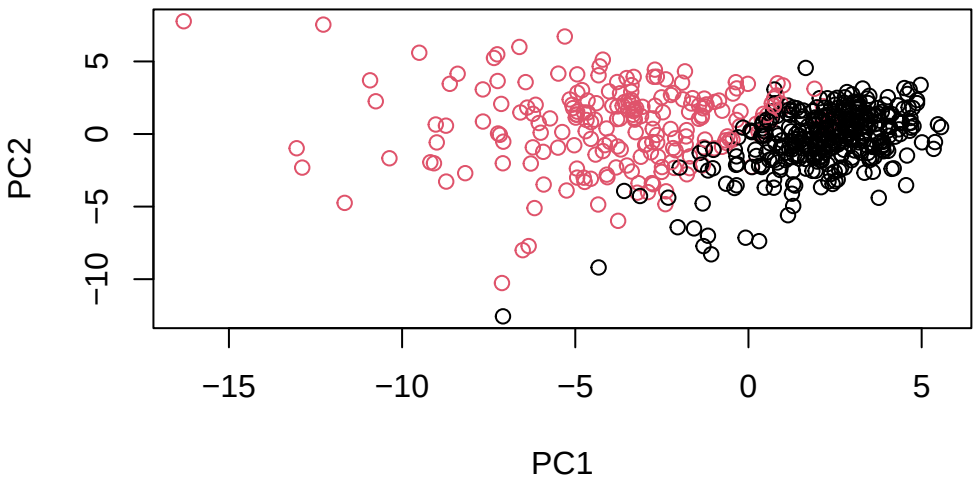
```
biplot(wisc.pr)
```



Question 7: What stands out to you about this plot? Is it easy or difficult to understand? Why?

What stands out is the main cluster of data in the middle of the plot, which makes it extremely difficult to understand due to the close proximity of the data points to one another.

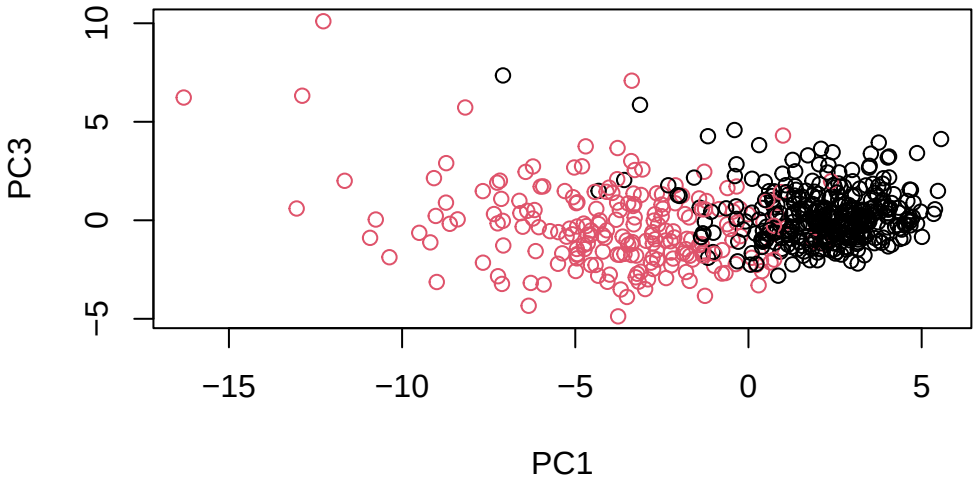
```
plot(wisc.pr$x, col = diagnosis, xlab = "PC1", ylab = "PC2")
```



Question 8: Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

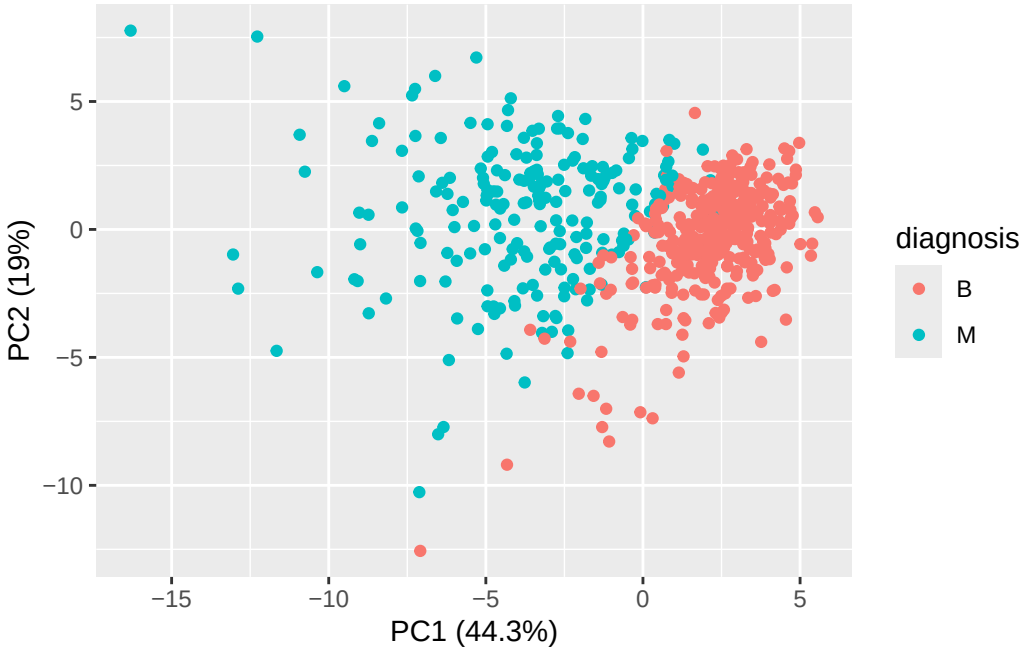
These plots very similar in their data points but the plot for PC1 and PC3 has better grouping compared to the first plot where there is less intermingling of benign and malignant data points.

```
plot(wisc.pr$x[,-2], col=diagnosis, xlab = "PC1", ylab = "PC3")
```



Let's make the main PC1 vs PC2

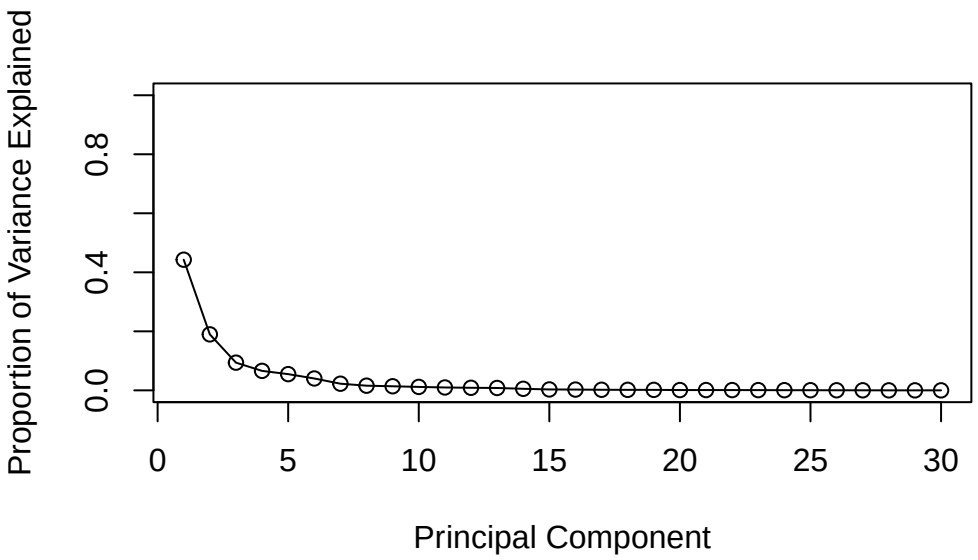
```
ggplot(wisc.pr$x) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point() +
  xlab("PC1 (44.3%)") +
  ylab("PC2 (19%)")
```




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

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

```
pve <- pr.var/30
plot(pve, xlab="Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0,1), type="o")
```

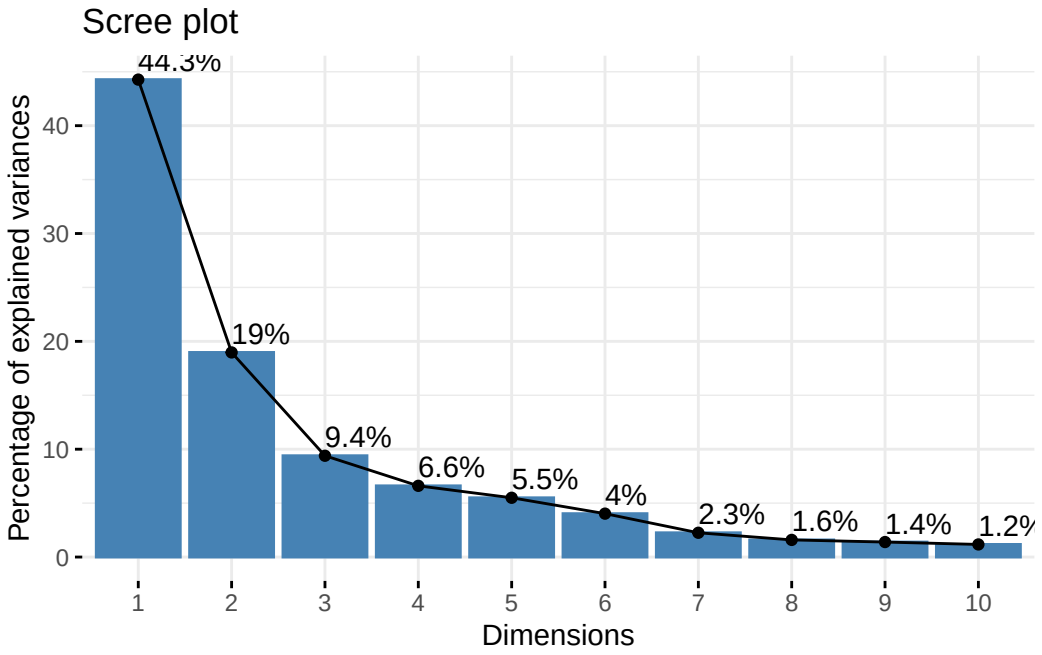



```
#install.packages("factoextra")
library(factoextra)
```

```
Warning: package 'factoextra' was built under R version 4.3.3
```

```
Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
```

```
fviz_eig(wisc.pr, addlabels = TRUE)
```



Question 9: For the first principal component, what is the component of the loading vector for the feature `concave.points_mean`?

```
wisc.pr$rotation[,1]
```

```
            radius_mean            texture_mean          perimeter_mean
             -0.21890244              -0.10372458              -0.22753729
              area_mean          smoothness_mean         compactness_mean
             -0.22099499              -0.14258969              -0.23928535
        concavity_mean     concave.points_mean           symmetry_mean
             -0.25840048              -0.26085376              -0.13816696
fractal_dimension_mean               radius_se              texture_se
             -0.06436335              -0.20597878              -0.01742803
          perimeter_se                area_se           smoothness_se
             -0.21132592              -0.20286964              -0.01453145
       compactness_se             concavity_se        concave.points_se
             -0.17039345              -0.15358979              -0.18341740
          symmetry_se     fractal_dimension_se            radius_worst
             -0.04249842              -0.10256832              -0.22799663
        texture_worst          perimeter_worst               area_worst
             -0.10446933              -0.23663968              -0.22487053
      smoothness_worst         compactness_worst           concavity_worst
```

```
          -0.12795256             -0.21009588             -0.22876753
concave.points_worst          symmetry_worst fractal_dimension_worst
          -0.25088597             -0.12290456             -0.13178394
```

-0.26

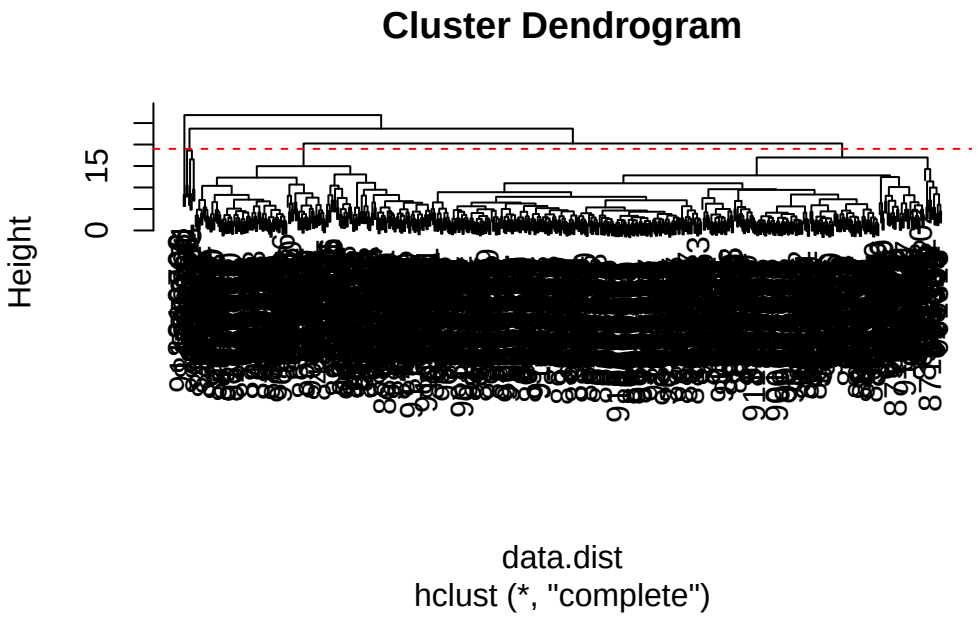
Question 10: Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

```
data.scaled <- scale(wisc.data)
```

```
data.dist <- dist(data.scaled)
```

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

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



At height 19 the clustering model has 4 clusters.

Question 12: Which method gives your favorite results for the same data.dist dataset?

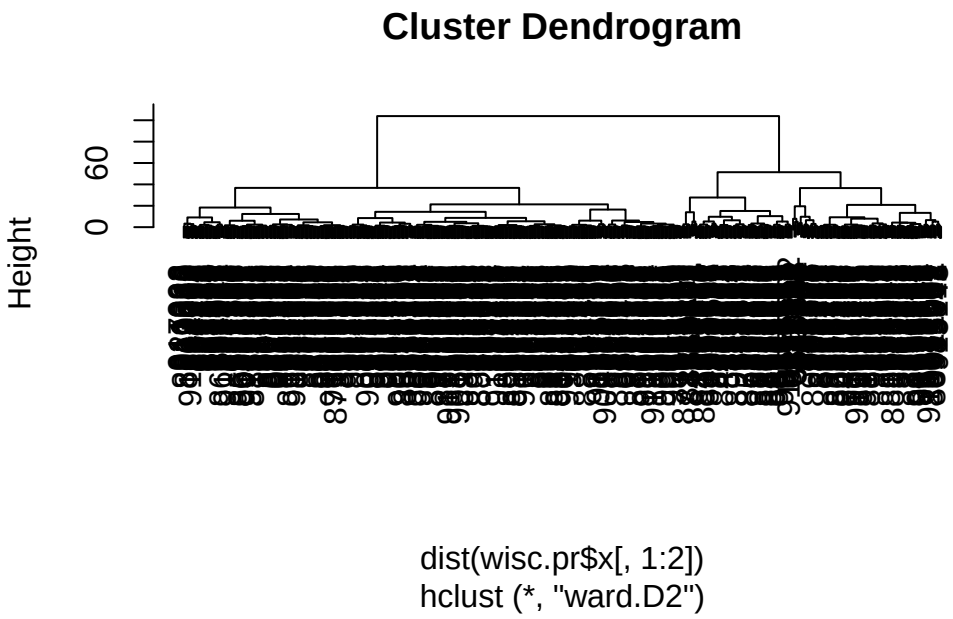
The method = "complete" gives our favorite results because it is sensitive to noise in the data set and can help create compact clusters.

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 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
```

> Question 13: How well does the newly created model with four clusters seperate out the two diagnoses?

The newly created model with four clusters separates out the two diagnoses very clearly and makes a more easy to read dendrogram with the same amount of information.

> Qustion 14: How well do the hierarchical clustering models you created in previous sections do in terms of separitng the diagnoses? Again, use the table() function to compare the output of each model with the vector containing the actual diagrams

They did really baddly. 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

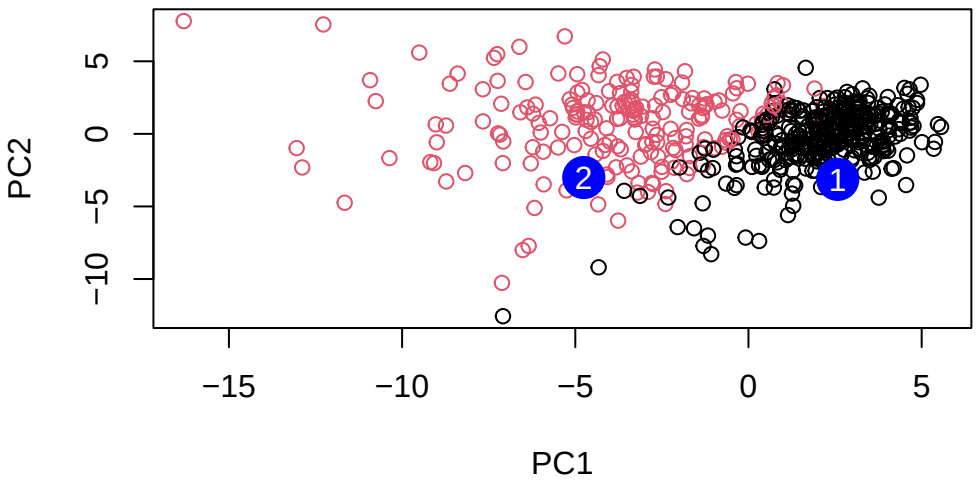
7. Prediction

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

```
#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
```

```r
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")
```



QUESTION 16: Which of these new patients should we prioritize for follow up based on your results?

PATIENT 2