Class 08: Machine Learning Mini Project

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Function focus for today: grep(), kmeans(), hclust(), prcomp()

#Import the dataset

Before we can begin our analysis we first have to download and import our data correctly into our R ression.

```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 samples are in this dataset?

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

```
[1] 569
```

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

```
[1] 31
```

> Q. How many variables (columns)?

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

```
[1] 31
```

> Q2. How many M and B samples are there?

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

```

  B   M 
357 212 
```

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

```r
txt <- c("_mean")
length(grep(txt, colnames(wisc.df), value =TRUE))
```

```
[1] 10
```

Q. what feathers are "mean" values?

```r
txt <- c("_mean")
grep(txt, colnames(wisc.df), value =TRUE)
```

```
 [1] "radius_mean"            "texture_mean"           "perimeter_mean"        
 [4] "area_mean"              "smoothness_mean"        "compactness_mean"      
 [7] "concavity_mean"         "concave.points_mean"    "symmetry_mean"         
[10] "fractal_dimension_mean"
```

I need to remove the first diagnosis column from my data before doing any analysis. I will store it for later.

```
# We can use -1 here to remove the first column
wisc.data <- wisc.df[,-1]
```

```
# Create diagnosis vector for later
diagnosis <- as.factor(wisc.df$diagnosis)
```

#2. Principal Component Analysis

The main PCA function in base R is called `prcom()`.

Before doing anything like PCA, it is important to check if the data need to be scaled before performing PCA. Recall two common reasons for scaling data include:

-The input variables use different units of measurement. -The input variables have significantly different variances.

```
#checking sd of data
round(apply(wisc.data, 2, sd), 2)
```

```
            radius_mean            texture_mean          perimeter_mean
                   3.52                    4.30                   24.30
              area_mean         smoothness_mean        compactness_mean
                 351.91                    0.01                    0.05
         concavity_mean     concave.points_mean           symmetry_mean
                   0.08                    0.04                    0.03
 fractal_dimension_mean               radius_se              texture_se
                   0.01                    0.28                    0.55
           perimeter_se                 area_se           smoothness_se
                   2.02                   45.49                    0.00
         compactness_se            concavity_se       concave.points_se
                   0.02                    0.03                    0.01
            symmetry_se    fractal_dimension_se            radius_worst
                   0.01                    0.00                    4.83
          texture_worst         perimeter_worst              area_worst
                   6.15                   33.60                  569.36
       smoothness_worst       compactness_worst         concavity_worst
                   0.02                    0.16                    0.21
   concave.points_worst          symmetry_worst fractal_dimension_worst
                   0.07                    0.06                    0.02
```

Looks like we need to scare by setting `scale = TRUE` in our `prcomp()` function call.

#Time for PCA

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

```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
                           PC8    PC9    PC10   PC11    PC12    PC13    PC14
Standard deviation     0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 0.39624
Proportion of Variance 0.01589 0.0139 0.01169 0.0098 0.00871 0.00805 0.00523
Cumulative Proportion  0.92598 0.9399 0.95157 0.9614 0.97007 0.97812 0.98335
                          PC15    PC16    PC17    PC18    PC19    PC20   PC21
Standard deviation     0.30681 0.28260 0.24372 0.22939 0.22244 0.17652 0.1731
Proportion of Variance 0.00314 0.00266 0.00198 0.00175 0.00165 0.00104 0.0010
Cumulative Proportion  0.98649 0.98915 0.99113 0.99288 0.99453 0.99557 0.9966
                          PC22    PC23   PC24    PC25    PC26    PC27    PC28
Standard deviation     0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 0.03987
Proportion of Variance 0.00091 0.00081 0.0006 0.00052 0.00027 0.00023 0.00005
Cumulative Proportion  0.99749 0.99830 0.9989 0.99942 0.99969 0.99992 0.99997
                          PC29    PC30
Standard deviation     0.02736 0.01153
Proportion of Variance 0.00002 0.00000
Cumulative Proportion  1.00000 1.00000
```

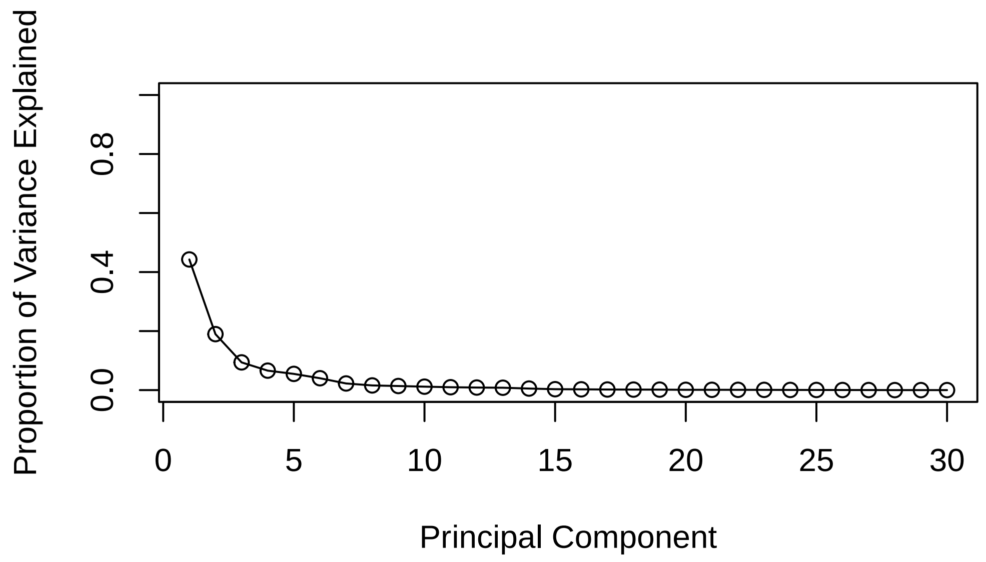
It’s good practice to make a SCREE plot and look for inflection point.

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

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

$class
[1] "prcomp"
```

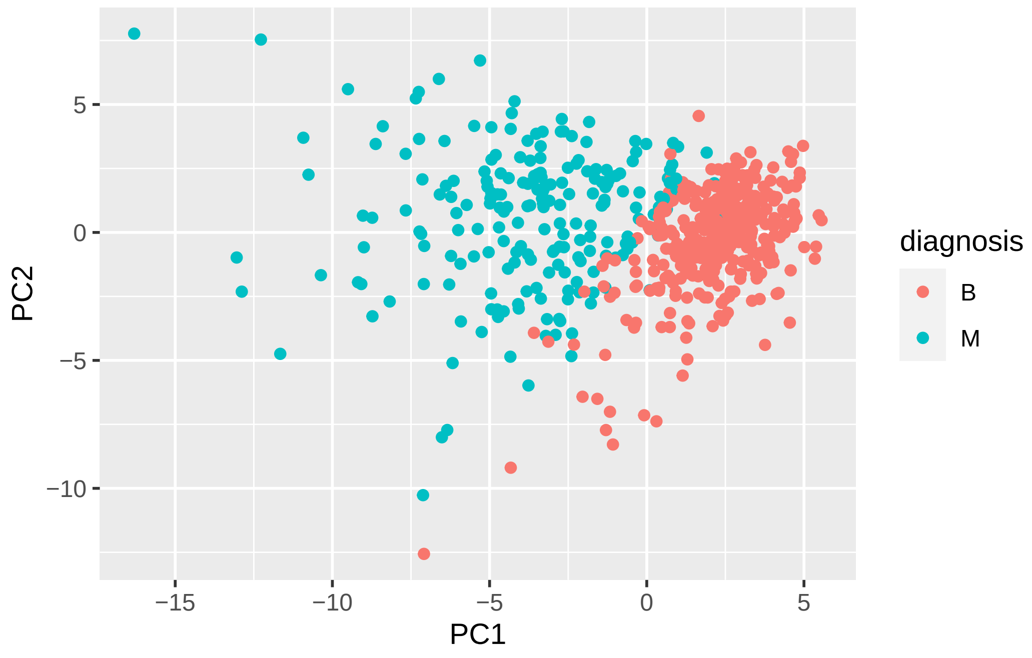
```r
pr.var <- wisc.pr$sdev^2
#proportion of variance
pve <- pr.var/sum(pr.var)
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



Let's make our main results figure from our PCA - our score plot (a.k.a "PC plot","PC1vsPC2 plot", etc)

```
library(ggplot2)
pc <- as.data.frame(wisc.pr$x)

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



#Hierachical clustering

Preparation for hierachical clustering, the distance between all pairs of observations are computed. Futhhermore, there are different ways to link clusters together, with single, complete, and average being teh most common "linkage methods.

We can try clustering the original data with `hclut()` or `kmeans()`

First scale wisc.data and and assign the result to data.scaled.

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

```
head(apply(data.scaled,2, sd))
```

```
    radius_mean      texture_mean    perimeter_mean         area_mean 
              1                 1                 1                 1 
smoothness_mean compactness_mean 
              1                 1 
```

Calculate the (Euclidean) distance between all pairs of observations in teh new scaled dataset and assign the result to data.dist.

Create a hierarchical clustering model using complete linkage. Manually specify the method argument to hclust() and assign the results to wisc.hclust.

```r
wisc.hclust <- hclust(dist(data.scaled))
wisc.hclust
```

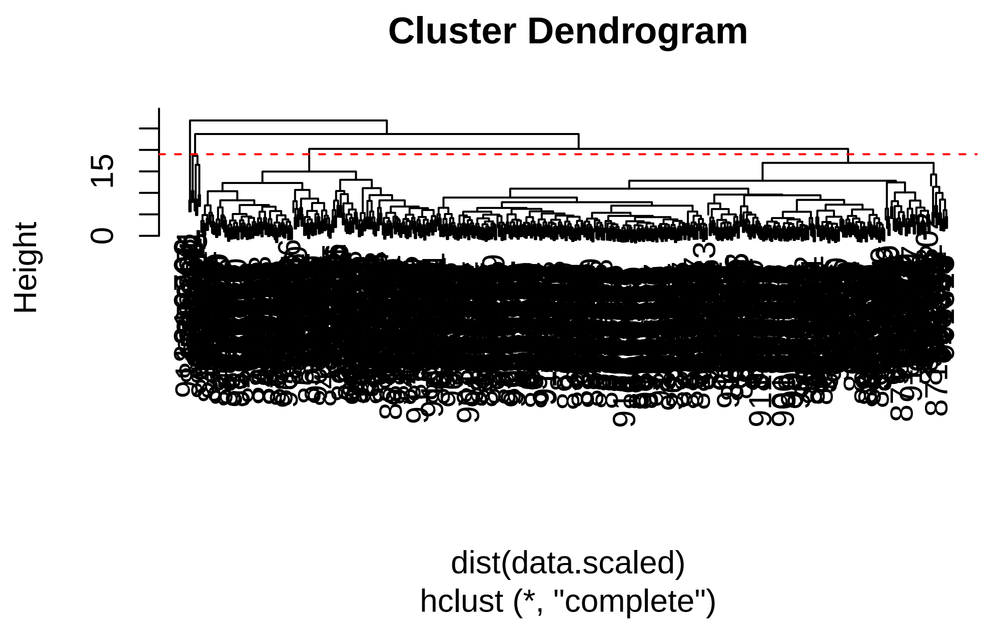
```

Call:
hclust(d = dist(data.scaled))

Cluster method   : complete 
Distance         : euclidean 
Number of objects: 569 
```

Let's use the hierarchical clustering model you just created to determine a height (or distance between clusters) where a certain number of clusters exists.

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



To get a cluster membership vector I will use the `cutree()` function and "cut" into 4 or so grps or clusters.

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

```
grps
  1   2   3   4 
177   7 383   2 
```

I can also use the `table()` to cross tabulate…

```r
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

We can use the table() function to compare the cluster membership to the actual diagnoses.

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

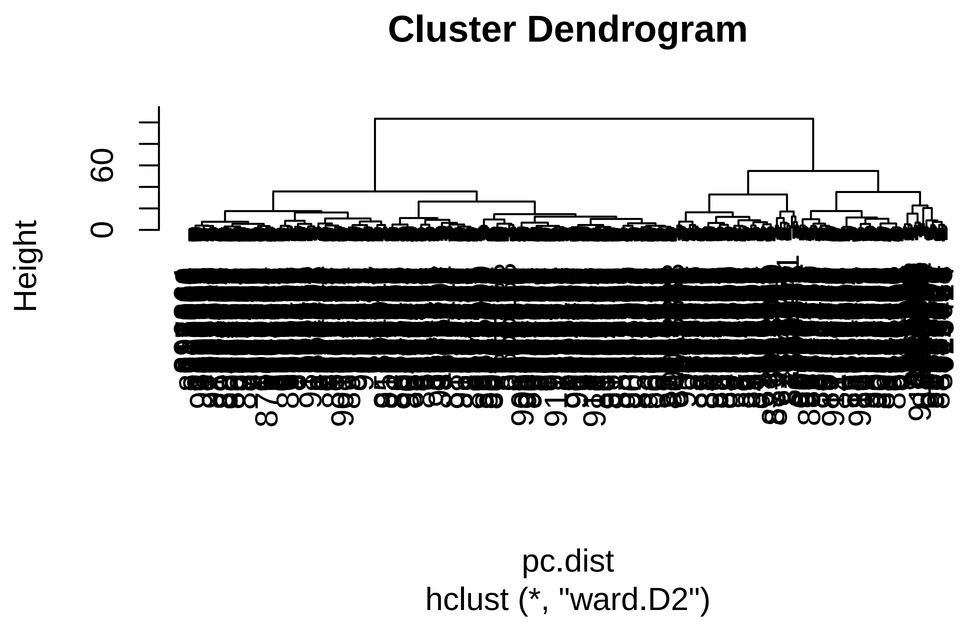
```
    diagnosis
grps   B   M
   1  12 165
   2   2   5
   3 343  40
   4   0   2
```

#Clustering on PCA results

I can cluster in PC-space and use as many or as few PCs as I want.

To start with I will use 3 PCs, that is I will cluster along PC1, PC2, and PC3. Those 3 PCs capture about 70% of variance.

```r
#calculate distance and select columns 1:3 for PC1-3.
pc.dist <- dist(wisc.pr$x[,1:3])
#use hclust
wisc.pr.hclust <- hclust(pc.dist, method = "ward.D2")
#plot
plot(wisc.pr.hclust)
```



This looks much nicer than our previous clustering result. Let's find the two major clusters wiht `cutree` function.

This looks much more promising than our previous clustering results on the original scaled data. Note the two main branches of or dendrogram indicating two main clusters - maybe these are malignant and benign. Let's find out!

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

```
    diagnosis
grps   B   M
   1  24 179
   2 333  33
```

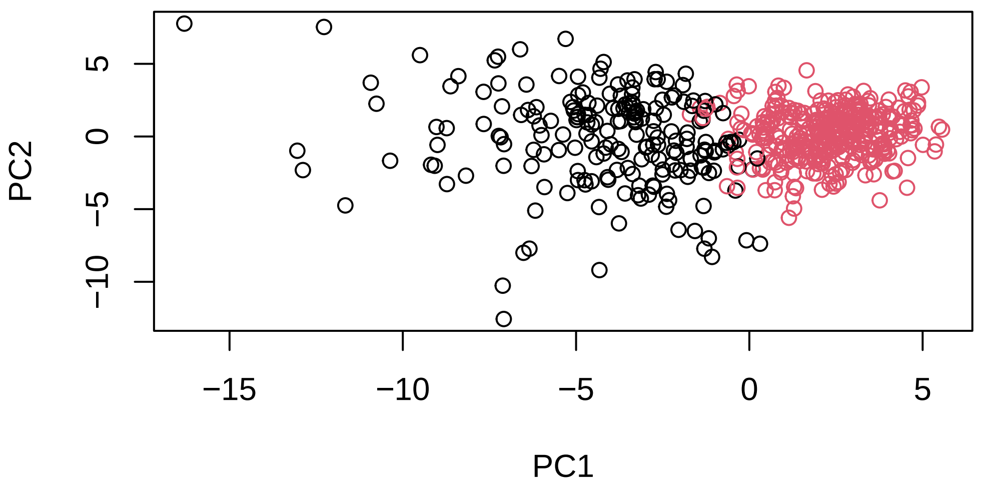
```
#According to our clustering. Cluster 1 groups is associated with malignancy and Cluster 2
```

We could calculate accuracy - the proportion of samples we got correct if we take cluster 1 to represent all M and cluster 2 to represent all B.

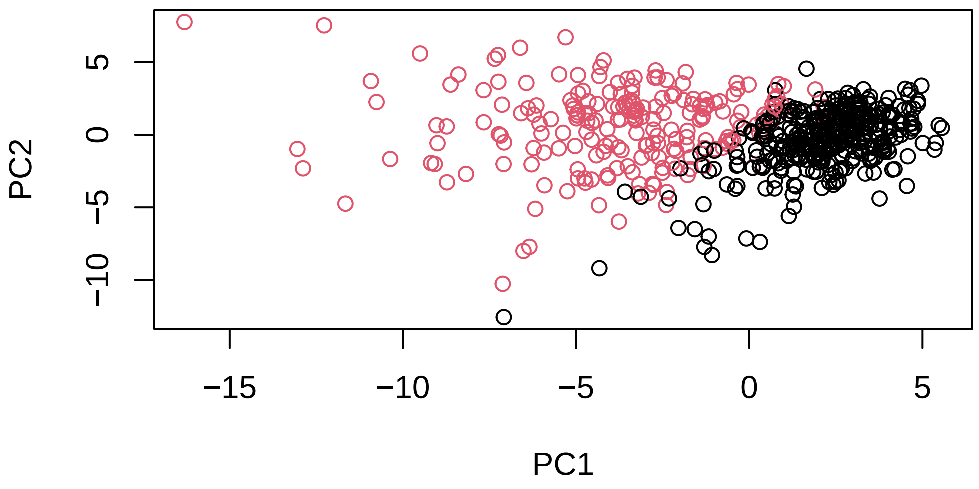
```
(179+333)/nrow(wisc.data)
```

```
[1] 0.8998243
```

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



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



> Q.14 How well do the 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

We could calculate accuracy - the proportion of samples we got correct if we take cluster 1 to represent all M and cluster 2 to represent all B.

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

```
[1] 0.8998243
```

#Sensitivity/Specificity

Sensitivity refers to a test's ability to correctly detect ill patients who do have the condition. In our example here the sensitivity is the total number of samples in the cluster identified as predominantly malignant (cancerous) divided by the total number of known malignant samples. In other words: TP/(TP+FN).

#According to our clustering. Cluster 1 groups is associated with malignancy and Cluster 2 groups is associated with benign. When we table our clusters and sort by diagnosis, we notice that in Cluster 1 and Cluster 2 we have patients that are B/M, so false positives or flase negatives and this can be used to calculate sensitivity/specificity

```r
TP = 179
FN = 24

table(grps, diagnosis)
```

```
    diagnosis
grps   B   M
   1  24 179
   2 333  33
```

```r
sensitivity <- TP/(TP+FN)
sensitivity
```

```
[1] 0.8817734
```

Specificity relates to a test's ability to correctly reject healthy patients without a condition. In our example specificity is the proportion of benign (not cancerous) samples in the cluster identified as predominantly benign that are known to be benign. In other words: TN/(TN+FN)

```r
TN = 333
FN = 33
specificity <- TN/(TN+FN)
specificity
```

```
[1] 0.9098361
```

Specificity relates to a test's ability to correctly reject healthy patients without a condition. In our example specificity is the proportion of benign (not cancerous) samples in the cluster identified as predominantly benign that are known to be benign. In other words: TN/(TN+FN).

> Q15. OPTIONAL: Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

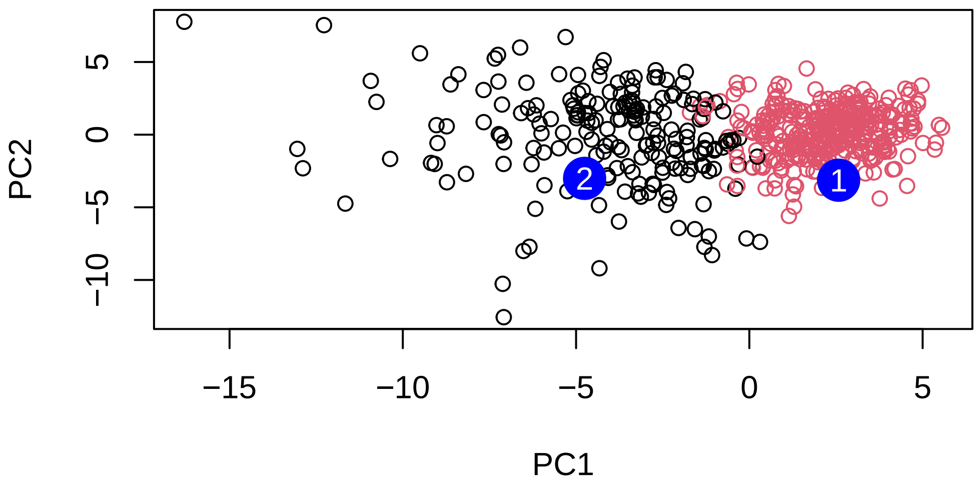
#Prediction We will use the predict() function that will take our PCA model from before and new cancer cell data and project that data onto our PCA space.

```r
#url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
```

```r
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
```

```r
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")
```



Q16. Which of these new patients should we prioritize for follow up based on your results? patient 2