class 08 mini project

Lawrence Adhinatha

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In today's mini-project we will explore a complete analysis using the unsupervised learning techniques covered in class (clustering and PCA for now).

The data itself comes from the Wisconsin Breast Cancer Diagnostic data set FNA biopsy data.

Exploratory Data Analysis

Data import

```
wisc.df <- read.csv("WisconsinCancer.csv", 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
```

Remove the diagnosis column and keep it in a separate vector for later.

```
diagnosis <- as.factor(wisc.df[,1])
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
```

Q1. How many observations are in this dataset?

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

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

There are 569 cells observed in this dataset.

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

```
table(diagnosis)
```

```
## diagnosis
##   B   M
## 357 212
```

212 cells have a malignant diagnosis.

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

First find the column names

```
colnames(wisc.data)
```

```
##  [1] "radius_mean"             "texture_mean"
##  [3] "perimeter_mean"          "area_mean"
##  [5] "smoothness_mean"         "compactness_mean"
##  [7] "concavity_mean"          "concave.points_mean"
##  [9] "symmetry_mean"           "fractal_dimension_mean"
## [11] "radius_se"               "texture_se"
## [13] "perimeter_se"            "area_se"
## [15] "smoothness_se"           "compactness_se"
## [17] "concavity_se"            "concave.points_se"
## [19] "symmetry_se"             "fractal_dimension_se"
## [21] "radius_worst"            "texture_worst"
## [23] "perimeter_worst"         "area_worst"
## [25] "smoothness_worst"        "compactness_worst"
## [27] "concavity_worst"         "concave.points_worst"
## [29] "symmetry_worst"          "fractal_dimension_worst"
```

Next, I need to search within the column names for "_mean" pattern The `grep()` function might be of use.

```
length(grep("_mean", colnames(wisc.data)))
```

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

There are 10 features in the data suffixed with _mean.

> Q. How many dimensions are in this dataset?

```
ncol(wisc.data)
```

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

Principal Component Analysis

First, check if the variables are all on the same scale: Do we need to scale the data before performing PCA?

```
round(apply(wisc.data, 2, sd), 3)
```

```
##             radius_mean            texture_mean          perimeter_mean
##                   3.524                   4.301                  24.299
##               area_mean         smoothness_mean        compactness_mean
##                 351.914                   0.014                   0.053
##          concavity_mean     concave.points_mean           symmetry_mean
##                   0.080                   0.039                   0.027
##  fractal_dimension_mean               radius_se              texture_se
##                   0.007                   0.277                   0.552
##            perimeter_se                 area_se           smoothness_se
##                   2.022                  45.491                   0.003
##          compactness_se            concavity_se       concave.points_se
##                   0.018                   0.030                   0.006
##             symmetry_se    fractal_dimension_se            radius_worst
##                   0.008                   0.003                   4.833
##           texture_worst         perimeter_worst              area_worst
##                   6.146                  33.603                 569.357
##        smoothness_worst       compactness_worst         concavity_worst
##                   0.023                   0.157                   0.209
##    concave.points_worst          symmetry_worst fractal_dimension_worst
##                   0.066                   0.062                   0.018
```

Looks like we need to scale.

```
# Perform PCA on wisc.data
wisc.pr <- prcomp(wisc.data, 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 PCs (PC3)

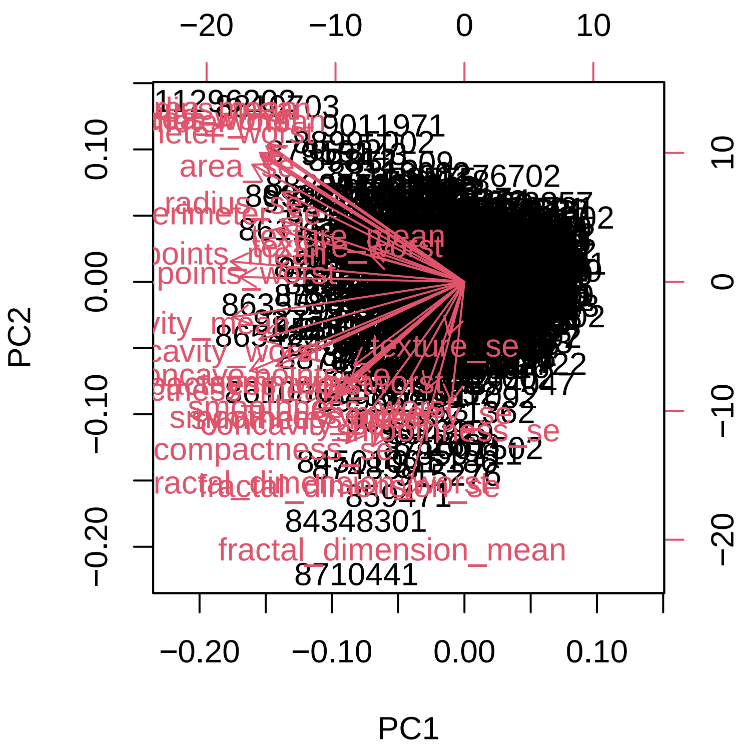
> Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

7 PCs (PC7)

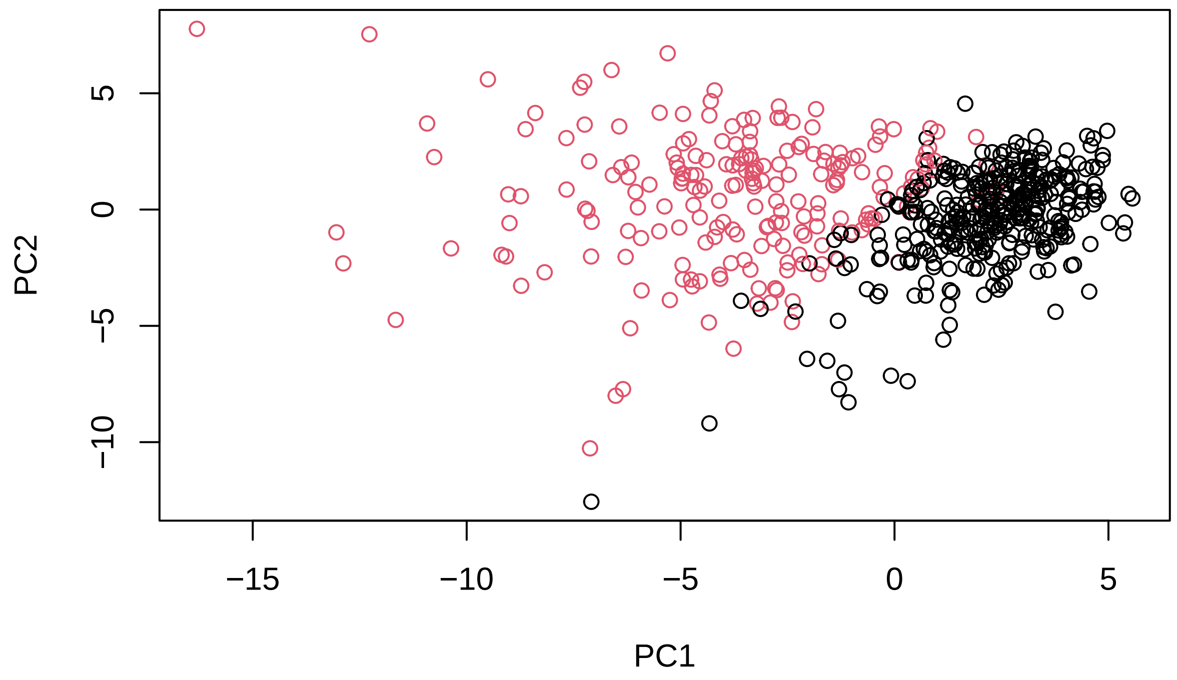
> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

This plot is difficult to understand, as the points are too close together to see any meaningful correlation.

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

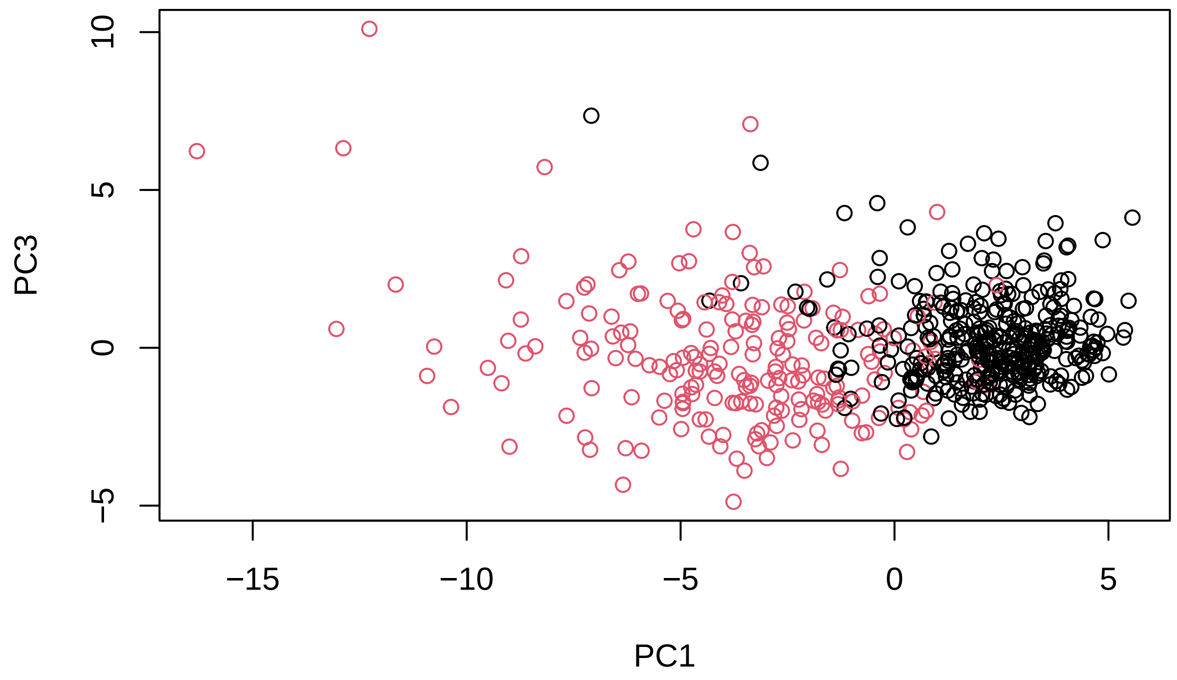


```
# Plot PC2 vs PC1
plot(wisc.pr$x[,1:2], col=diagnosis, xlab="PC1", ylab="PC2")
```



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

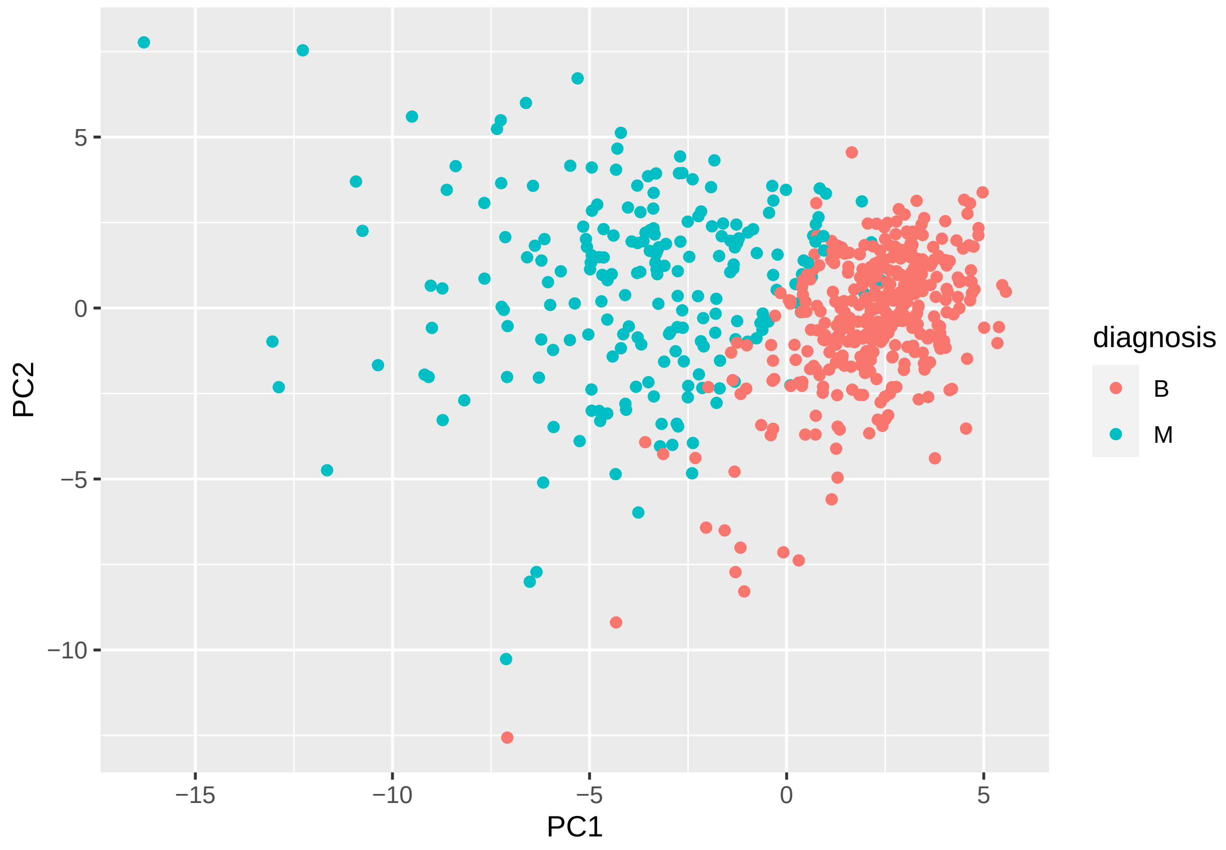
```r
plot(wisc.pr$x[,c(1, 3)], col=diagnosis, xlab="PC1", ylab="PC3")
```



These plots display a distinction between two subgroups. There is a relatively clean separation between Benign and Malignant cell groups in the PC2 vs PC1 plot, while there is a less clean but still visible distinction in the PC3 vs PC1 plot. This is due to the fact that PC2 explains more variance in the data than PC3.

We can also create a plot using ggplot:

```r
library(ggplot2)
wisc.df <- as.data.frame(wisc.pr$x)
ggplot(wisc.df, aes(wisc.pr$x[,1], wisc.pr$x[,2], col=diagnosis)) +
  geom_point() +
  labs(x="PC1", y="PC2")
```



Making scree plots to show how much variance is explained as the PC number increases:

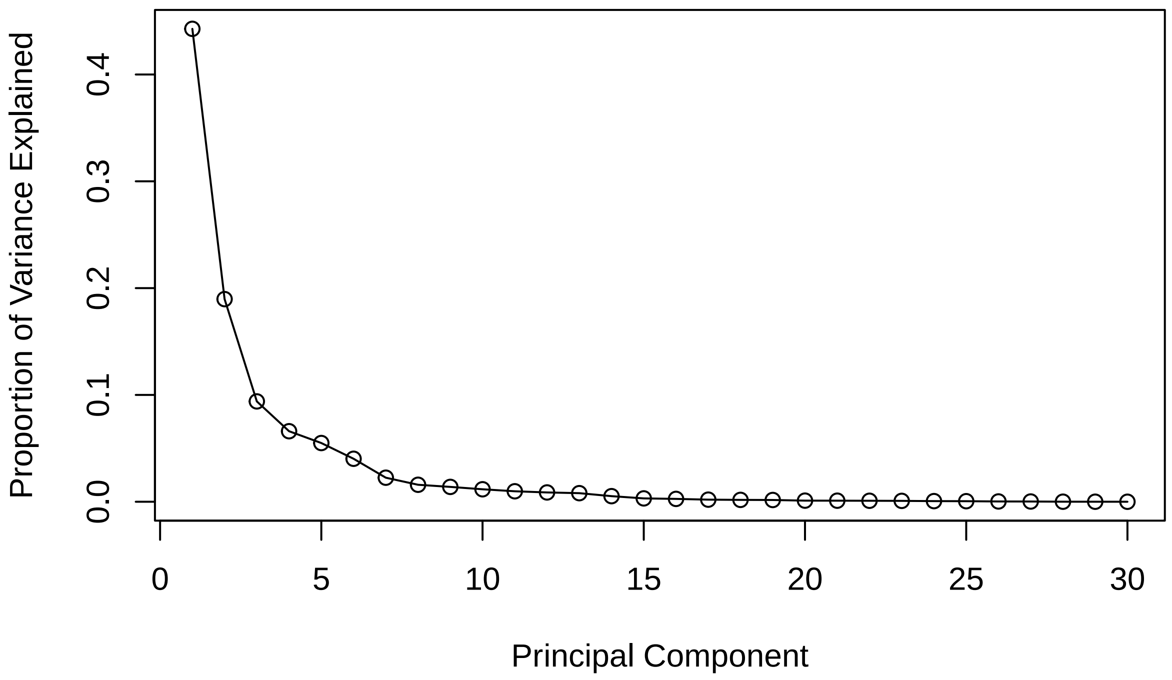
First, store the variance in a variable.

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

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

Next, calculate the variance described by each PC vs that of all PCs.

```
pve <- (wisc.pr$sdev^2)/sum(wisc.pr$sdev^2)
plot(pve,
     xlab="Principal Component", ylab="Proportion of Variance Explained", type="o")
```

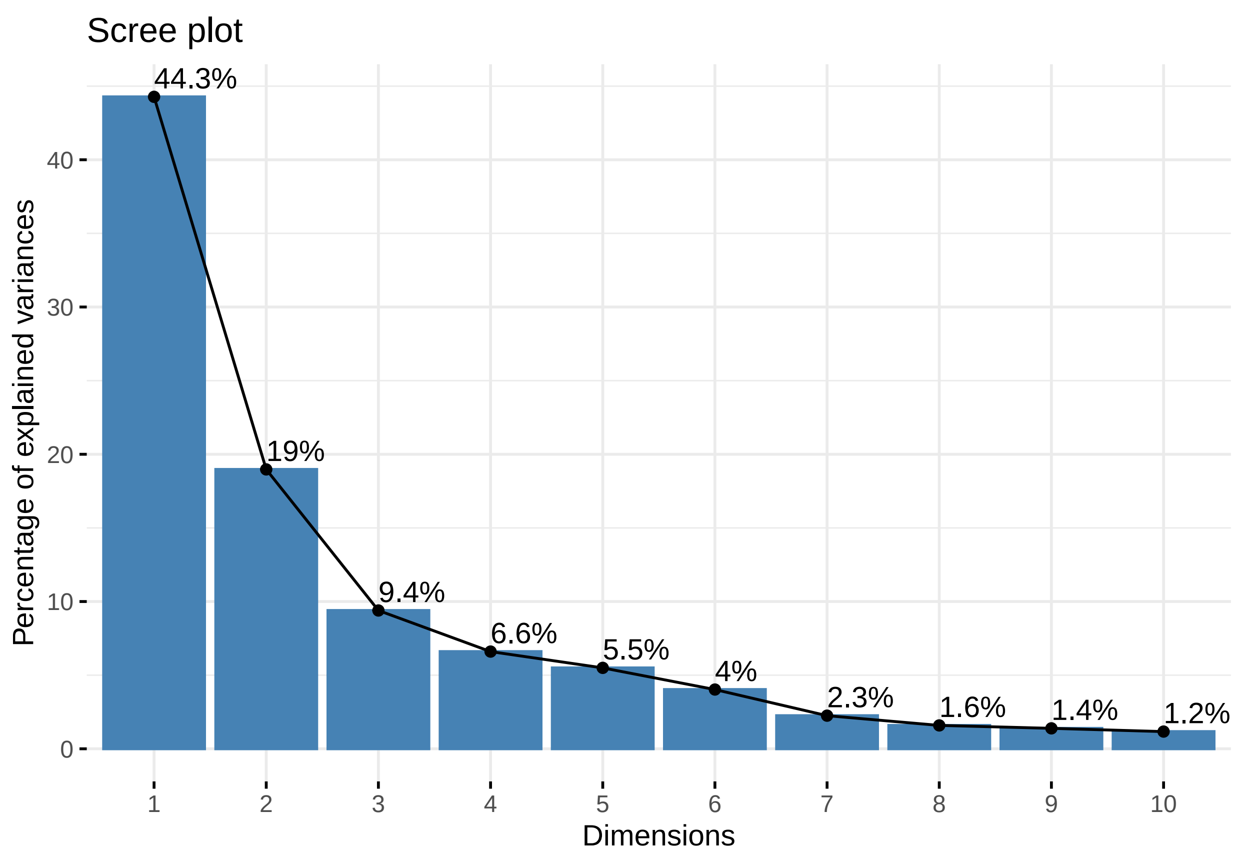


We can also use a barplot to represent this variance; this time we'll use the CRAN package factoextra.

```
library(factoextra)
```

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

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



Examine the PC loadings

How much do the original variables contribute ot the new PCs that we have calculated? to get at the is at we can look at the `$rotation` componentn of the returned PCA object.

```
head(wisc.pr$rotation[,1:3])
```

```
##                          PC1         PC2          PC3
## radius_mean      -0.2189024  0.23385713 -0.008531243
## texture_mean     -0.1037246  0.05970609  0.064549903
## perimeter_mean   -0.2275373  0.21518136 -0.009314220
## area_mean        -0.2209950  0.23107671  0.028699526
## smoothness_mean  -0.1425897 -0.18611302 -0.104291904
## compactness_mean -0.2392854 -0.15189161 -0.074091571
```

Focus in on PC1

```
head(wisc.pr$rotation[,1])
```

```
##      radius_mean     texture_mean   perimeter_mean        area_mean 
##       -0.2189024       -0.1037246       -0.2275373       -0.2209950 
##  smoothness_mean compactness_mean 
##       -0.1425897       -0.2392854
```

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?

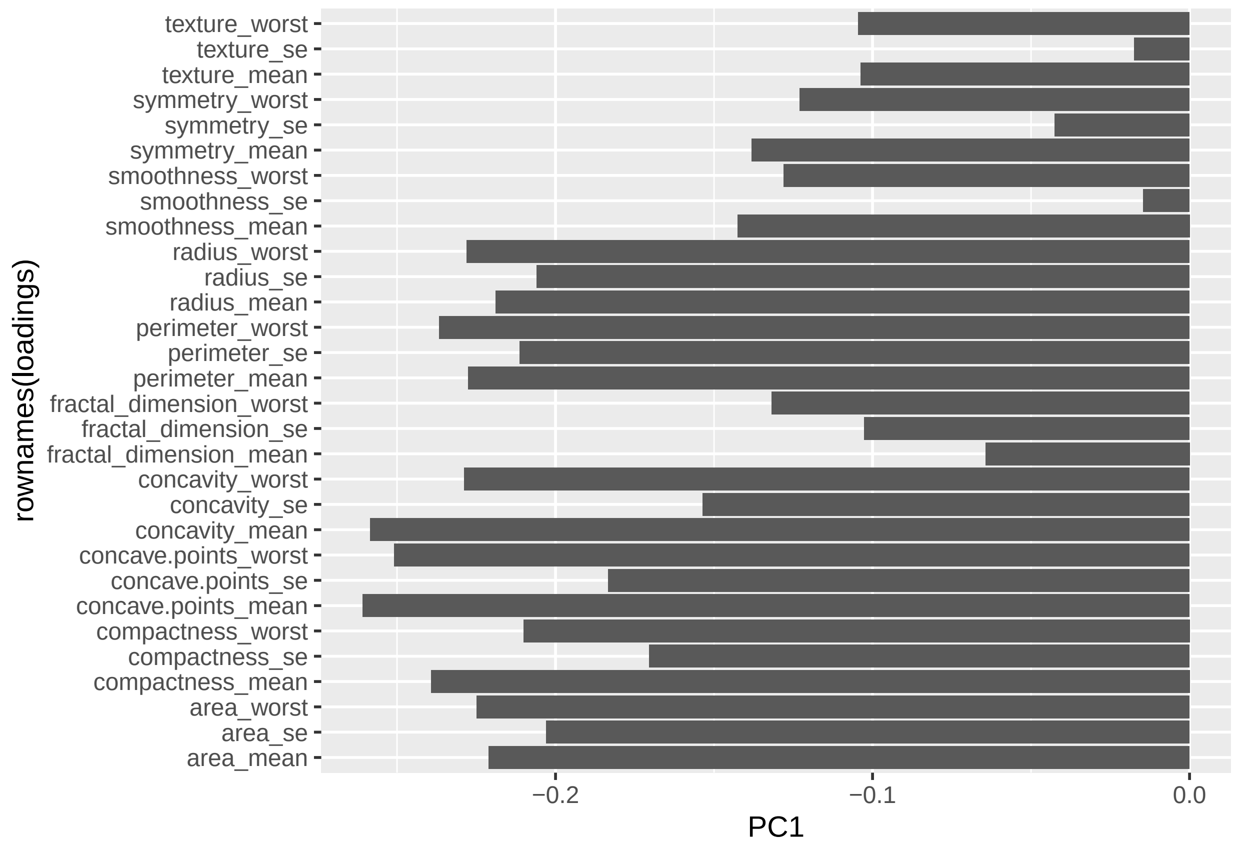
```
wisc.pr$rotation["concave.points_mean",1]
```

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

There is a complicated mix of variables that go together to make up PC1 (i.e. there are many of the original variables that together contribute highly to PC1).

```
loadings <- as.data.frame(wisc.pr$rotation)

ggplot(loadings) +
  aes(PC1, rownames(loadings)) +
  geom_col()
```



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

```
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
```

5 PCs (PC5)

Hierarchical Clustering

Scale the data

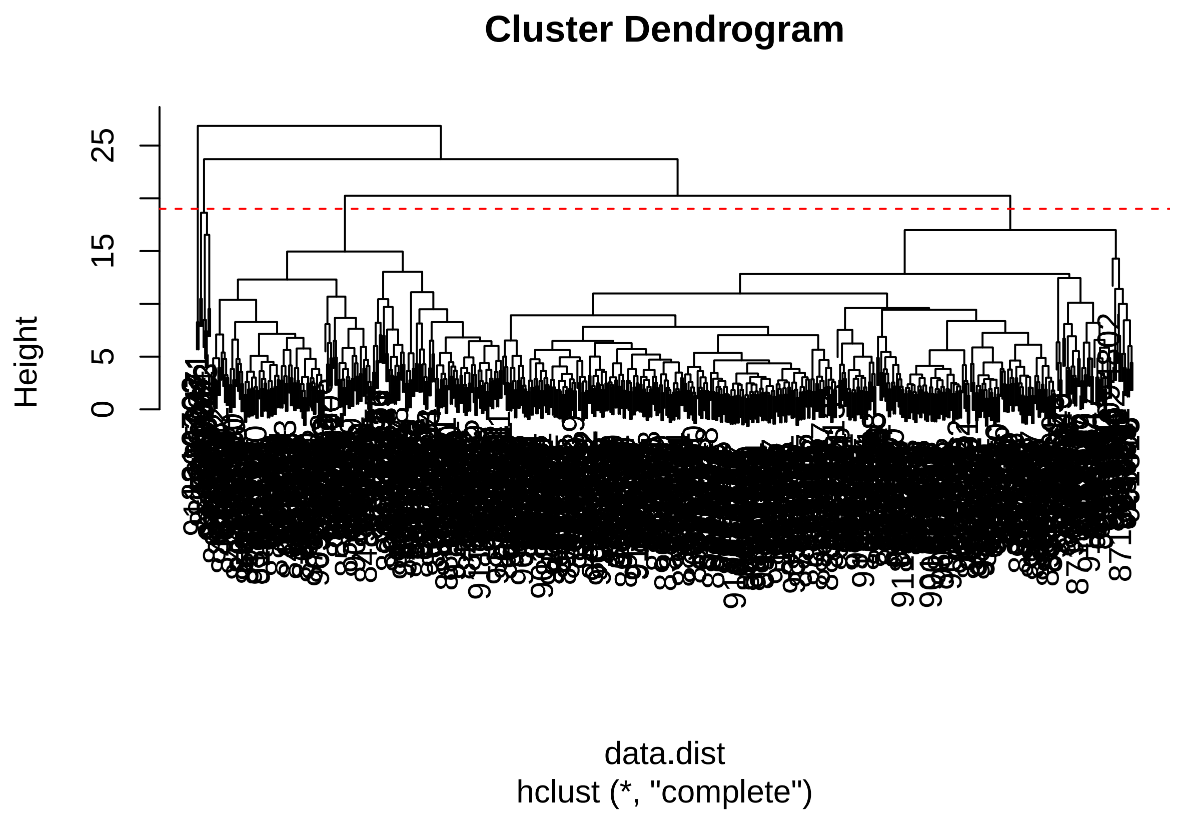
```
data.scaled <- scale(wisc.data)
```

Calculate Euclidean distances between all pairs of observations

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

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

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



A height of 19 yields 4 clusters for the model.

Cut this tree to yield cluster membership vector using `cutree()` function.

```
wisc.hclust.clusters <- cutree(wisc.hclust, h=19)
table(wisc.hclust.clusters)
```

```
## wisc.hclust.clusters
##   1   2   3   4
## 177   7 383   2
```

```
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?

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

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

The best cluster vs diagnosis match is at k=4 clusters, as it is the lowest number of groupings necessary to separate the benign and malignant groups accurately enough, before the increase in accuracy tapers off as the value of `k` increases.

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

```
methods <- function(x) {
  table(cutree(hclust(data.dist, method=x), k=4), diagnosis)
}

methods("single")
```

```
##    diagnosis
##       B   M
##   1 356 209
##   2   1   0
##   3   0   2
##   4   0   1
```

```
methods("complete")
```

```
##    diagnosis
##       B   M
##   1  12 165
##   2   2   5
##   3 343  40
##   4   0   2
```

```
methods("average")
```

```
##    diagnosis
##       B   M
##   1 355 209
##   2   2   0
##   3   0   1
##   4   0   2
```

```
methods("ward.D2")
```

```
##    diagnosis
##       B   M
##   1   0 115
##   2   6  48
##   3 337  48
##   4  14   1
```

method="complete" and method="ward.D2" give my favorite results. "ward.D2" generally separates B and M into two groups, with some overlap and increased clustering in other groups; "complete" in this case is the best method, since it keeps clustering mostly within two groups, 1 and 3, and separates B and M about as well as "ward.D2". In contrast, "single" and "average" both leave nearly all the data points in one group, failing to separate the diagnoses at all.

K-means clustering

```
wisc.km <- kmeans(data.scaled, centers=2, nstart=50)
table(wisc.km$cluster, diagnosis)
```

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

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

K-means does a good job of separating the two diagnoses, producing very similar results to the hclust results. There is a consistently high amount of false positives and a lower amount of false negatives in both models.

Comparing clusters using k-means model with clusters using hierarchical clustering model:

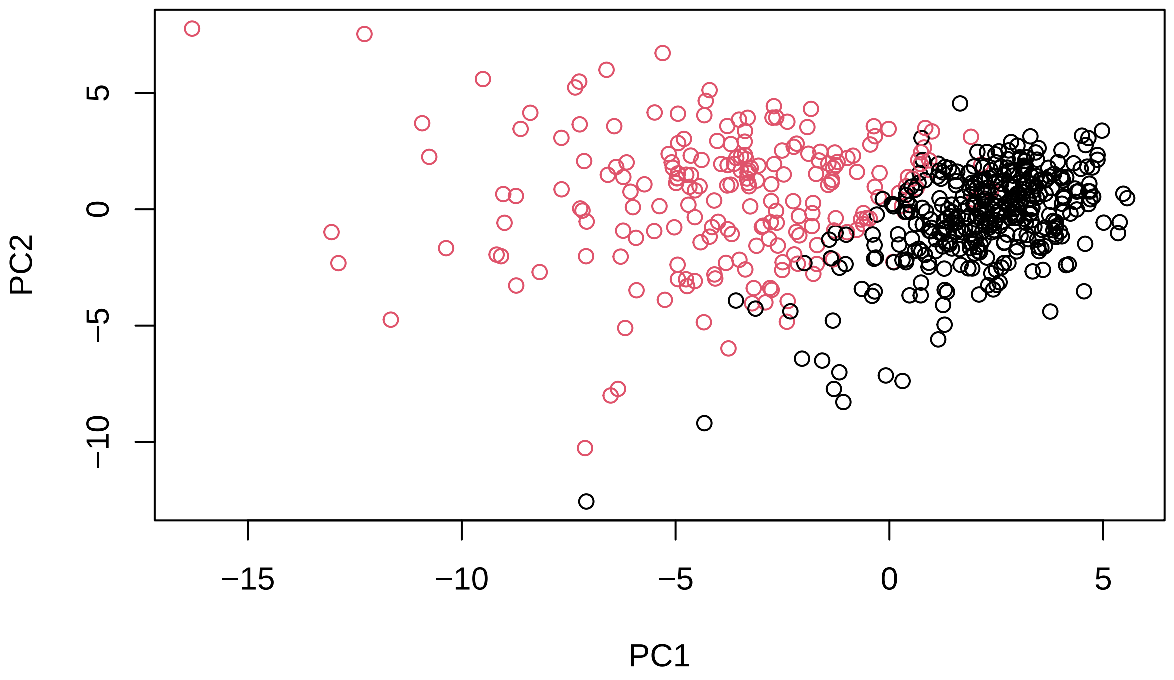
```
table(wisc.hclust.clusters, diagnosis)
```

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

Combine methods: PCA and HCLUST

My PCA results were interesting as they showed a separation of M and B samples along PC1.

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



I want to cluster my PCA results - that is use `wisc.pr$x` as input to `hclust`.

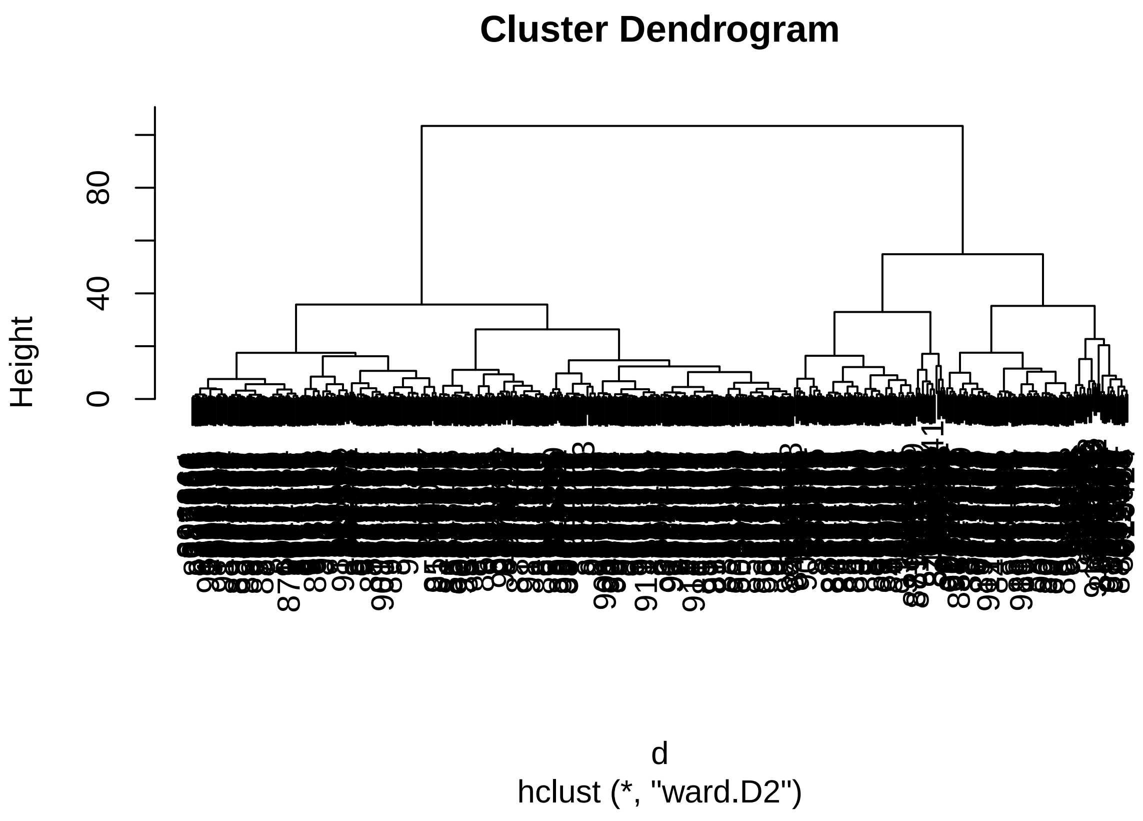
Try clustering in 3 PCs, that is PC1, PC2, PC3 as input

```
d <- dist(wisc.pr$x[,1:3])

wisc.pr.hclust <- hclust(d, method="ward.D2")
```

Tree result figure:

```
plot(wisc.pr.hclust)
```

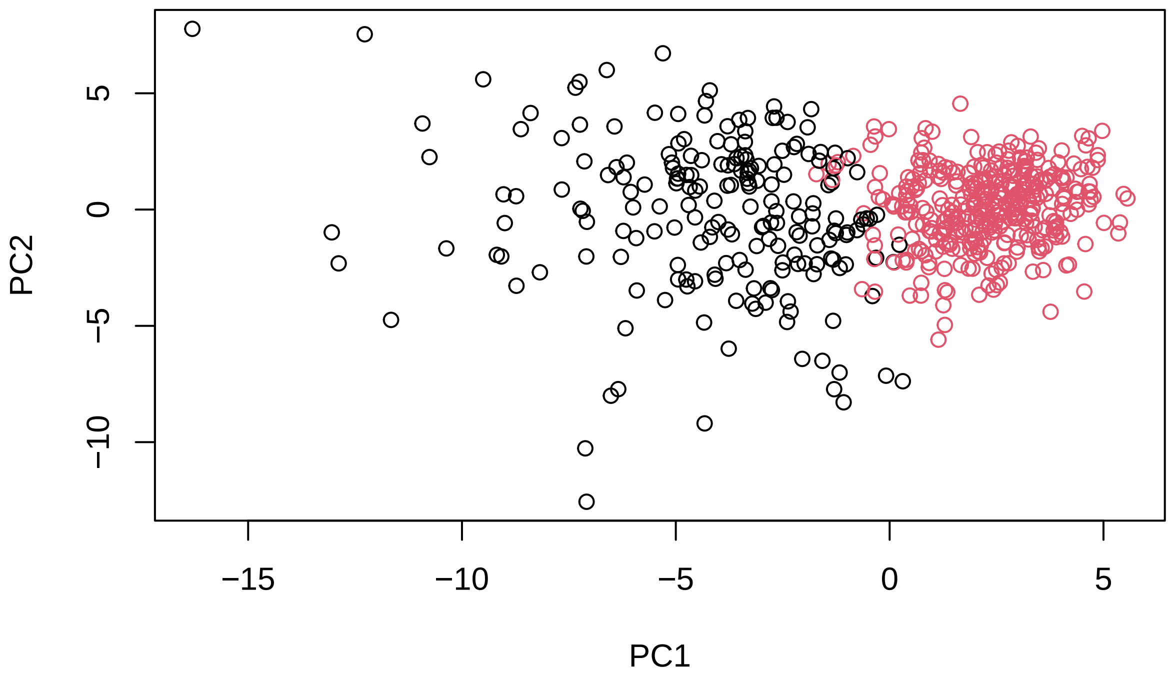


Let’s cut this tree into two groups/clusters

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

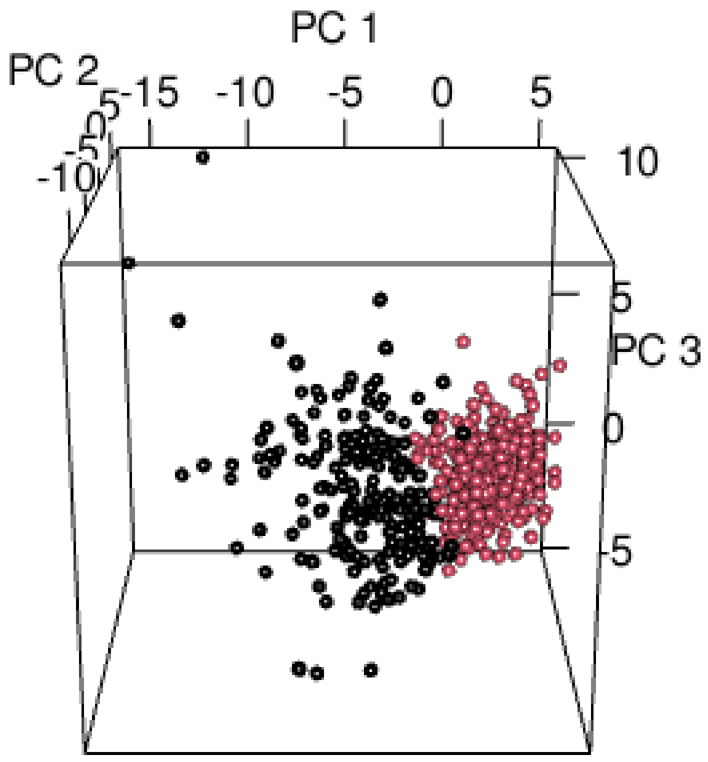
```
## wisc.hclust.clusters
##   1   2
## 203 366
```

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



```
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=wisc.hclu
rglwidget(width = 400, height = 400)
```

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



How well do the two clusters separate the M and B diagnosis?

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

```
##                     diagnosis
## wisc.hclust.clusters   B   M
##                    1  24 179
##                    2 333  33
```

Calculate the accuracy of our results

```
(179+333)/nrow(wisc.data)
```

```
## [1] 0.8998243
```

Nearly 90% of our results are accurate. However, a 10% false positive could potentially be dangerous to patients.

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

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

```
##                            diagnosis
## wisc.pr.hclust.clusters.4   B   M
##                         1   0 111
##                         2  24  68
##                         3 184  32
##                         4 149   1
```

With four clusters, this new model produces a group with too much of each diagnosis to be as useful as with 2 clusters.

> Q16. How well do the k-means and hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.km$cluster and wisc.hclust.clusters) with the vector containing the actual diagnoses.

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

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

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

```
##                            diagnosis
## wisc.pr.hclust.clusters.2   B   M
##                         1  24 179
##                         2 333  33
```

The k-means and hierarchical clustering combination separated the diagnoses with similar accuracy as the PCA clustering model.

Sensitivity and specificity

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

```r
# function for sensitivity and specificity calculations
sens.spec <- function(tp, fn, tn, fp) {
  sens <- tp/(tp+fn)
  spec <- tn/(tn+fp)
  results <- c(sens, spec)
  names(results) <- c("Sensitivity", "Specificity")
  results
}
```

```
# results for each method
## table(wisc.hclust.clusters, diagnosis)
hclust <- sens.spec(165, 12, 343, 40)

## table(wisc.km$cluster, diagnosis)
kmeans <- sens.spec(175, 14, 343, 37)

## table(wisc.pr.hclust.clusters.2, diagnosis)
pca <- sens.spec(179, 24, 333, 33)

# data frame of all method results
sens.spec.df <- data.frame(hclust, kmeans, pca)
sens.spec.df
```

```
##                hclust    kmeans       pca
## Sensitivity 0.9322034 0.9259259 0.8817734
## Specificity 0.8955614 0.9026316 0.9098361
```

```
# calculate colnames of max sensitivity and max specificity
sens.spec.df$max <- colnames(sens.spec.df)[apply(sens.spec.df, 1, which.max)]
best <- sens.spec.df$max
names(best) <- c("Best Sensitivity", "Best Specificity")
best
```

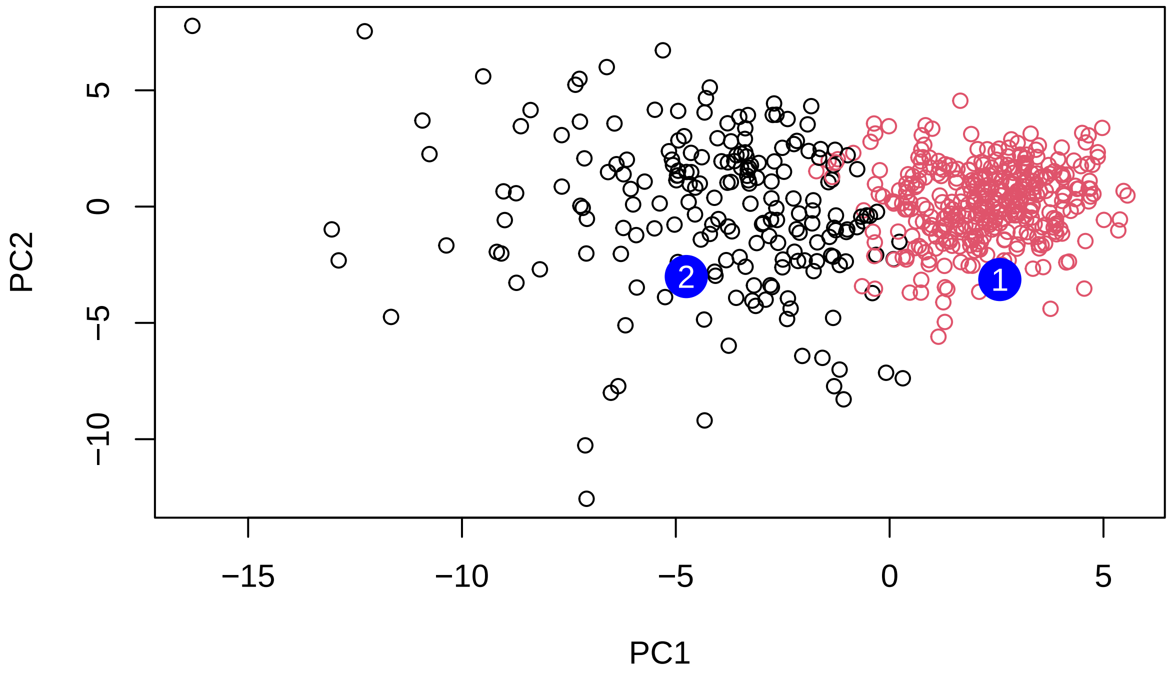
```
## Best Sensitivity Best Specificity
##         "hclust"            "pca"
```

Prediction

```
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=wisc.hclust.clusters)
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?

We should prioritize patient 2, as their cell data seem to correspond to the PCA group denoting a malignant diagnosis.