Class 8: Breast Cancer Mini Project

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Background

In today’s class we will be employing all the R techniques for data analysis that we have learned thus far - including machine learning methods of clustering and PCA - to analyze real breast cancer biopsy data.

Importing Our Data

Before we start analyzing we need to make sure the data is uploaded into the project so we can access it.

```r
fna.data <- "WisconsinCancer.csv"
wisc.df <- read.csv(fna.data, row.names=1)
head(wisc.df, 4)
```

```
         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
         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
         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
         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
         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
         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
         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
         fractal_dimension_worst
842302                   0.11890
842517                   0.08902
84300903                 0.08758
84348301                 0.17300
```

We don’t want the diagnosis column in our data so we have to remove it and create a new vectors `diagnosis` so we can access both if needed. We can compare our findings to the experts with it after we are done.

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

> Q1. How many observations are in this dataset?

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

```
[1] 569
```

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

```
sum(diagnosis == "M")
```

```
[1] 212
```

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

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

```
[1] 10
```

Performing PCA!

The main function in base R is called `prcomp()` we will use the optional argument `scaling=T` here as the data columns/features/dimensions are on very different scales in the orginal data set.

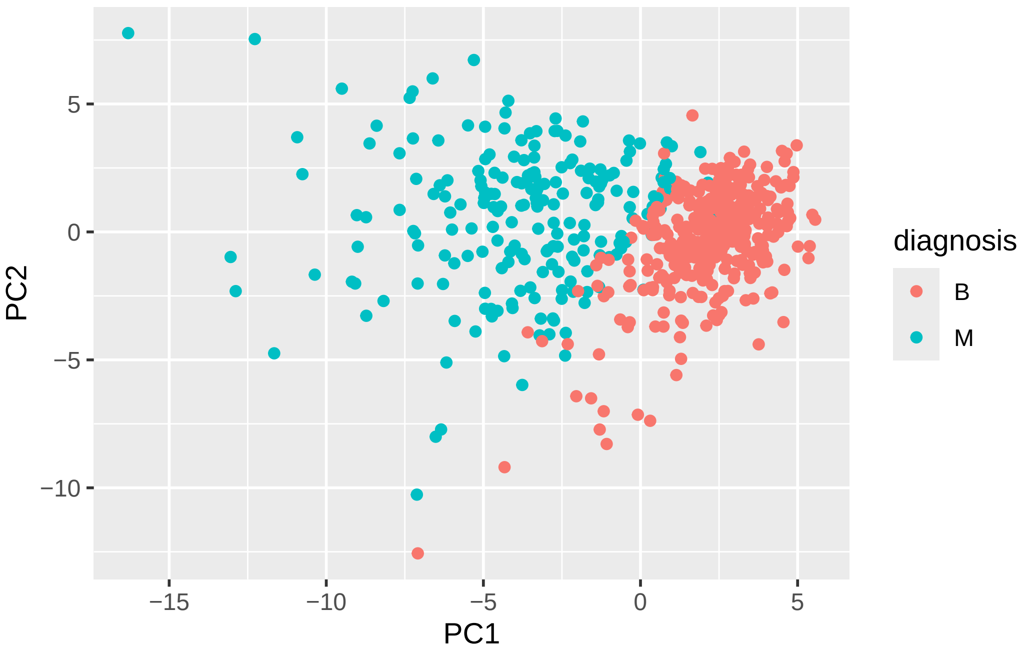
```
wisc.pr <- prcomp(wisc.data, scale = T)
summary(wisc.pr)
```

```
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
```

```r
library(ggplot2)

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



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

0.44272 is captured within PC1

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

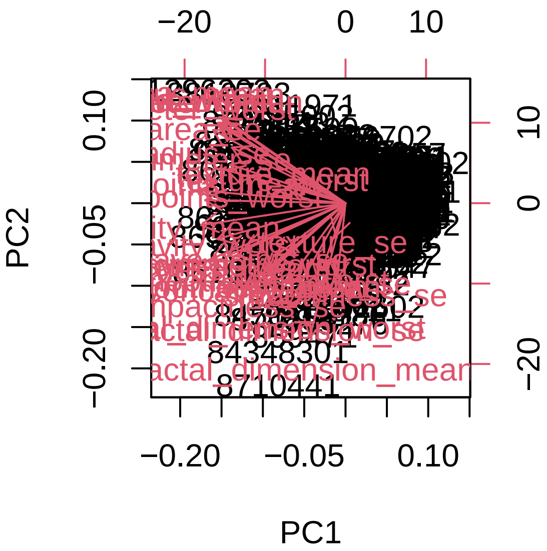
It took 3 PCs to describe at least 70% of the original variance in the data.

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

It takes 7 PCs to describe at least 90% of the original variance.

Interpreting PCA results

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



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

This plot is very confusing to understand and interpret as it is all overlapped. What stands out to me is the tight spread in the plot, all within +- 0.20.

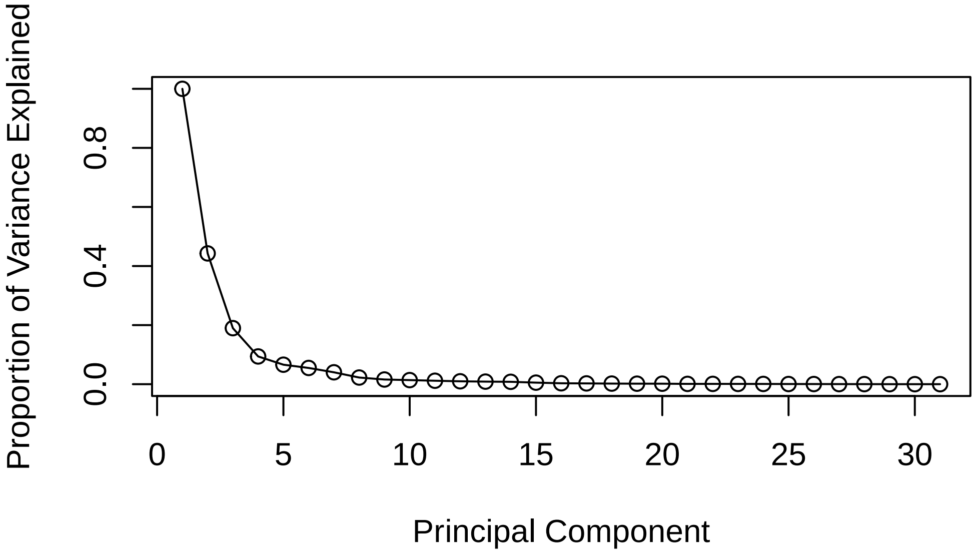
Explaining our Variance with a screen plot

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



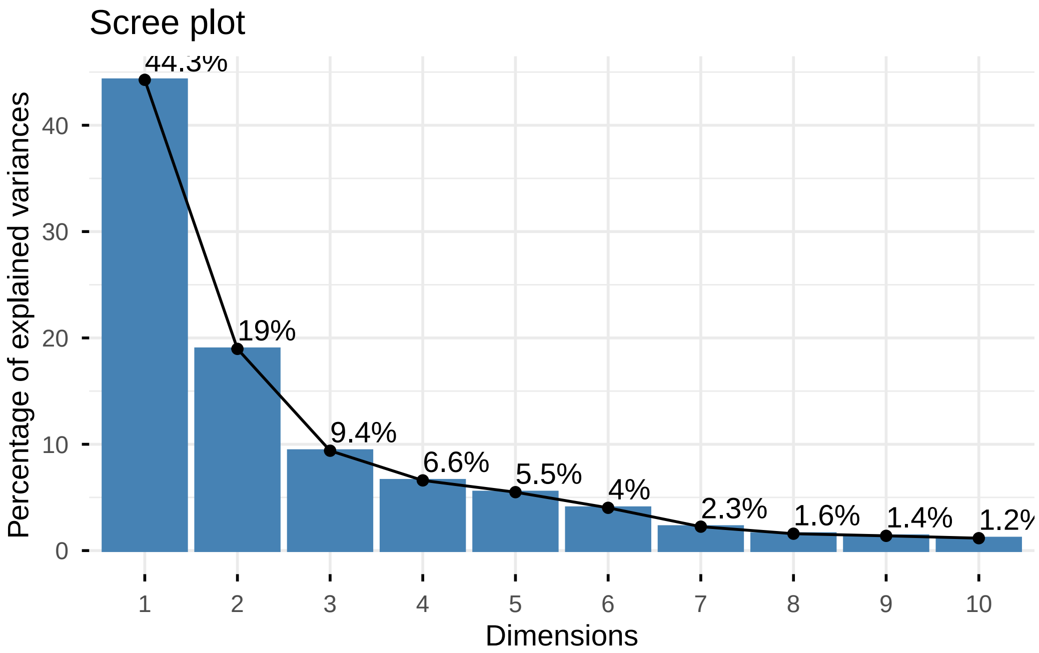
Screen plot

```
library(factoextra)
```

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

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

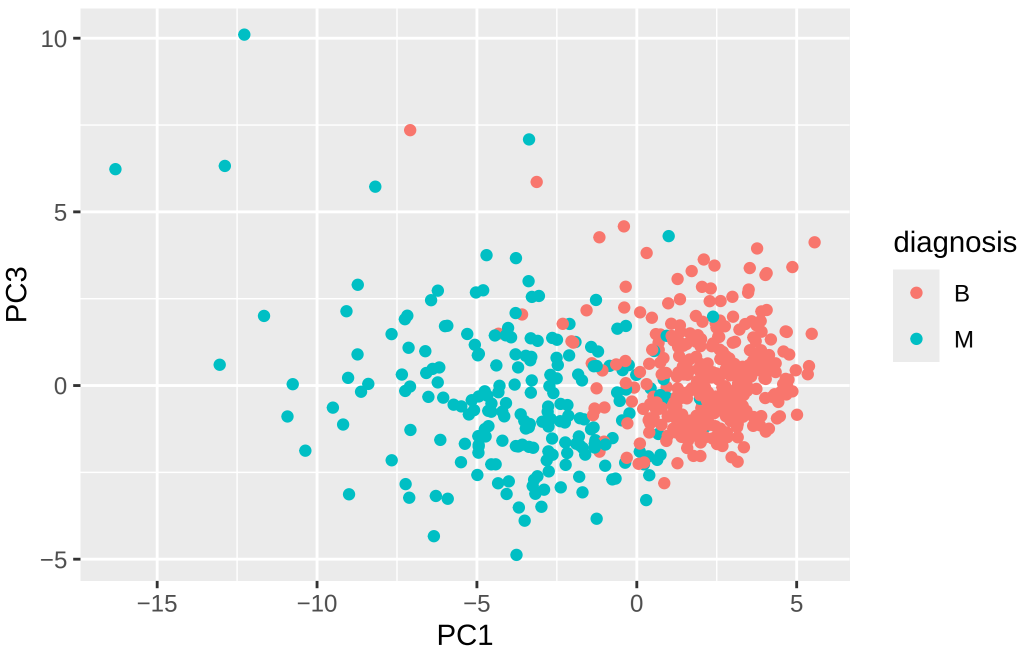
```
Warning in geom_bar(stat = "identity", fill = barfill, color = barcolor, :
Ignoring empty aesthetic: `width`.
```



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

```
library(ggplot2)

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



I notice there is still a pretty strong divide between M and B and it is fairly clear where there is a difference

> 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", "PC1"]
```

```
[1] -0.2608538
```

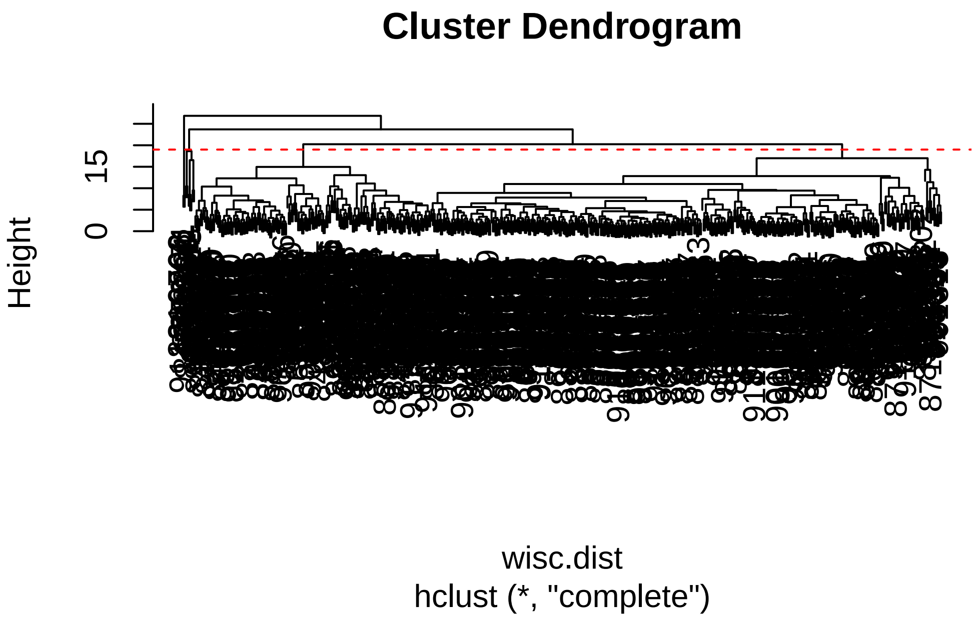
I could not find any feature with larger contributions.

4. Hierarchal Clustering

The goal of this section is to do hierarchical clustering of the original data to see if there is any obvious grouping into malignant and benign clusters.

First we will scale our `wisc.data` then calculate a distance matrix then pas to `hclust()`

```r
wisc.dist <- dist( scale(wisc.data))
wisc.hclust <- hclust(wisc.dist)
plot(wisc.hclust)
abline(h = 19, col = "red", lty = 2)
```



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

~19

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

```
wisc.hclust.clusters
  1   2 
567   2 
```

> Q12. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

Ward.D2 hierarchical clustering on the PCA-transformed data, the separation between diagnoses is much better than when clustering the original variables.

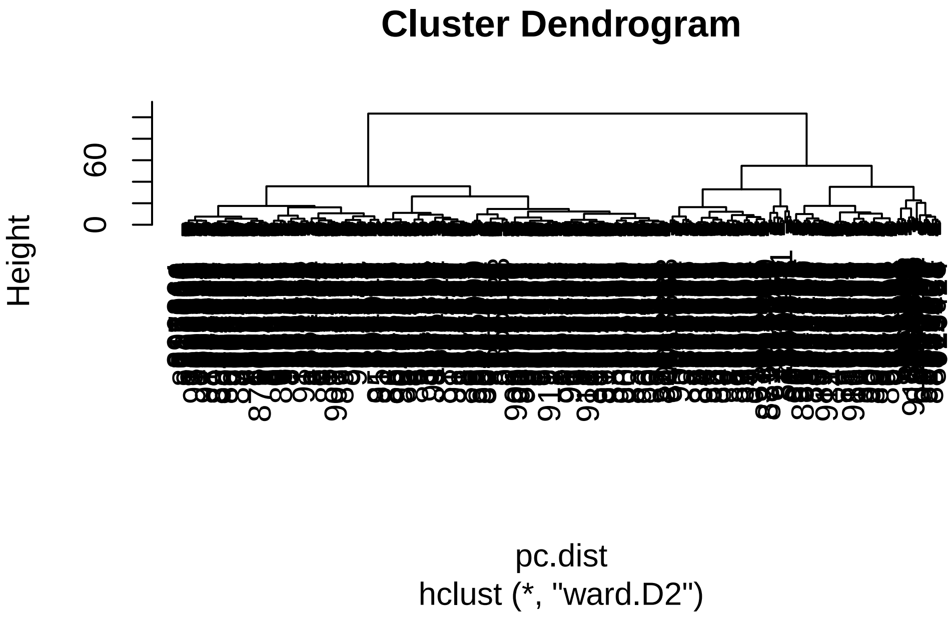
Combining Method

The idea here is that I can take my new variables (i.e. the scores PCs `wisc.pr$x`) that are better descriptors of the data-set than the original features (i.e. the 30 columns in `wisc.data`) and use these as a basis for clusting.

```
pc.dist<- dist(wisc.pr$x[,1:3])

wisc.pr.hclust <- hclust(pc.dist, method = "ward.D2")

plot(wisc.pr.hclust)
```



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

```
grps
  1   2
203 366
```

```
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

> Q13. How well does the newly created hclust model with two clusters separate out the two "M" and "B" diagnoses?

I can now run `table()` with both my clustering `grps` and the expert diagnoses

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

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

Our cluster "1" has 179 "M" diagnosis

However, cluster "2" has 333 "B" diagnosis

Group 1: 179 = True positive 24 = False positives

Group 2: 333 = True negative 33 = False negative

Sensitivity: TP/(TP+FN)

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

```
[1] 0.8443396
```

Specificity: TN(TN+FP)

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

```
[1] 0.9327731
```

> Q14. How well do the hierarchical clustering models you created in the previous sections (i.e. without first doing PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.hclust.clusters and wisc.pr.hclust.clusters) with the vector containing the actual diagnoses.

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

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1 357 210
                   2   0   2
```

This means the clustering largely fails to distinguish between benign and malignant tumors

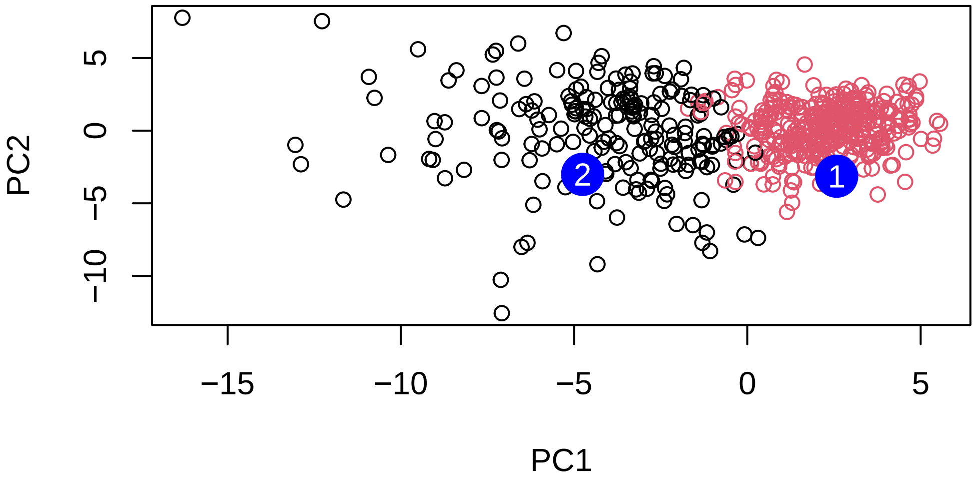
Prediction

We can use our PCA model for prediction of new un-seen cases!

```
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?

Patient 2 is malignant and 1 is benign so we would want to follow up with patient 2 most likely first.