Class 8: Mini Project

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Preparing the Data

```
r = getOption("repos")
r["CRAN"] = "http://cran.us.r-project.org"
options(repos = r)

# 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)
```

Checking that my dataframe was uploading correctly.

> use the head() function to see the first 6 rows of the dataframe

```
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  X
## 842302                   0.11890 NA
## 842517                   0.08902 NA
## 84300903                 0.08758 NA
## 84348301                 0.17300 NA
## 84358402                 0.07678 NA
## 843786                   0.12440 NA
```

We will not be using the column labelled 'Diagnosis'

```
# We can use -1 here to remove the first column
wisc.data <- wisc.df[,-1]
```

Create diagnosis vector for later

```
diagnosis <- as.numeric(wisc.df$diagnosis =="M")
```

Exploratory Data Analysis

[Q1] How many observations are in this data set?

```r
# Use nrow() to get the number of rows. This is the number of observations in the data set.
nrow(wisc.data)
```

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

There are 569 observations. ### [Q2] How many of the observations have a malignant diagnosis?

```r
# Use grep() to find all rows in the diagnosis column with "M"
malignant <- grep("M", wisc.df$diagnosis)
# find the length of this vector to know how many rows
length(malignant)
```

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

There are 212 observations with a malignant diagnosis.

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

```r
wisc_col_mean <- wisc.data[,grepl("_mean",colnames(wisc.data))]
ncol(wisc_col_mean)
```

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

There are 10 variables/features in the data suffixed with _mean.

Principal Component Analysis

Performing PCA

```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
##                      X
##                     NA
```

```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
##                      X
##                     NA
```

```r
# Perform PCA on wisc.data by completing the following code
install.packages("dplyr")
```

```
##
## The downloaded binary packages are in
##  /var/folders/9r/2f14lwsd285gxhxcsztcvzp40000gn/T//RtmpHn37H6/downloaded_packages
```

```r
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
```

```r
wisc.data2 <- dplyr :: select(wisc.data, -c(X))
wisc.pr <- prcomp(na.omit(wisc.data2),  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% of the original variance is captured by the first principal components.

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

Three. PC1-PC3 describe 72.63% of the original variance in the data.

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

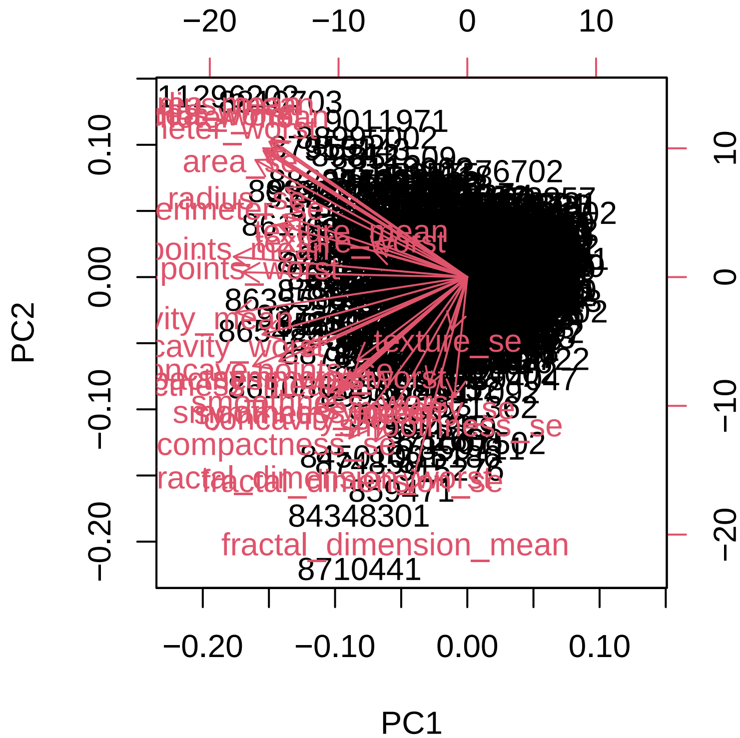
Five. PC1-PC5 describe 91.01% of the original variance in the data.

```r
#Adding Proportion of Variance of PC1-PC5
0.4427+0.1897+0.09393+0.06602+0.05496+0.04025+0.02251
```

```
## [1] 0.91007
```

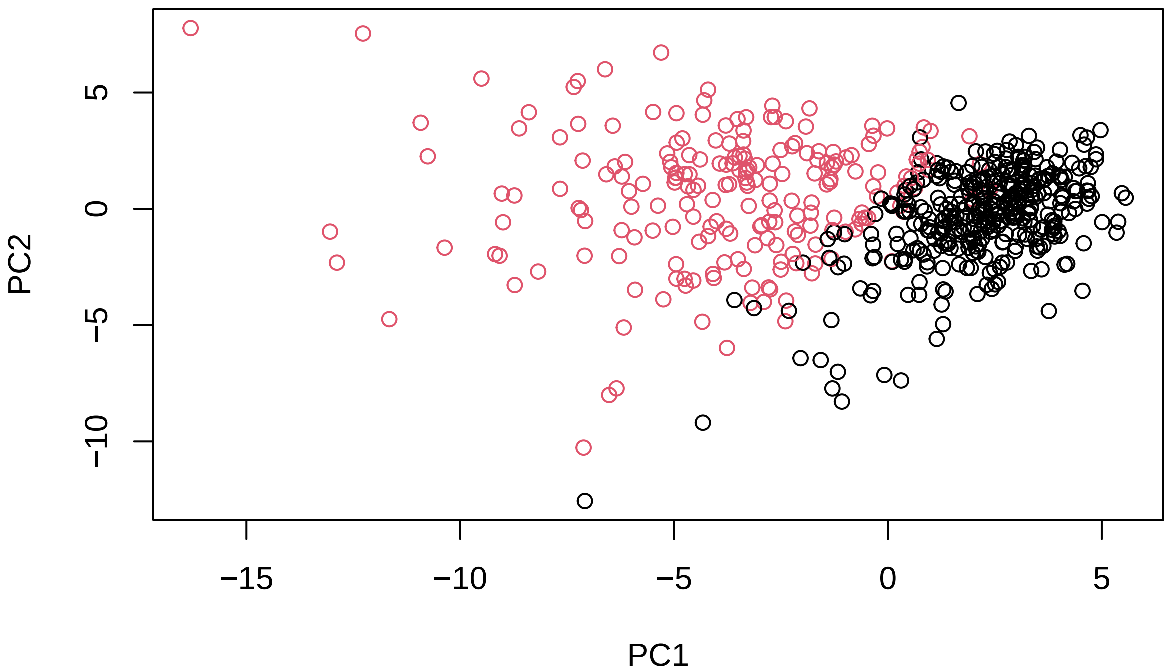
Interpreting PCA Results

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

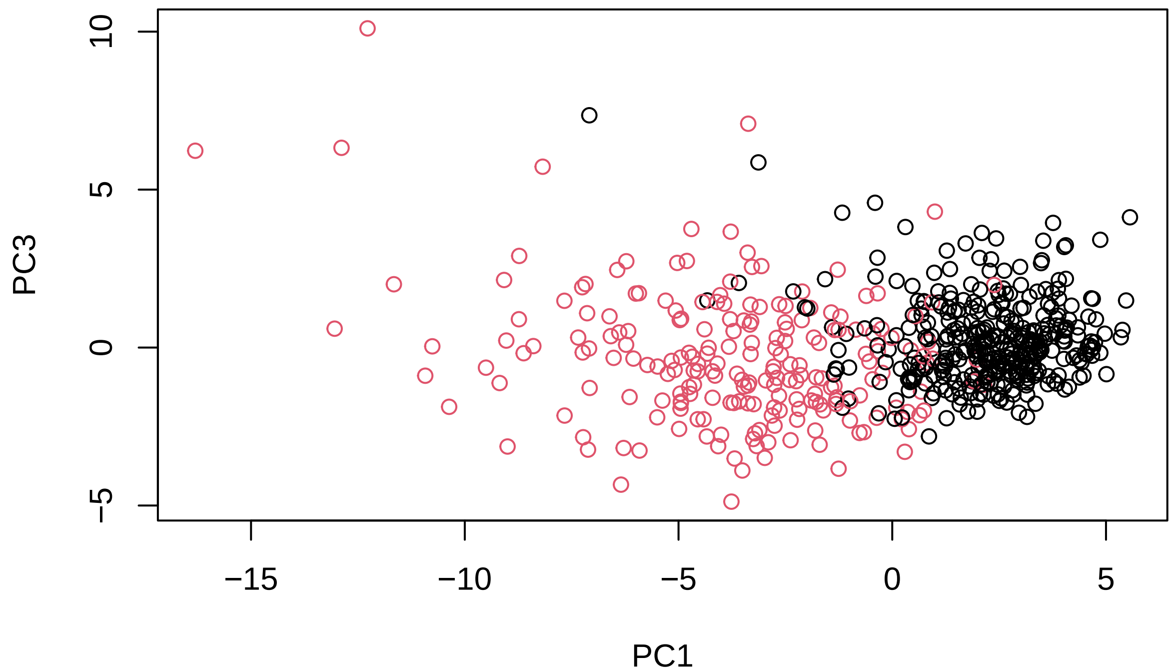


[Q7] What stands out to you about this plot? Is it easy or difficult to understand? Why? This plot is very difficult to read due to the density of the samples and size of the labels.Additionally, it is impossible to tell which labels are being assigned where.

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




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



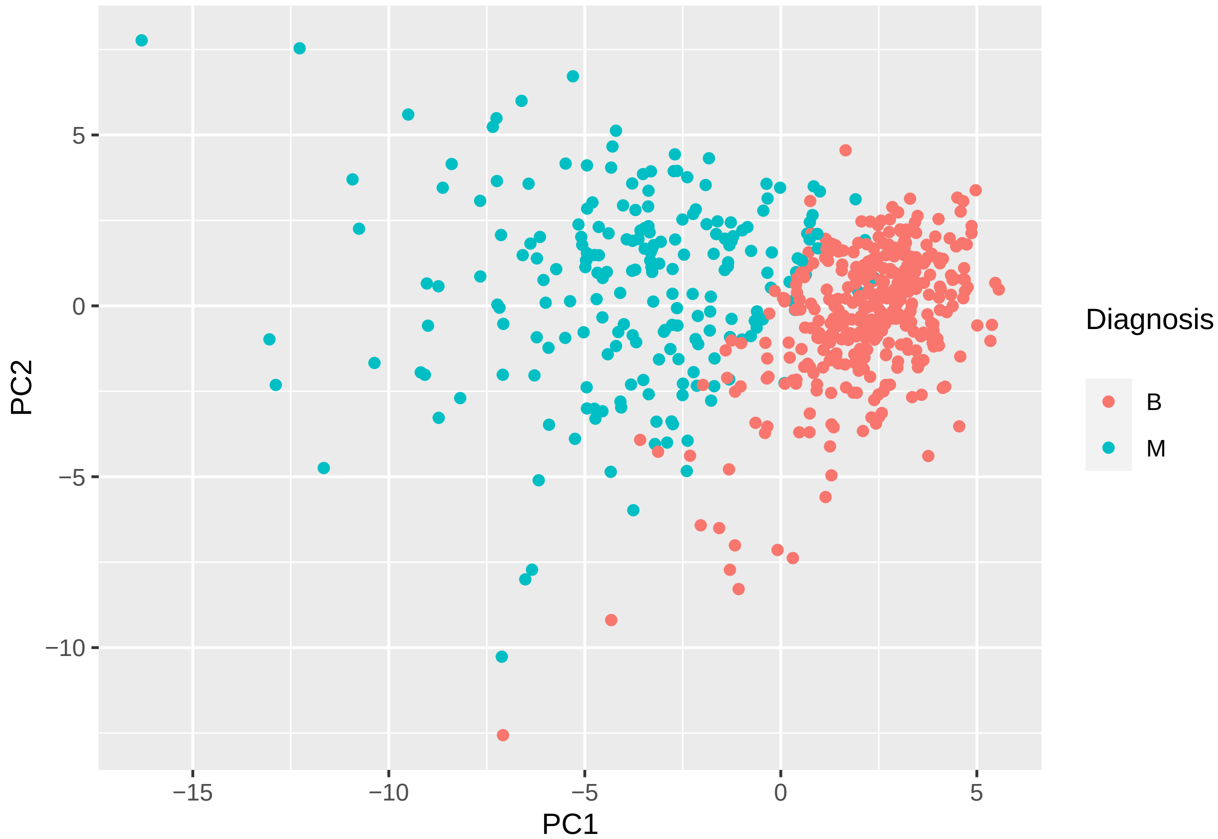
[Q8] Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

The plot comparing components 1 and 2 have less overlapping than the plots comparing 1 and 3. This is because principal component 2 explains more of the variance in the data than principle component 3.

```
# 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 = as.factor(diagnosis)) +
  geom_point() +
  labs(color="Diagnosis\n") +
  scale_color_hue(labels=c("B","M"))
```



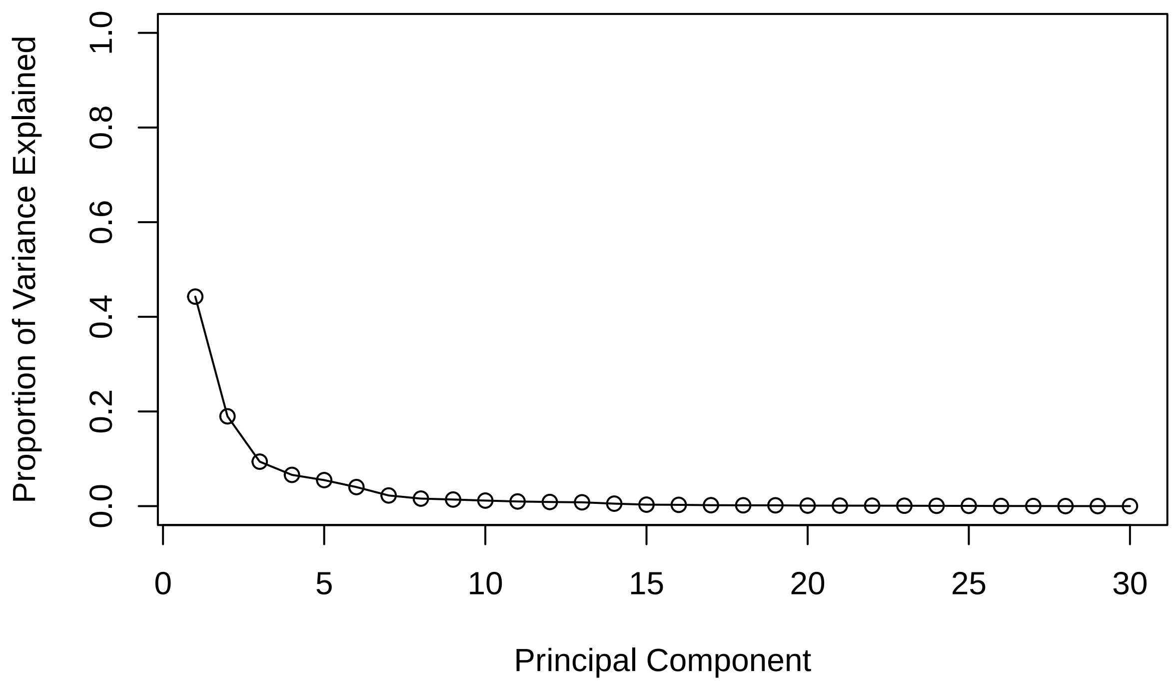
Variance Explained

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

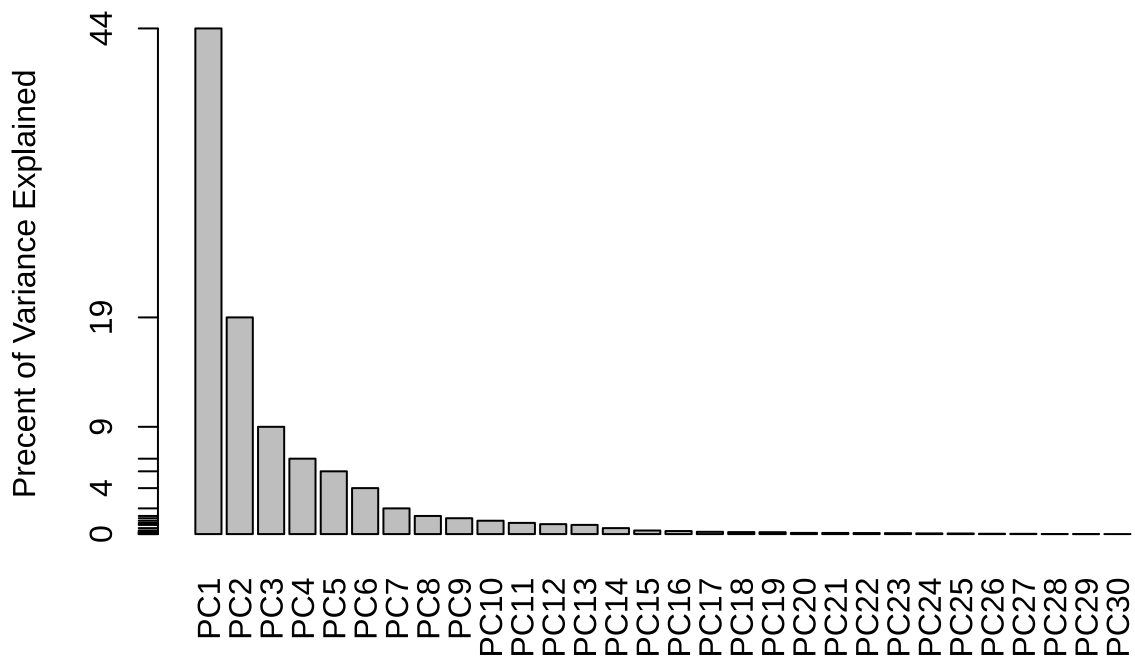
```
## [1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

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



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?

```
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
```

Concave.points_mean is -0.26085376

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

Five principal components is the minimum number required to explain 80% of the variance of the data.

Hierarchical Clustering

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

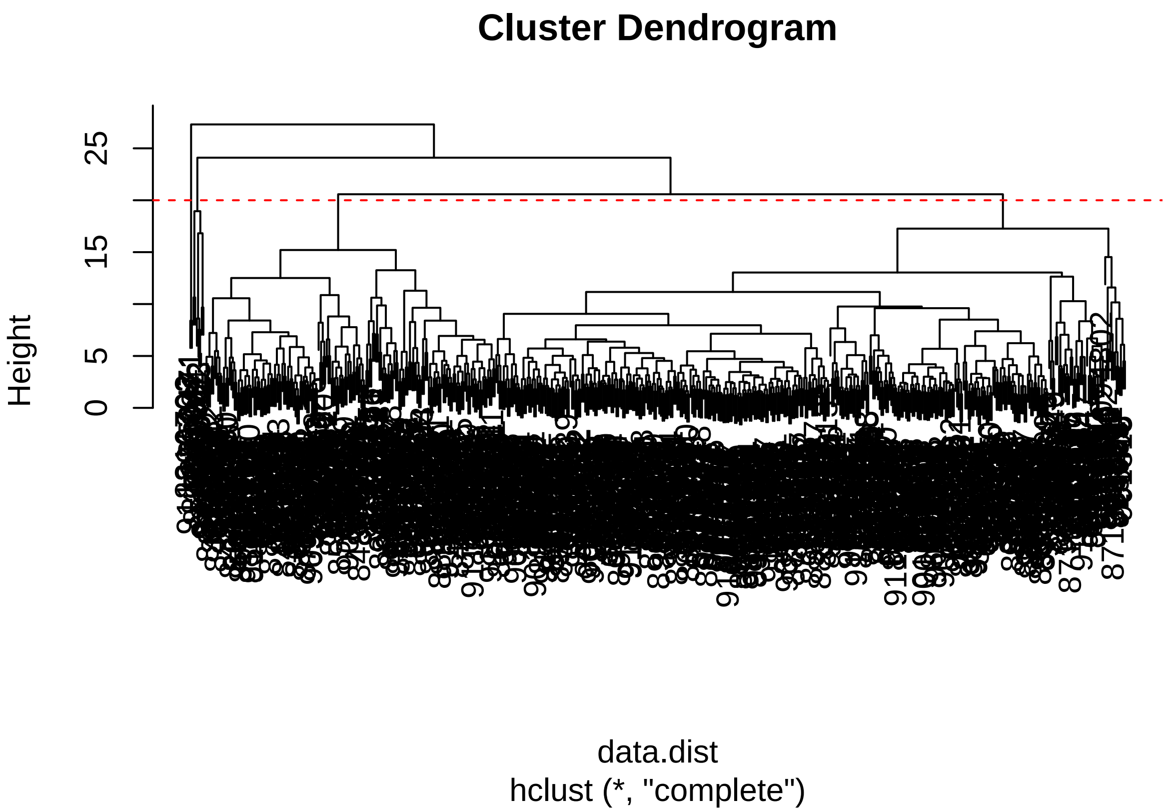
```
# Calculating the euclidean distance
data.dist <- dist(data.scaled, method= 'euclidean')
```

```
# Create a hierarchical clustering model
wisc.hclust <- hclust(data.dist, method = 'complete')
```

Results of Hierarchical Clustering

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

```
plot(wisc.hclust)
abline(h = 20, col="red", lty=2)
```



At height 20 the model has 4 clusters.

Selecting Number of Clusters

```
# Cut tree so that it has 4 clusters: wisc.hclust.clusters
wisc.hclust.clusters <- cutree(wisc.hclust, k = 4)
```

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

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

Exploring different clusters

```
wisc.hclust.clusters2 <- cutree(wisc.hclust, k = 8)
```

```
table(wisc.hclust.clusters2, diagnosis)
```

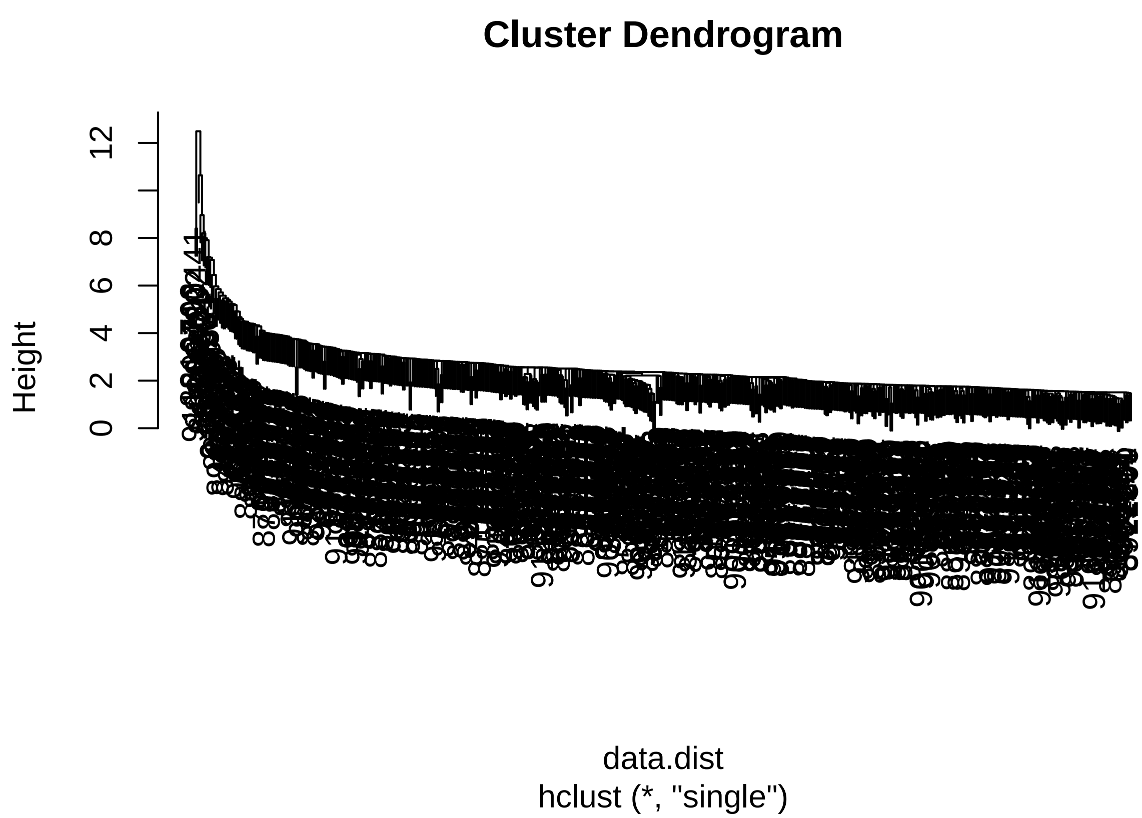
```
##                      diagnosis
```

```
## wisc.hclust.clusters2   0   1
##                      1  12  86
##                      2   0  79
##                      3   0   3
##                      4 331  39
##                      5   2   0
##                      6  12   1
##                      7   0   2
##                      8   0   2
```

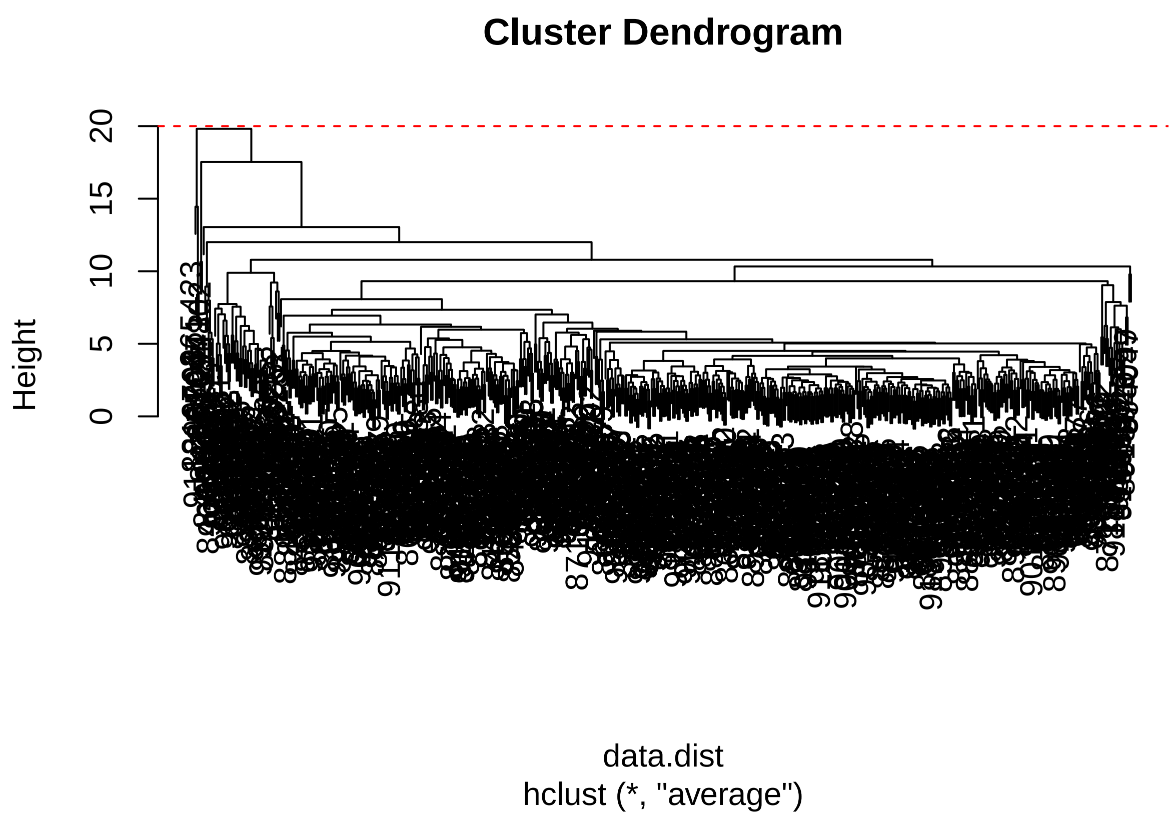
A cluster of 8 further breaks up the malignant diagnosis. Other clusters have little effect on separating the different diagnoses

Using Different Methods

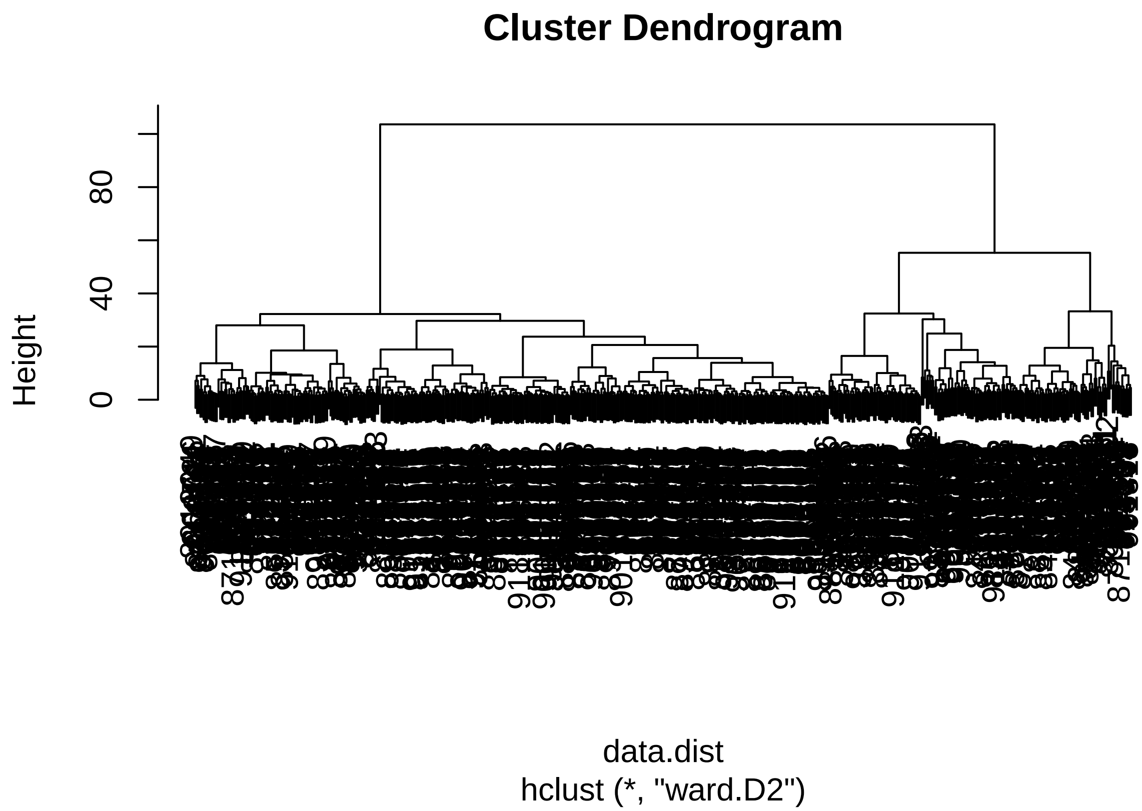
```
wisc.single <- hclust(data.dist, method = 'single')
plot(wisc.single)
abline(h = 20, col="red", lty=2)
```




```
wisc.average <- hclust(data.dist, method = 'average')
plot(wisc.average)
abline(h = 20, col="red", lty=2)
```




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



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

My favorite method for this data set was the 'Complete' method used originally. The dendrogram is most easy and visually pleasing to read, and the clustering is very clear.

Combining Methods

Clustering on PCA Results

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

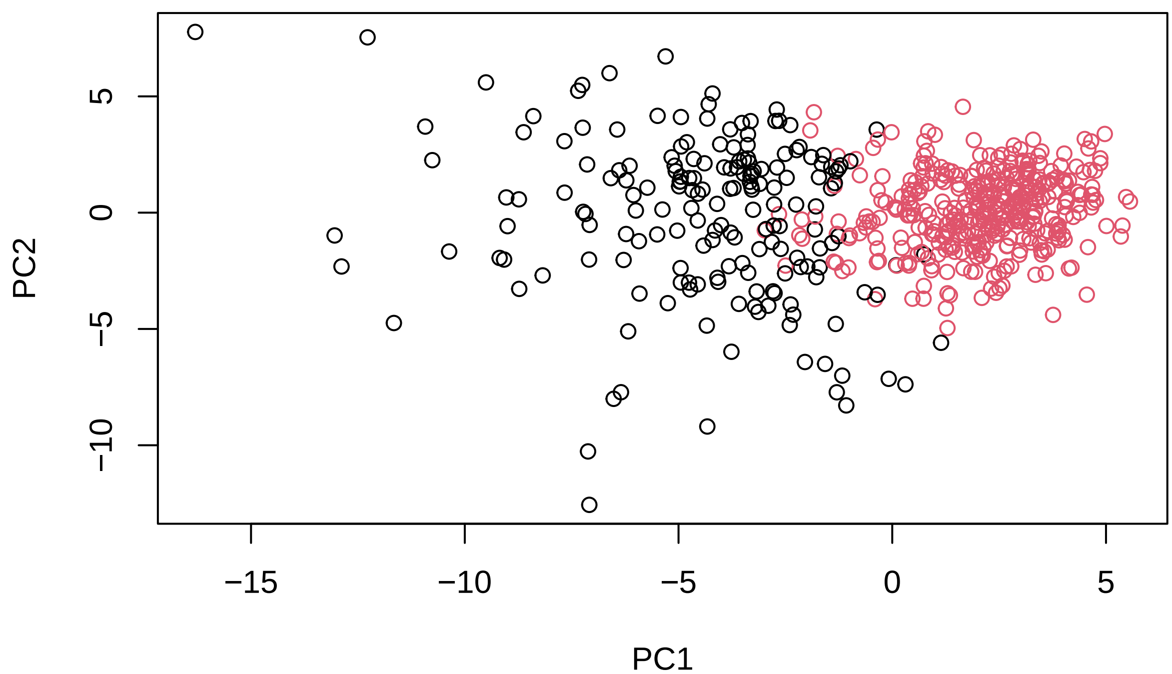
```
## grps
##   1   2
## 184 385
```

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

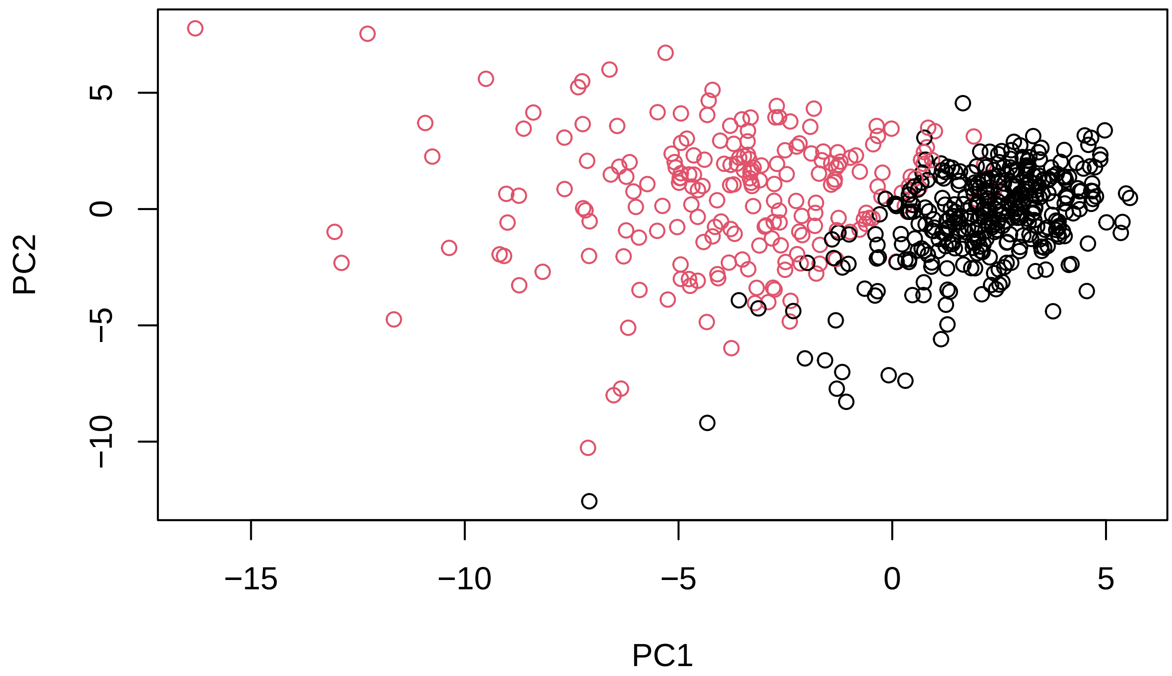
```
##     diagnosis
## grps   0   1
```

```
##     1  20 164
##     2 337  48
```

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




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



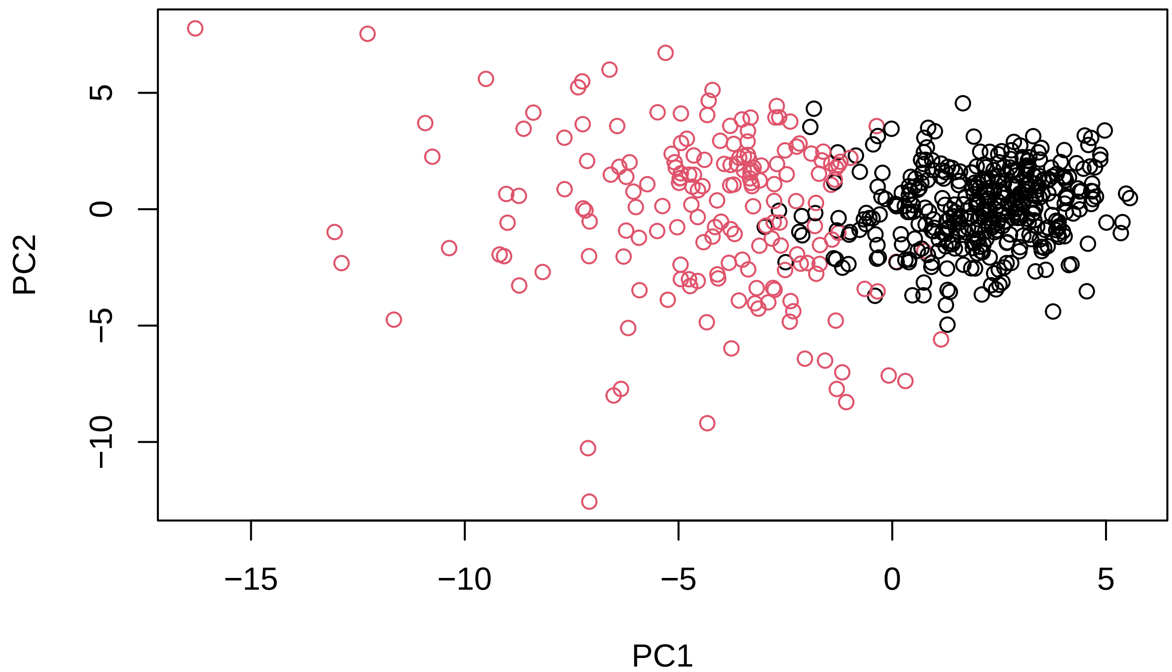

```
g <- as.factor(grps)
levels(g)
```

```
## [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)
```




```
## 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")
```

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

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

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

```
##                          diagnosis
## wisc.pr.hclust.clusters   0   1
##                       1  28 188
##                       2 329  24
```

[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.

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

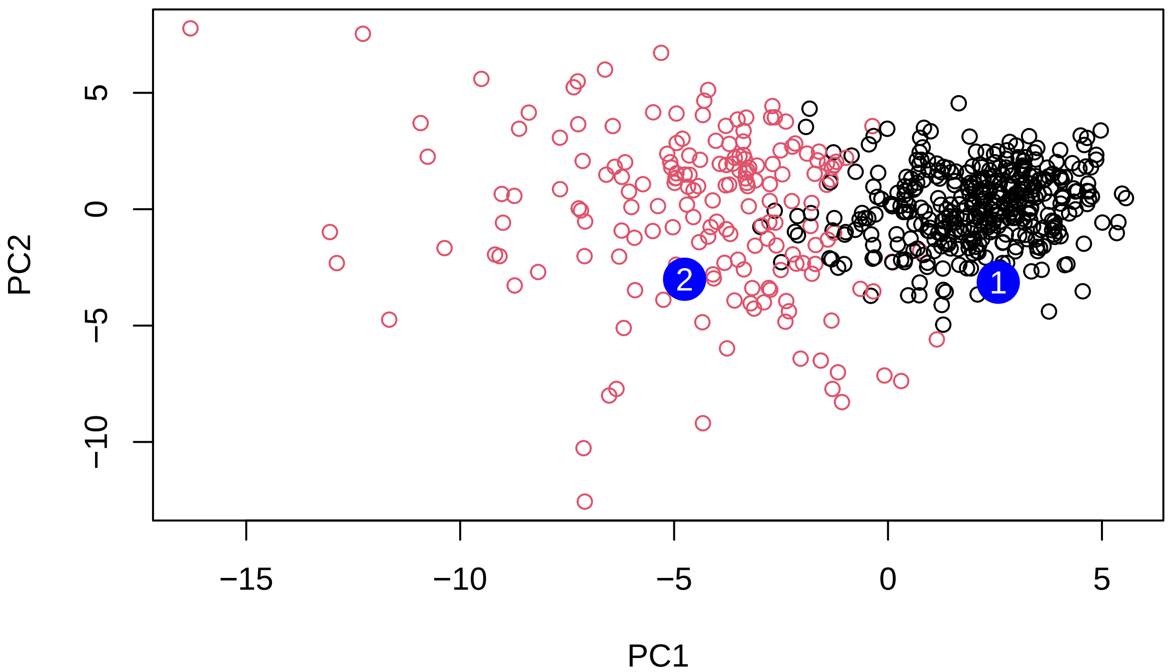
```
##                     diagnosis
## wisc.hclust.clusters   0   1
##                    1  12 165
##                    2   2   5
##                    3 343  40
##                    4   0   2
```

Prediction

```
#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? Patient 2 which has been predicted to have a malignant sample.