Lab_08

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Lab08

1. Exploratory data analysis

```
# Save your input data file into your Project directory
fna.data <- "WisconsinCancer.csv"

# Complete the following code to input the data and store as wisc.df
wisc.df <- read.csv(fna.data, row.names=1)
```

```
#hide the diagnosis result so we can proceed with the unsupervised learning
wisc.data <- wisc.df[,-1]
diagnosis <- as.factor(wisc.df[,1])

dim(wisc.df)
```

```
[1] 569  31
```

```
View(wisc.df)
```

Q1. How many observations are in this dataset?

```
nrow(wisc.data)
```

```
[1] 569
```

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

```
sum(diagnosis=="M")
```

```
[1] 212
```

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

```
sum( grepl( "_mean", colnames(wisc.data), ignore.case=T) )
```

```
[1] 10
```

2. Principal Component Analysis

check mean and standard deviation to see whether data should be scaled

```
# Check column means and standard deviations
colMeans(wisc.data)
```

```
            radius_mean            texture_mean          perimeter_mean 
           1.412729e+01            1.928965e+01            9.196903e+01 
              area_mean         smoothness_mean        compactness_mean 
           6.548891e+02            9.636028e-02            1.043410e-01 
         concavity_mean     concave.points_mean           symmetry_mean 
           8.879932e-02            4.891915e-02            1.811619e-01 
 fractal_dimension_mean               radius_se              texture_se 
           6.279761e-02            4.051721e-01            1.216853e+00 
           perimeter_se                 area_se           smoothness_se 
           2.866059e+00            4.033708e+01            7.040979e-03 
         compactness_se            concavity_se       concave.points_se 
           2.547814e-02            3.189372e-02            1.179614e-02 
            symmetry_se    fractal_dimension_se            radius_worst 
           2.054230e-02            3.794904e-03            1.626919e+01 
          texture_worst         perimeter_worst              area_worst 
           2.567722e+01            1.072612e+02            8.805831e+02 
       smoothness_worst       compactness_worst         concavity_worst 
           1.323686e-01            2.542650e-01            2.721885e-01 
   concave.points_worst          symmetry_worst fractal_dimension_worst 
           1.146062e-01            2.900756e-01            8.394582e-02 
```

```r
apply(wisc.data,2,sd)
```

```
            radius_mean            texture_mean          perimeter_mean 
           3.524049e+00            4.301036e+00            2.429898e+01 
              area_mean         smoothness_mean        compactness_mean 
           3.519141e+02            1.406413e-02            5.281276e-02 
         concavity_mean     concave.points_mean           symmetry_mean 
           7.971981e-02            3.880284e-02            2.741428e-02 
 fractal_dimension_mean               radius_se              texture_se 
           7.060363e-03            2.773127e-01            5.516484e-01 
           perimeter_se                 area_se           smoothness_se 
           2.021855e+00            4.549101e+01            3.002518e-03 
         compactness_se            concavity_se       concave.points_se 
           1.790818e-02            3.018606e-02            6.170285e-03 
            symmetry_se    fractal_dimension_se            radius_worst 
           8.266372e-03            2.646071e-03            4.833242e+00 
          texture_worst         perimeter_worst              area_worst 
           6.146258e+00            3.360254e+01            5.693570e+02 
       smoothness_worst       compactness_worst         concavity_worst 
           2.283243e-02            1.573365e-01            2.086243e-01 
```

```
   concave.points_worst          symmetry_worst fractal_dimension_worst
           6.573234e-02            6.186747e-02            1.806127e-02
```

```r
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp(wisc.data, scale=TRUE)
# Look at summary of results
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
```

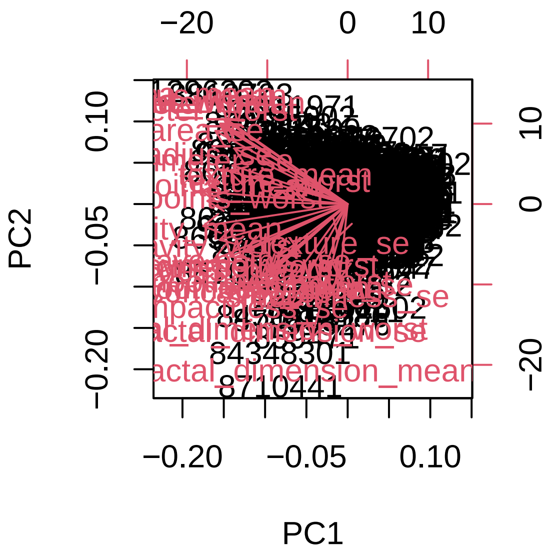
Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)? A: 44.27%

Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data? A: 3 PCs are required for capuring at least 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? A: 7

Interpreting PCA results

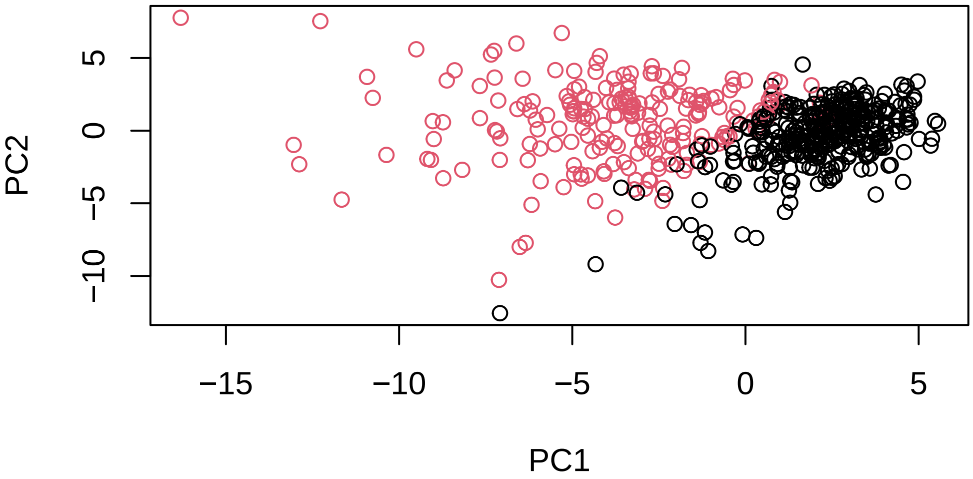
```r
biplot(wisc.pr)
```



Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why? A: This plot is not too informative because it's messy

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

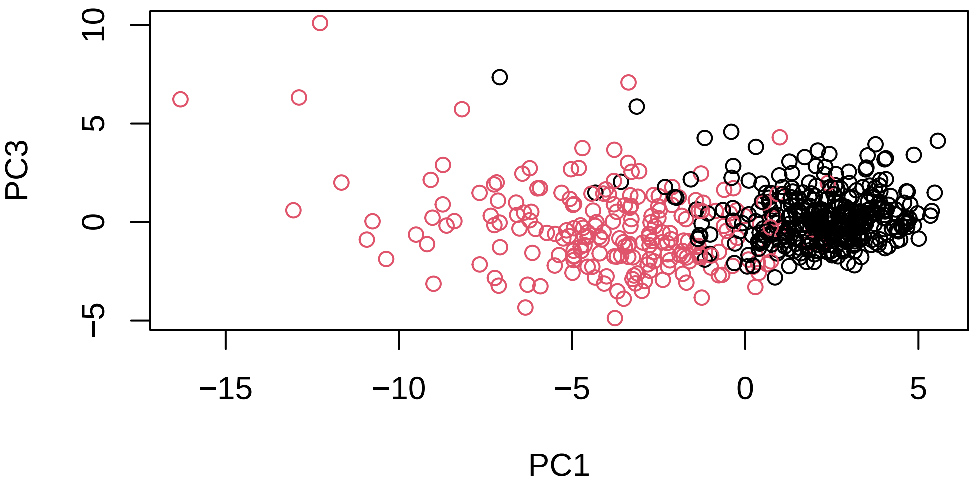
```r
# Scatter plot observations by components 1 and 2
plot( wisc.pr$x[,1], wisc.pr$x[,2], col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



A: there is now a better seperation between the points.

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

```
# Scatter plot observations by components 1 and 3
plot( wisc.pr$x[,1], wisc.pr$x[,3], col = diagnosis ,
     xlab = "PC1", ylab = "PC3")
```



A: PC1&3 is not as clear as PC1&2, which makes sense because PC2 explains more variations than PC3

creat a ggplot

```
library(ggplot2)
library(dplyr)
```

```
Attaching package: 'dplyr'
```

```
The following objects are masked from 'package:stats':

    filter, lag
```

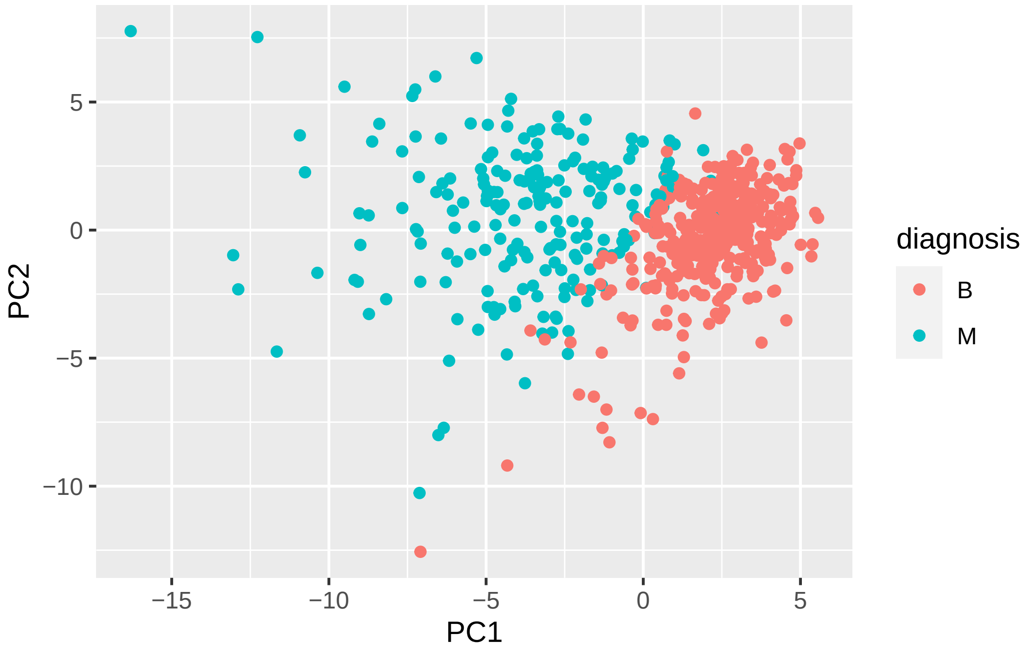
```
The following objects are masked from 'package:base':

    intersect, setdiff, setequal, union
```

first convert wisc.pr from list to dataframe so it can be read by ggplot

```
df <- as.data.frame(wisc.pr$x)

ggplot(df, aes(PC1, PC2, col=diagnosis)) +
  geom_point()
```

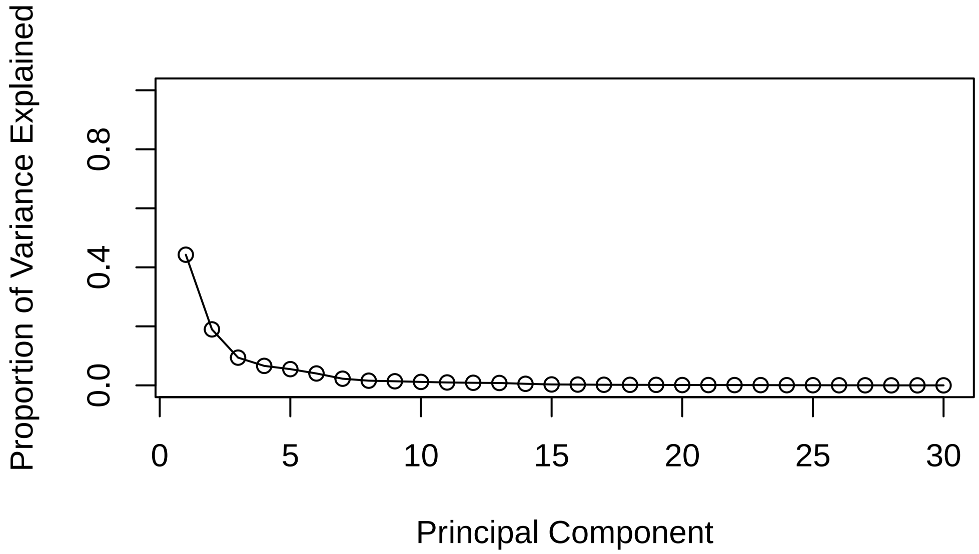


Variance explained

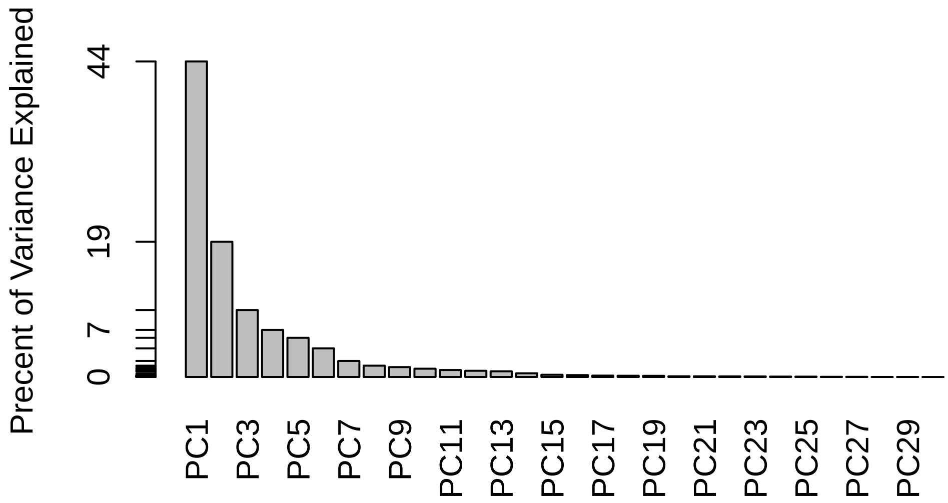
```
# Calculate variance of each component
pr.var <- (wisc.pr$sdev^2)
head(pr.var)
```

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

```
# Variance explained by each principal component: pve
pve <- pr.var / sum(pr.var)
# Plot variance explained for each principal component
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), typ = "o")
```



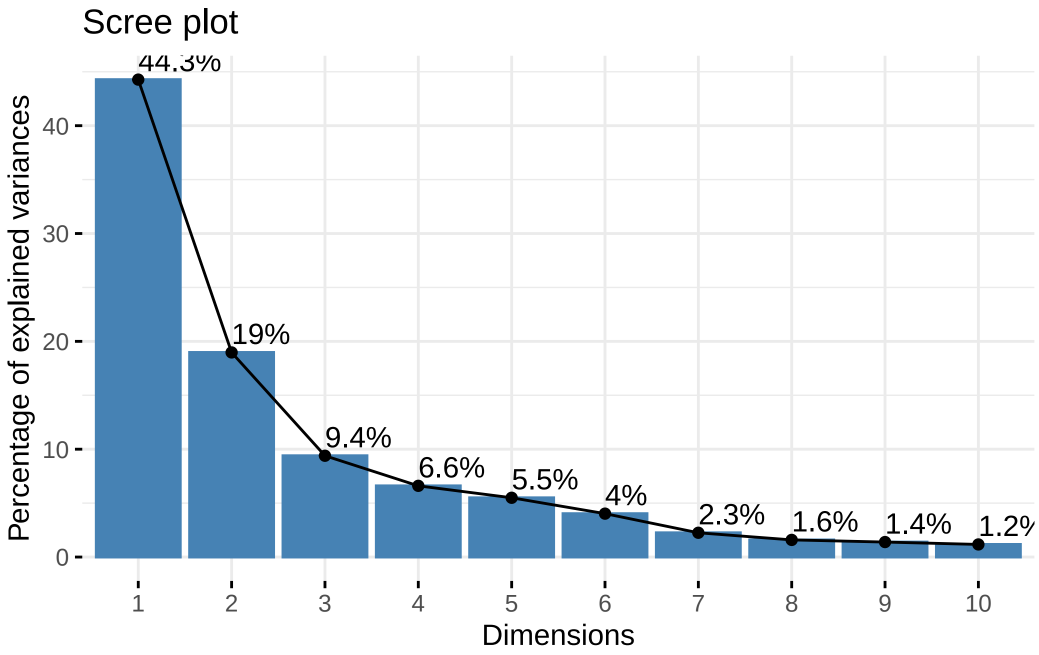
```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```



```
## ggplot based graph
#install.packages("factoextra")
library(factoextra)
```

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

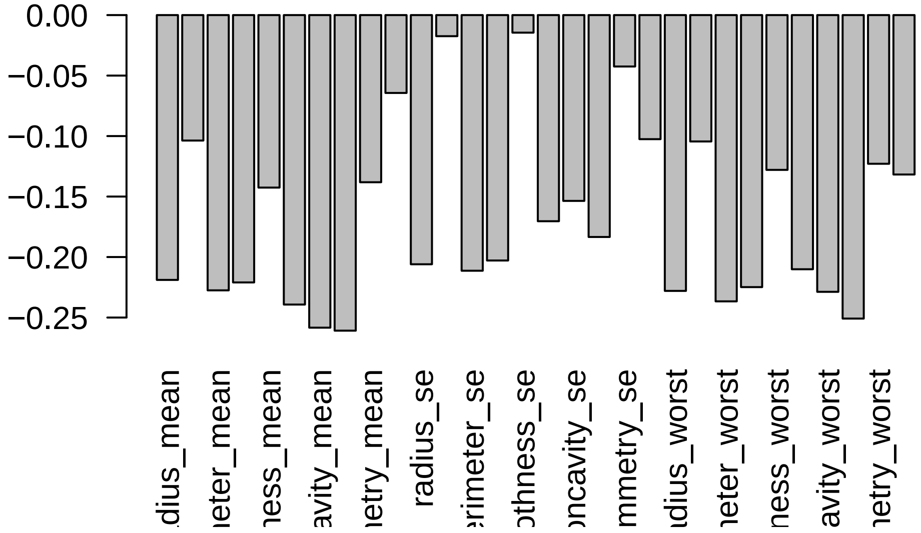
```
fviz_eig(wisc.pr, addlabels = TRUE)
```



Communicating PCA results

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?

```
barplot(wisc.pr$rotation[,1], las=2)
```



```
wisc.pr$rotation[,1][ names( wisc.pr$rotation[,1])=="concave.points_mean"]
```

```
concave.points_mean
         -0.2608538
```

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

```
y<-summary(wisc.pr)
attributes(y)
```

```
$names
[1] "sdev"       "rotation"   "center"     "scale"      "x"
[6] "importance"

$class
[1] "summary.prcomp"
```

```
sum(y$importance[3,] <=0.8)
```

```
[1] 4
```

A: 5 PCs are reqruired to explain 80% of the variance

3. Hierarchical clustering

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

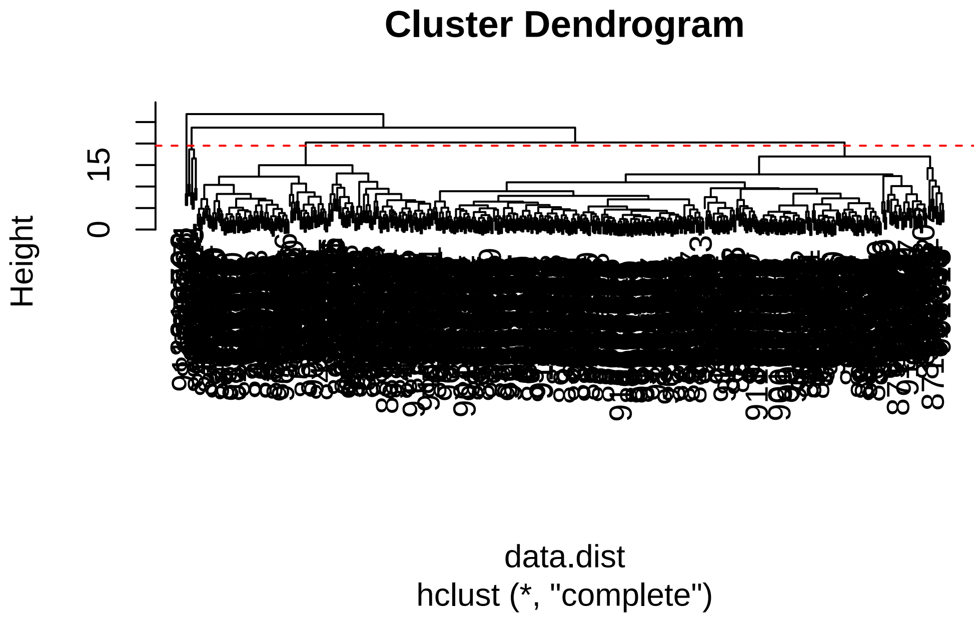
Calculate the (Euclidean) distances between all pairs of observations in the new scaled dataset and assign the result to data.dist.

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

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

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

```
plot(wisc.hclust)
abline(h=19.5, col="red", lty=2)
```



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

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   2   5
                   3 343  40
                   4   0   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=10)
table(wisc.hclust.clusters, diagnosis)
```

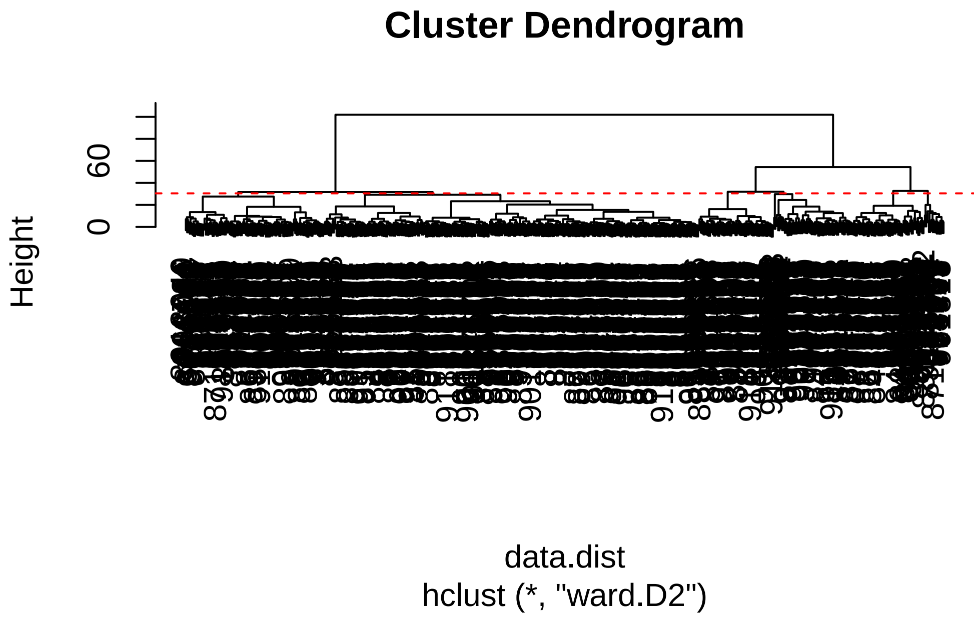
```
                    diagnosis
wisc.hclust.clusters   B   M
                  1   12  86
                  2    0  59
                  3    0   3
                  4  331  39
                  5    0  20
                  6    2   0
                  7   12   0
                  8    0   2
                  9    0   2
                  10   0   1
```

A: clusters of 10 returned a better match

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

ward.D2

```r
wisc.hclust <- hclust(data.dist, "ward.D2")
plot(wisc.hclust)
abline(h=30.5, col="red", lty=2)
```



```
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
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
```

average

```
wisc.hclust <- hclust(data.dist, "average")
wisc.hclust.clusters <- cutree(wisc.hclust, k=4)
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1 355 209
                   2   2   0
                   3   0   1
                   4   0   2
```

ward.D

```
wisc.hclust <- hclust(data.dist, "ward.D")
wisc.hclust.clusters <- cutree(wisc.hclust, k=4)
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1   6 131
                   2  23  53
                   3 149  24
                   4 179   4
```

A: ward.D2 gives the favorite results. Compared with other method, ward.D2 led to a better seperation between B and M groups.

4. OPTIONAL: K-means clustering

```
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
wisc.km <- kmeans(data.dist, centers=2 , nstart= 20)
table(wisc.km$cluster, diagnosis)
```

```
   diagnosis
      B   M
  1  20 134
  2 337  78
```

Q14. How well does k-means separate the two diagnoses? How does it compare to your hclust results?

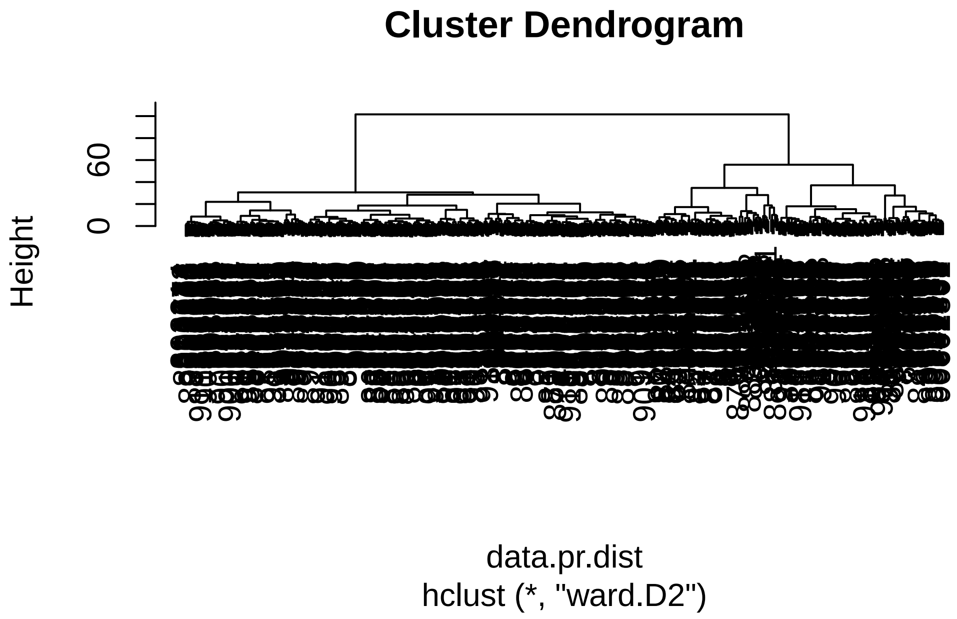
A: k-means did not do as well as ward.D2

```
table(wisc.hclust.clusters, wisc.km$cluster)
```

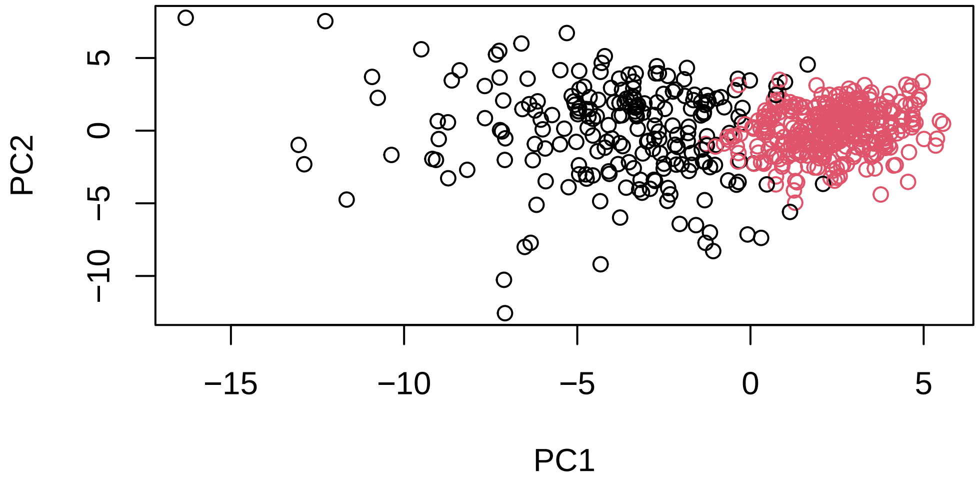
```
wisc.hclust.clusters   1   2
                   1  93  44
                   2  52  24
                   3   7 166
                   4   2 181
```

5. Combining methods

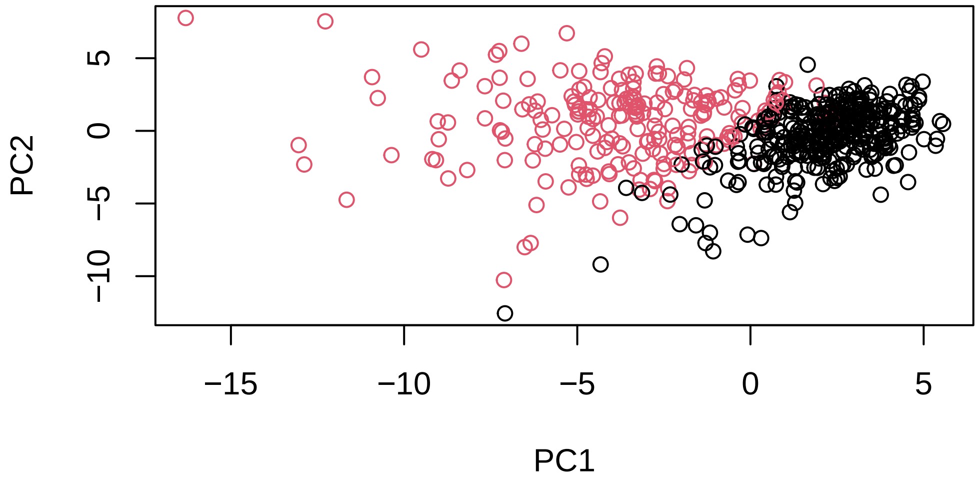
```
data.pr.dist <- dist(wisc.pr$x[, 1:7])
wisc.pr.hclust <- hclust(data.pr.dist, "ward.D2")
plot(wisc.pr.hclust)
```



```
grps <- cutree(wisc.pr.hclust, k=2)
plot(wisc.pr$x[,1:2], col=grps)
```



```r
plot(wisc.pr$x[,1:2], col=diagnosis)
```



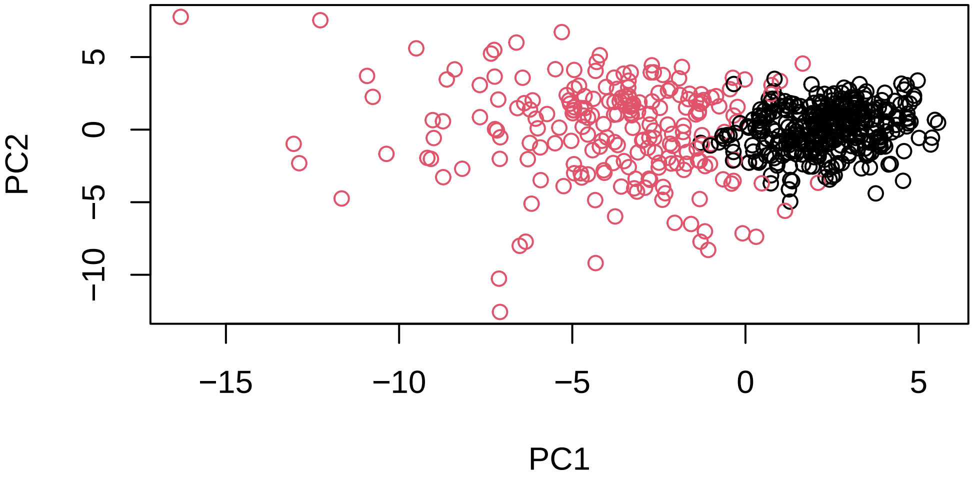
```
g <- as.factor(grps)
levels(g)
```

```
[1] "1" "2"
```

```
g <- relevel(g,2)
levels(g)
```

```
[1] "2" "1"
```

```
plot(wisc.pr$x[,1:2], col=g)
```



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

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

```
    diagnosis
grps   B   M
   1  28 188
   2 329  24
```

A: the newly created model with the first 7 PCs separated the data pretty well. The separation largely agreed with the diagnosis result, however, it is still not perfect.

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.

```
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(data.dist, "complete")
wisc.hclust.clusters <- cutree(wisc.hclust, k=4)
table(wisc.hclust.clusters, diagnosis)
```

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

```
table(wisc.km$cluster, diagnosis)
```

```
   diagnosis
      B   M
  1  20 134
  2 337  78
```

A:hcluster('complete') performed better in terms of separating the diagnoses

6. Sensitivity/Specificity

Q17. Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

```r
sum(diagnosis=="M")
```

```
[1] 212
```

```r
sum(diagnosis=="B")
```

```
[1] 357
```

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

```
    diagnosis
grps   B   M
   1  28 188
   2 329  24
```

A: sensitivity specificity PCA & h-cluster: .887 .922

h-clutser alone: .811 .961

k-means alone: .632 .944

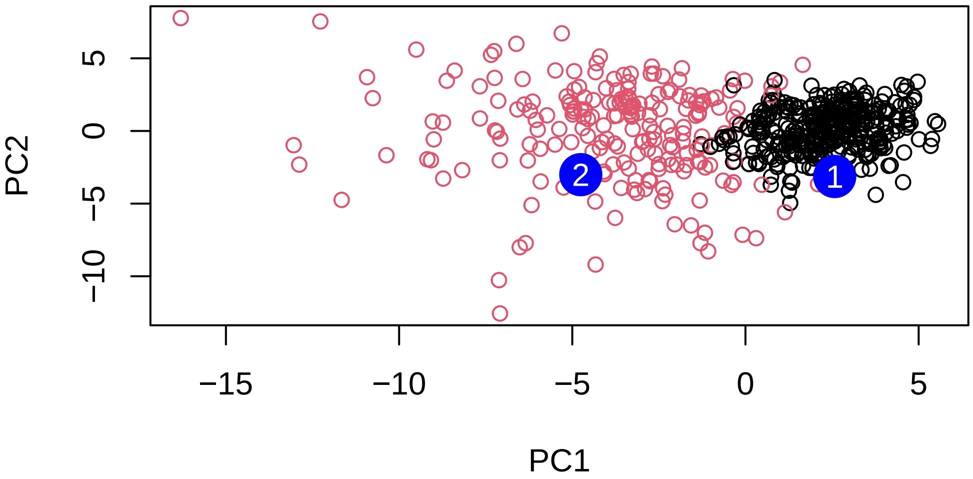
to conclude, the combined method has the highest sensitivity, and the h-cluster when performed alone has the highest specificity.

```r
#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")
```



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

A: we should prioritize the patients who fall under group 2; When patients' information are plotted in the PCA planes constructed using past diagnosis, the patients from group 2 appeared to be more likely to get a malignant diagnosis.