Class 8: PCA mini project

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Today we will do a. omplete analysis of some breast cancer biopsy data but first let's revist 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 and sd 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 
```

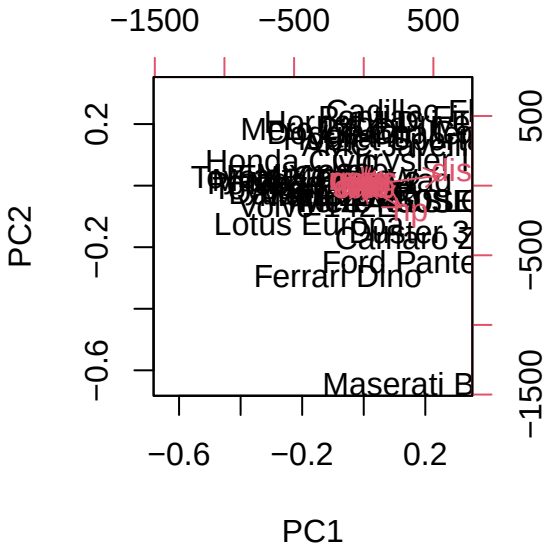
```
apply(mtcars, 2, sd)
```

```
       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 "disp" and "hp" have the highest mean values and the highest standard deviation. They will likely dominate any analysis I do on this dataset. Let's see:

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

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



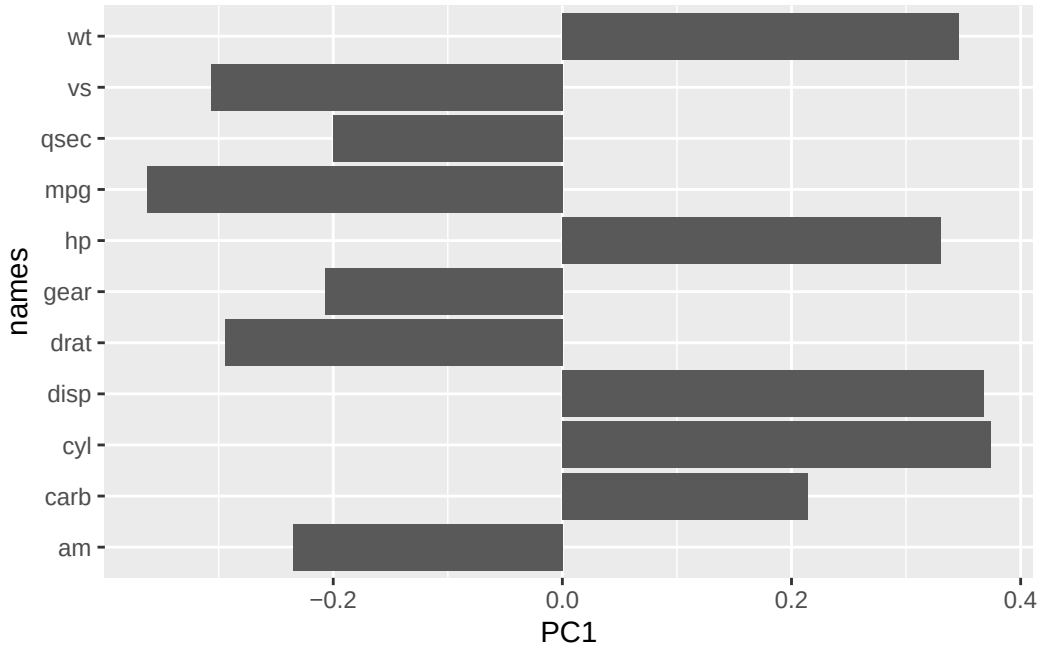

```
pc.noscale$rotation[,1]
```

```
         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
```

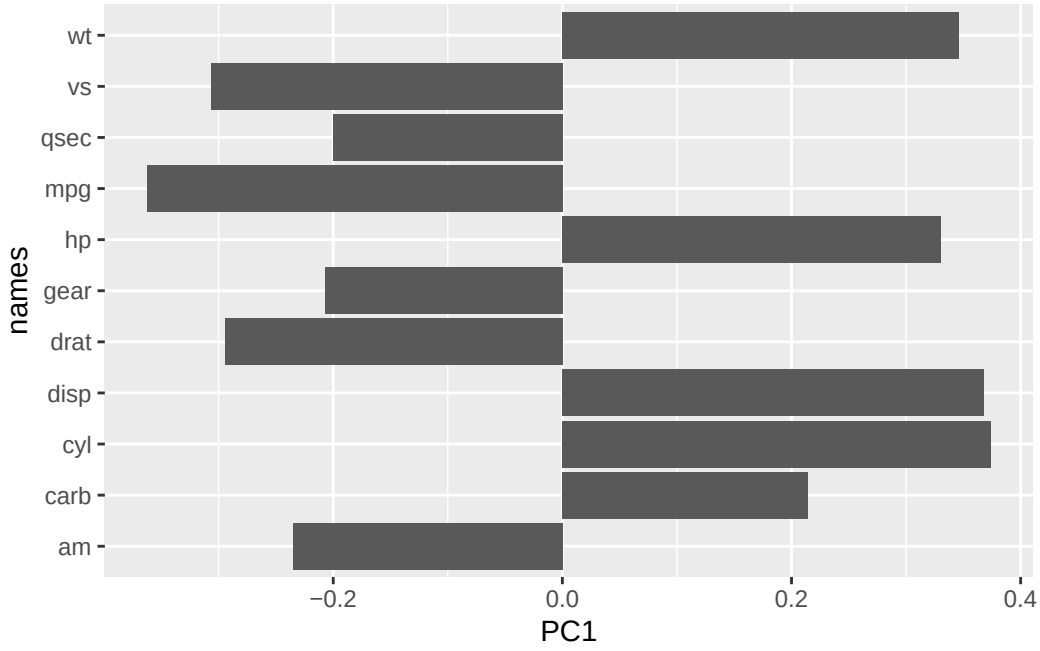
Plot the loadings:

```
library(ggplot2)

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

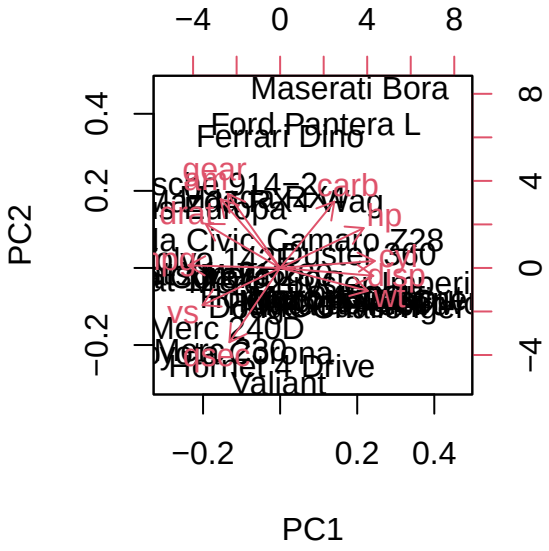
```
ggplot(r2) +
  aes(PC1, names) +
  geom_col()
```




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

ggplot(r1) +
  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 ebing dominated by individual variables with the largest variance just due to their unit of measurment.

FNA breast cancer data

Preparing the 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
```

Exploratory data analysis

Q1. How many observations are in this data-set?

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

```
[1] 569
```

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

The `table()` function is super useful here:

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

```
  B   M
357 212
```

or you could do...

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

```
[1] 212
```

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

First how many columns do we have?

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

```
[1] 31
```

Now we want to know the names of the columns.

```
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()` function.

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

```
[1] 10
```

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

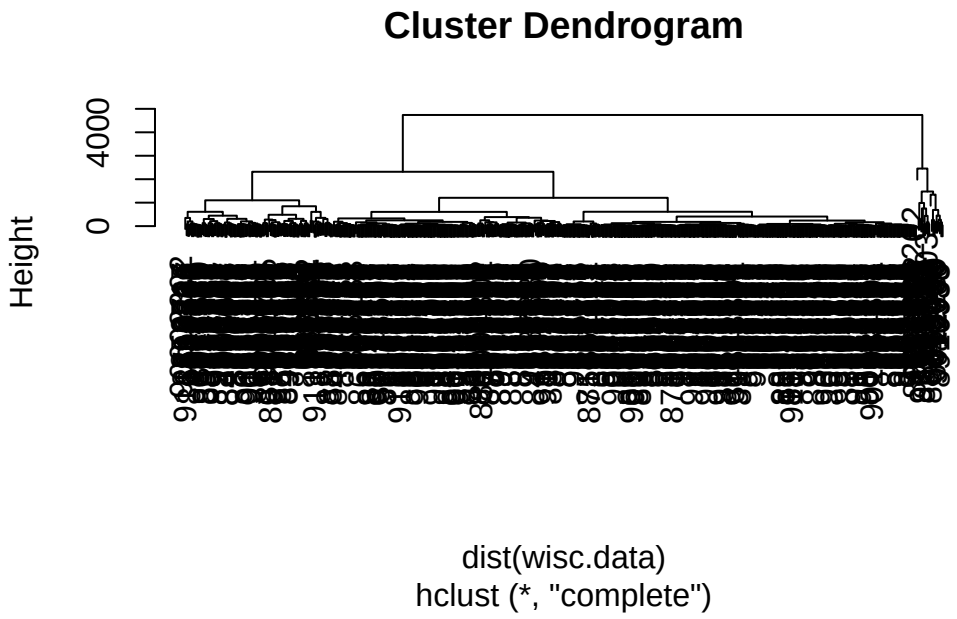
```
diagnosis <- as.factor(wisc.df$diagnosis)
head(diagnosis)
```

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

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

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

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



Principal Component Analysis (PCA)

Performing 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)?

```
pr.var <- wisc.pr$sdev^2
pve <- pr.var/sum(pr.var)
pve[1]
```

```
[1] 0.4427203
```

Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in 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
```

```
which(cumsum(pve) > 0.7)[1]
```

```
[1] 3
```

```
sum(pve[1:3])
```

```
[1] 0.7263637
```

Three PCs are required to describe at least 70% of the original variance in the data.

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

```
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
```

```
which(cumsum(pve) > 0.9)[1]
```

```
[1] 7
```

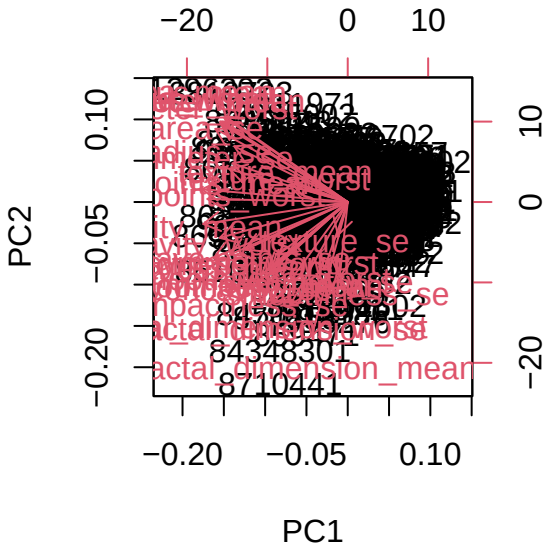
```
sum(pve[1:7])
```

```
[1] 0.9100953
```

Seven PCs are required to describe at least 90% of the original variance in the data

Interpreting PCA results

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



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

The overlapping of text and numbers stands out to me about this plot. It is very difficult to understand because of the excessive overlapping of data points.

This biplot sucks! We need to build our own PCA score plot of PC1 vs PC2.

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

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

$class
[1] "prcomp"
```

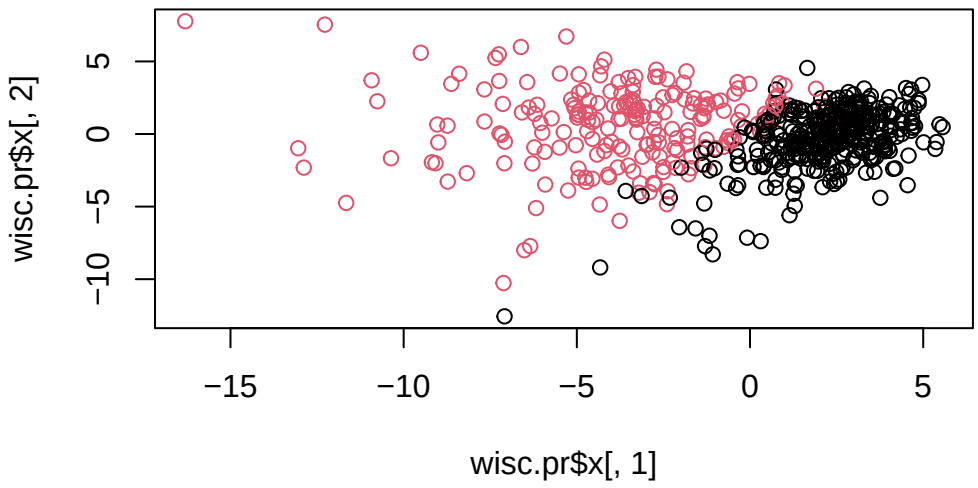
```
head(wisc.pr$x)
```

```
               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
```

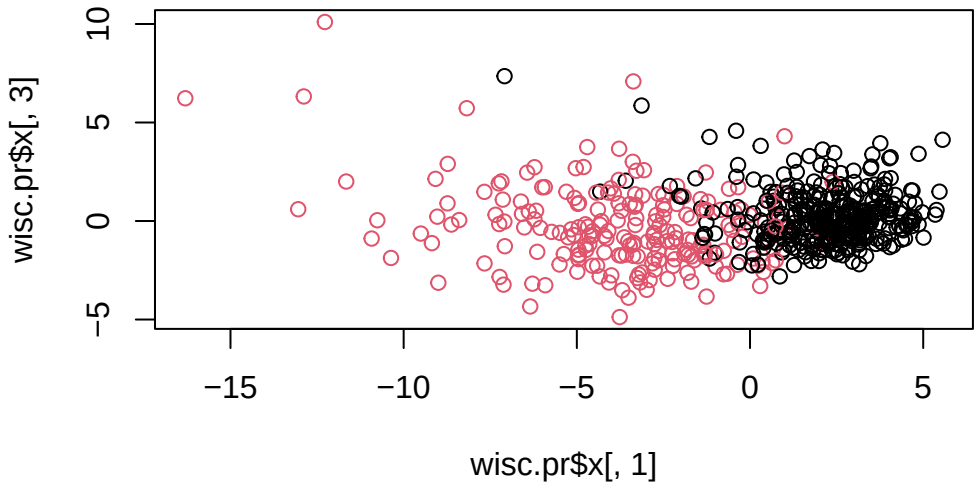
Plot of PC1 vs PC2 the first two columns

```
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?

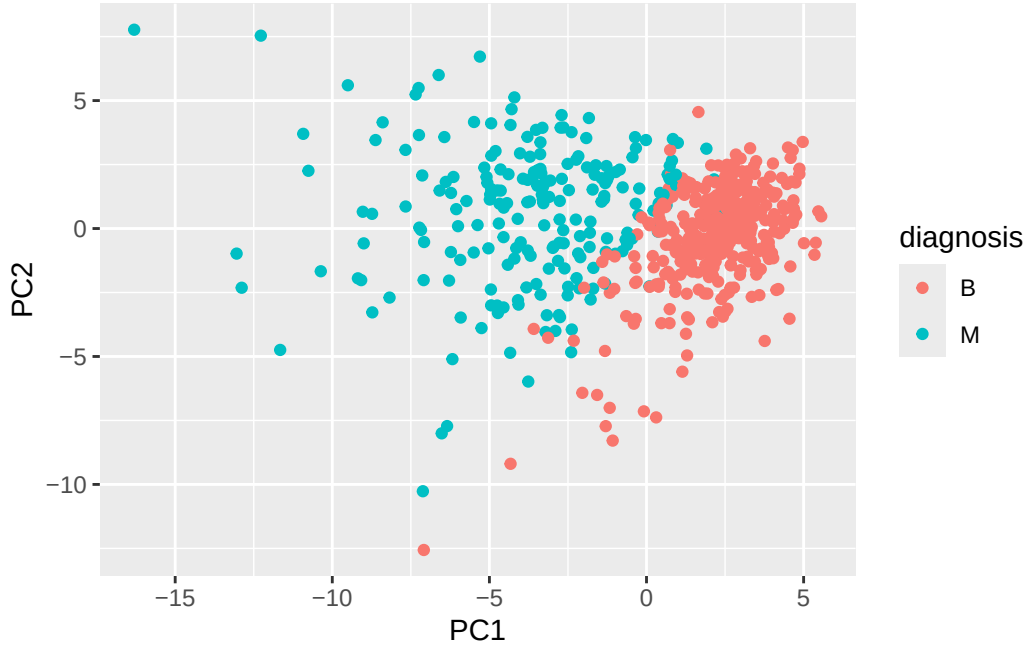
```
plot( wisc.pr$x[,1], wisc.pr$x[,3], col=diagnosis )
```



The values on the y-axis of this plot are much lower than the values on the y-axis of the other plot. PC3 is much different from PC2.

Make a ggplot version of the first score plot

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

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



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?

```
which(cumsum(pve) > 0.8)[1]
```

```
[1] 5
```

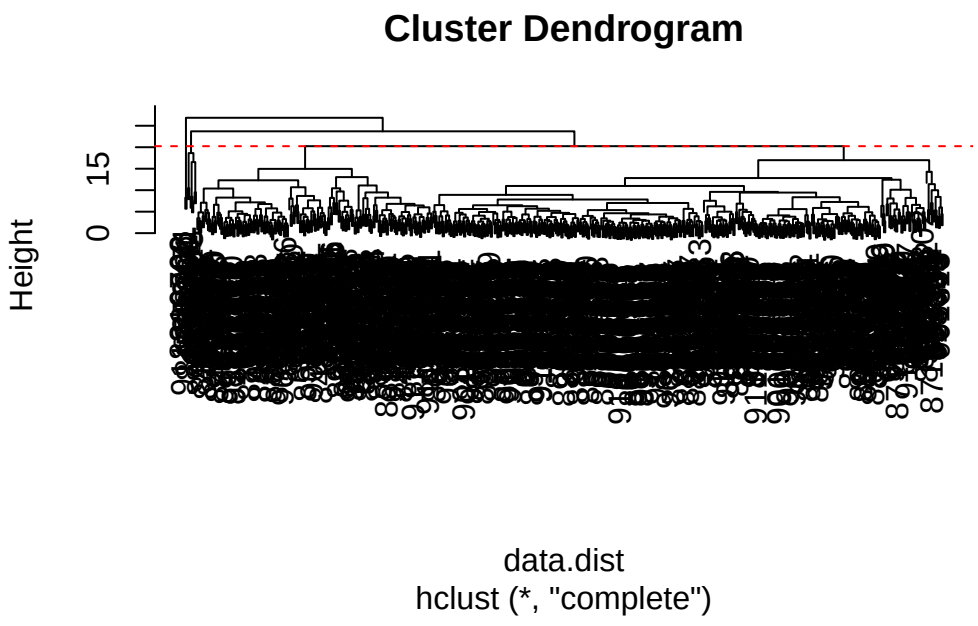
Hierarchical clustering

Results of 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)
heights <- sort(wisc.hclust$height, decreasing = TRUE)
height_for_4_clusters <- heights[3]
abline(h = height_for_4_clusters, col="red", lty=2)
```



At height 3, is the height at which the clustering model has 4 clusters.

Selecting number of clusters

```
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?

```
for (k in 2:10) {
  clusters <- cutree(wisc.hclust, k = k)
  cat("\nNumber of Clusters:", k, "\n")
  print(table(clusters, diagnosis))
}
```

```
Number of Clusters: 2
        diagnosis
clusters   B   M
       1 357 210
       2   0   2

Number of Clusters: 3
        diagnosis
clusters   B   M
       1 355 205
       2   2   5
       3   0   2

Number of Clusters: 4
        diagnosis
clusters   B   M
       1  12 165
       2   2   5
```

```
       3 343  40
       4   0   2

Number of Clusters: 5
        diagnosis
clusters   B   M
       1  12 165
       2   0   5
       3 343  40
       4   2   0
       5   0   2

Number of Clusters: 6
        diagnosis
clusters   B   M
       1  12 165
       2   0   5
       3 331  39
       4   2   0
       5  12   1
       6   0   2

Number of Clusters: 7
        diagnosis
clusters   B   M
       1  12 165
       2   0   3
       3 331  39
       4   2   0
       5  12   1
       6   0   2
       7   0   2

Number of Clusters: 8
        diagnosis
clusters   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

Number of Clusters: 9
        diagnosis
clusters   B   M
       1  12  86
       2   0  79
       3   0   3
       4 331  39
       5   2   0
       6  12   0
       7   0   2
       8   0   2
       9   0   1

Number of Clusters: 10
        diagnosis
clusters   B   M
      1   12  86
      2    0  59
      3    0   3
      4  331  39
      5    0  20
      6    2   0
      7   12   0
      8    0   2
      9    0   2
      10   0   1
```

Using different methods

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

Ward.D2 method is my favorite method because it creates compact, evenly-sized clusters. This method also reduces variance within each cluster and aligns better with classifications like, benign vs. malignant tumors in this data set.

OPTIONAL: K-means clustering

K-means clustering and comparing results

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

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

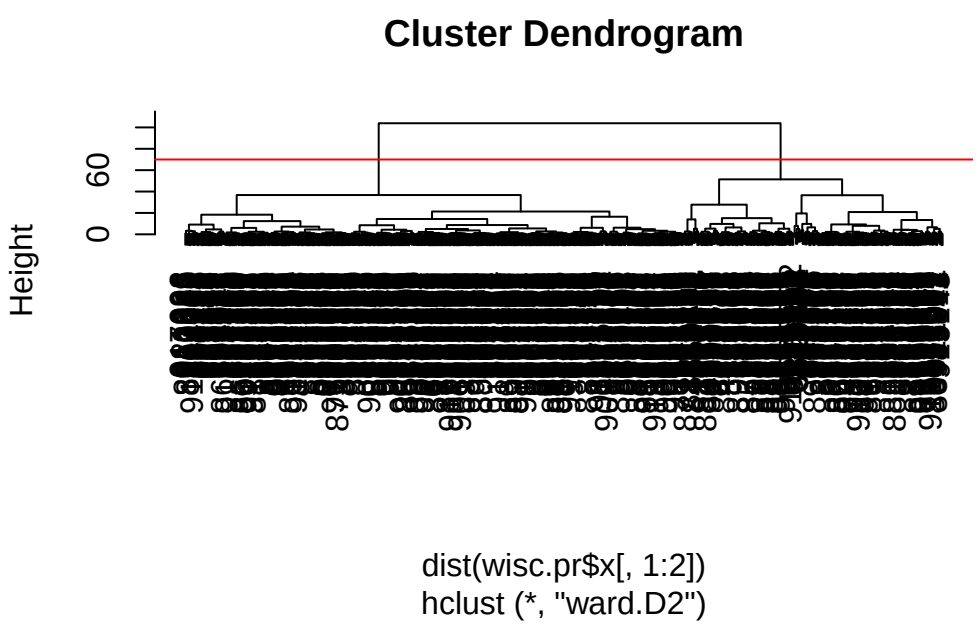
```
table(wisc.km$cluster, wisc.hclust.clusters)
```

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

Combining methods

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

```
grps <- cutree(hc, h=70, k=2)
table(grps)
```

```
grps
  1   2
195 374
```

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

Cross-table to see how my clustering groups correspond to the expert diagnosis vector of M and B values.

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

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

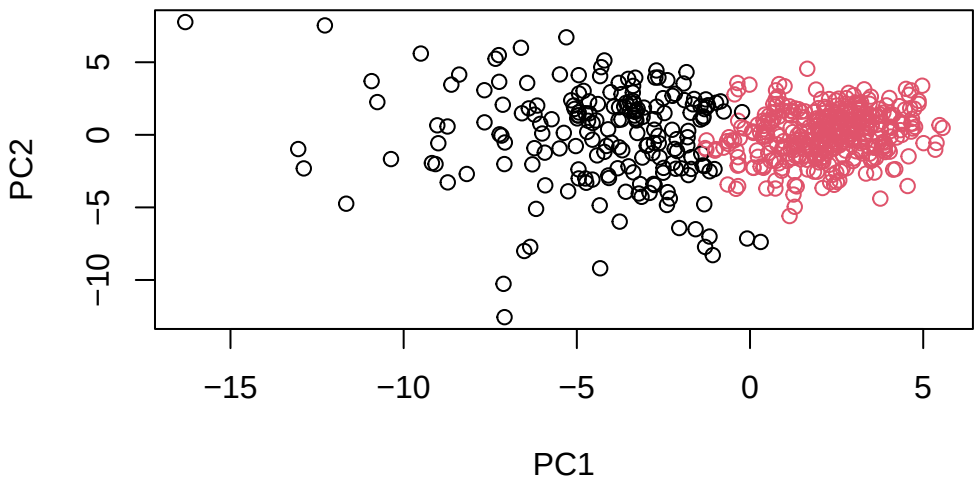
Positive => cancer M Negative => non-cancer B

True = cluster/grp 1 False = grp 2

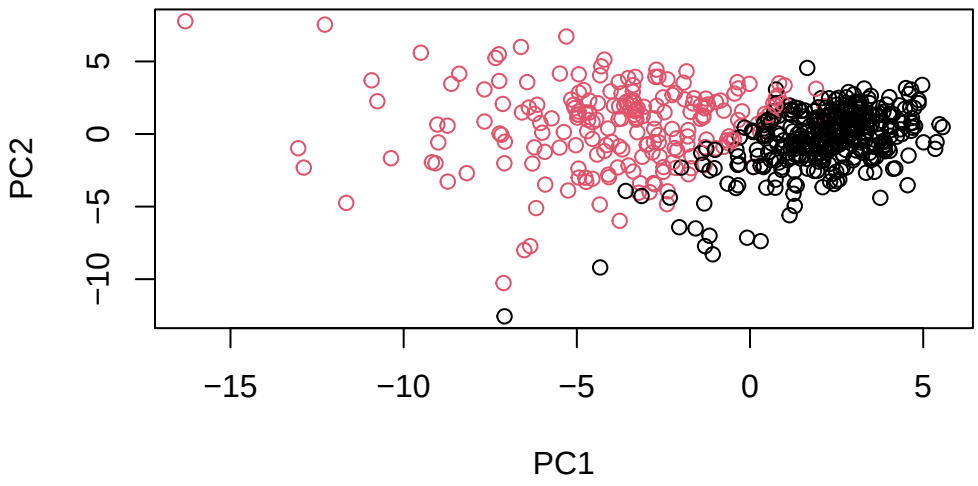
True Positive 177 False Positive 18 True Negative 339 False Negative 35

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

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




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



Clustering on PCA results

```
wisc.pr.dist <- dist(wisc.pr$x[, 1:7])
wisc.pr.hclust <- hclust(wisc.pr.dist, method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=4)
```

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

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

```
                    diagnosis
wisc.pr.hclust.clusters   B   M
                      1   0  45
                      2   2  77
                      3  26  66
                      4 329  24
```

The newly created model with four clusters separates out the two diagnoses shows a different distribution of diagnoses compared to the original model. Cluster 4 contains the majority of

the benign diagnoses, whereas the malignant diagnoses are more spread out between clusters 1, 2, and 3. This suggests the original clustering model is more efficient in separating the diagnoses.

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
```

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

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

The k-means clustering model provides a better separation between the two diagnoses, compared to the hierarchical clustering model. K-means effectively grouped most malignant cases into one cluster and most benign cases into another, despite some mis-classifications. Hierarchical clustering created four clusters, leading to more overlap between benign and malignant diagnoses, and thus a less distinct separation less.

Sensitivity/Specificity

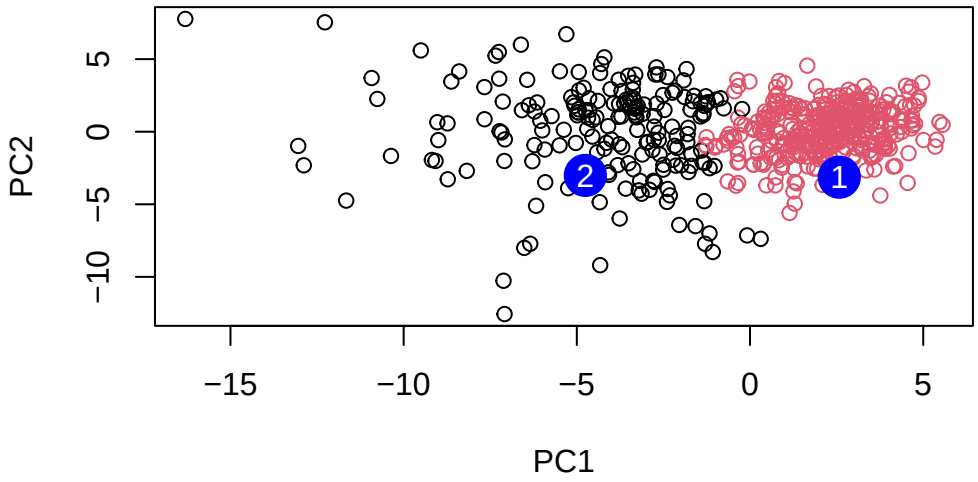
Q17. Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

The hierarchical clustering model with four clusters had better specificity in detecting benign cases compared to the k-means model. But, the k-means clustering model is better in sensitivity than the hierarchical clustering.

Prediction

```
#url <- "new_samples.csv"
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?

Based on these results, patient #2 should be prioritized for a follow up. This is because they are in the group of malignant.