# class 08: Brest Cancer Mini Project

## Background

In today's class we will apply the methods and techniques clustering and PCA to help make sense of a real world breast cancer FNA biopsy data set.

## Data Import

We start by importing our data. It is a CSV file so we will use the `read.csv()` function.

```
wisc.df <- read.csv("wisconsinCancer.csv", row.names = 1)
```

have a wee peak at the first few rows

```
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
```

Make sure to remove the first `diagnosis` colum - I dont want to use this for my mashine learning models. We weill use it later to compare our results to the expert diagnosis.

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

### Exploratory data analysis

> Q1. How many observations are in this dataset?

```
nrow(wisc.data)
```

```
[1] 569
```

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

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

```
[1] 212
```

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

```

  B   M 
357 212 
```

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

```
#colnames(wisc.data)
length(grep("_mean", colnames(wisc.data)))
```

```
[1] 10
```

### Principal Component Analysis

The main data function here is `prcomp()` and we want to make sure we set the optional argument `scale=TRUE`:

```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
```

> Q4. From your results, what proportion of the original variance is captured by the first principal component (PC1)? 0.4427 or 44%

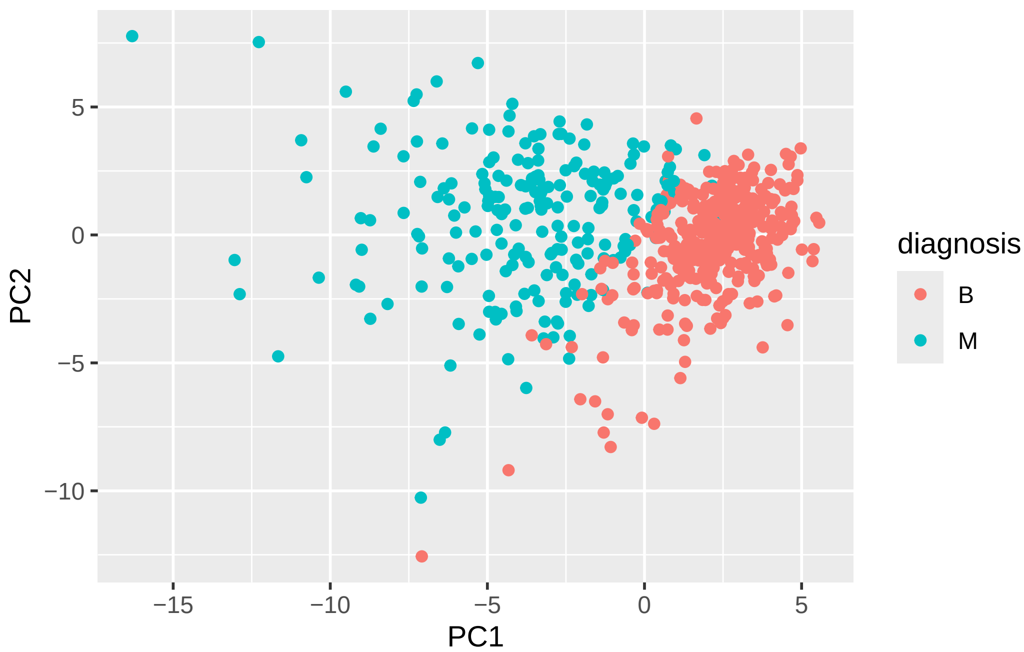
> Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data? at least 3 PC's would be 72%

> Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data? at least 7 PC's would yeild 91%

Our main PCP "score plot" of results:

```r
library(ggplot2)
```

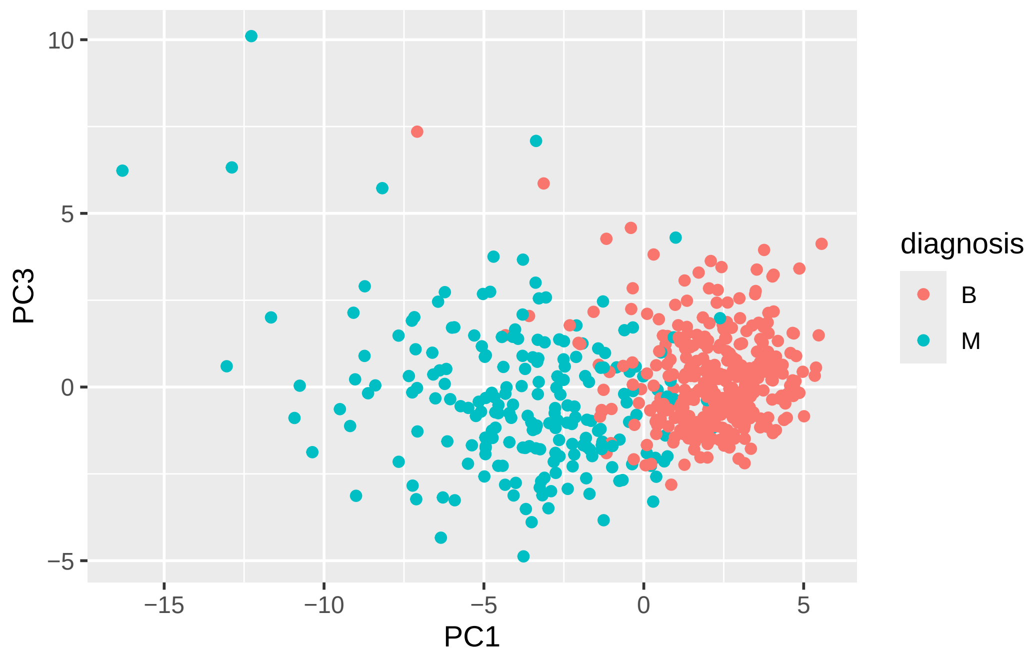
```r
ggplot(wisc.pr$x) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point()
```




Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why? I notice that the similar compnets cluster together either B or M but it is dificult to understand because we need to make our own plots so we can make sense of these PCA's. The low weight PC dont contrubute as much.

Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots? I notice they are more toweds the bottom of the graph now

```
ggplot(wisc.pr$x) +
  aes(PC1, PC3, col=diagnosis) +
  geom_point()
```



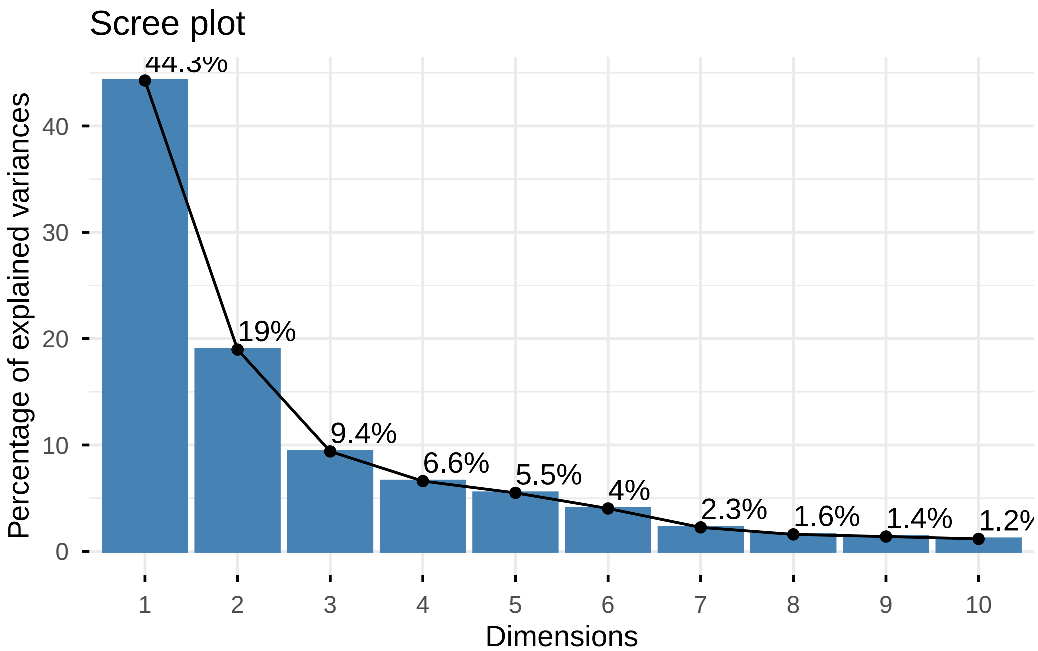

Scree-plot:

```
library(factoextra)
```

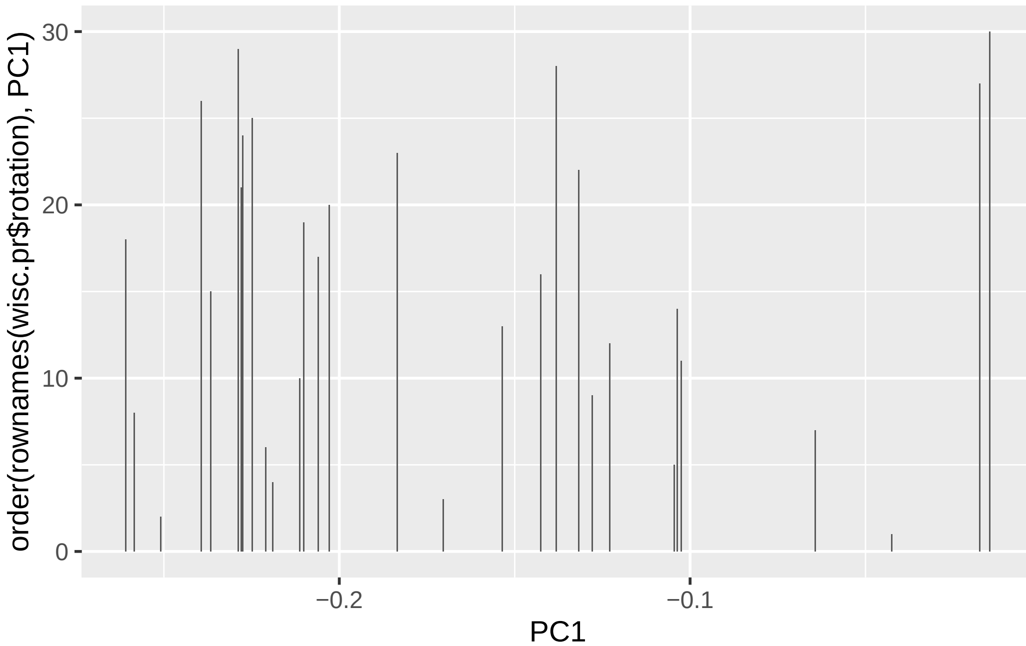
```
Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
```

```
fviz_eig(wisc.pr, addlabels = TRUE)
```

```
Warning in geom_bar(stat = "identity", fill = barfill, color = barcolor, :
Ignoring empty aesthetic: `width`.
```




```
ggplot(wisc.pr$rotation) +
  aes(PC1,
      order( rownames(wisc.pr$rotation), PC1) ) +
  geom_col()
```




Collectively these two plots ("score plot" and "loading plot") tell us that if cells nucleus are deeply indented ("concave"), irregular non circular ("compactness"), and have large "perimeter" values they tend to be malignant….

> 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? This tells us how much this original feature contributes to the first PC. Are there any features with larger contributions than this one?

```
wisc.pr$rotation["concave.points_mean", 1]
```

```
[1] -0.2608538
```

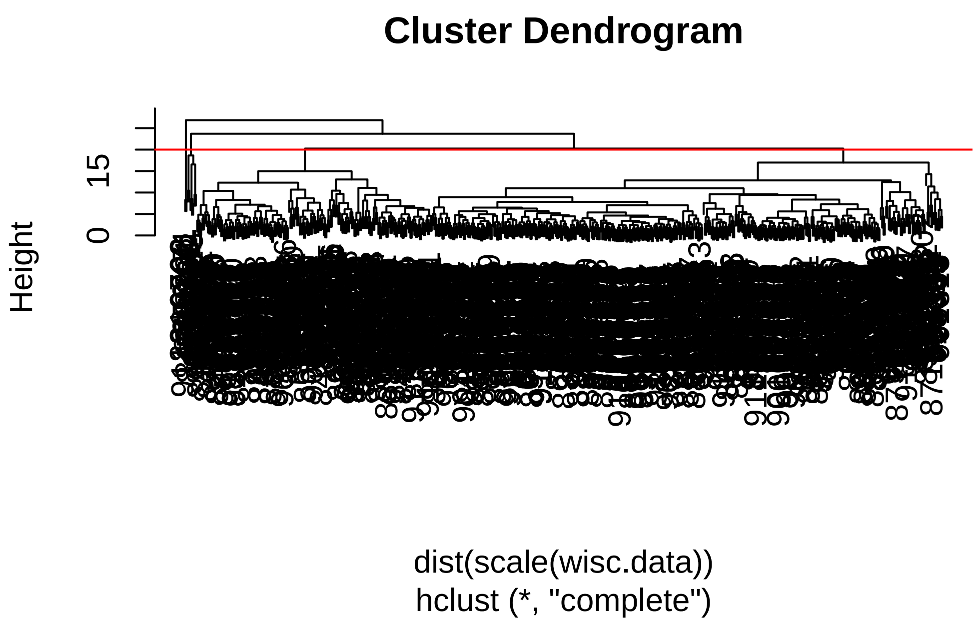
## Hierarchical clustering

First scale the data (with the `scale()` function), then calculate a distance matrix (with the `dist()` function). Then cluster with the `hclust()` function and plot:

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

> Q10. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

```r
plot(wisc.hclust)
abline(h=20, col="red")
```




you can also use `cutree()` function with argument `k=4` rather than`h=hight`

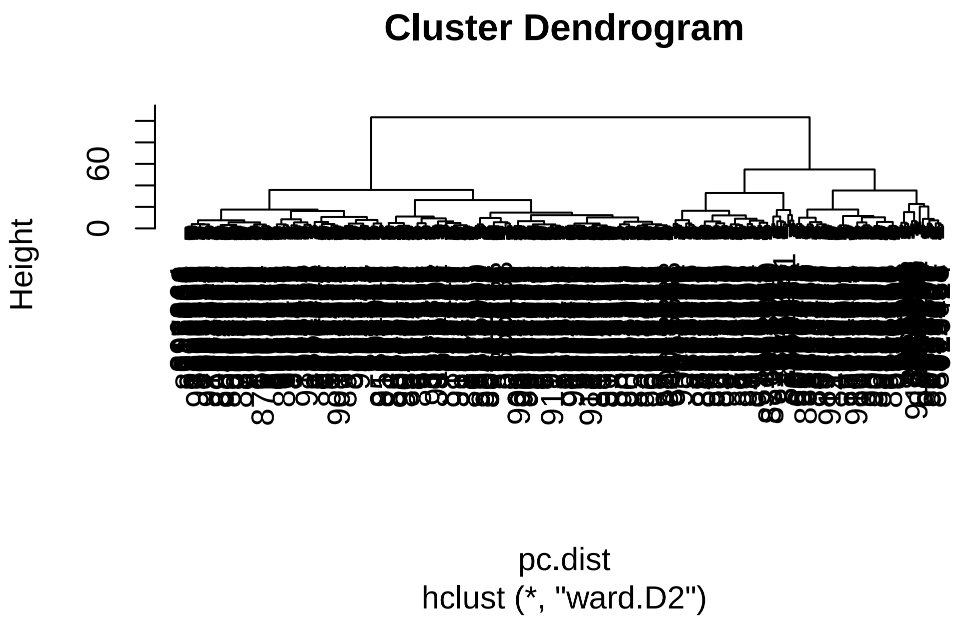
```r
wisc.hclust.clusters <- cutree(wisc.hclust, k=4)
table(wisc.hclust.clusters)
```

```
wisc.hclust.clusters
  1   2   3   4 
177   7 383   2 
```

### Combining methods

Here we will taek out PCA results and use thoes as input for clustering. i other words our `wisc.pr$x` scores that we plotted above (the main output from PCA - how the data lie on our new principal componet axis/variables) and use the subset of these PC's that capture the most variance as input for `hclust()`.

```r
pc.dist <- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <- hclust(pc.dist, method= "ward.D2")
plot(wisc.pr.hclust)
```




Cut the deprogram/tree into two main groups/clusters:

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

```
grps
  1   2 
203 366 
```

I wan to know how the clustering in **grps** with values of 1 or 2 correspond to the expert **diagnosis**

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

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

My clustering **groups 1** are mostly "M" diagnosis (179) and my clustering **group 2** are mostly "B" diagnosis

24 FP 179 TP 333 TN 33 FN

Sensitivity TP/(TP+FN)

```
179/(179+33)
```

```
[1] 0.8443396
```

Specificity TN/(TN+FP)

```
333/(333+24)
```

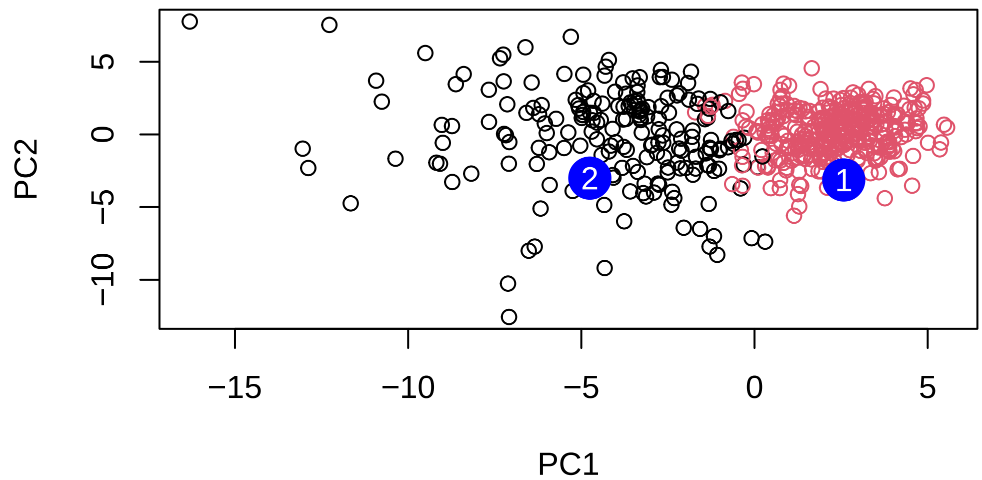
```
[1] 0.9327731
```

> Q15. OPTIONAL: Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity? There is high specificity and strong sensitivity compared to clustering on the orignial 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=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? Cluster 1 should be prioritized for a follow up because they are malignant.