Class08 - PCA Mini Project

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Today we will do a complete analysis of some breast cancer biopsy data. First, let's revisit the main PCA finction 'prcomp()' and see what 'scale=TRUE/FALSE' does.

```
head(mtcars)
```

```
                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

Find the mean value per column.

```
apply(mtcars, 2, sd)
```

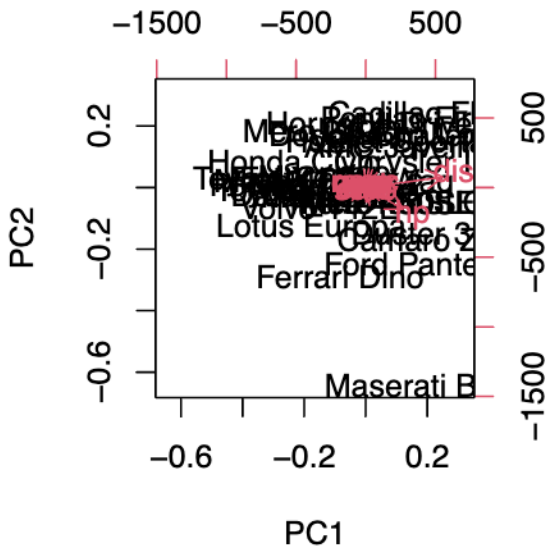
```
       mpg        cyl       disp         hp       drat         wt 
 6.0269481  1.7859216 123.9386938 68.5628685  0.5346787  0.9784574 
      qsec         vs         am       gear       carb 
 1.7869432  0.5040161  0.4989909  0.7378041  1.6152000 
```

```
#2 refers to columns
```

It's clear that displacement (disp) and horsepower (hp) have the highest mean values and highest standard deviations. They will likley dominate any analysis I do on this dataset.

```
pc.noscale <- prcomp(mtcars)
pc.scale <- prcomp (mtcars, scale=TRUE)
```

```
biplot(pc.noscale)
```

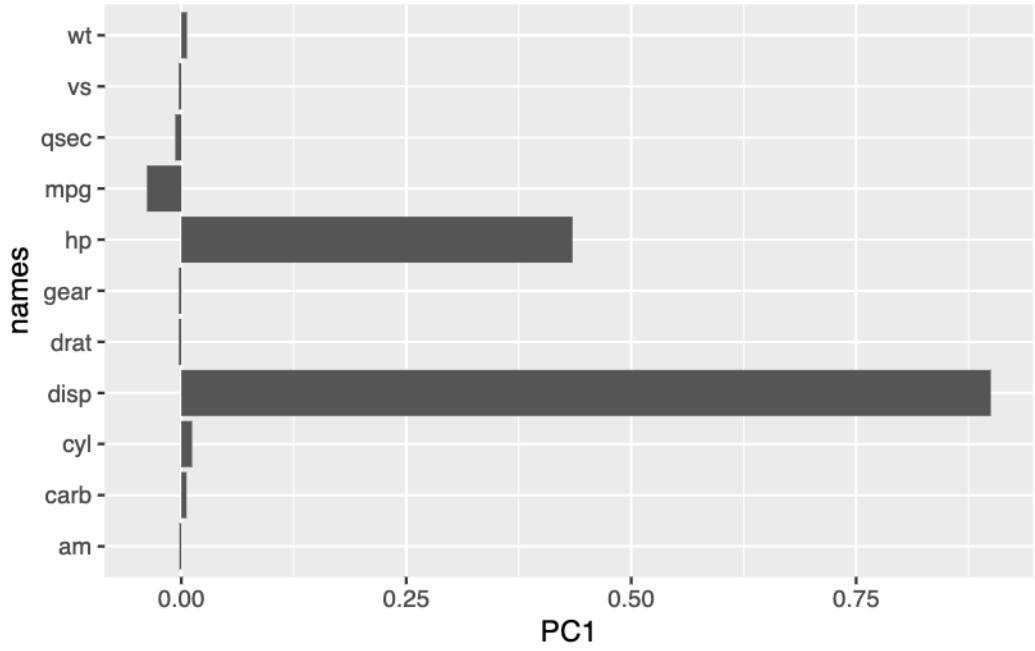



```
pc.noscale$rotation [,1]
```

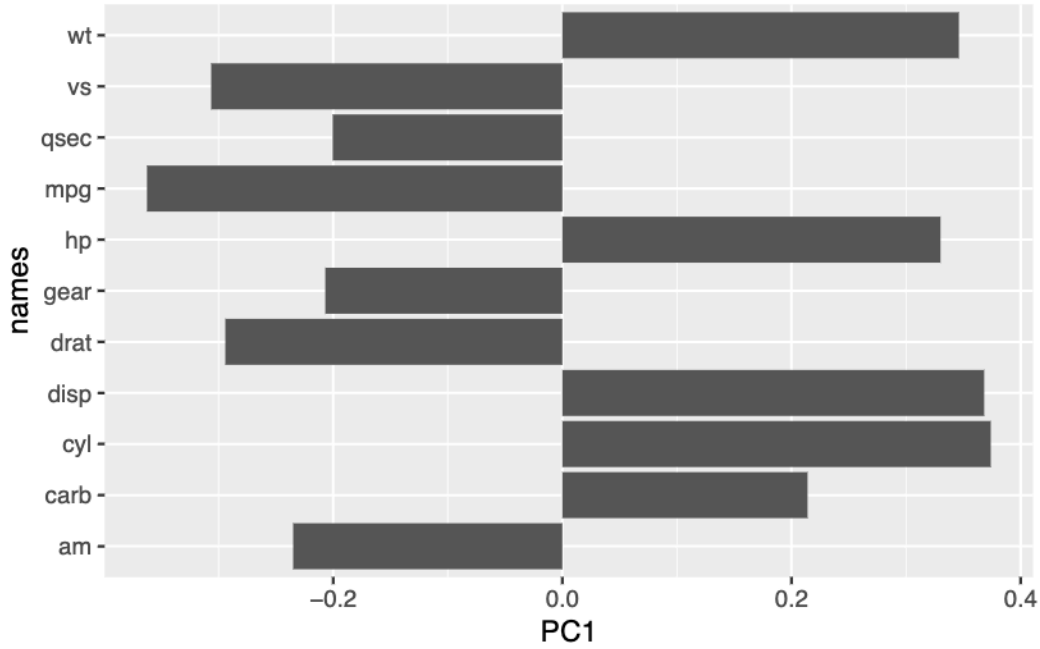
```
         mpg          cyl         disp           hp         drat           wt
-0.038118199  0.012035150  0.899568146  0.434784387 -0.002660077  0.006239405
        qsec           vs           am         gear         carb
-0.006671270 -0.002729474 -0.001962644 -0.002604768  0.005766010
```

Plot the loadings

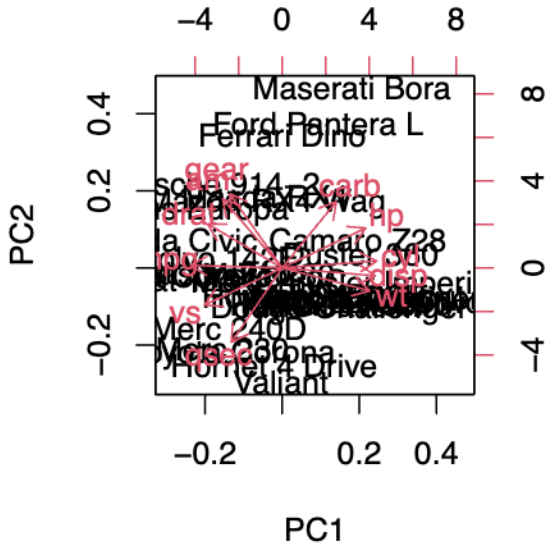
```
library(ggplot2)

r1<- as.data.frame(pc.noscale$rotation)
r1$names <- row.names (pc.noscale$rotation)

ggplot (r1) +
  aes(PC1, names) +
  geom_col()
```




```
r2<- as.data.frame(pc.scale$rotation)
r2$names <- row.names (pc.scale$rotation)

ggplot (r2) +
  aes(PC1, names) +
  geom_col()
```




```
biplot(pc.scale)
```



Take-home: Generally, you always want to set `scale=TRUE` when we do this type

of analysis to avoid having our analysis be dominated by individual variables with the largest variance due to their unit of measurment.

FNA breast cancer data

Load the data into R, save data to same folder for it to be able to read.

```
fna.data <- "WisconsinCancer.csv"

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
```

Q1. How many observations are in this dataset?

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

```
[1] 569
```

```
#how many people are being measured?
```

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

```
wisc.df$diagnosis == "M" -> 'is this values equal to M, returns TF'
sum (wisc.df$diagnosis == "M")
```

```
[1] 212
```

The `table()` function is quicker and easier

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

```
  B   M
357 212
```

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

```
ncol(wisc.df)
```

```
[1] 31
```

```
colnames(wisc.df)
```

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

A useful function for this is `grep()`

```
grep ("_mean", colnames(wisc.df))
```

```
 [1]  2  3  4  5  6  7  8  9 10 11
```

```
#If you use sum, it will add the values of the numerical column outputs

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

```
[1] 10
```

Before we go any further we need to exclude the diagnosis column from future analysis as to not bias our predictions. Diagnosis give the 'answer', benign versus malignant.

```
#Store this data separately so we don't lose it
diagnosis <- as.factor(wisc.df$diagnosis)
#Store as a factor because the variable has multiple factors
head(diagnosis)
```

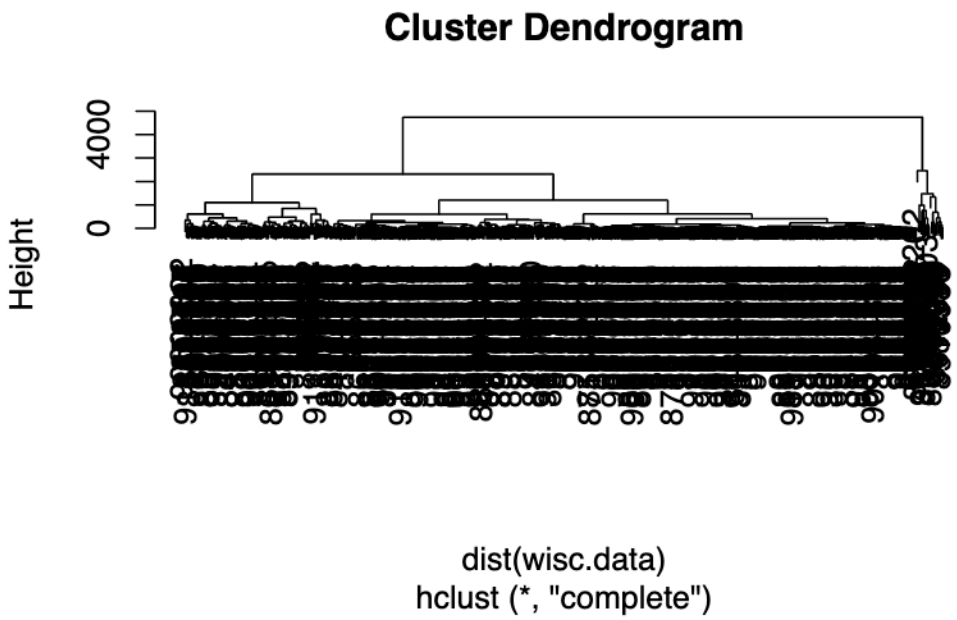
```
[1] M M M M M M
Levels: B M
```

Create data minus diagnosis

```
wisc.data <- wisc.df[, -1]
```

Let's see if we can cluster the 'wisc.data' to find some structure in the dataset.

```
hc <- hclust(dist(wisc.data))
plot(hc)
```



Principal Component Analysis (PCA)

Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)? 44% is captured in PC1, which is significantly higher than the other PCs.

Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data? Three - could be a combination of PC1 (44%), PC2 (19%), and PC3 (9%).

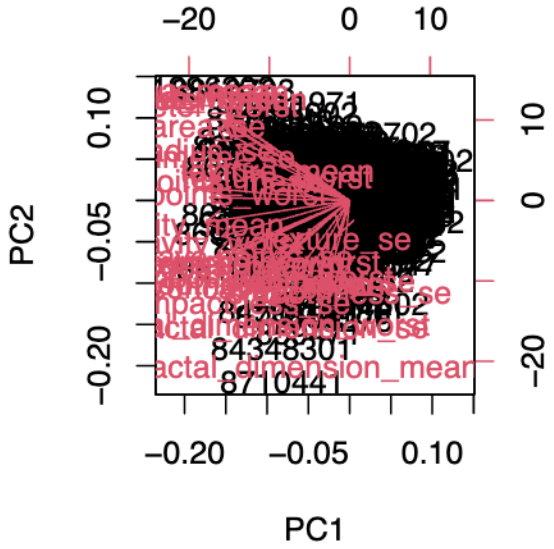
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data? You would need to incorporate 7 PCs.

```
wisc.pr <- prcomp (wisc.data, scale=T)
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
```

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



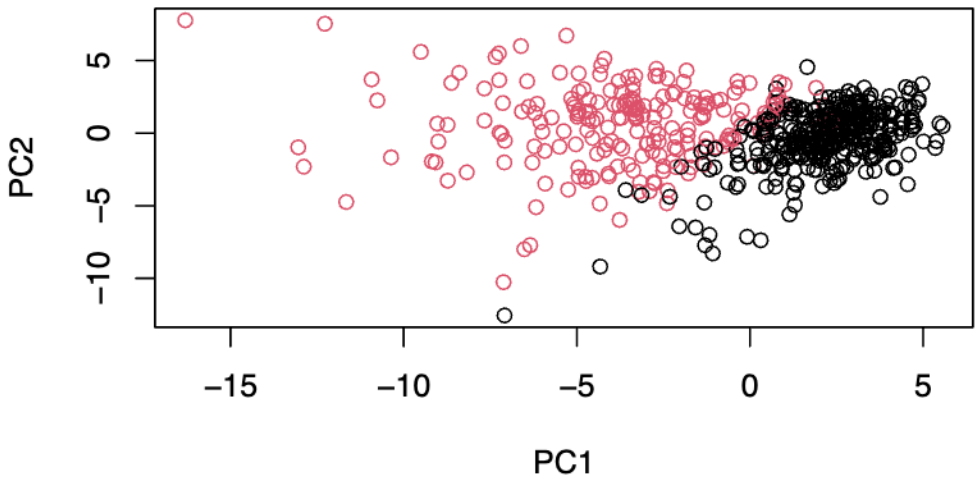
Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why? This plot has far too much information to interpret. I noticed that all the values seem to clump in a circle.

This biplot suck. We need to build our own PCA score plot of PC1 v PC2.

```
attributes(wisc.pr)
```

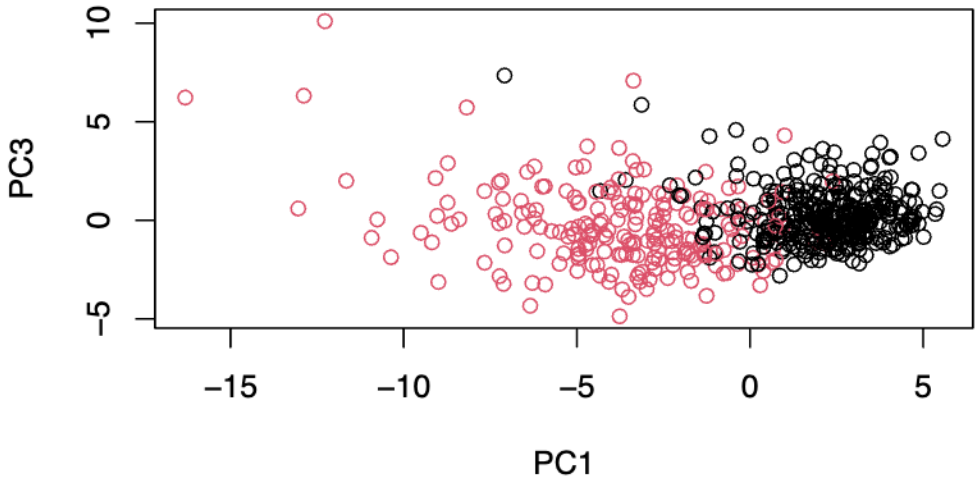
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

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



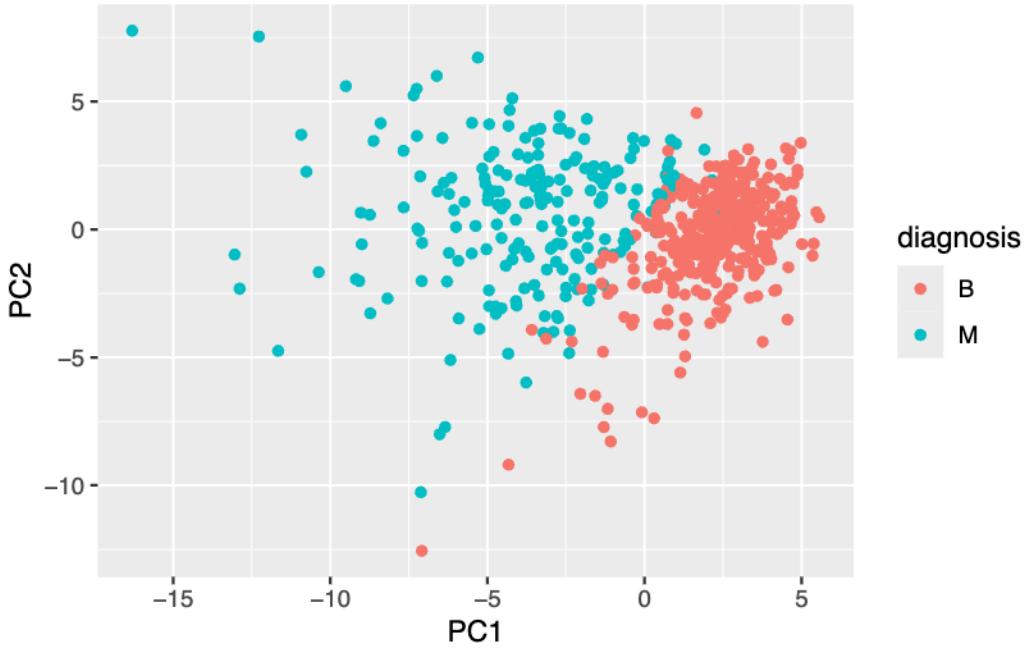
Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots? The shape of these plots feels very similar. The points appear to have moved slighlty down and right as a group. There is slightly more overlap in the center of the dots.

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



This is nice, make a ggplot of this data

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

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



PCA tries to find meaningful ways to flatten data with many inputs so that it can be analyzed reasonably.

Variance

Calculate the variance of each component. This is the variability among a group of data. This is done by squaring the stdev of the data.

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

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

Calculate the variance explained by each PC. This is done by dividing total variance by the PCs.

```
pve <- pr.var/wisc.pr$x
head(pve)
```

```
              PC1           PC2           PC3           PC4           PC5
842302   -1.4460492 -0.0000683378 -6.672761e-04 4.377694e-04  5.778995e-03
```

```
842517   -2.3856094  3.5277835000 -2.515846e-04 6.702014e-04 -2.558379e-03
84300903 -0.4918869  5.2980852242 -2.409307e+01 1.459976e-04  4.232194e-03
84348301 -0.2783092 -0.2744785181 -1.762058e+00 8.714227e+01  4.497378e-05
84358402 -0.4193277  1.0176131423  2.029426e+00 1.937117e+00 -2.431341e+01
843786   -0.5076863 -0.4177749272 -6.754571e-01 2.997150e+00  5.394068e+00
                 PC6           PC7          PC8          PC9         PC10
842302    5.798989e-03  0.0071756550  0.045357845 -0.155056705 -0.03130099
842517    2.410124e-01  0.6127248096 -0.064297242 -0.025383862  0.02200756
84300903  2.937907e-03 -0.0103365489 -0.084055881  0.643859521  0.03977960
84348301  2.454499e-04  0.0011124725 -0.006518273 -0.005823683 -0.01387219
84358402 -1.085711e-04 -0.0008005254 -0.002499680 -0.026180411  0.02166995
843786   -2.947263e+01  0.0002715123  0.004530007 -0.011918029 -0.01302061
               PC11        PC12        PC13        PC14        PC15
842302   -0.11408498 -0.03630535  0.47898487 -0.07623736  0.09879027
842517   -0.03377553  0.18996185 -0.03305337 -0.07578117 -5.86806264
84300903  0.04022803  0.22079102 -0.07305729  1.86974044 -0.10243919
84348301  0.01569317  0.02408966 -0.02942719 -0.06154745  0.18470370
84358402 -0.02378854 -0.16351466  0.06279774 -0.05093571 -0.09667220
843786   -0.07456600  0.19025796 -0.68777438  7.76683989 -0.15376730
               PC16       PC17       PC18       PC19       PC20        PC21
842302    0.10727604 -0.3549083 -0.2859508  1.8058935  0.7564170   3.0479681
842517   -0.09163148 -4.6439767  0.2960056 -0.6347752 -2.1165631  -3.3803143
84300903  0.16199132  0.3113963 -0.9085892 -0.2399681 -0.7683282   0.7765854
84348301  0.96400407  0.1091201 -1.6571898 -2.9884186 -0.2027350   0.3619306
84358402 -0.20436194  0.3719413 -2.8141714  0.1288398  1.2204381  -0.8084247
843786   -2.35901940  0.1584000 -0.1664360 -0.4056133 -0.8345546 -33.2736930
              PC22      PC23       PC24       PC25       PC26      PC27
842302   -5.0980745  4.936921   2.721937   4.474997  -5.997014 -6.533172
842517    3.1103735 -1.612186 -36.958129   2.797700 -16.431661  6.666397
84300903  4.3341960 -3.959750  -3.415687  -2.437872 100.738130 13.633689
84348301  1.1884435 -2.106216  -1.917324  -4.529310  -1.516076  2.600192
84358402  8.9036390  1.732259  49.024962 -96.070644   8.941750 12.971387
843786    0.9312878  4.694117 -85.052439  -2.135717  -9.709053 -4.156081
              PC28       PC29        PC30
842302   -58.45246   61.78684   120.76443
842517    50.58154 -348.55554  1509.96537
84300903  25.69692  524.55038 -2641.29438
84348301  15.90738  -17.43882    82.76806
84358402 -13.71338  134.14575   -56.96390
843786   571.35589  -24.18886  -195.35171
```

```
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
```

```
attributes(wisc.pr)
```

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

$class
[1] "prcomp"
```

```
# Variance isn't one of them, so we need to manipulate sdev to create variance
```

```
#pr.var <- wisc.pr$sdev^2
#pve <- round(pr.var/sum(pr.var),2)
#pve
#Round to 2 decimal points to make more sense of the results
```

```r
#cumsum(pve)
#Cumulative Sum. This adds up the total variance gotten by each PC. Ie by the 4th PC, 79% of
```

```r
pve <- pr.var/sum(pr.var)
pve
```

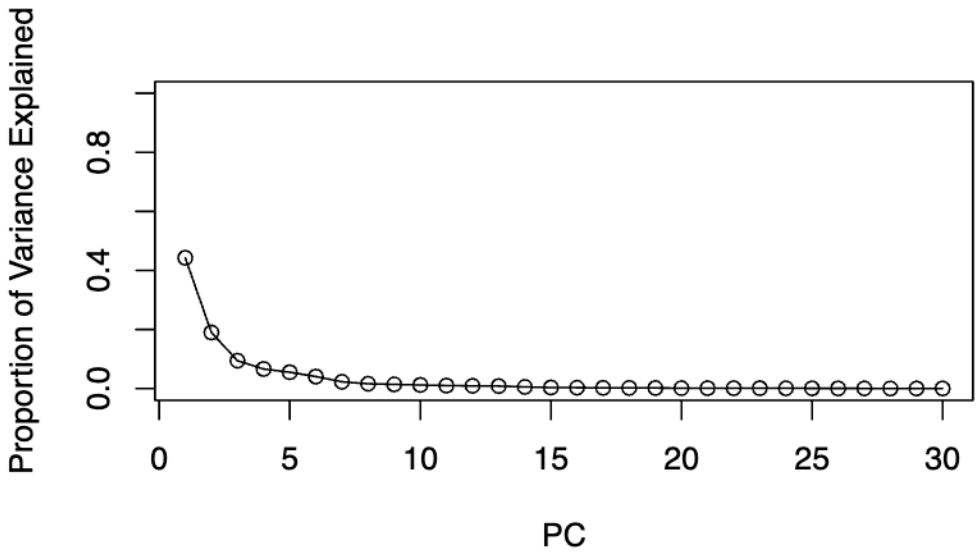
```
 [1] 4.427203e-01 1.897118e-01 9.393163e-02 6.602135e-02 5.495768e-02
 [6] 4.024522e-02 2.250734e-02 1.588724e-02 1.389649e-02 1.168978e-02
[11] 9.797190e-03 8.705379e-03 8.045250e-03 5.233657e-03 3.137832e-03
[16] 2.662093e-03 1.979968e-03 1.753959e-03 1.649253e-03 1.038647e-03
[21] 9.990965e-04 9.146468e-04 8.113613e-04 6.018336e-04 5.160424e-04
[26] 2.725880e-04 2.300155e-04 5.297793e-05 2.496010e-05 4.434827e-06
```

```r
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
```

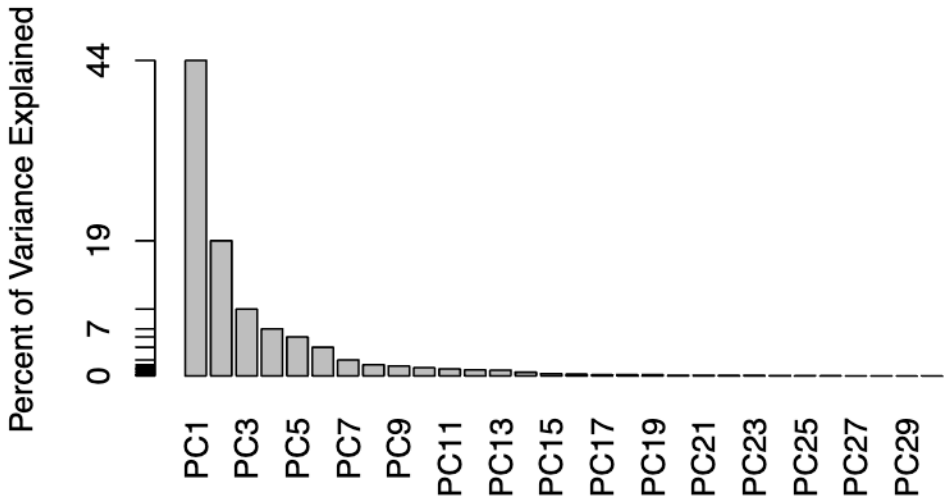
```r
# compare
```

```r
# When you call plot, check your data type and how many inputs you're giving it

plot(pve, xlab= "PC",
     ylab= "Proportion of Variance Explained",
     ylim = c(0,1), type= "o")
```



Another plot of the same data

```r
barplot(pve, ylab = "Percent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```



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?

```
#isolate pc1, find the vector you fed in to the equation to create the PCA that contributes l

comp.load.vect <- wisc.pr$rotation["concave.points_mean",1]

comp.load.vect
```

```
[1] -0.2608538
```

Q10. What is the minimum number of principal components required to explain 80% of the variance of the data? 5 principal components

```
pve <- round(pr.var/sum(pr.var),2)
pve
```

```
 [1] 0.44 0.19 0.09 0.07 0.05 0.04 0.02 0.02 0.01 0.01 0.01 0.01 0.01 0.01 0.00
[16] 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
```

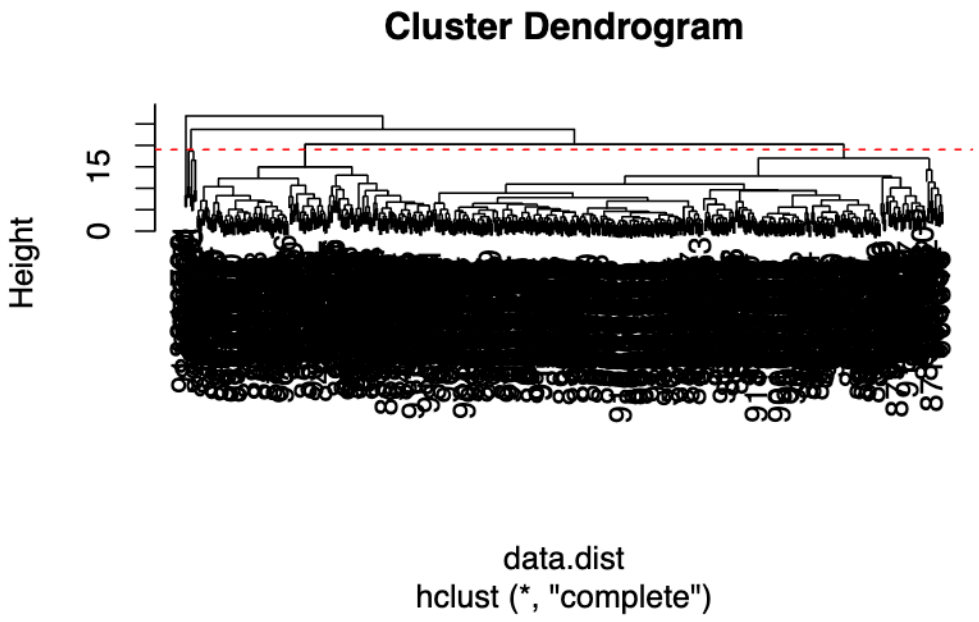
```
cumsum (pve)
```

```
 [1] 0.44 0.63 0.72 0.79 0.84 0.88 0.90 0.92 0.93 0.94 0.95 0.96 0.97 0.98 0.98
[16] 0.98 0.98 0.98 0.98 0.98 0.98 0.98 0.98 0.98 0.98 0.98 0.98 0.98 0.98 0.98
```

Hierarchical Clustering

First, scale the data. Calculate distances between all pairs of observations. Create a hierarchical clustering model with complete linkage.

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

data.dist <- dist(data.scaled)

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

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



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

H=19

Selecting number of clusters

Use 'cutree()' to cut into 4 clusters and compare with diagnosis data.

```
wisc.hclust.clusters <- cutree(wisc.hclust, 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?

You need at least 4 clusters to separate benign and malignant data - anything less yields almost all data in cluster 1. I like the distribution at 8 clusters as it separates the large group of 'M' results in cluster 1 in two different groups, one of which has no 'B' results.

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

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

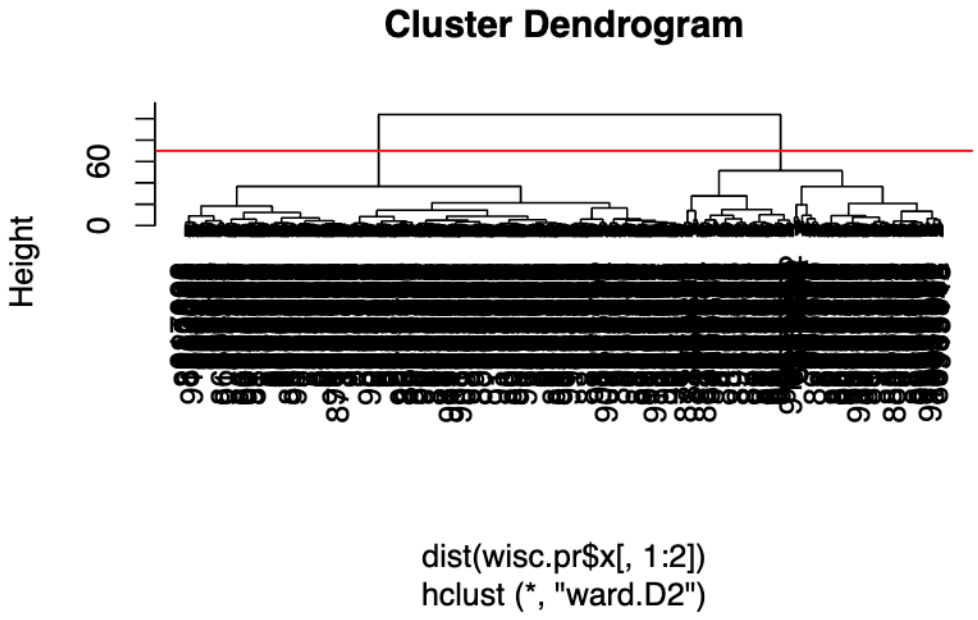
```
                     diagnosis
wisc.hclust.clusters2   B   M
                    1  12  86
                    2   0  79
                    3   0   3
                    4 331  39
                    5   2   0
                    6  12   1
                    7   0   2
                    8   0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

Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning. Options:"single", "complete", "average" and "ward.D2"

I like the ward.D2 method because it creates a smaller number of cleanly separated groups. This makes it easier to make more generalized predictions by the split between defined groups.

Clustering in PC space

```
hc <- hclust(dist(wisc.pr$x[,1:2]), method= "ward.D2")
plot(hc)

abline(h=70, col="red")
```



Cluster membership vector, clustering on PCA results

```
grps <- cutree(hc, h=70)
table(grps)
```

```
grps
  1   2
195 374
```

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

Cross-table to see how my clustering groups compare to the expert diagnosis vector.

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

```
    diagnosis
grps   B   M
   1  18 177
   2 339  35
```

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

The new model does a fairly good job at separating the diagnoses. However, there are still a significant amount of false positive results (18, are diagnosed with cancer but don't have it) and false negative results (35, are not diagnosed with cancer but do have it).

Positive => cancer M Negative => non-cancer B

True = cluster/grp 1 False = grp 2

True Pos = 177 False Pos = 18 True Neg = 339 False Neg = 35

So we captured 177/212 of the cancer positive patients. –> sensitivity

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

Our new method does about as well at splitting up results as the hierarchical clustering method, with slight increases in some areas and slight decreases in values of others. K-means is optional component

Sensitivity/Specificity

Sensitivity: True Pos/ (true pos + false neg)
Specificity: True Neg/ (true neg + false pos)

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

```
# for hierarchical clustering method
#1,2,4 -> B: 12+2+0 (FP), M: 165+5+2 (TP)
#3 -> B: 343 (TN), M:40 (FN)
TP1 = sum(165+2+5)
FP1 = sum(12+2+0)
TN1 = 343
FN1 = 40

sens2 <- TP1/(TP1+FN1)
sens2
```

```
[1] 0.8113208
```

```
spec2 <- TN1 / (TN1+FP1)
spec2
```

```
[1] 0.9607843
```

```
# for new created method
TP1 = 177
FP1 = 18
TN1 = 339
FN1 = 35

sens1 <- TP1/(TP1+FN1)
sens1
```

```
[1] 0.8349057
```

```
spec1 <- TN1 / (TN1+FP1)
spec1
```

```
[1] 0.9495798
```

```
#hierarchical clustering- 1, 2, and 4 are M, 3 is B
#newly created method groups
```

Based on these calculations, our new method displays greater sensitivity (83% v 81%) and the hierarchical clustering methods shows greater specificity (96% v 95%). Overall, the differences are pretty minimal and insignificant between the two techniques.

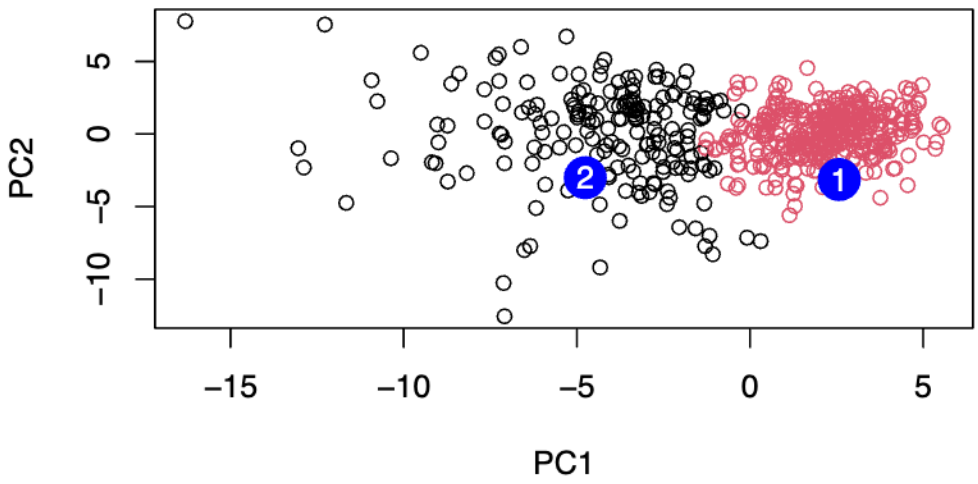
Predictions

We can use our PCA results (wisc.pr) to make predictions on new unseen data.

```
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=grps)
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?

I would prioritize patient number 2, as they fall much closer to the cluster of malignant data points.