Class 8: PCA miniproject

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Today we will complete analysis of some breast cancer biopsy data but first let's revisit the main PCA function 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 data set

```
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 
```

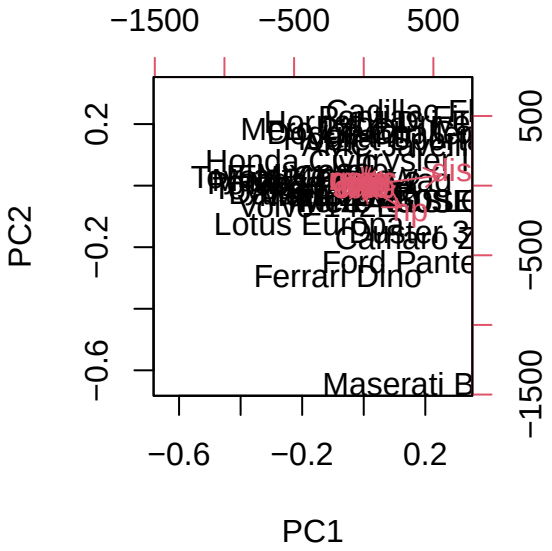
```
apply(mtcars,2, sd)
```

```
       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 displacement and horsepower have the highest mean values and the highest standard deviation. They will likely dominate any analysis I do on this data-set. Let's see:

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

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



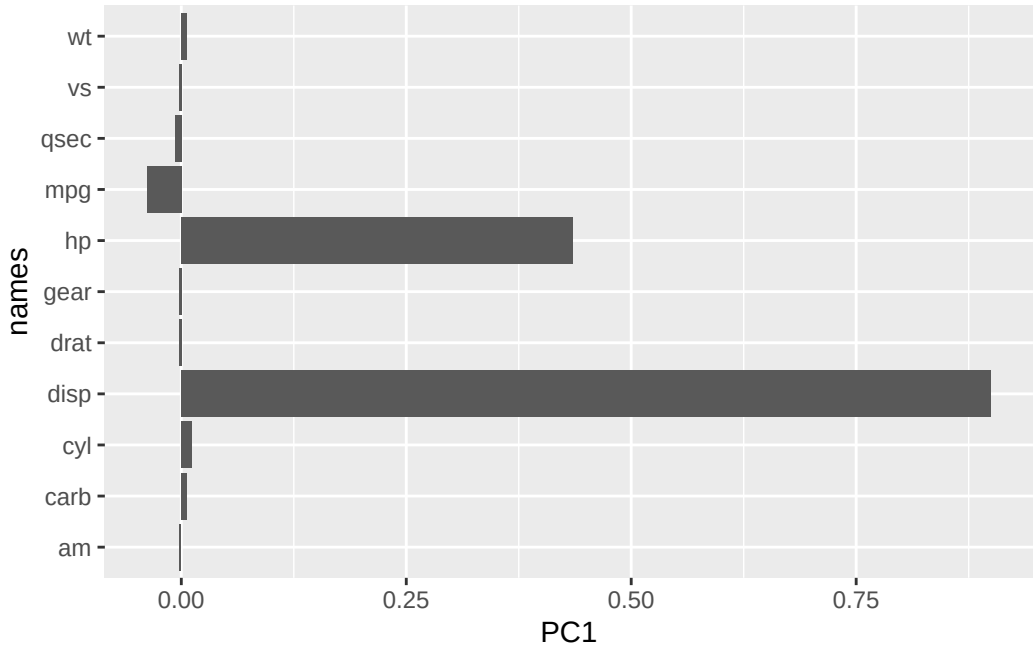

```
pc.noscale$rotation[,1]
```

```
         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
```

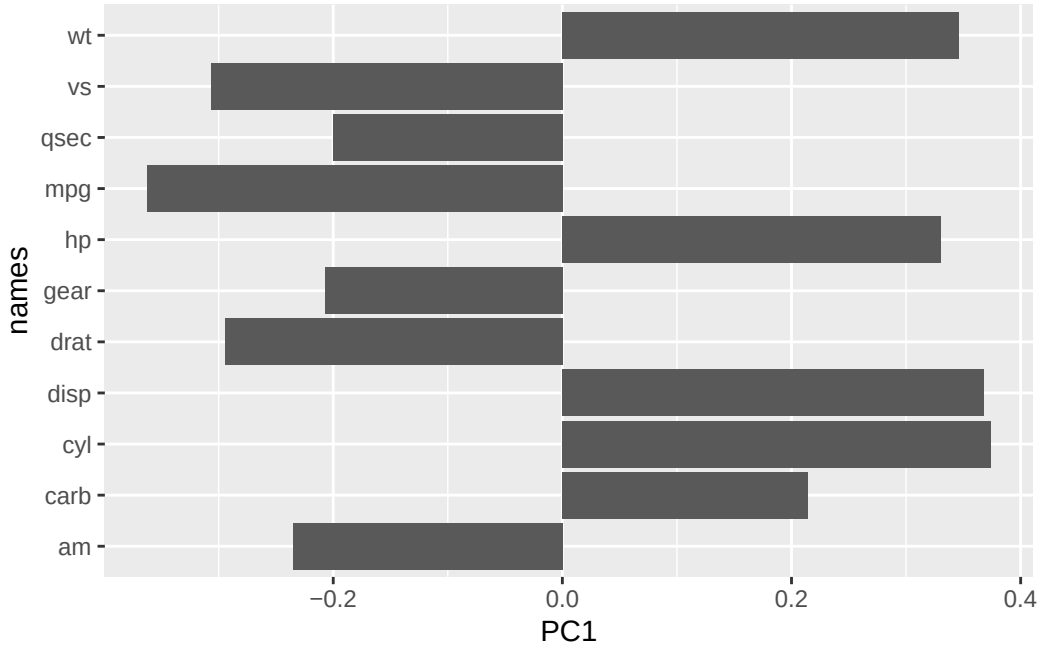
plot the loadings

```
library(ggplot2)

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

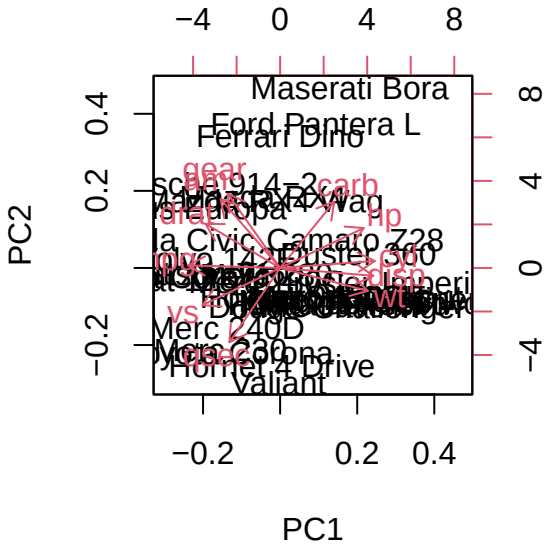
```
ggplot(r1)+
  aes(PC1,names)+
  geom_col()
```




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

ggplot(r2)+
  aes(PC1,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 variables with the largest variance just due to their unit of measurement.

#FNA breast cancer data

Load the data in 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?

```
sum(wisc.df$diagnosis =="M")
```

```
[1] 212
```

The `table()` function is super 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 the `grep()`

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

```
[1] 10
```

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

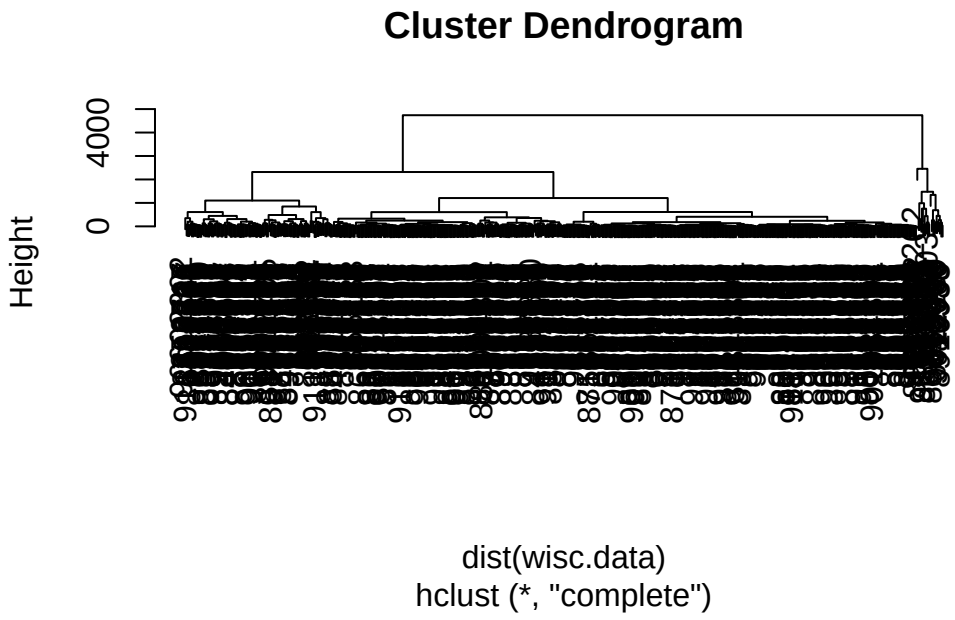
```
diagnosis <- as.factor(wisc.df$diagnosis)
head(diagnosis)
```

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

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

Lets 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)

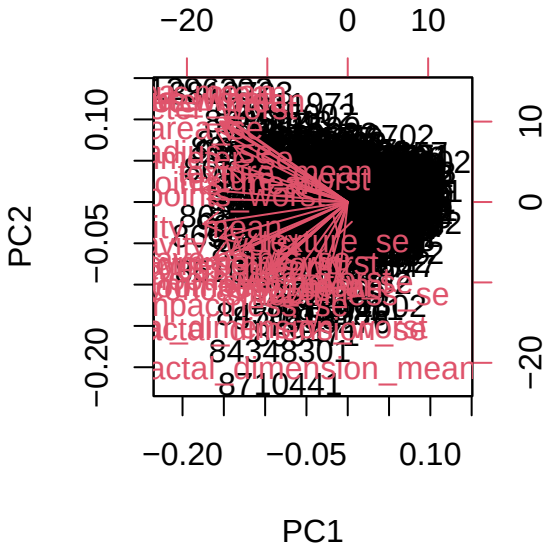
```
wisc.pr <- prcomp (wisc.data, scale=T)
summary(wisc.pr)
```

```
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)? 0.4427 or (44.27%) Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data? Three Principal Components Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data? Seven Principal Components

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



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

This biplot stinks! We need to build our PCA score plot of Pc1vsPC2

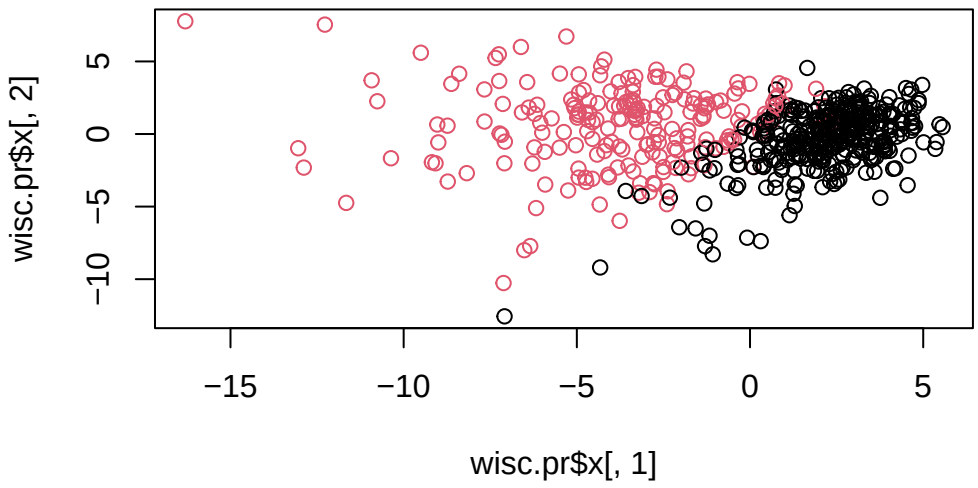
```
head(wisc.pr$x)
```

```
               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
```

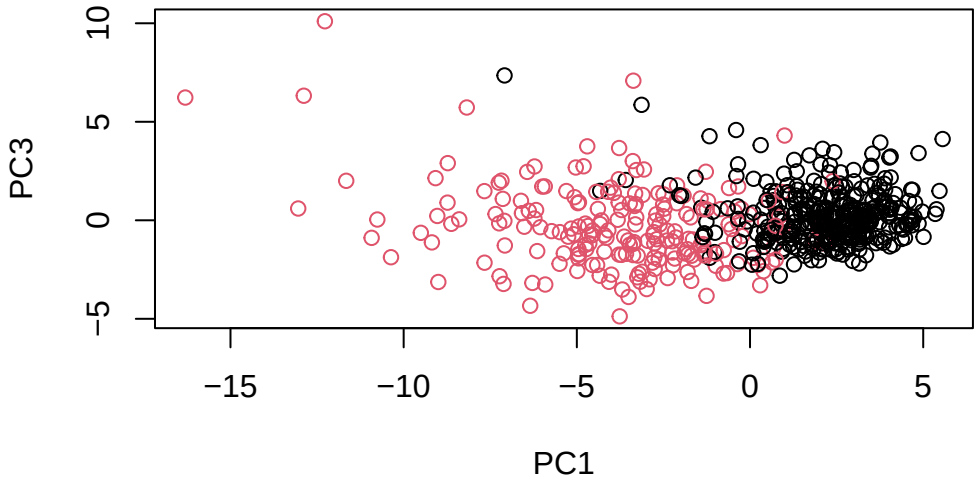
Plot of PC1 vs PC2 the first two columns

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



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

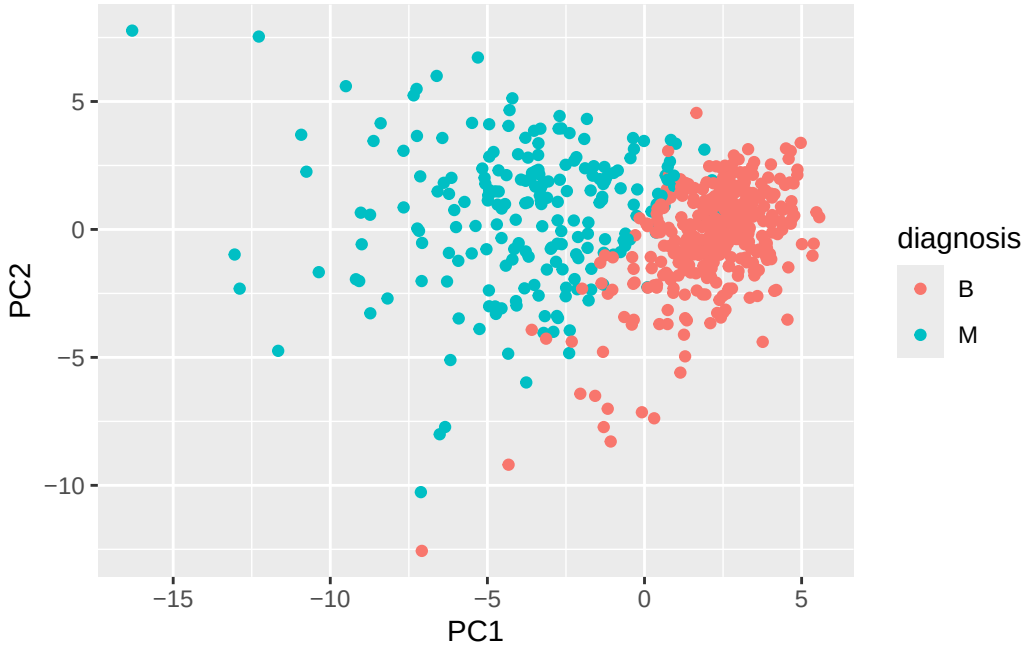
```
plot(wisc.pr$x[,1 ],wisc.pr$x[,3], col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```



Answer: There exist a clear distinct between these two. As well as, malignant and benign being clearly seperate from each other.

Make a ggplot version of this score plot:

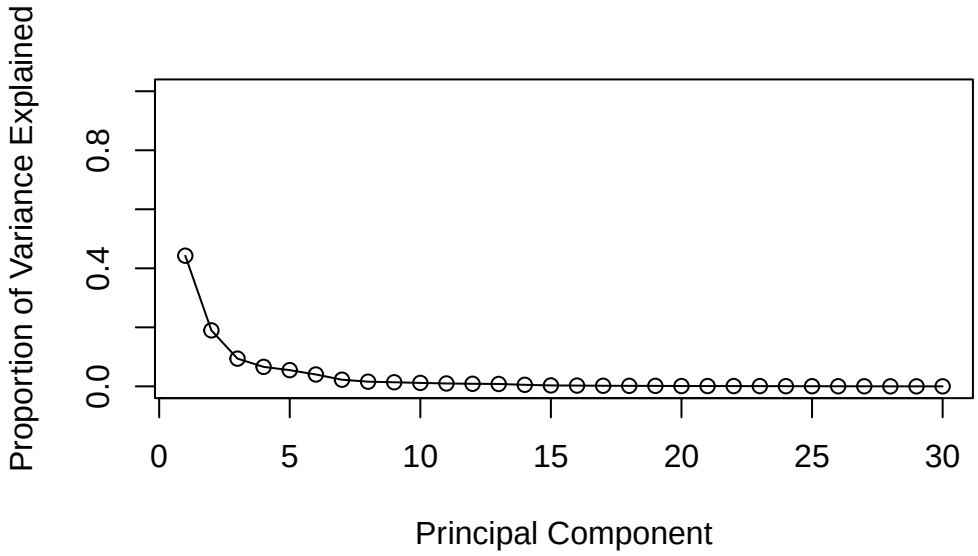
```
pc<-as.data.frame(wisc.pr$x)

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




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

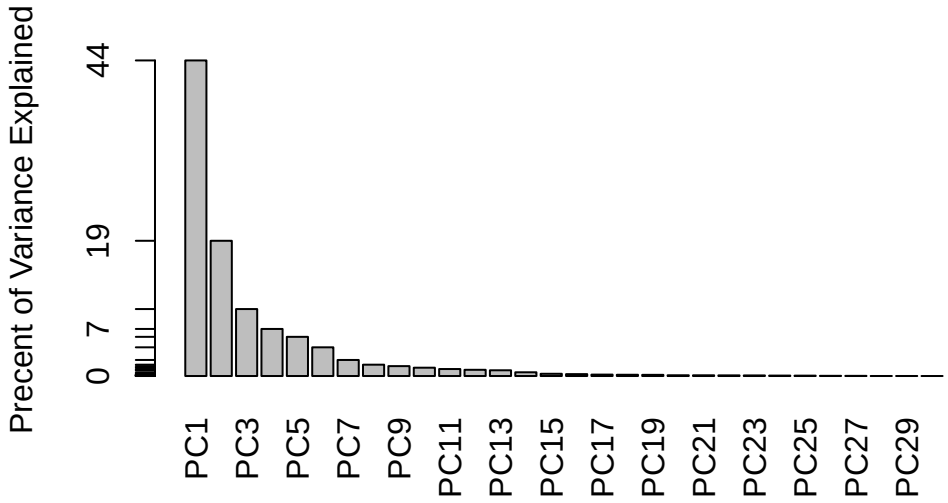
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

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


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



(Same Data)

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



Communicating PCA Results

Q9. For the first principal component, what is the component of the loading vector (i.e. wisc.pr$rotation[,1]) for the feature concave.points_mean?

```
wisc.pr$rotation["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?

```
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
```

Answer: 5 PCA required to explain 80% of variance data.

Hierarchical Clustering

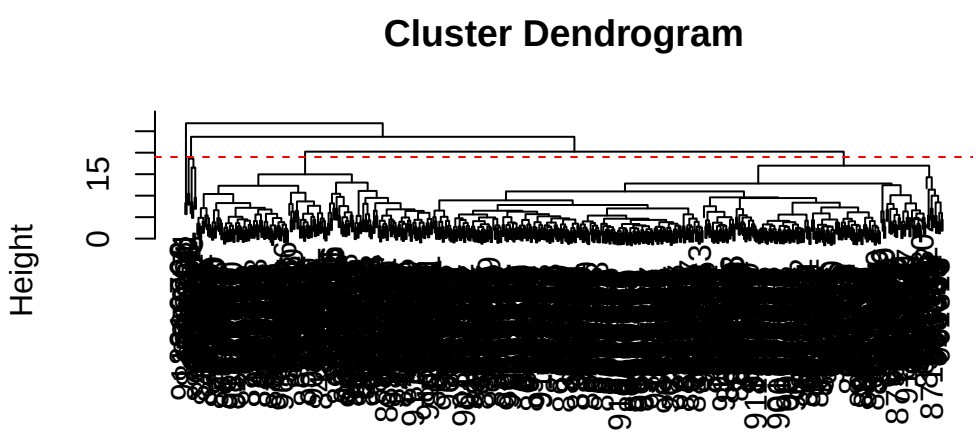
```
data.scaled <- scale((wisc.data))
```

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

```
wisc.hclust <- hclust(data.dist, )
```

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, col="red", lty=2)
```



Answer: 19

```
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?

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

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

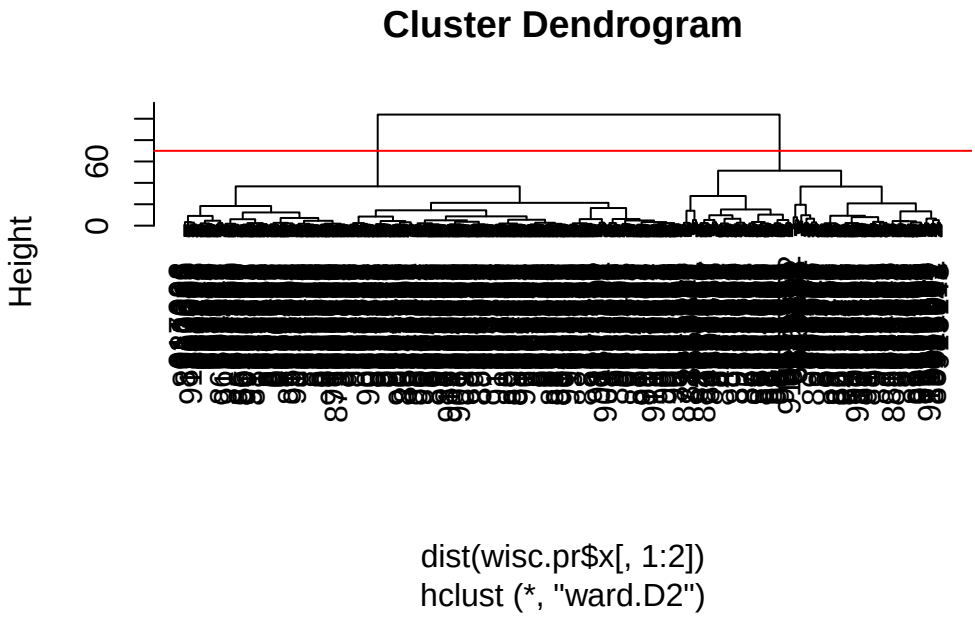
```
                    diagnosis
wisc.hclust.clusters   B   M
```

```
1  12 165
2   2   5
3 343  40
4   0   2
```

Answer: I believe that the best cluster vs diagnoses match is 10, since it has the most definitive clusters. However, there is always a trade off, since is there not one single cluster grouping that doesn't create false positives.

Clustering on PCA results

```
hc<-hclust(dist(wisc.pr$x[,1:2]), method= "ward.D2")
plot(hc)
abline(h=70,col="red")
```



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

Answer: Ward.2 is the my personal favorite for this specific data set since it minimizes the variance of the data set and makes it easier to understand.

K-means clustering and comparing results

```
wisc.km <- kmeans(scale(wisc.data), centers= 2, nstart= 20)
```

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

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

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

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

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

Answer: I would say it is a little bit better however, overall the clustering for both would not give confidence in all diagnosis except for some clusters.

Cluster membership vector

```
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 corresponded to the expert diagnosis vvector of M and B values

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

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

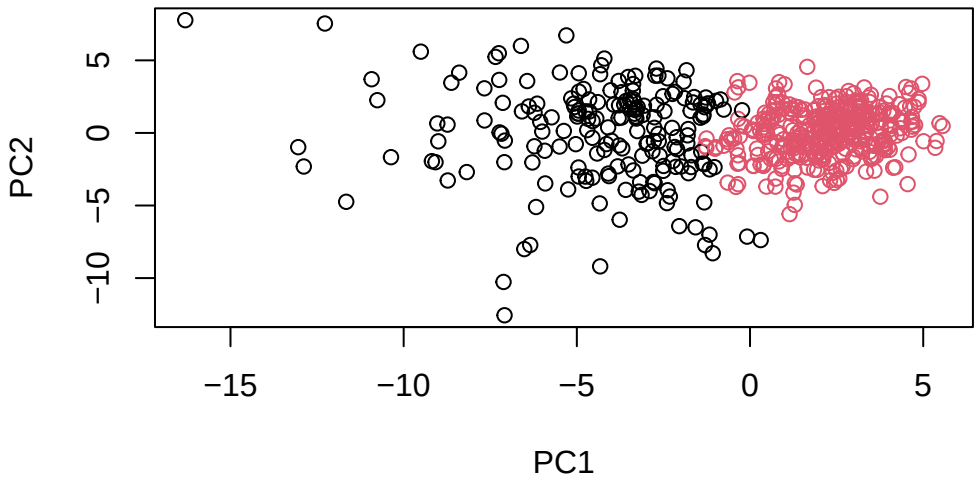
positive=> cancer M Negative=> non-cancer B

True=cluster/grp1 False= grp 2

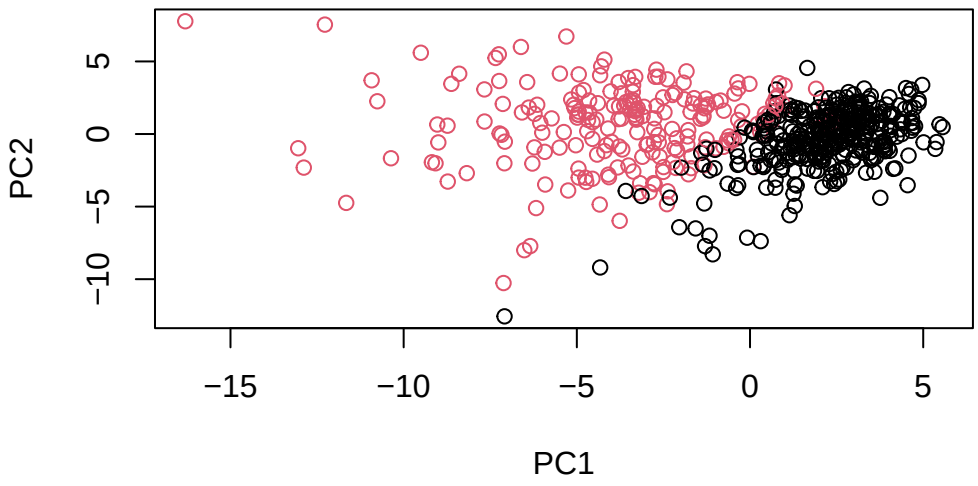
True Positive 177 False Positive 18 True Negative 339 False Negative 35

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

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




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



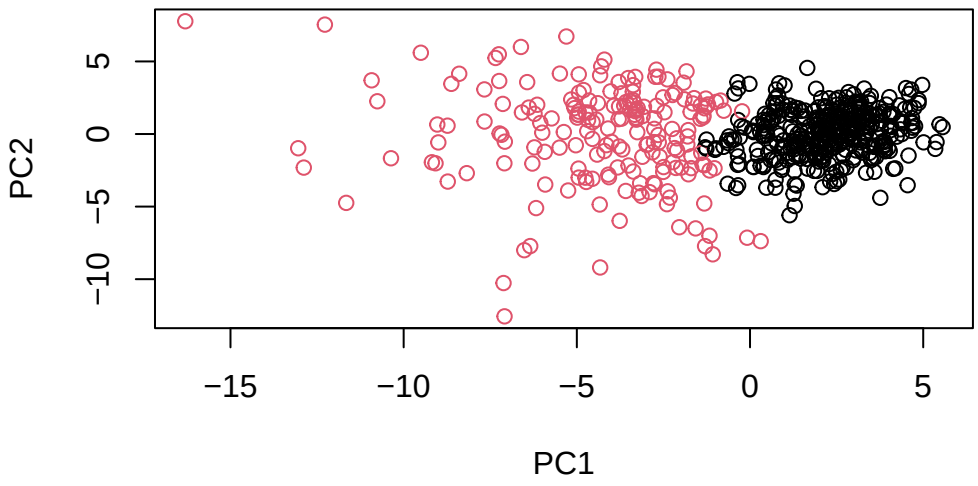

```
g <- as.factor(grps)
levels(g)
```

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

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

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

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




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

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

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

```
table(cutree(wisc.pr.hclust,k=4), diagnosis)
```

```
   diagnosis
      B   M
  1   0  45
  2   2  77
  3  26  66
  4 329  24
```

Answer: The first two clusters are pretty good at determining diagnosis. However, the third and fourth clusters are not good at determining diagnosis. That makes this model pretty bad at determining diagnosis.

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

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

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

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

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

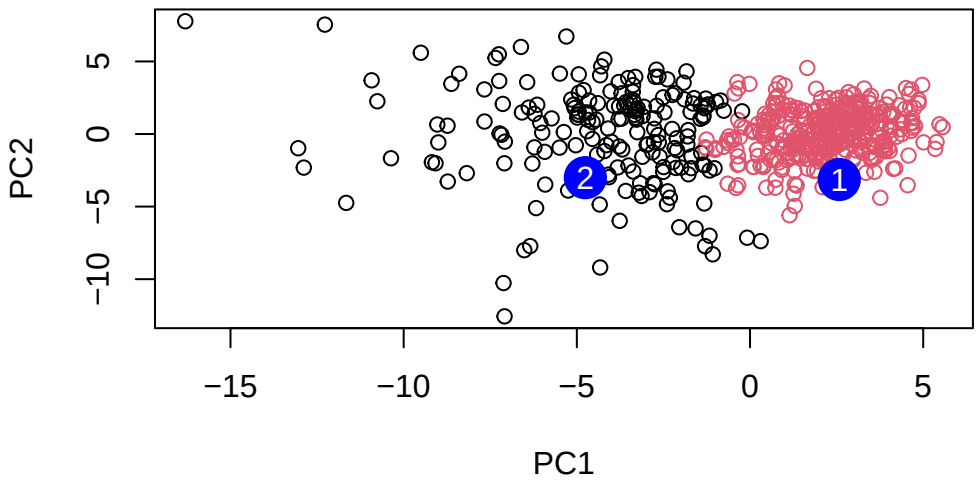
Answer: They are both bad. However, k-means is a simpler 2-cluster set up, with significantly more errors. Hclust, is more accurate, but also more complex. This makes both inadequate for clincial use.

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

Answer: Each method is good at its owns thing. Hierarchical gave more benign results than malignant. Hierarchical combined with PCA gave more malignant than benign. Meaning combined was more sensitive, and hierarchical was more specific. **7. Prediction**

```
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
```

```
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?

Answer: Patient 1 should be prioritized for a follow up since they lie in a predominantly malignant (red) cluster.