Class8: Mini Project

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Today we will do a complete analysis of some breast cancer biopsy data, but first, let's revisit the main PCA functions in R, `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 of this dataset.

```
apply(mtcars, 2, mean)
```

```
      mpg        cyl       disp         hp       drat         wt       qsec
20.090625   6.187500 230.721875 146.687500   3.596563   3.217250  17.848750
       vs         am       gear       carb
 0.437500   0.406250   3.687500   2.812500
```

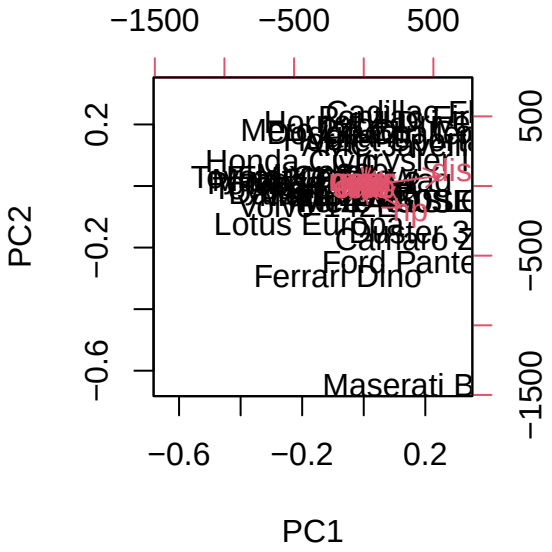
```
apply(mtcars, 2, sd)
```

```
       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
```

It is clear that "disp" and "hp" have the highest mean values and the highest standard deviation. They will dominate any analysis we do on this dataset. Let's see.

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

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

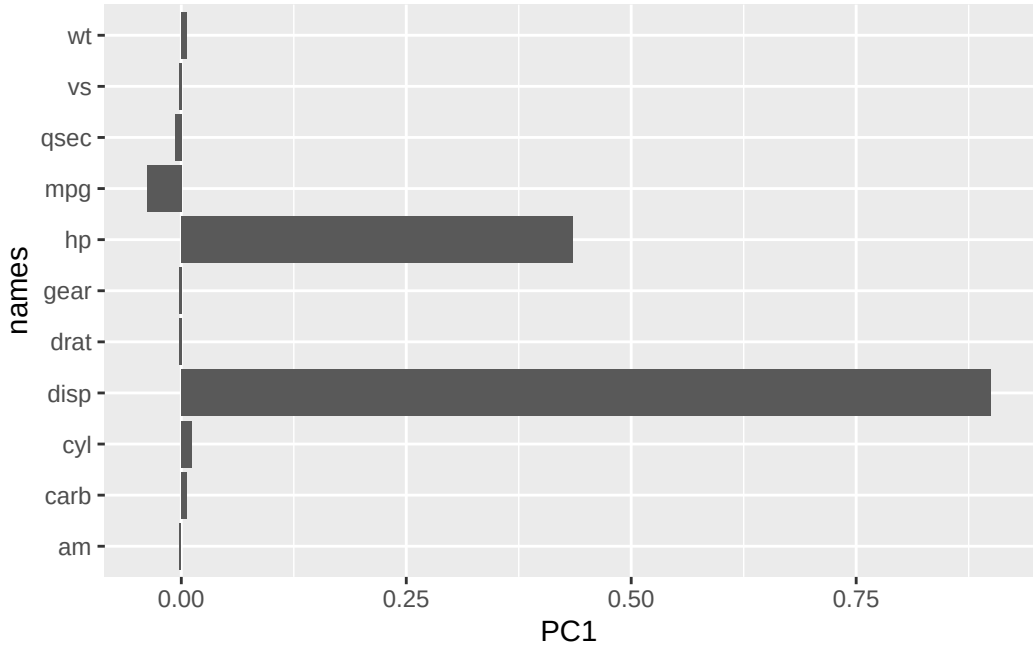



```
pc.noscale$rotation[,1]
```

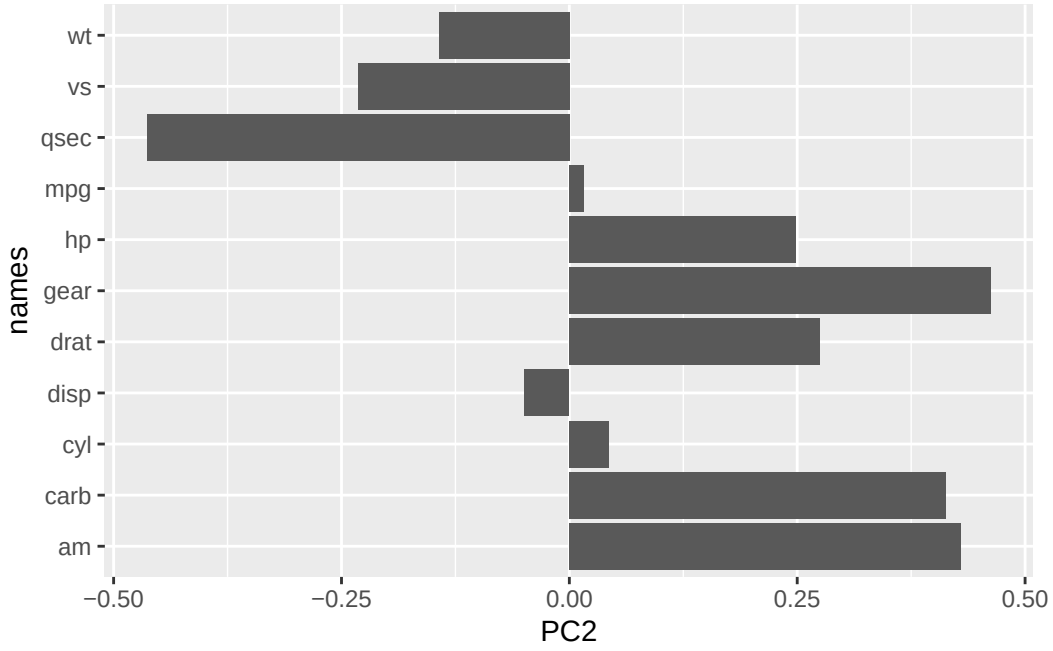
```
         mpg          cyl         disp           hp         drat           wt
-0.038118199  0.012035150  0.899568146  0.434784387 -0.002660077  0.006239405
        qsec           vs           am         gear         carb
-0.006671270 -0.002729474 -0.001962644 -0.002604768  0.005766010
```

Plot the loadings

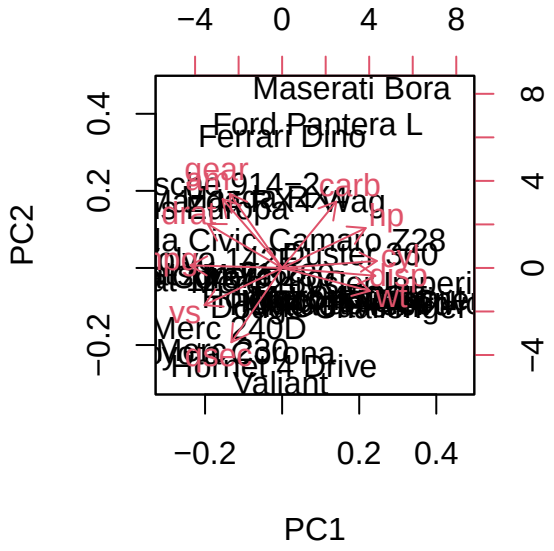
```
library(ggplot2)
r1 <- as.data.frame(pc.noscale$rotation)
r1$names <- rownames(pc.noscale$rotation)

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




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

ggplot(r2)+
    aes(PC2, names) +
    geom_col()
```




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



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

of analysis to avoid our analysis being dominated by individual varibles with the largest variance just due to their unit of measurement.

1. Exploratory data analysis - FNA breast cancer data

Load the data into R.

```
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
```

Q1. How many observations are in this dataset?

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

```
[1] 569
```

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

The table function is really useful here.

```
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()`

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

```
[1] 10
```

2. Principal Component Analysis

Exclude diagnosis

Before we go any further, we need to exclude the diagnosis column from any future analysis - this tells us whether a sample is cancer or non-cancer.

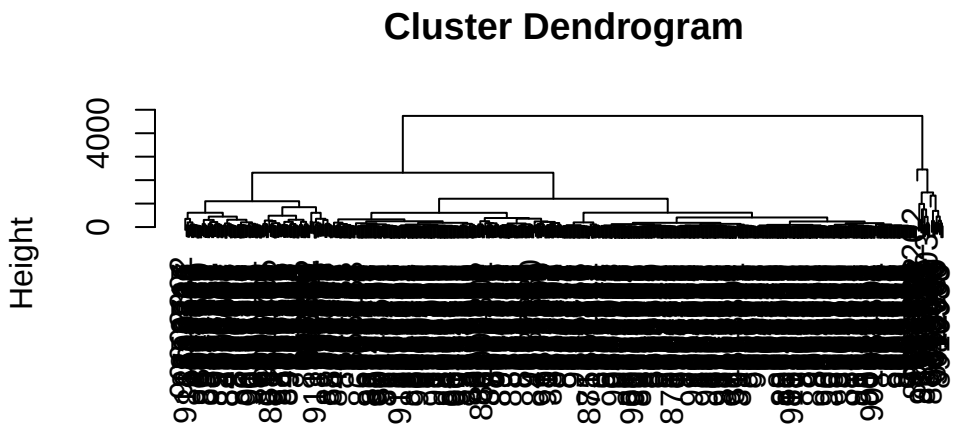
```
diagnosis <- as.factor(wisc.df$diagnosis)
head(diagnosis)
```

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

```
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)

```
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
```

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?

```
sum(0.4427, 0.1897, 0.09393)
```

```
[1] 0.72633
```

PC1 to PC3

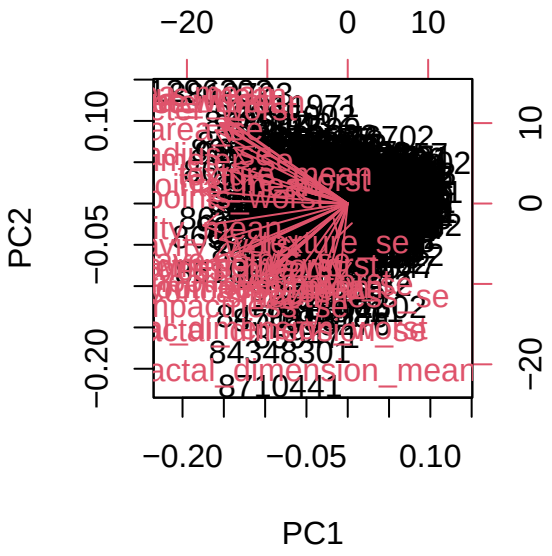
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

```
sum(0.4427, 0.1897, 0.09393, 0.06602, 0.05496, 0.04025, 0.02251)
```

```
[1] 0.91007
```

PC1 to PC7

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



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

All the arrows are pointing toward the left or pointing down on the plot. This biplot is too messy. The letters and numbers overlapping makes it too hard to interpret.

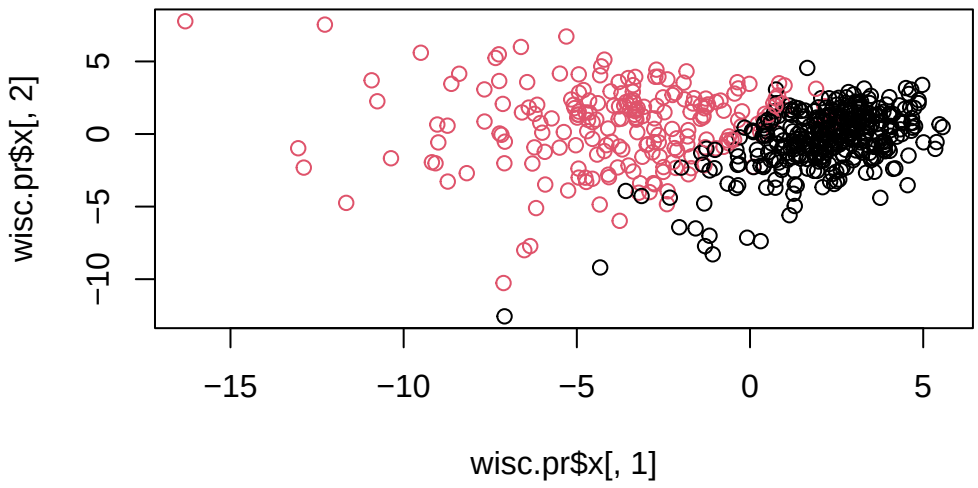
```
head(wisc.pr$x)
```

```
               PC1        PC2        PC3        PC4        PC5         PC6
842302   -9.184755  -1.946870 -1.1221788  3.6305364  1.1940595  1.41018364
842517   -2.385703   3.764859 -0.5288274  1.1172808 -0.6212284  0.02863116
84300903 -5.728855   1.074229 -0.5512625  0.9112808  0.1769302  0.54097615
84348301 -7.116691 -10.266556 -3.2299475  0.1524129  2.9582754  3.05073750
84358402 -3.931842   1.946359  1.3885450  2.9380542 -0.5462667 -1.22541641
843786   -2.378155  -3.946456 -2.9322967  0.9402096  1.0551135 -0.45064213
                PC7         PC8         PC9        PC10        PC11        PC12
842302   2.15747152  0.39805698 -0.15698023 -0.8766305 -0.2627243 -0.8582593
842517   0.01334635 -0.24077660 -0.71127897  1.1060218 -0.8124048  0.1577838
84300903 -0.66757908 -0.09728813  0.02404449  0.4538760  0.6050715  0.1242777
84348301  1.42865363 -1.05863376 -1.40420412 -1.1159933  1.1505012  1.0104267
```

```
84358402 -0.93538950 -0.63581661 -0.26357355  0.3773724 -0.6507870 -0.1104183
843786    0.49001396  0.16529843 -0.13335576 -0.5299649 -0.1096698  0.0813699
                PC13         PC14         PC15        PC16        PC17
842302    0.10329677 -0.690196797  0.601264078  0.74446075 -0.26523740
842517   -0.94269981 -0.652900844 -0.008966977 -0.64823831 -0.01719707
84300903 -0.41026561  0.016665095 -0.482994760  0.32482472  0.19075064
84348301 -0.93245070 -0.486988399  0.168699395  0.05132509  0.48220960
84358402  0.38760691 -0.538706543 -0.310046684 -0.15247165  0.13302526
843786   -0.02625135  0.003133944 -0.178447576 -0.01270566  0.19671335
                PC18        PC19        PC20         PC21        PC22
842302   -0.54907956  0.1336499  0.34526111  0.096430045 -0.06878939
842517    0.31801756 -0.2473470 -0.11403274 -0.077259494  0.09449530
84300903 -0.08789759 -0.3922812 -0.20435242  0.310793246  0.06025601
84348301 -0.03584323 -0.0267241 -0.46432511  0.433811661  0.20308706
84358402 -0.01869779  0.4610302  0.06543782 -0.116442469  0.01763433
843786   -0.29727706 -0.1297265 -0.07117453 -0.002400178  0.10108043
                PC23         PC24         PC25         PC26         PC27
842302    0.08444429  0.175102213  0.150887294 -0.201326305 -0.25236294
842517   -0.21752666 -0.011280193  0.170360355 -0.041092627  0.18111081
84300903 -0.07422581 -0.102671419 -0.171007656  0.004731249  0.04952586
84348301 -0.12399554 -0.153294780 -0.077427574 -0.274982822  0.18330078
84358402  0.13933105  0.005327110 -0.003059371  0.039219780  0.03213957
843786    0.03344819 -0.002837749 -0.122282765 -0.030272333 -0.08438081
                 PC28         PC29          PC30
842302   -0.0338846387  0.045607590  0.0471277407
842517    0.0325955021 -0.005682424  0.0018662342
84300903  0.0469844833  0.003143131 -0.0007498749
84348301  0.0424469831 -0.069233868  0.0199198881
84358402 -0.0347556386  0.005033481 -0.0211951203
843786    0.0007296587 -0.019703996 -0.0034564331
```

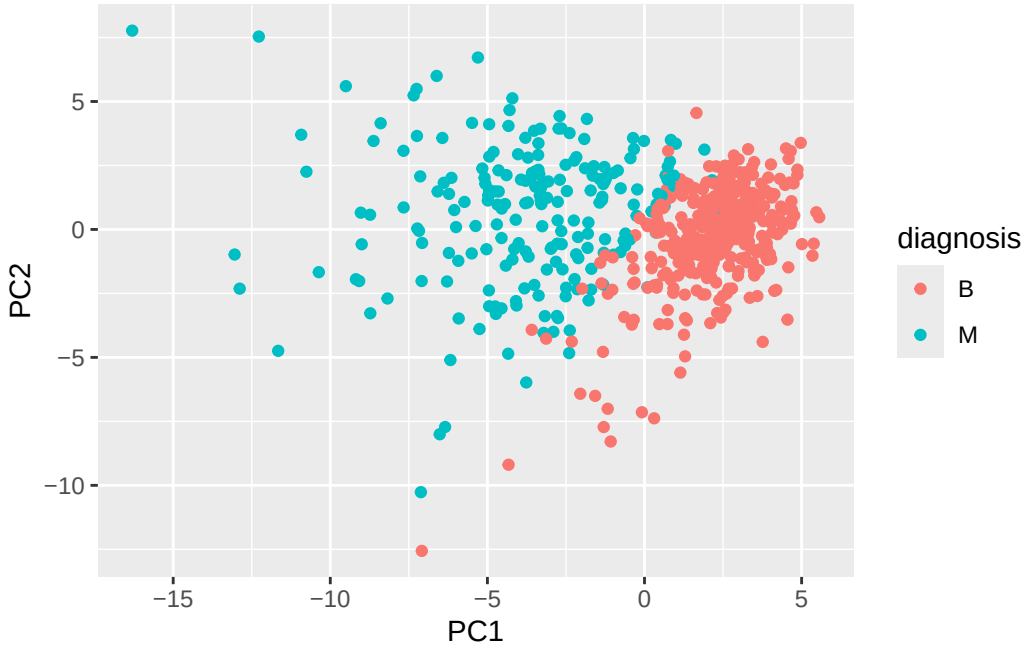
Plot of PC1 vs PC2, the first 2 columns.

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



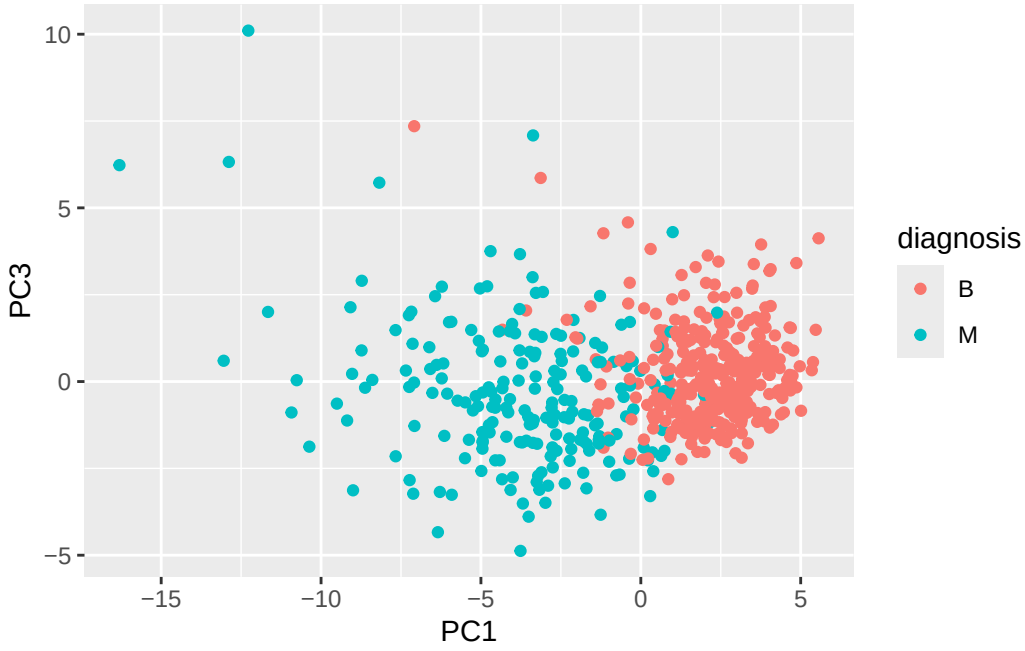
Make a ggplot version of this score plot, PC2 vs PC1.

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

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



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

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

ggplot(pc) +
  aes(PC1, PC3, col=diagnosis) +
  geom_point()
```



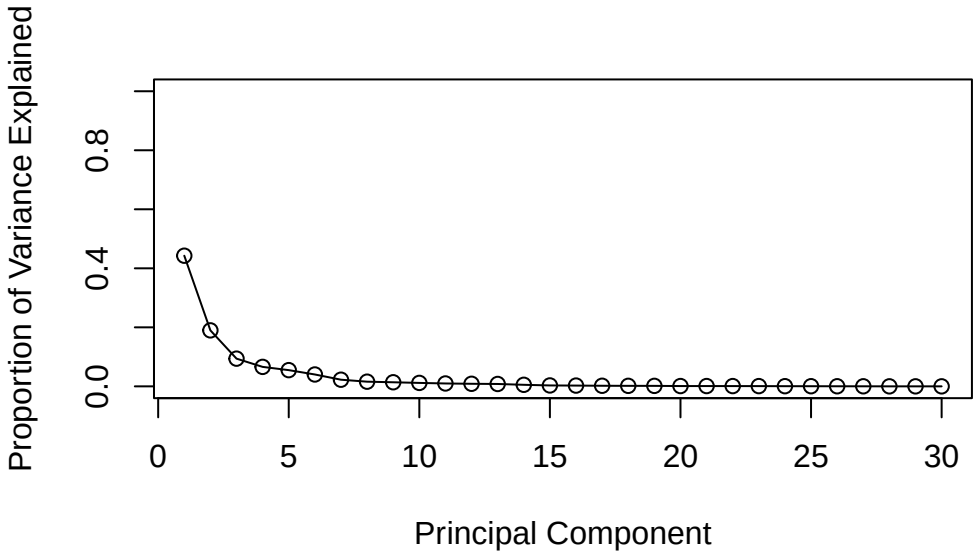
Both of the plots have similar scattering pattern for the benign and malignant clusters. For PC1 vs PC2, there is a more clear separation between the clusters. For PC1 vs PC3, there is more overlapping at the verge of two clusters.

Variance explained

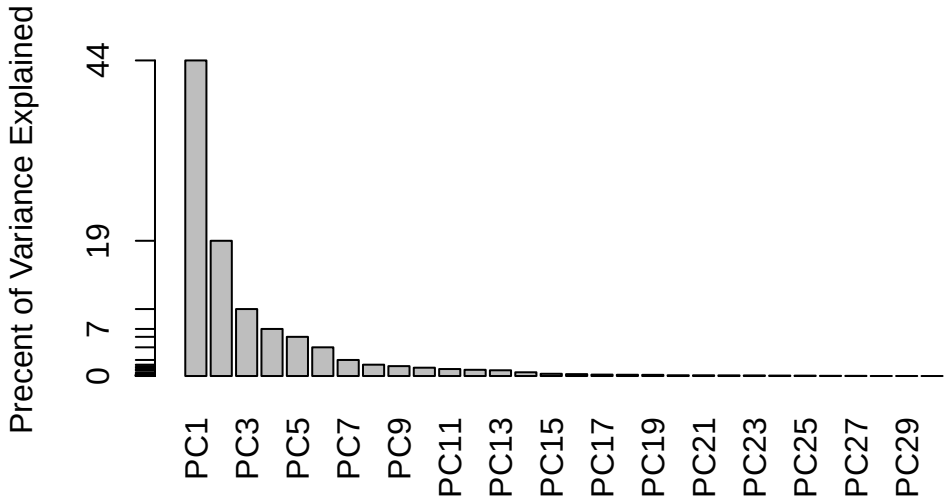
```
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

```
#variance explained by each principal component / total variance explained of all principal c
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 )
```



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
```

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
```

```
sum(0.4427, 0.1897, 0.09393, 0.06602, 0.05496)
```

```
[1] 0.84731
```

PC1 to PC5

3. Hierarchical Clustering

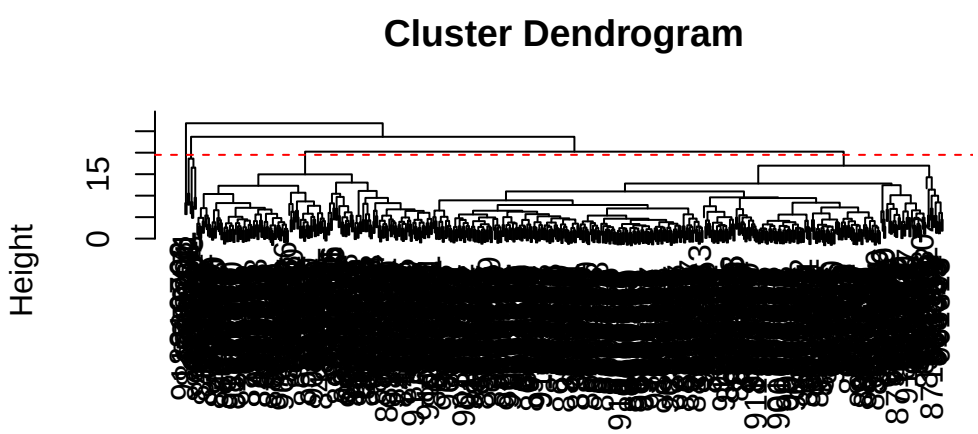
```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
```

```
#Calculate the (Euclidean) distances
data.dist <- dist(data.scaled)
```

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

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

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



height is about 19.5

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

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

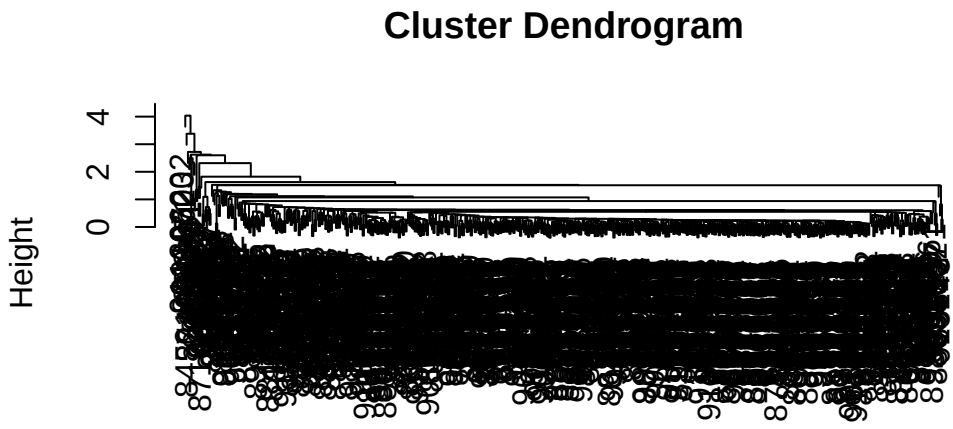
> Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

No. Any other cluster amount between 2 and 10 cannot give a cluster with more than 343 benign in a cluster or more than 165 malignant in a cluster.

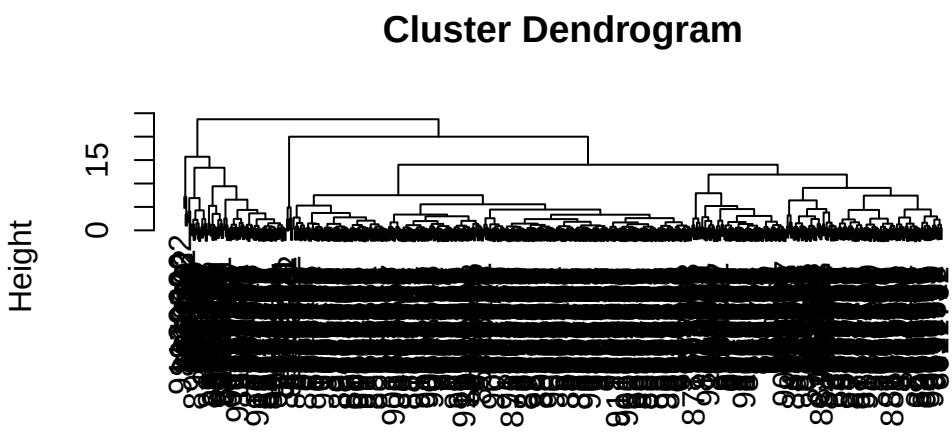
Clustering in PC space

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

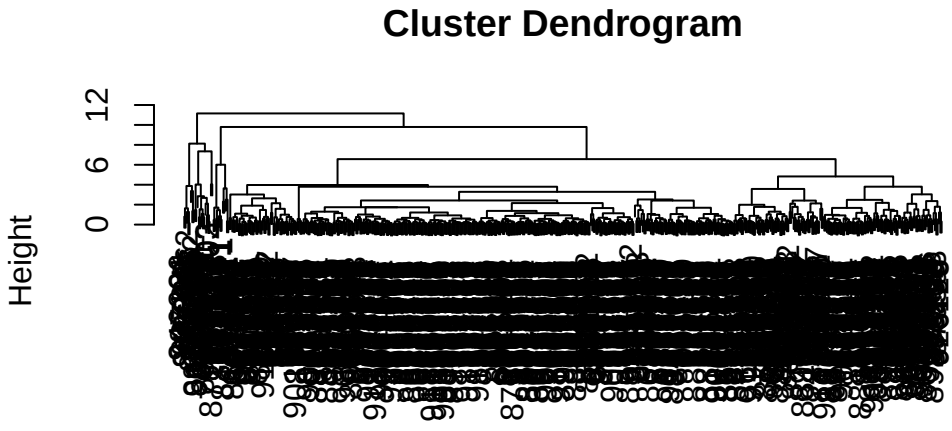
```
#single
hc1 <- hclust(dist(wisc.pr$x[,1:2]), method = "single")
plot(hc1)
```



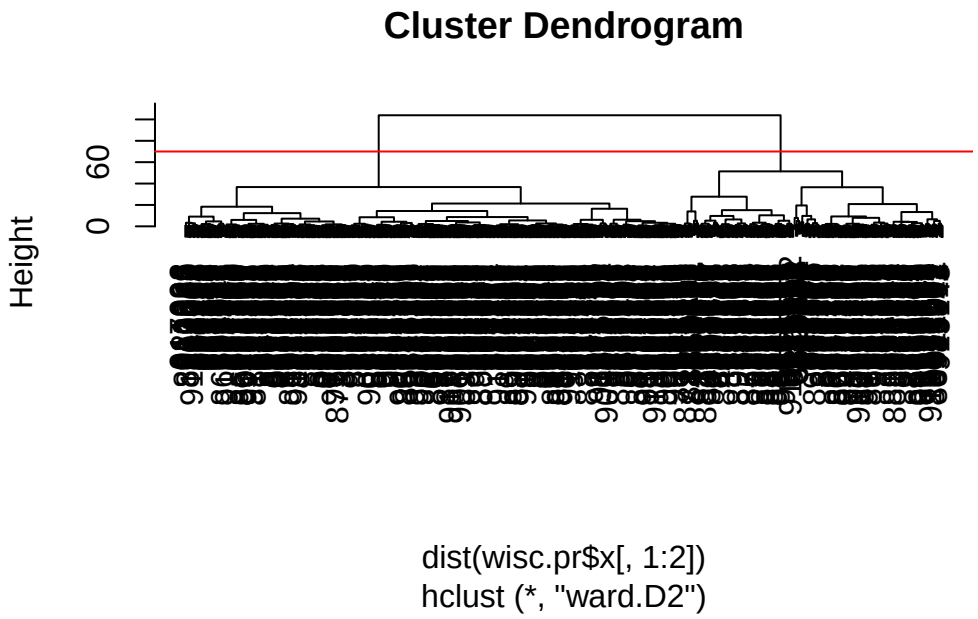

```
#complete
hc2 <- hclust(dist(wisc.pr$x[,1:2]), method = "complete")
plot(hc2)
```




```
#average
hc3 <- hclust(dist(wisc.pr$x[,1:2]), method = "average")
plot(hc3)
```



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

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



I like "ward.D2" the most, because the branches are more symmetrical, instead of more compacted on the left side like the others. It is thus easier to read.

4. OPTIONAL: K-means clustering

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

```
   diagnosis
      B   M
  1 356  82
  2   1 130
```

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

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

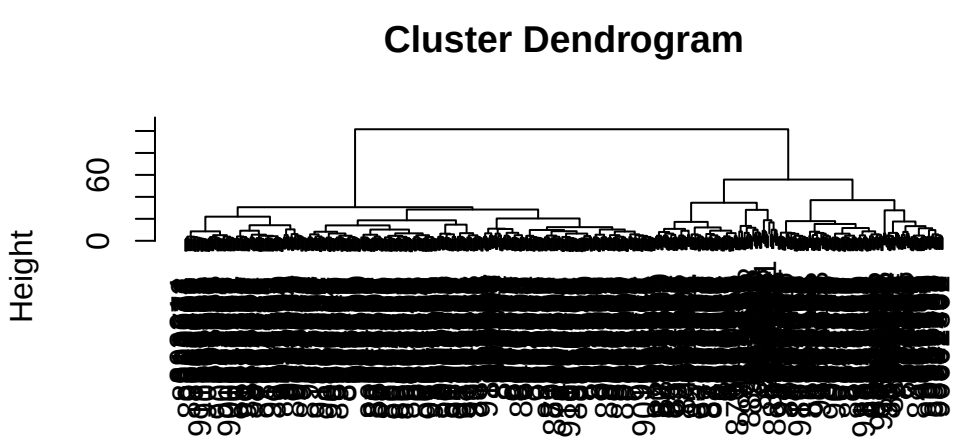
```
wisc.hclust.clusters   1   2
                   1  68 109
                   2   5   2
                   3 365  18
                   4   0   2
```

I think k-means separated the diagnoses well. It results in 2 clusters, corresponding to the two types of diagnoses. Majority of benign is in one cluster, and majority of malignant is in the other cluster. Compared to the hclust results, k-means clustering is better. Hclust results have 4 clusters, which do not match the diagnoses groups that well.

5. Combining methods

Cluster PC1~7

```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")

plot(wisc.pr.hclust)
```



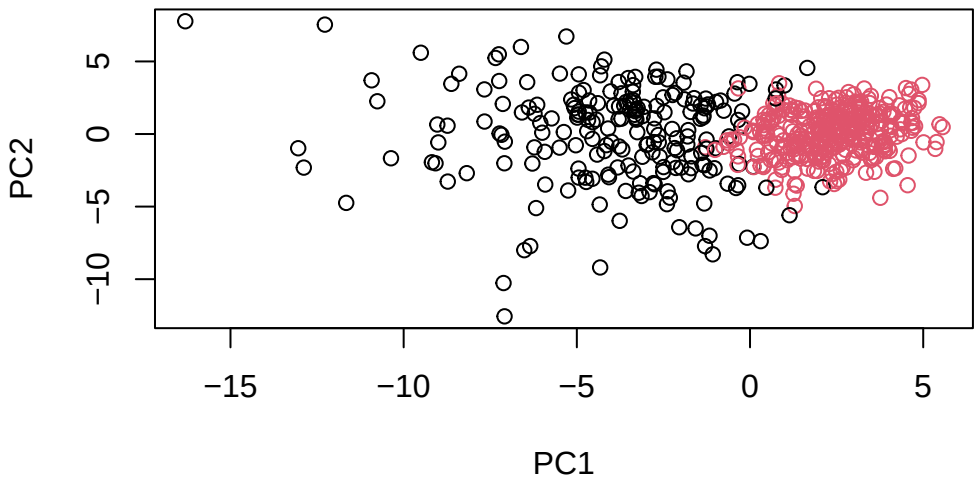

```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
216 353
```

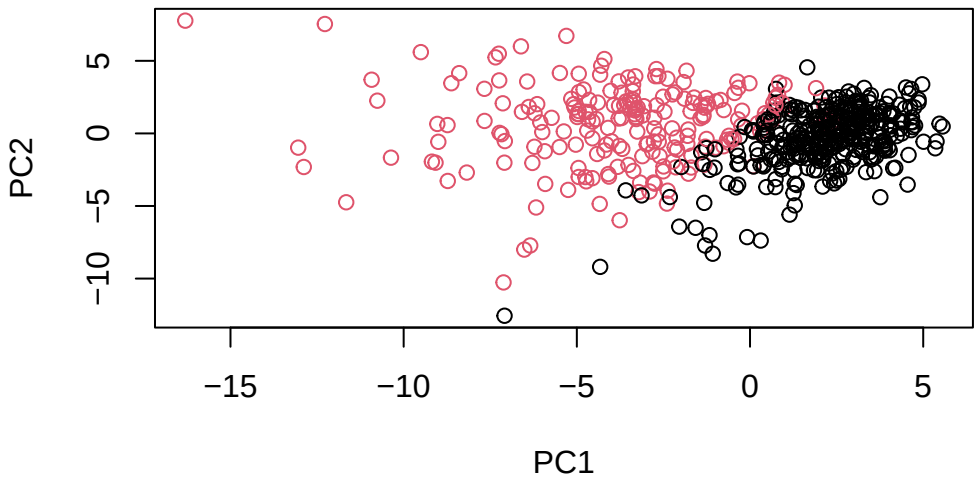
```
table(grps, diagnosis)
```

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

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




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



These two ways of plotting have opposite color for each group. To make is consistent, we can convert the data into factor:

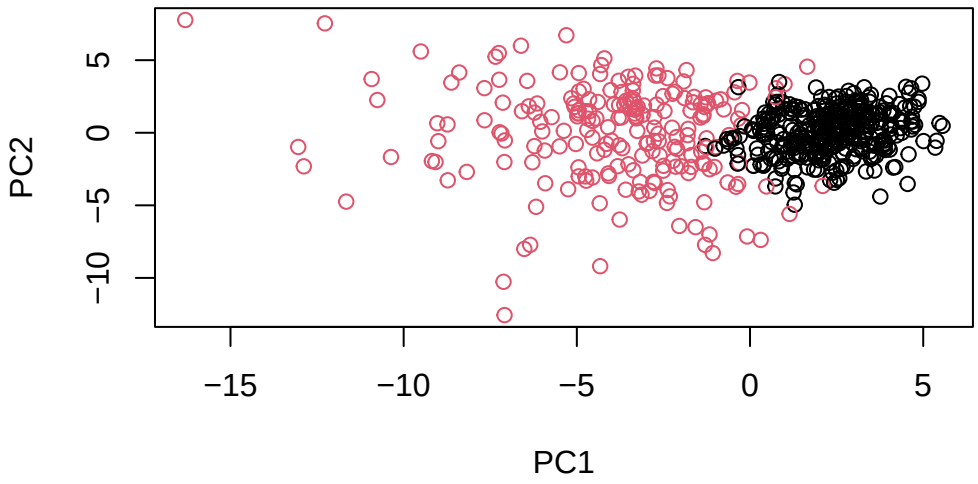
```
g <- as.factor(grps)
levels(g)
```

```
[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)
```



Now the red is malignant, black is benign.

```
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  45
2   2  77
3  26  66
4 329  24
```

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

```
# Compare to actual diagnoses
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
table(wisc.pr.hclust.clusters)
```

```
wisc.pr.hclust.clusters
  1   2
216 353
```

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

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

If the new model separate the two diagnoses into 4 clusters, the malignant is spread out into four clusters, instead of grouping the majority into one cluster. Most of the benign is still in one cluster. Compare to the actual dianoses, the new model is worse.

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.

```
# k-means
table(wisc.km$cluster, diagnosis)
```

```
   diagnosis
      B   M
  1 356  82
  2   1 130
```

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

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

K-means separate the diagnoses well, as the number of clusters match the number of diagnoses groups. Hierarchical clustering separate the dignoses into 4 clusters. Thus is does not work as well as k-means.

6. Sensitivity/Specificity

Hierarchical clustering

```
grps1 <- cutree(hc, h=70) #hc from Q13, hc <- hclust(dist(wisc.pr$x[,1:2]), method = "ward.D2
table(grps1)
```

```
grps1
  1   2
195 374
```

```
#same in Q2
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

Crosstable to see how my clustering groups correspond to the expert diagnosis vector of M an B values.

```
table(grps1, diagnosis)
```

```
     diagnosis
grps1   B   M
    1  18 177
    2 339  35
```

Positive => Malignant, Cancer Negative => Benign, non-cancer

True => cluster group 1 False => cluster grp 2

True Positive = 177 (want to optimize) False positive = 18 (minimize)

True Negative = 339 (want to optimize) (sensitivity) False Negative = 35 (minimize)

```
Sensitivity = 177/(177+35)
Sensitivity
```

```
[1] 0.8349057
```

```
Specificity = 339/(339+18)
Specificity
```

```
[1] 0.9495798
```

K-means

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

```
   diagnosis
      B   M
  1 356  82
  2   1 130
```

True Positive = 130 False positive = 1

True Negative = 356 False Negative = 82

```
Sensitivity = 130/(130+82)
Sensitivity
```

```
[1] 0.6132075
```

```
Specificity = 356/(356+1)
Specificity
```

```
[1] 0.9971989
```

Combining PCA & hierarchical

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

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

True Positive = 188 False positive = 28

True Negative = 329 False Negative = 24

```
Sensitivity = 188/(188+24)
Sensitivity
```

```
[1] 0.8867925
```

```
Specificity = 329/(329+28)
Specificity
```

```
[1] 0.9215686
```

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

Combining PCA and hierarchical clustering gives the highest sensitivity. K-means gives the best specificity.

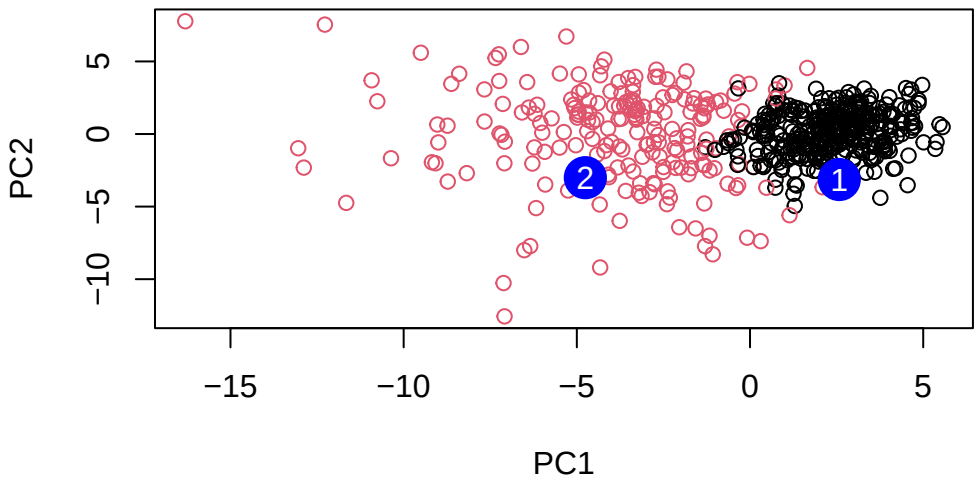
7. Prediction

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

```
#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 1 is clustered with benign. Patient 2 is clustered with malignant. Thus we should prioritize patient 2.