Lab 9: Mini Project

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1. Explorotory Data Analysis

Before starting the project, I downloaded the WisconsinCancer.csv file from the class website and moved it into the Lab9 folder (same directory as my R markdown file)

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

# input the data and store as wisc.df
wisc.df <- read.csv(fna.data, 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
```

```r
dim(wisc.df)
```

```
## [1] 569  31
```

```r
# Creating a new data frame what omits the diagnosis column
wisc.data <- wisc.df[,-1]
head(wisc.data)
```

```
##          radius_mean texture_mean perimeter_mean area_mean smoothness_mean
## 842302         17.99        10.38         122.80    1001.0         0.11840
## 842517         20.57        17.77         132.90    1326.0         0.08474
## 84300903       19.69        21.25         130.00    1203.0         0.10960
## 84348301       11.42        20.38          77.58     386.1         0.14250
## 84358402       20.29        14.34         135.10    1297.0         0.10030
## 843786         12.45        15.70          82.57     477.1         0.12780
##          compactness_mean concavity_mean concave.points_mean symmetry_mean
## 842302            0.27760         0.3001             0.14710        0.2419
## 842517            0.07864         0.0869             0.07017        0.1812
## 84300903          0.15990         0.1974             0.12790        0.2069
## 84348301          0.28390         0.2414             0.10520        0.2597
## 84358402          0.13280         0.1980             0.10430        0.1809
## 843786            0.17000         0.1578             0.08089        0.2087
##          fractal_dimension_mean radius_se texture_se perimeter_se area_se
## 842302                  0.07871    1.0950     0.9053        8.589  153.40
## 842517                  0.05667    0.5435     0.7339        3.398   74.08
## 84300903                0.05999    0.7456     0.7869        4.585   94.03
## 84348301                0.09744    0.4956     1.1560        3.445   27.23
## 84358402                0.05883    0.7572     0.7813        5.438   94.44
## 843786                  0.07613    0.3345     0.8902        2.217   27.19
##           smoothness_se compactness_se concavity_se concave.points_se
## 842302         0.006399        0.04904      0.05373           0.01587
## 842517         0.005225        0.01308      0.01860           0.01340
## 84300903       0.006150        0.04006      0.03832           0.02058
## 84348301       0.009110        0.07458      0.05661           0.01867
## 84358402       0.011490        0.02461      0.05688           0.01885
## 843786         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
```

```
# also create a factor using only the diagnosis column
diagnosis <- factor(wisc.df[,1])
head(diagnosis)
```

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

```


dim(wisc.data)
```

Q1. How many observations are in this dataset?

```
## [1] 569  30
```

The data frame has **569** observations.

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

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

```
## [1] 212
```

Out of the 569 observations, **212** are malignant.

```
# save column names as a new vector
wisc.colnames <- c(colnames(wisc.df))
wisc.colnames
```

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

```
##  [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"
```

```
# find the number of elements in wisc.colnames that contains _mean
length(grep("_mean", wisc.colnames))
```

```
## [1] 10
```

10 features from the data are suffixed with "_mean".

2. Principle Component Analysis

```r
# 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, since the data are on different magnitudes upon first inspection, we set sc
wisc.pr <- prcomp( wisc.data, center = TRUE, scale. = TRUE )
summary(wisc.pr)
```

```
## Importance of components:
```

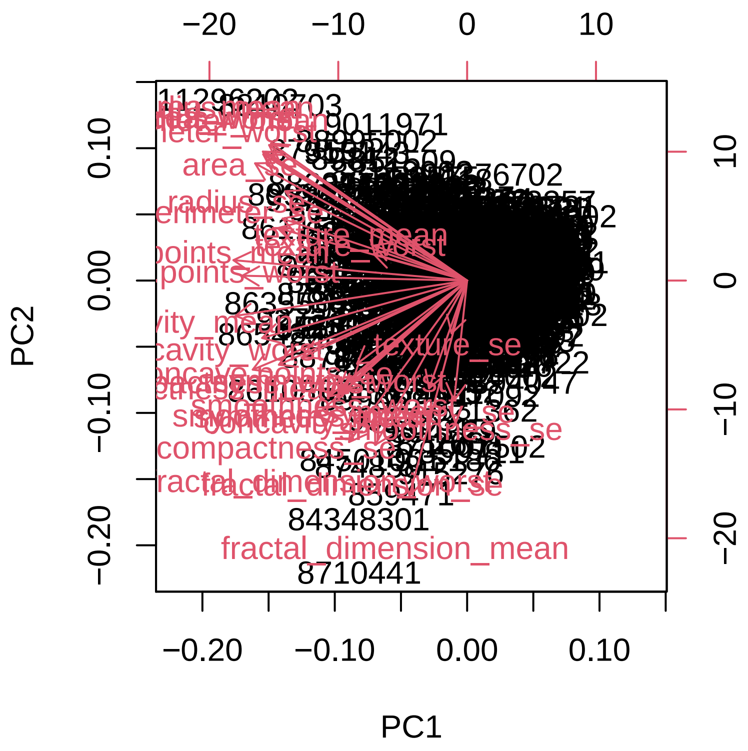
```
##                           PC1    PC2     PC3     PC4     PC5     PC6     PC7
## Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
## Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
## Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 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)? 44.27%

Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data? 3 (cumulative proportion achieves 72.6% at PC3)

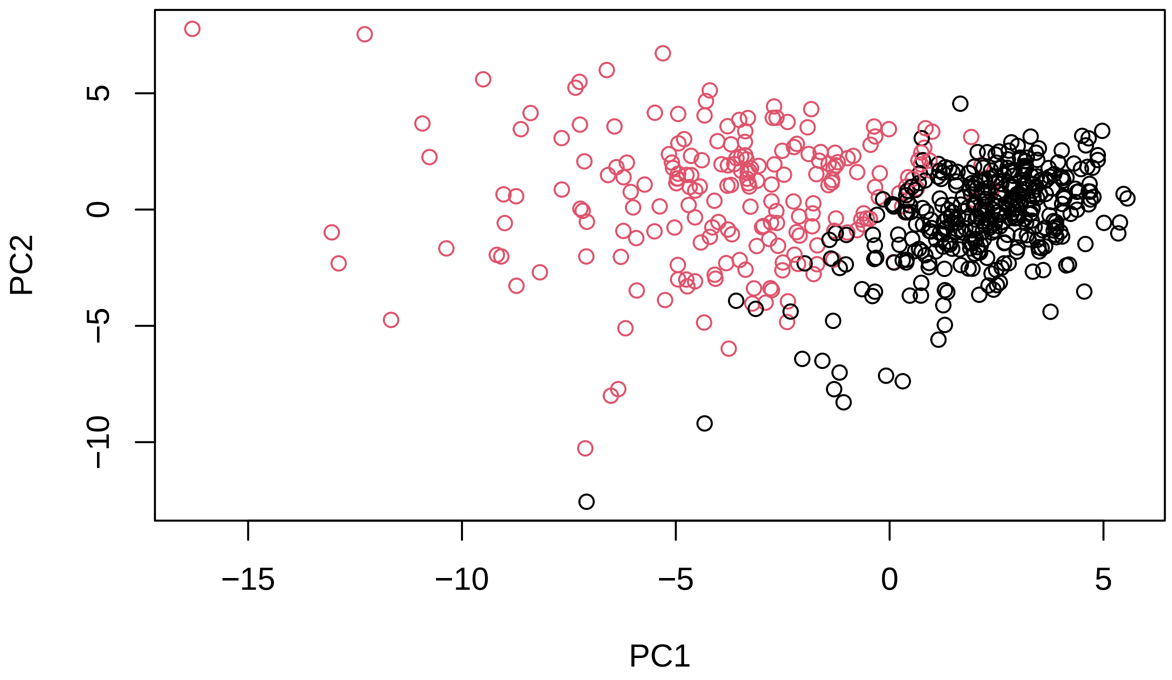
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data? 7 (cumulative proportion achieves 91% at PC7)

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



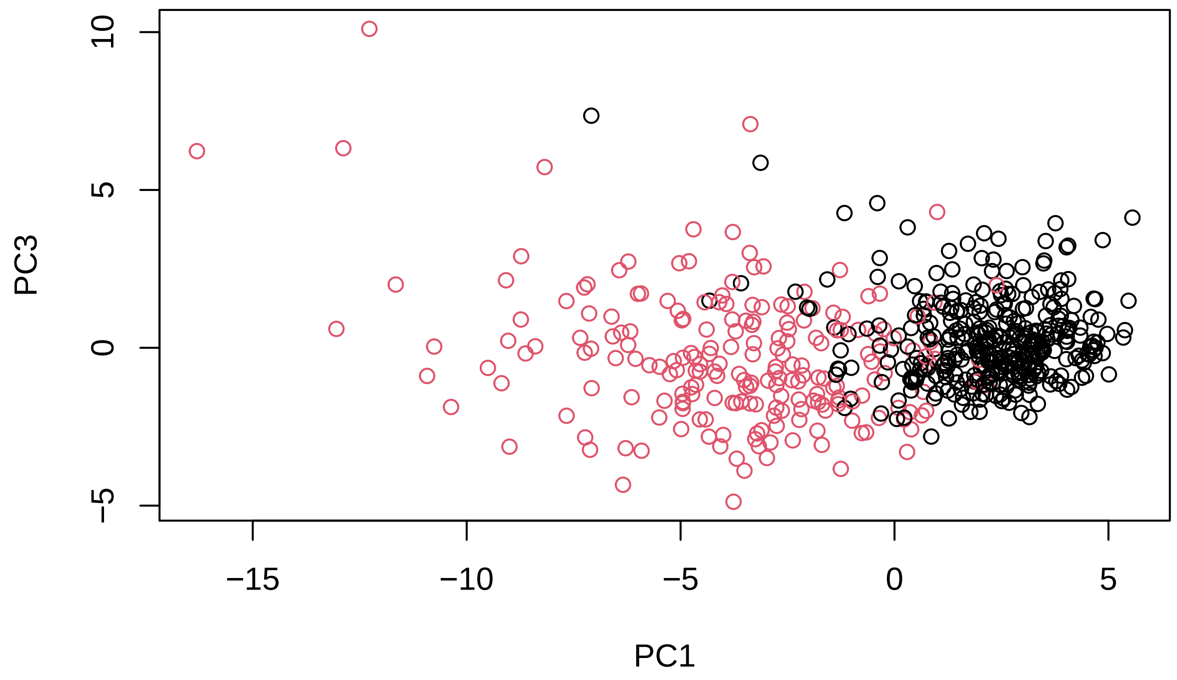
Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why? The plot is very difficult to understand because everything is on top of each other and we can't really see what is going on.(30PCs are too many!)

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



Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots? We see an overall **separation of "M"(red) from "B"(black) samples**. **The plot of PC1 vs. PC2 has better separation on the y-axis than that of the PC1 vs. PC3 plot**. This is reasonable because PC2 captures more variance in the data than PC3.

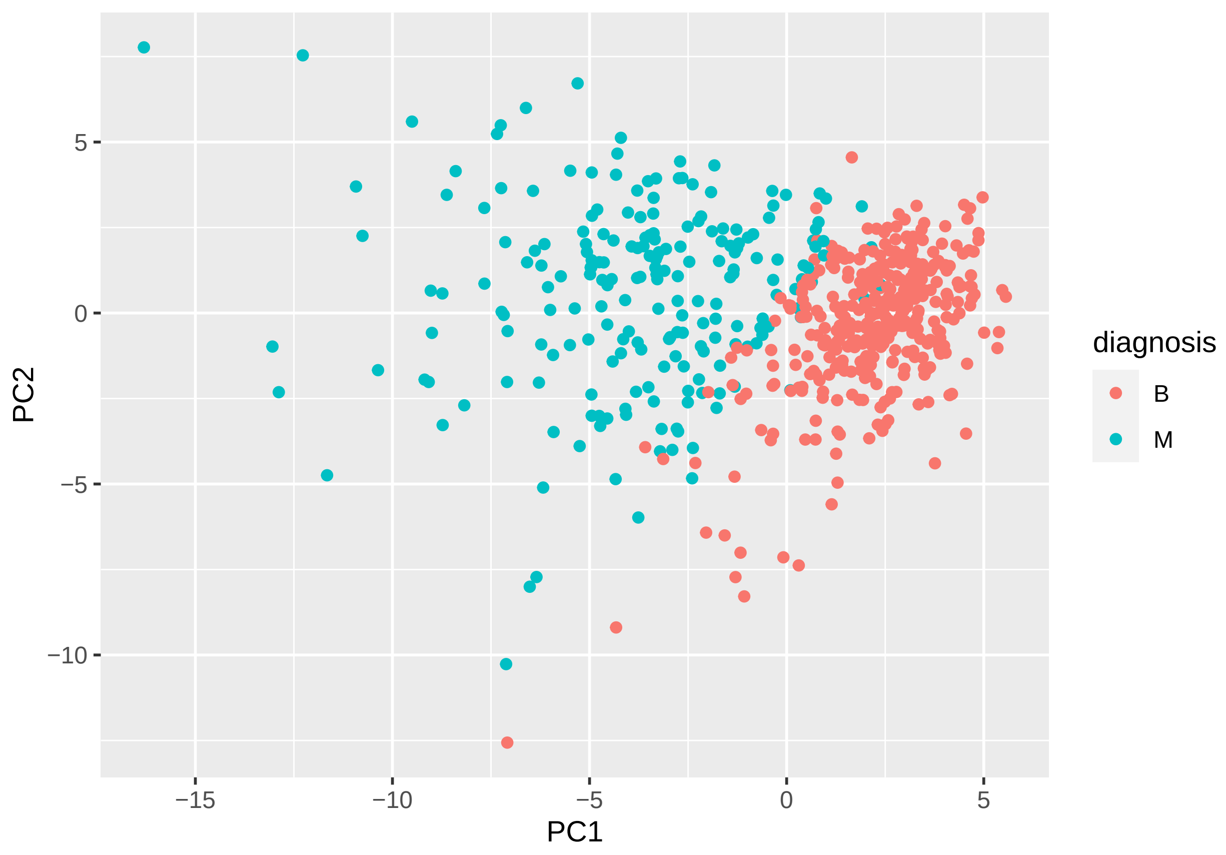
```r
# Repeat for components 1 and 3
plot(wisc.pr$x[,1], wisc.pr$x[,3], col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```



```
# Create a data.frame for ggplot
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis

# Load the ggplot2 package
library(ggplot2)

# Make a scatter plot colored by diagnosis
ggplot(df) +
  aes(PC1, PC2, col= diagnosis) +
  geom_point()
```

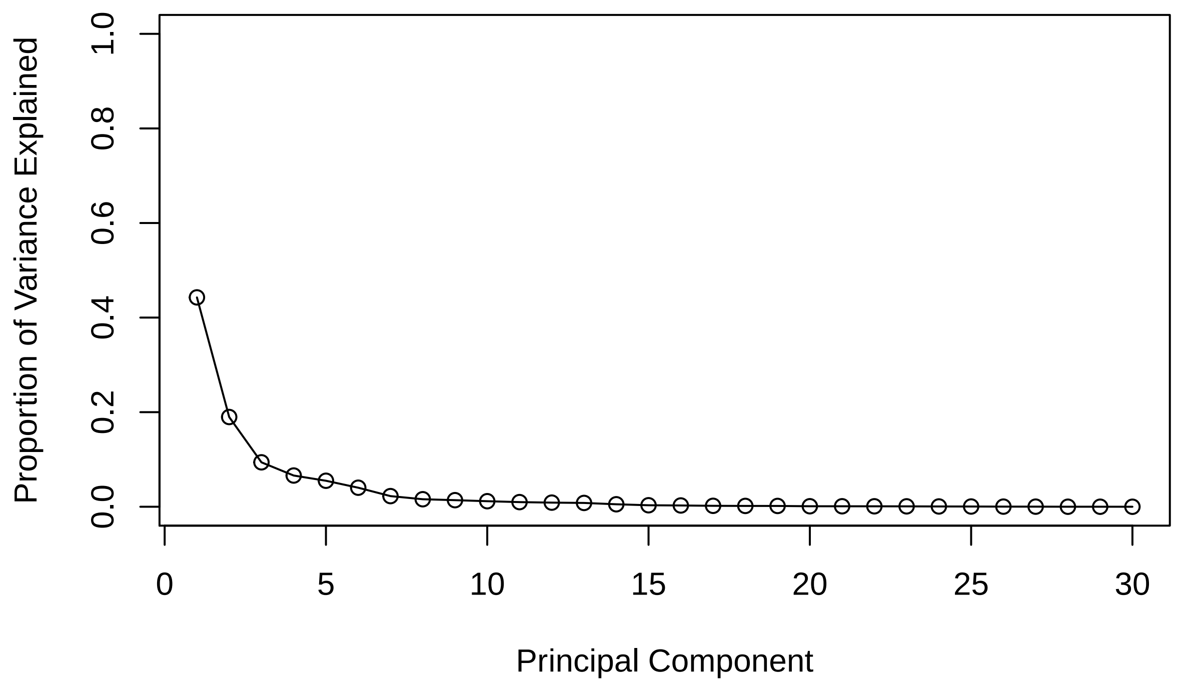


```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

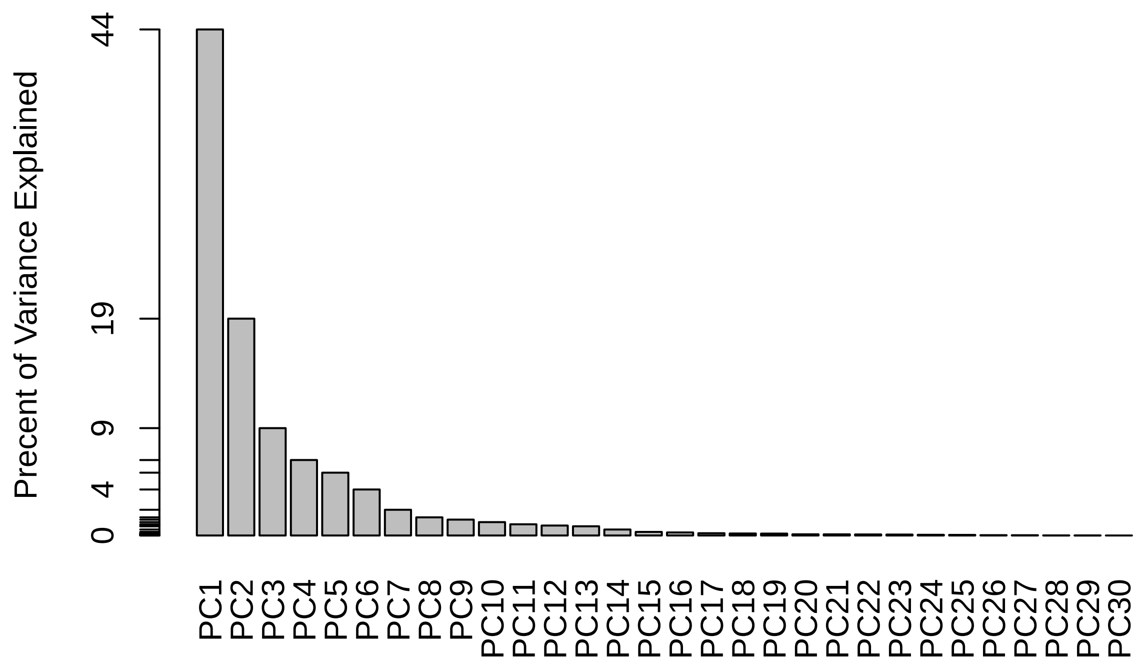
```
## [1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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), type = "o")
```



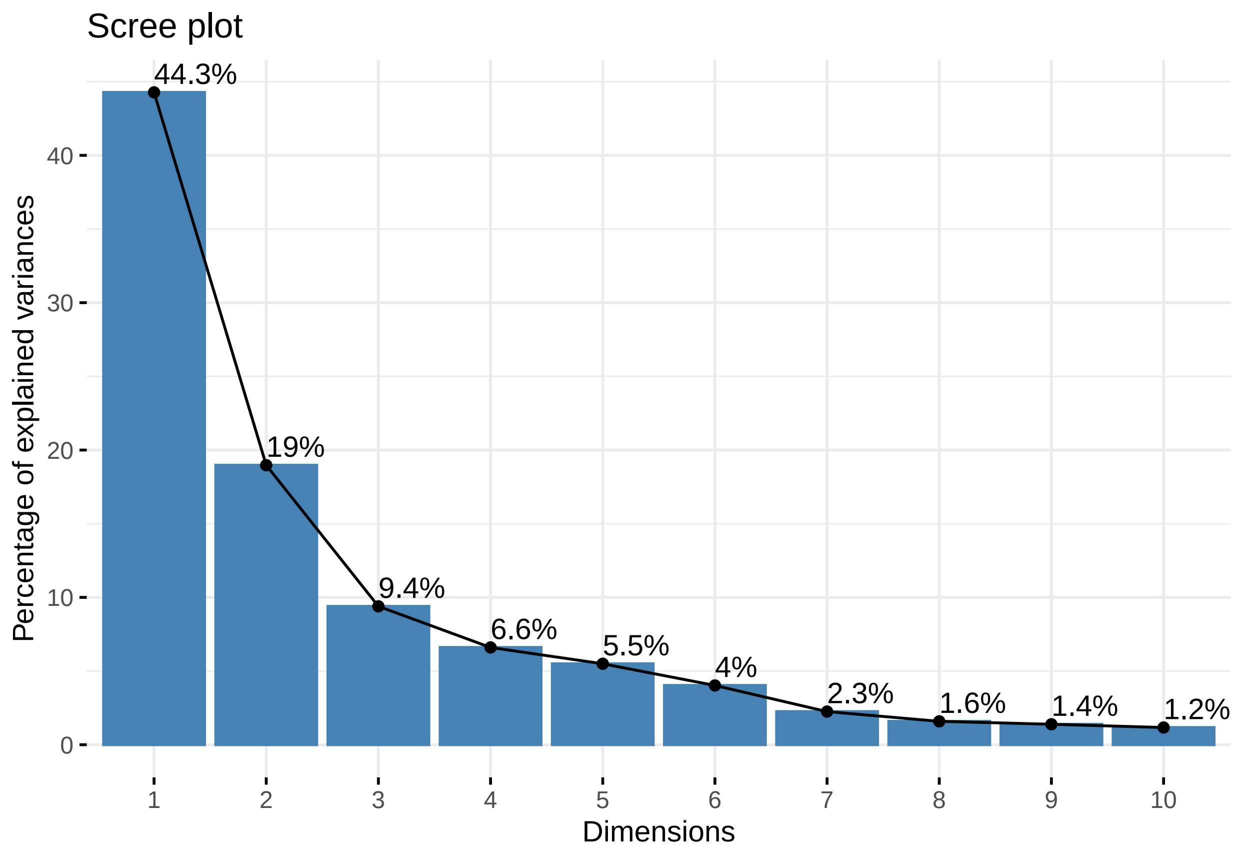
```r
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```



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

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

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



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

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?

```
## [1] -0.2608538
```

The loading vector of concave.points_mean for PC1 is about **-0.26**.

Q10. What is the minimum number of principal components required to explain 80% of the variance of the data? Based on the scree plots and the variance table, **5 PCs** are required to explain 80% of the data.

3. Hierarchical Clustering

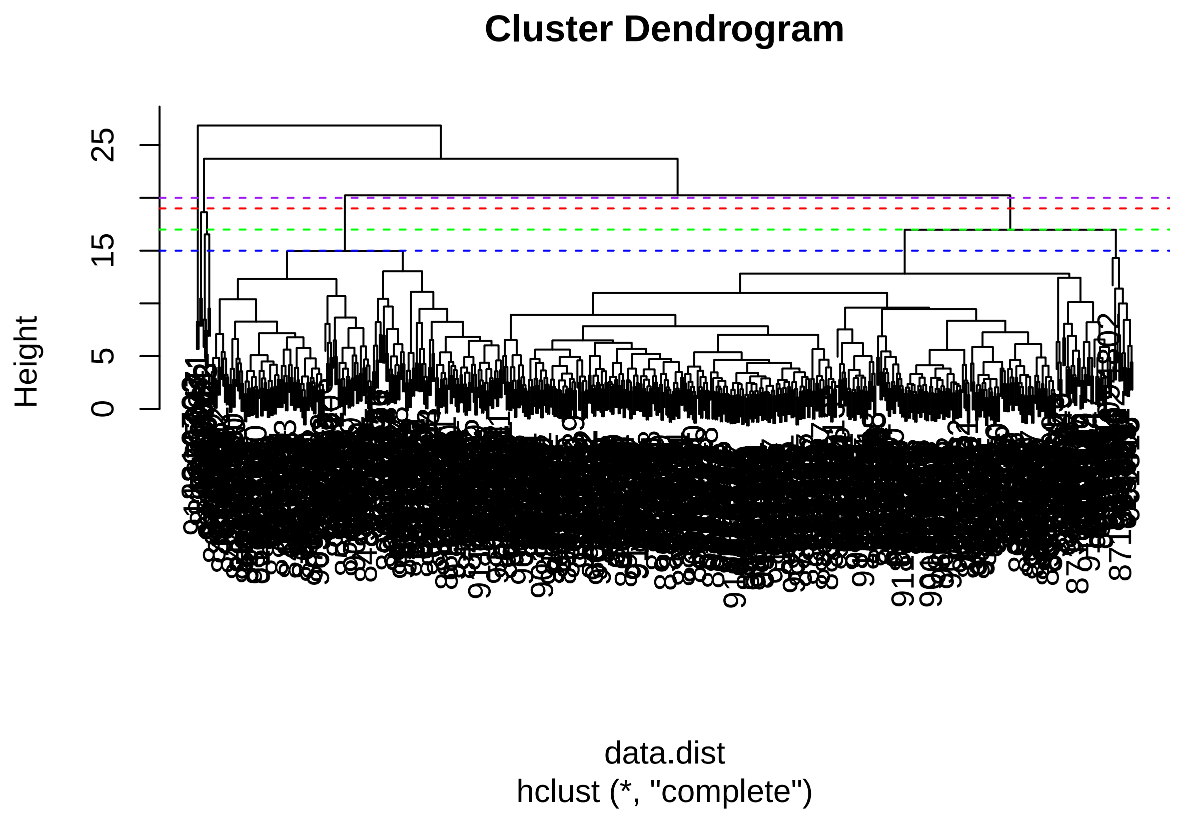
```r
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
```

```
# 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)
```

```
# Create a hierarchical clustering model using
# complete linkage. Manually specify the method
# argument to hclust() and assign the results to
# wisc.hclust
wisc.hclust.complete <- hclust(data.dist, method = "complete")
```

Q11. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters? As shown, at height **19**, the model has 4 cluster.

```
plot(wisc.hclust.complete)
abline(h = 15, col="blue", lty=2)
abline(h = 17, col="green", lty=2)
abline(h = 19, col="red", lty=2)
abline(h = 20, col="purple", lty=2)
```



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

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

```
wisc.hclust.clusters.complete9 <- cutree(wisc.hclust.complete, k = 9)
table(wisc.hclust.clusters.complete9, diagnosis)
```

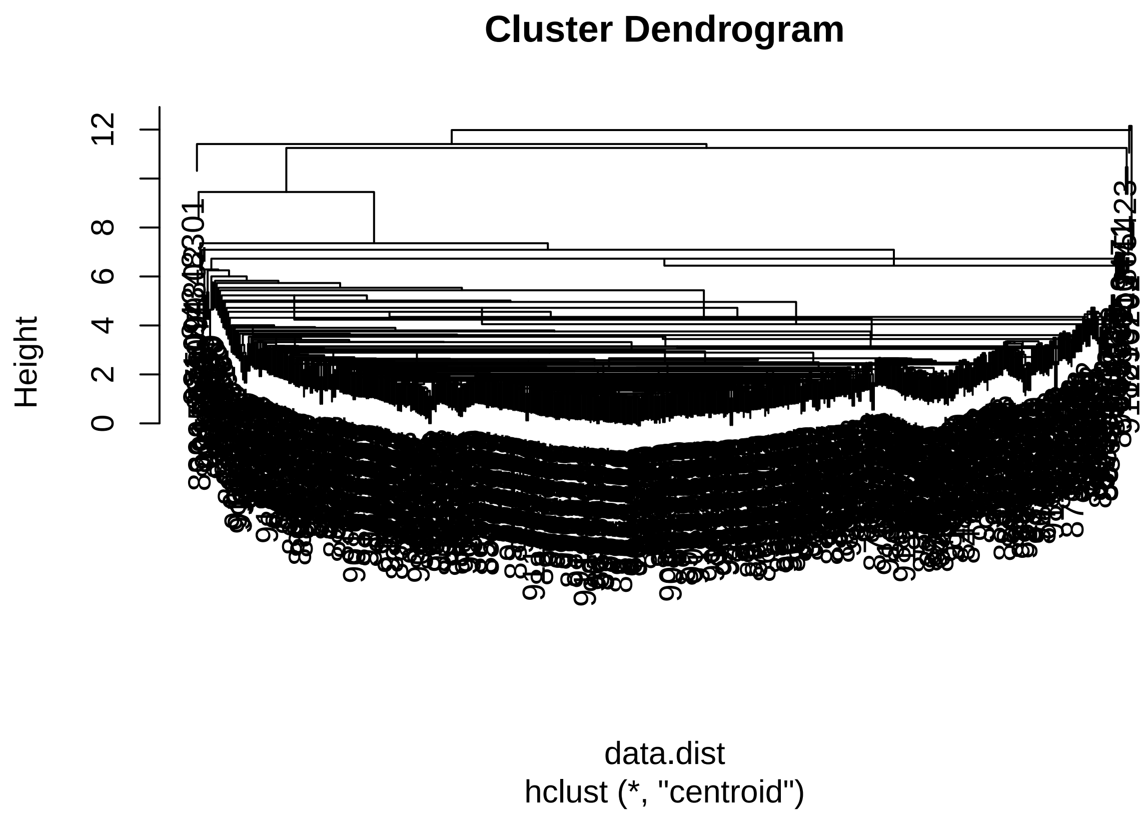
Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

```
##                                diagnosis
## wisc.hclust.clusters.complete9   B   M
##                               1  12  86
##                               2   0  79
##                               3   0   3
##                               4 331  39
##                               5   2   0
##                               6  12   0
##                               7   0   2
##                               8   0   2
##                               9   0   1
```

Using **k = 9**, the result is slightly better.

Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning. Side-note: The method="ward.D2"creates groups such that variance is minimized within clusters. This has the effect of looking for spherical clusters with the process starting with all points in individual clusters (bottom up) and then repeatedly merging a pair of clusters such that when merged there is a minimum increase in total within-cluster variance This process continues until a single group including all points (the top of the tree) is defined.

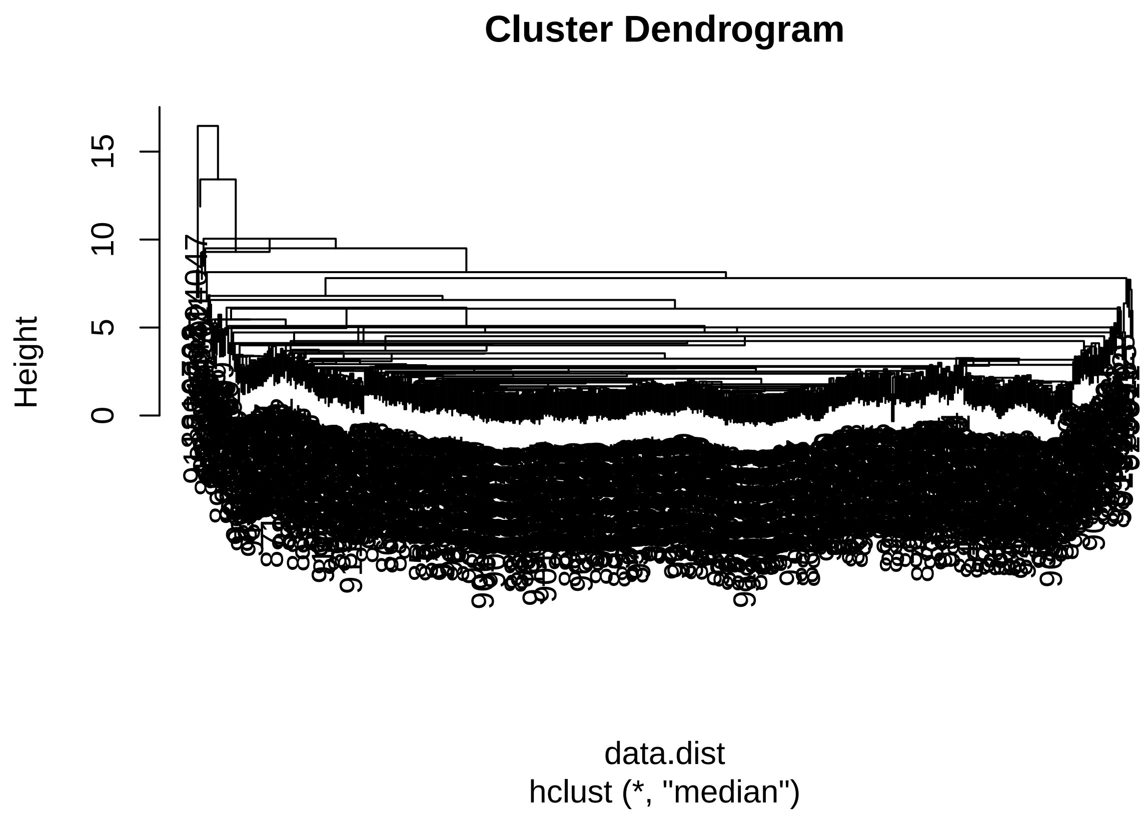
```
wisc.hclust <- hclust(data.dist, method = "centroid")
plot(wisc.hclust)
```



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

```
##                       diagnosis
## wisc.hclust.clusters   B   M
##                    1 357 208
##                    2   0   1
##                    3   0   1
##                    4   0   2
```

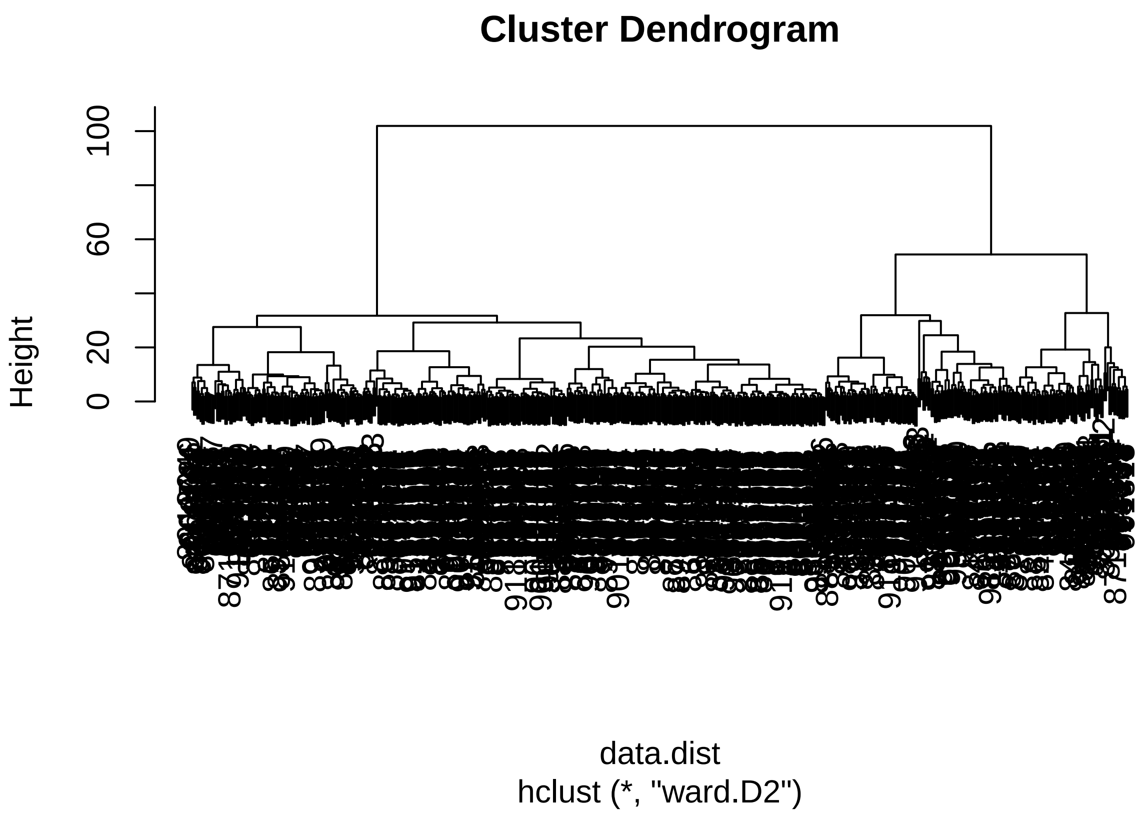
```
wisc.hclust <- hclust(data.dist, method = "median")
plot(wisc.hclust)
```



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

```
##                     diagnosis
## wisc.hclust.clusters   B   M
##                    1 355 210
##                    2   1   0
##                    3   0   2
##                    4   1   0
```

```
wisc.hclust <- hclust(data.dist, method = "ward.D2")
plot(wisc.hclust)
```



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

```
##                     diagnosis
## wisc.hclust.clusters   B   M
##                    1   0 115
##                    2   6  48
##                    3 337  48
##                    4  14   1
```

I like the **"ward.D2"** method the best for it gives the neatest graph.The bottom-up grouping is also suitable for this dataset for we are eventually looking at either benign/malignant samples.However, the "complete" method seems to give the cleanest separation of the two sample types.

4. K-means Clustering

```
# Create a k-means model on wisc.data, assigning the result to wisc.km.
wisc.km <- kmeans(scale(wisc.data), centers= 2, nstart= 20)

# Use the table() function to compare the cluster membership of the k-means model
table(wisc.km$cluster, diagnosis)
```

```
##    diagnosis
##       B   M
##   1  14 175
##   2 343  37
```

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

```
## 
## wisc.hclust.clusters.complete   1   2
##                             1 160  17
##                             2   7   0
##                             3  20 363
##                             4   2   0
```

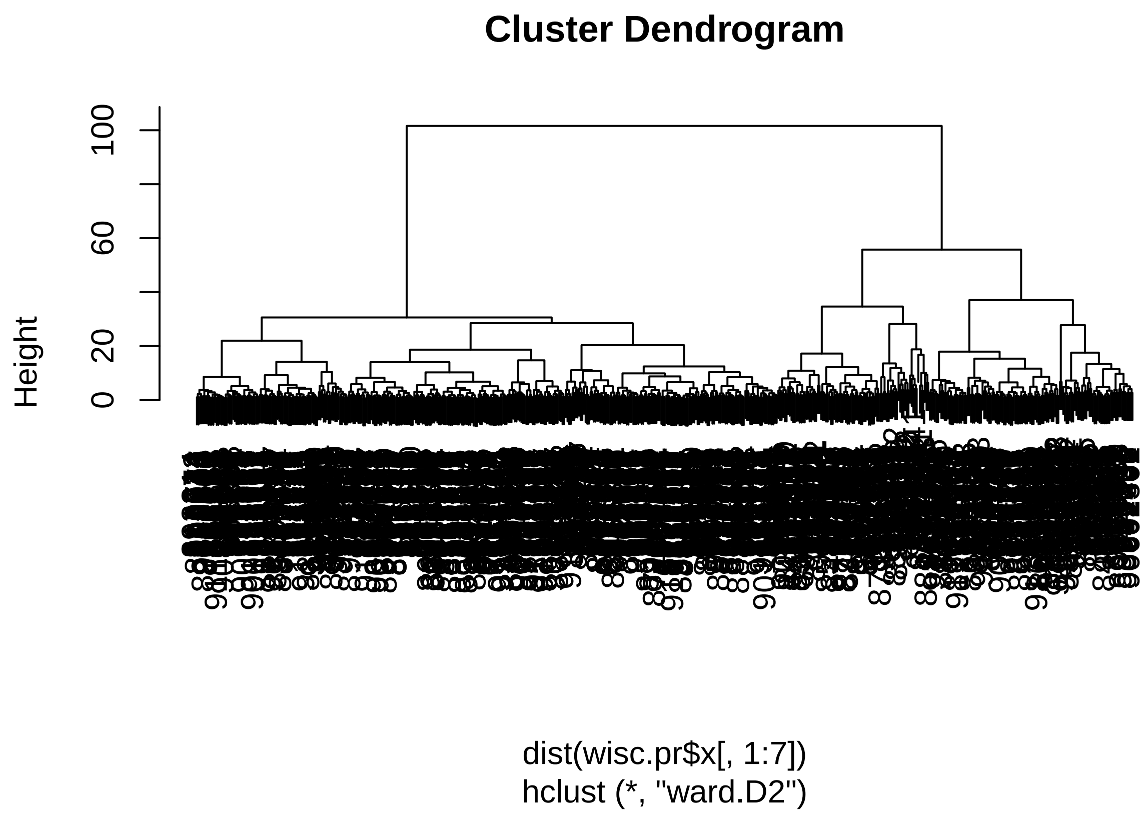
Q14. How well does k-means separate the two diagnoses? How does it compare to your hclust results? k-means seem to have done a better job than hclust by giving two clusters with very good separation based on diagnosis.

5. Combining Methods

Using the minimum number of principal components required to describe at least 90% of the variability in the data, create a hierarchical clustering model with the linkage method="ward.D2". We use Ward's criterion here because it is based on multidimensional variance like principal components analysis. Assign the results to wisc.pr.hclust.

```
# Using the minimum number of principal components
# required to describe at least 90% of the
# variability in the data (PC1-7), create a
# hierarchical clustering model with the linkage
# method="ward.D2". We use Ward's criterion here
# because it is based on multidimensional variance
# like principal components analysis. Assign the
# results to wisc.pr.hclust.

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



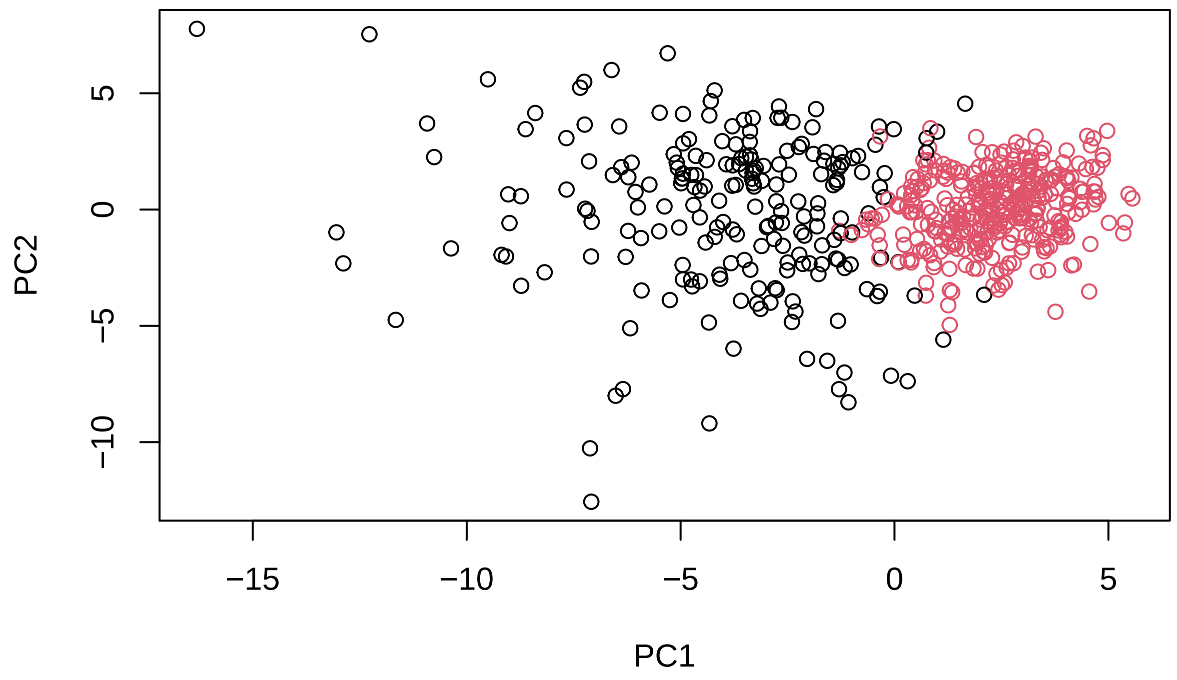
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
## grps
##   1   2
## 216 353
```

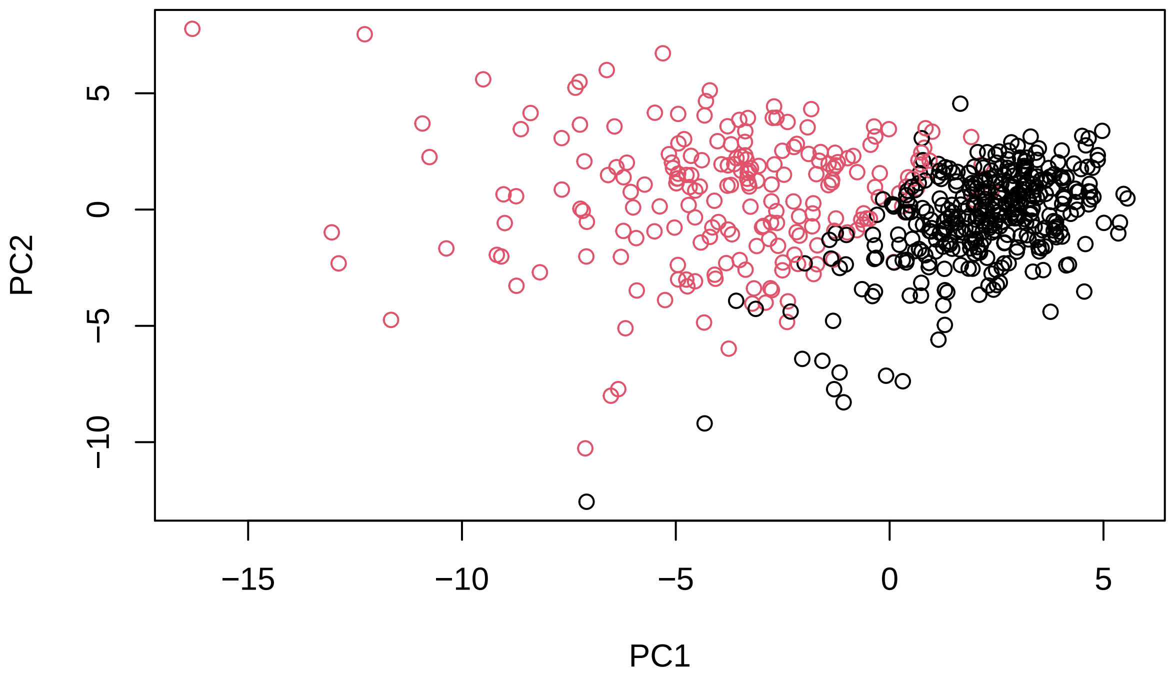
```
table(grps, diagnosis)
```

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

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



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



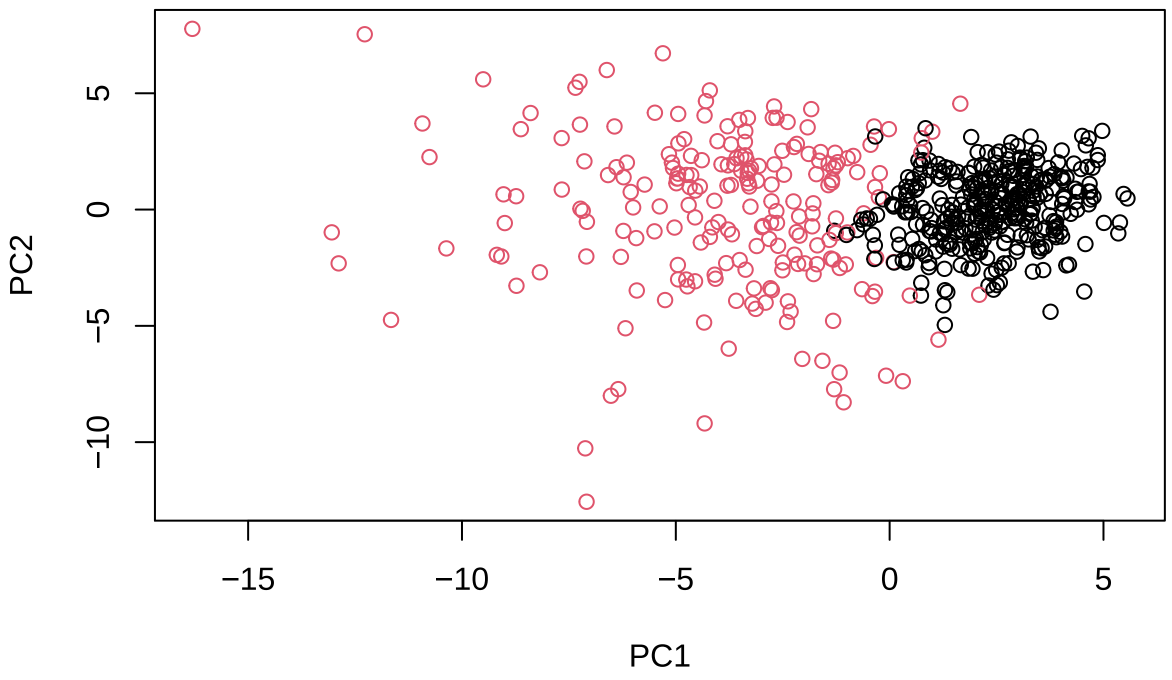
```
# Note the color swap here as the hclust cluster 1
# is mostly "M" and cluster 2 is mostly "B" as we
# saw from the results of calling table(grps,
# diagnosis). To match things up we can turn our
# groups into a factor and reorder the levels so
# cluster 2 comes first and thus gets the first
# color (black) and cluster 1 gets the second color
# (red).
g <- as.factor(grps)
levels(g)
```

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

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

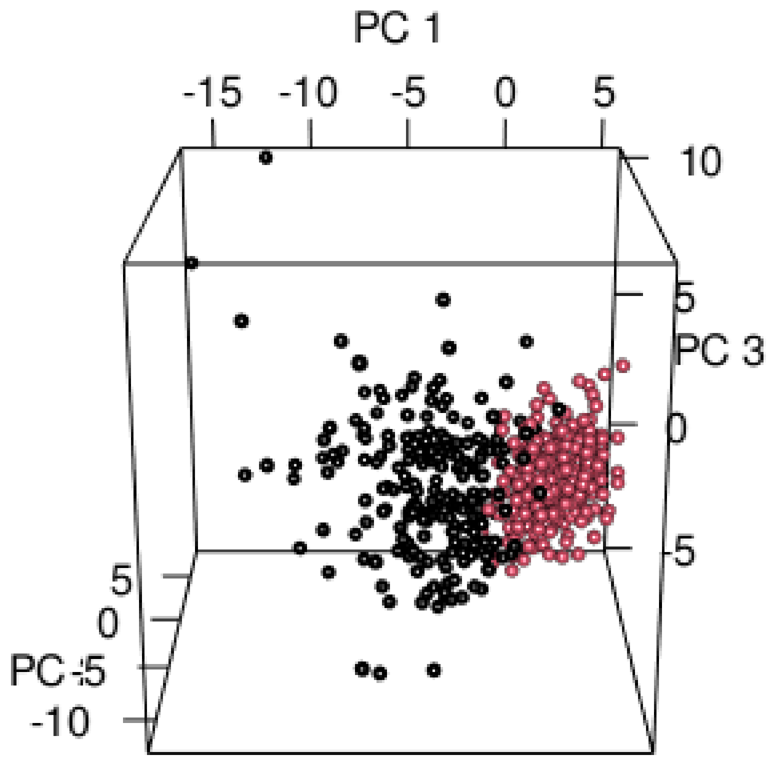
```
## [1] "2" "1"
```

```
# Plot using our re-ordered factor
plot(wisc.pr$x[,1:2], col=g)
```



```
# Fancy 3D plot
library(rgl)
plot3d(wisc.pr$x[,1:3], xlab="PC 1", ylab="PC 2", zlab="PC 3", cex=1.5, size=1, type="s", col=grps)
rglwidget(width = 400, height = 400)
```

```
## Warning in snapshot3d(scene = x, width = width, height = height): webshot = TRUE
## requires the webshot2 package; using rgl.snapshot() instead
```



```r
# Use the distance along the first 7 PCs for
# clustering i.e. wisc.pr$x[, 1:7]
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method="ward.D2")

# Cut this hierarchical clustering model into 2
# clusters and assign the results to
# wisc.pr.hclust.clusters.
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)

# Compare to actual diagnoses
table(wisc.pr.hclust.clusters, diagnosis)
```

```
##                        diagnosis
## wisc.pr.hclust.clusters   B   M
##                       1  28 188
##                       2 329  24
```

Q15. How well does the newly created model with two clusters separate out the two diagnoses?
It did a better job than before and is pretty similar to the k-means results.

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

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.

```
##    diagnosis
##       B   M
##   1  14 175
##   2 343  37
```

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

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

Before PCA, the clustering is a lot messier and requires more than two clusters to achieve decent separation of the 2 diagnosis. After PCA, the separation is much cleaner.

6. Sensitivity/Specificity

Q17. Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity? **Sensitivity** refers to a test's ability to correctly detect ill patients who do have the condition. In our example here the sensitivity is the total number of samples in the cluster identified as predominantly malignant (cancerous) divided by the total number of known malignant samples. In other words: **TP/(TP+FN)**.

```
TPFN <- sum(diagnosis == "M")
kmeans.sensi = 175/TPFN
prWard2.sensi = 188/TPFN
```

Specificity relates to a test's ability to correctly reject healthy patients without a condition. In our example specificity is the proportion of benign (not cancerous) samples in the cluster identified as predominantly benign that are known to be benign. In other words: **TN/(TN+FN)**.

```
TNFN <- sum(diagnosis == "B")
kmeans.speci = 343/TNFN
prWard2.speci = 329/TNFN
```

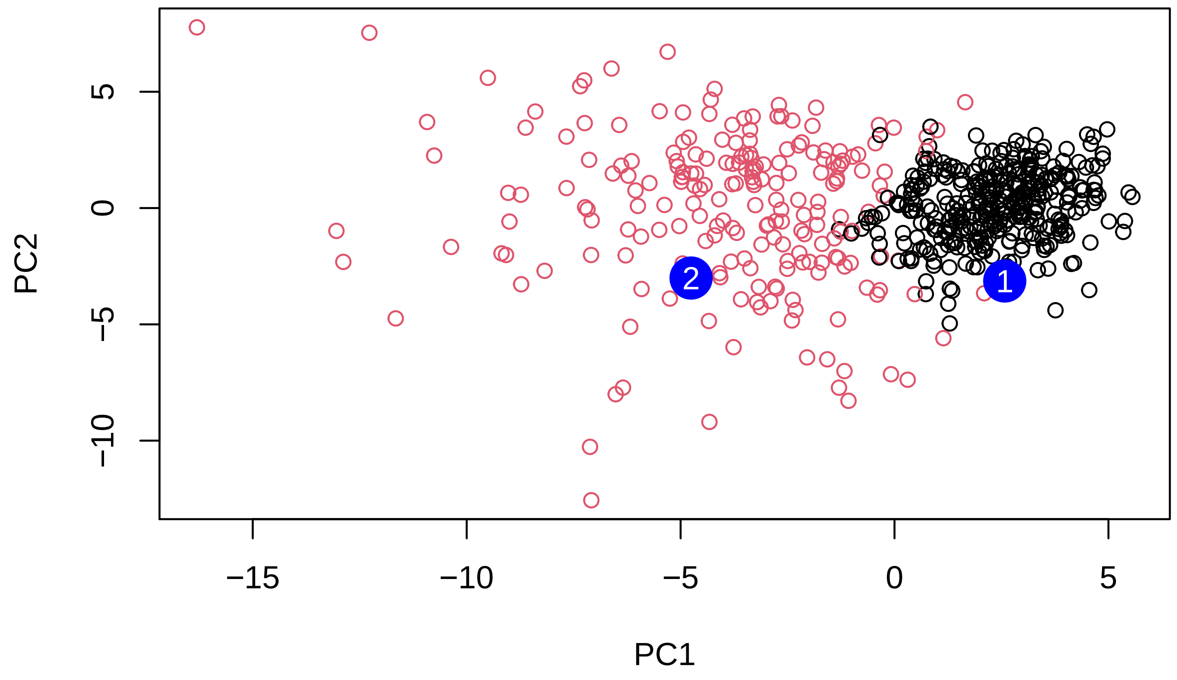
Based on the above calculations, the kmeans clustering has higher specificity while the h-clust after PCA method has higher sensitivity.

7. Prediction

```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
```

```r
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? Based on our clustering, patent 2 is located closer to the center of the maliganent cluster, therefore, we should give priority to **patient 2**.