Class08_Mini_Project

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Background

In today's class we will be using all the R techniques for data analysis that we have learned so far ,including the machine learning methods of clustering and PCA, to anlayze real breast cancer biopsy data.

Data Import

The data is in CSV format:

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

Let's look at the data

```r
head(wisc.df,3)
```

```
         diagnosis radius_mean texture_mean perimeter_mean area_mean
842302           M       17.99        10.38          122.8      1001
842517           M       20.57        17.77          132.9      1326
84300903         M       19.69        21.25          130.0      1203
         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
         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
         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
         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
         perimeter_worst area_worst smoothness_worst compactness_worst
842302             184.6       2019           0.1622            0.6656
842517             158.8       1956           0.1238            0.1866
84300903           152.5       1709           0.1444            0.4245
         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
         fractal_dimension_worst
842302                   0.11890
842517                   0.08902
84300903                 0.08758
```

Q1. How many observations are in this data set?

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

```
[1] 569
```

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

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

```

  B   M 
357 212 
```

Here we have 357 observations that are benign and 212 observations that are malignant.

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

```
sum(grepl(pattern = "_mean", x = colnames(wisc.df)))
```

```
[1] 10
```

We now need to remove the `diagnosis` column before we do any further analysis of this data set, we don't want to pass the is to PCA. WE will save it as a separate vector that we can use later to compare our fundings to those of experts.

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

Principal Component Analysis (PCA)

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

The main function in base R is called `prcomp()`

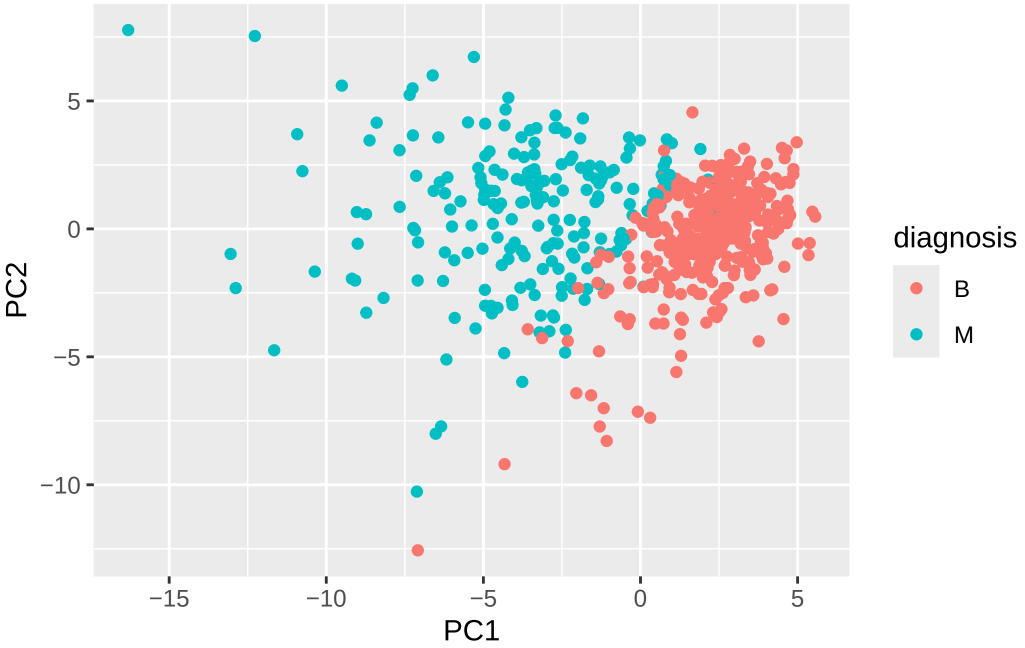
```
wisc.pr <- prcomp(wisc.data, scale=T)
```

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

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

$class
[1] "prcomp"
```

```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)?

```r
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
```

The proportion of variance captured by PC1 is 44.27% of the variance.

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

You need three principal components to describe at least 70% of the variance.

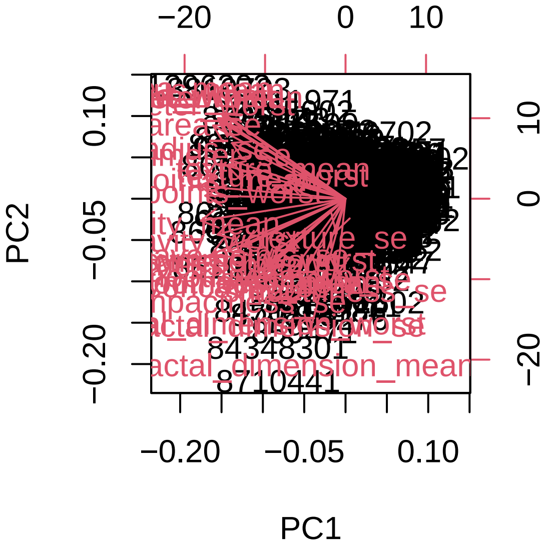
> Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

You need seven principal components to capture 90% of the data.

##Interpreting PCA results

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

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



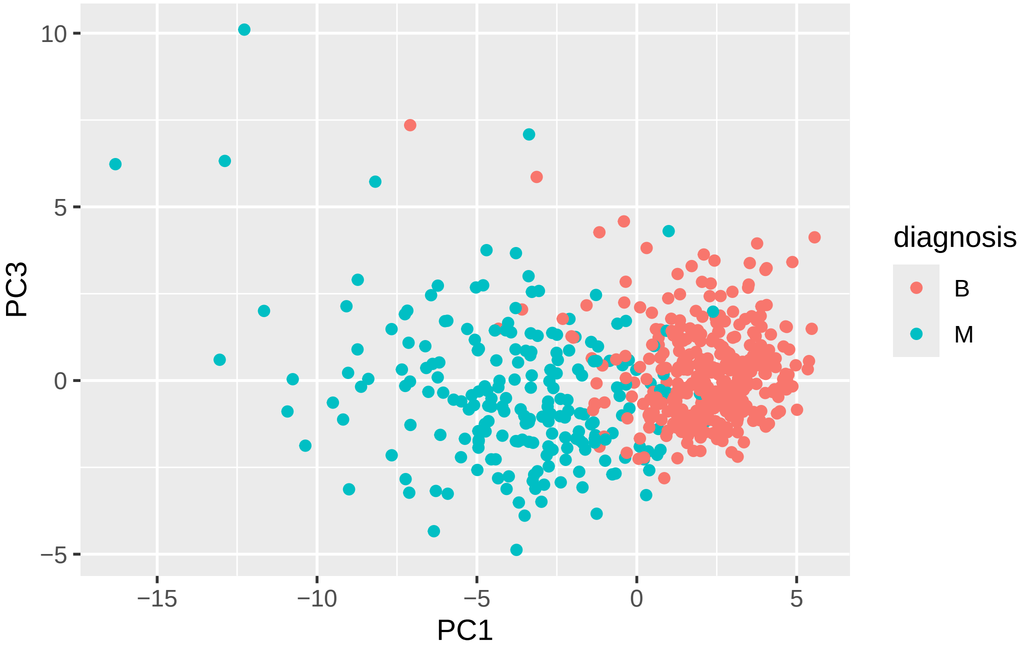
This plot is very hard to read there are too many data points and labels for anyone to tell what they are looking at.

Making it clear

We made it more clear earlier by using ggplot to plot PC1 vs PC2 to determine the trends seen in patients who had malignant and begnin masses.

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

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



The two plots are very similar in terms of the separation between malignant and benign observations but lie on a more linear scale.

##Variance Explained

A scree plot shows how much variance each PC captures. We typically look for an "elbow" — a point where adding more PCs gives diminishing returns. This can help us decide how many PCs to consider for further analysis.

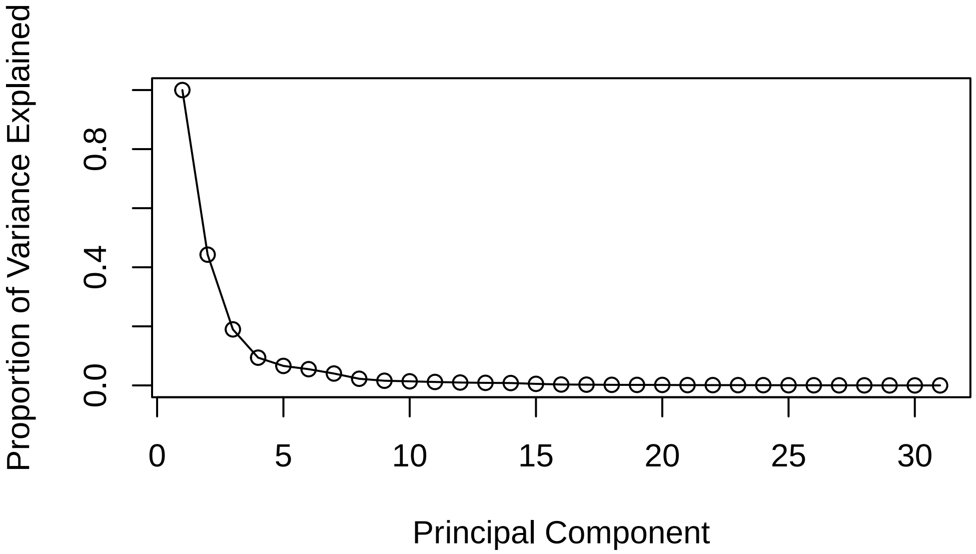
```
# Calculate variance of each component
pr.var <-wisc.pr$sdev^2
head(pr.var)
```

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

We will now calculate the variance explained by each principal component divided by the total variance explained of all principal components.

```
# Variance explained by each principal component: pve
pve <- pr.var / sum(pr.var)

# Plot variance explained for each principal component
plot(c(1,pve), xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



##Communicating PCA results

In this section we will check your understanding of the PCA results, in particular the "loadings" and "variance explained".

The loading vector `wisc.pr$rotation` tells us which original measurements contribute most to each PC.

> 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[,1]
```

```
            radius_mean            texture_mean          perimeter_mean 
            -0.21890244             -0.10372458             -0.22753729 
              area_mean         smoothness_mean        compactness_mean 
            -0.22099499             -0.14258969             -0.23928535 
         concavity_mean     concave.points_mean           symmetry_mean 
```

```
            -0.25840048             -0.26085376             -0.13816696
 fractal_dimension_mean               radius_se              texture_se
            -0.06436335             -0.20597878             -0.01742803
           perimeter_se                 area_se           smoothness_se
            -0.21132592             -0.20286964             -0.01453145
         compactness_se            concavity_se       concave.points_se
            -0.17039345             -0.15358979             -0.18341740
            symmetry_se    fractal_dimension_se            radius_worst
            -0.04249842             -0.10256832             -0.22799663
          texture_worst         perimeter_worst              area_worst
            -0.10446933             -0.23663968             -0.22487053
       smoothness_worst       compactness_worst         concavity_worst
            -0.12795256             -0.21009588             -0.22876753
   concave.points_worst          symmetry_worst fractal_dimension_worst
            -0.25088597             -0.12290456             -0.13178394
```

Concave.points_mean is the biggest driver of variance in each principal component since there is no other component with a larger absolute value of a loading vector.

Hierarchical clustering

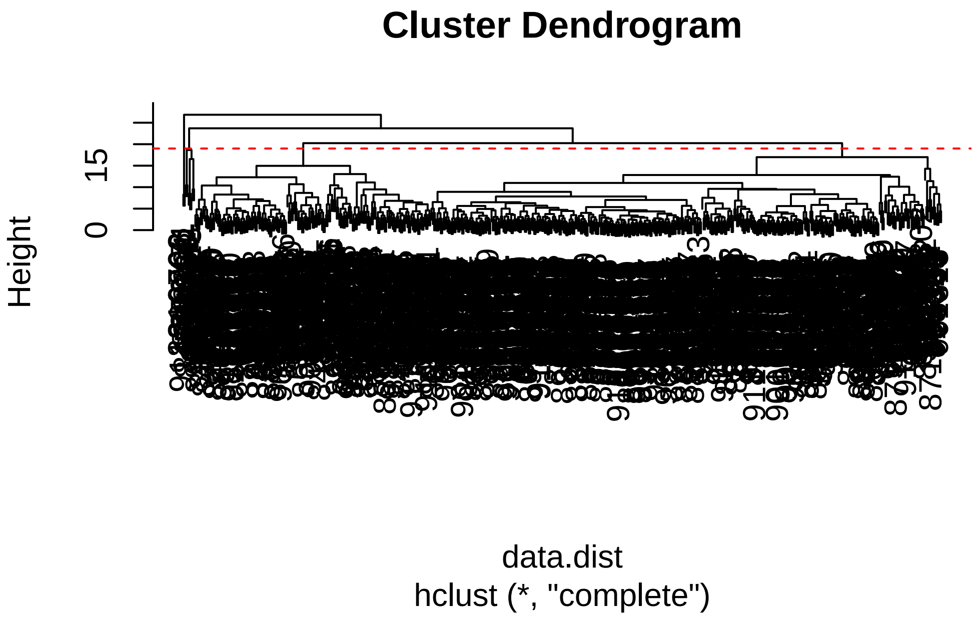
The goal of this section is to do hierarchical clustering of the original data to see if there is any obvious grouping into malignant and benign clusters.

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

Results of hierarchical clustering

Let’s use the hierarchical clustering model we 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)
```



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

We have 4 clusters at height 19.

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

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

Ward.D2 gave the most visually understandable results.

##Combining methods

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

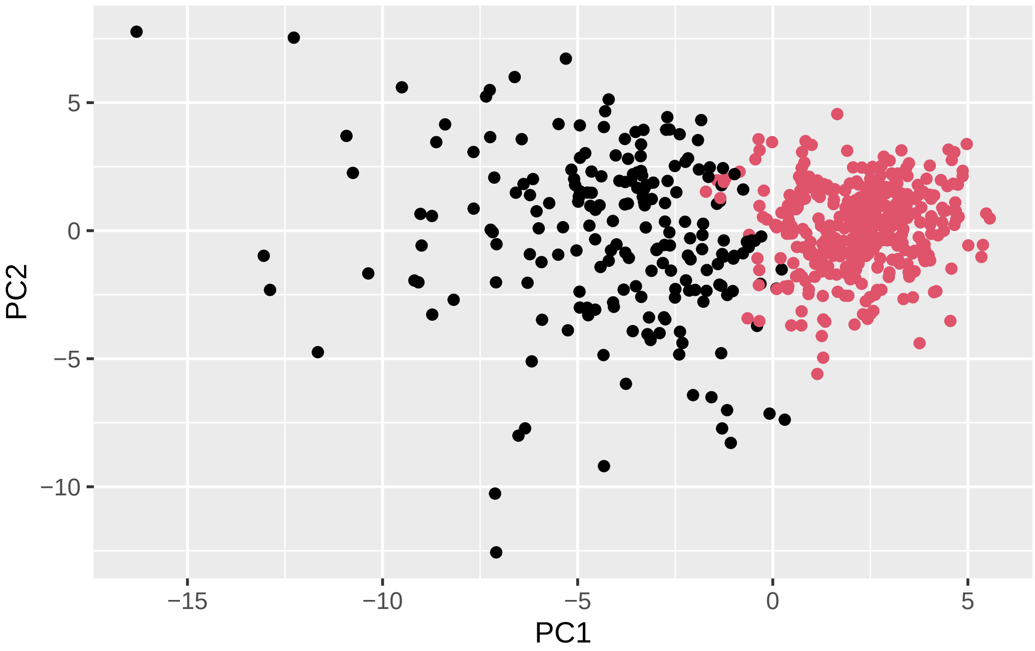
```r
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2 
203 366 
```

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

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

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



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

```
# Compare to actual diagnoses
table(grps, diagnosis)
```

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

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

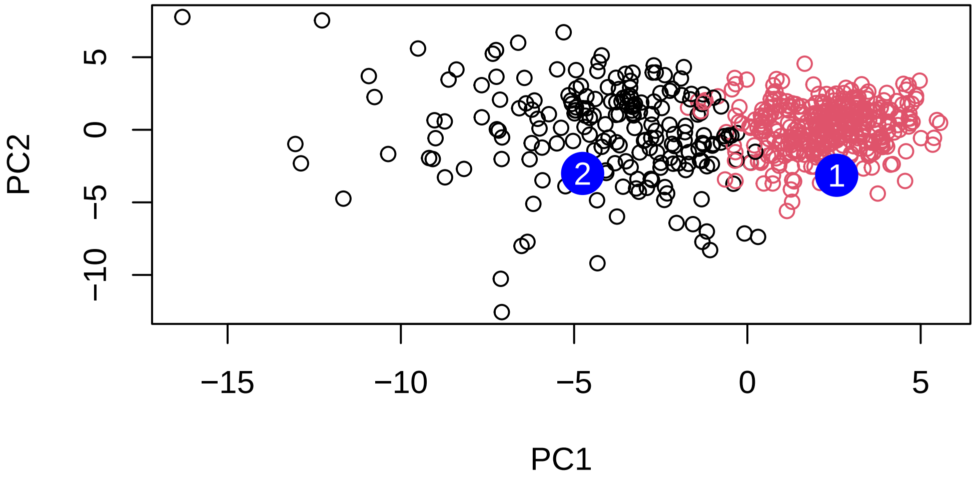
Prediction

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

```
#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?

Based on these results and compared to our PCA plot from earlier patient 2 more represents he malignant group meaning that they are a higher priority.