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 the machine learning methods of clustering and PCA - to analyze real breast cancer biopsy data.

Data Import

The data is in CSV format:

```
#read.csv("WisconsinCancer.csv")
```

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

wee peak at the data

```
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 dataset?

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

```
[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?

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

```
[1] 10
```

We need to remove the `diagnosis` column before we do any further analysis of this dataset - we don't want to pass this to PCA etc. We will save it as a seperate wee vector that we can use later to compare our findings 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 `prcomp()` we will use the optional argument `scake=TRUE` here as the data columns/features.dimensions are on very different scales in the original data set.

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

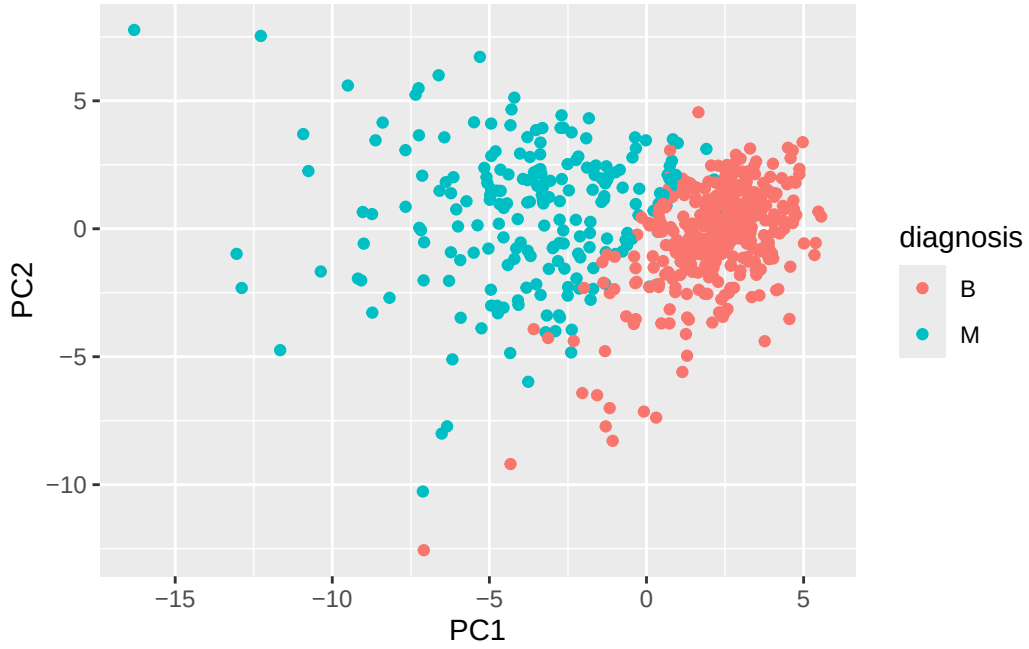
```
attributes(wisc.pr)
```

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

$class
[1] "prcomp"
```

```
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)?

```
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
```

44.27% of variance was captured

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

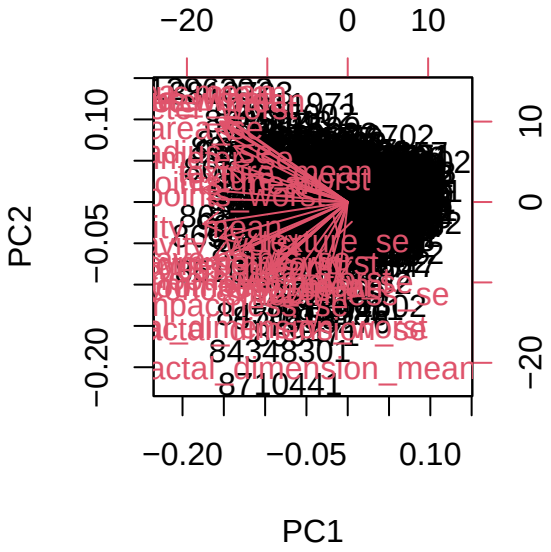
3 principal components (PCs 1 to 3) are needed to describe 70% of the original variance

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

7 principal components (PCs 1 to 7) are needed to describe 90% of the original variance

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

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

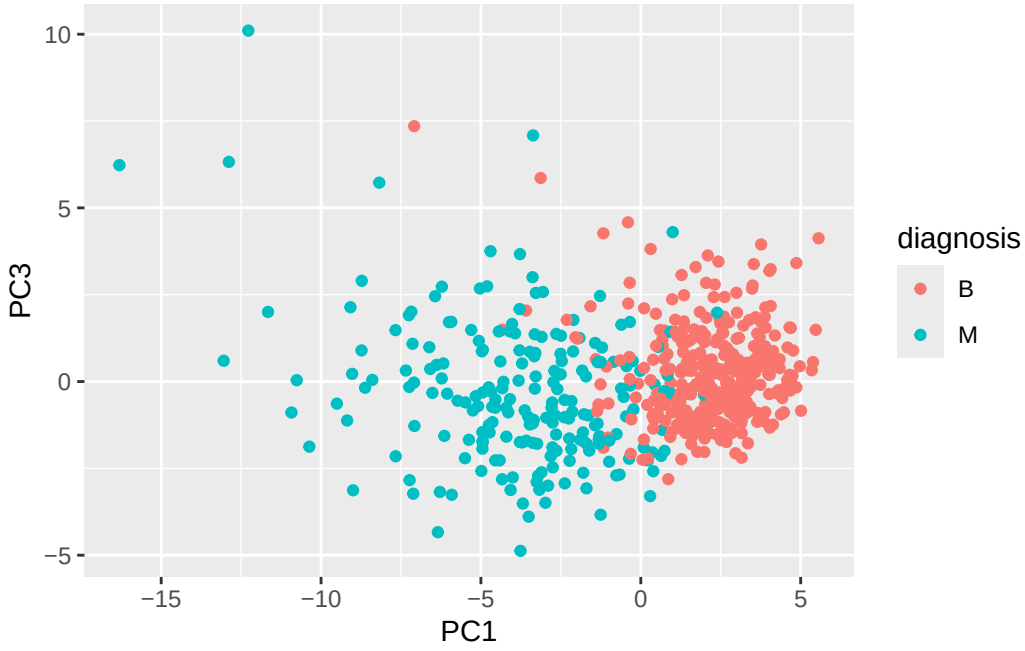


This plot is hard to read due to the large amount of labels on the graph making it difficult to distern what each label means as well as seeing the points on the graph

> 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()
```



this scatter plot has a similar spread to the PC1 vs PC2 plot but this plot has the points located generally at a lower y-axis area than the PC1 vs PC2 plot.

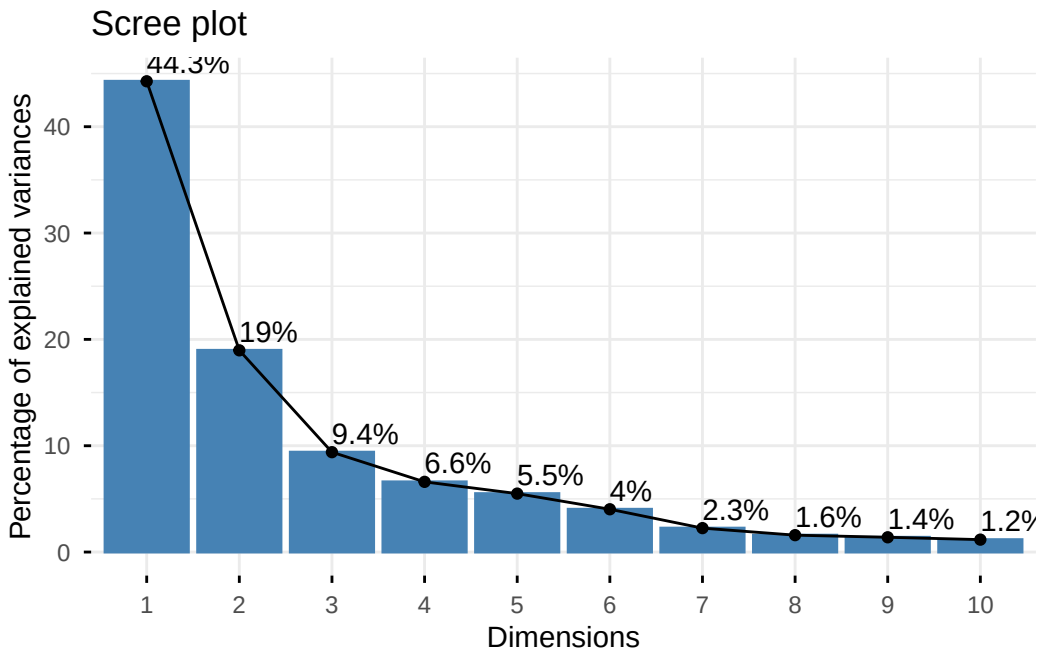
Scree plot

```
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`.
```



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?

```
pc1_loading_concave <- wisc.pr$rotation["concave.points_mean", "PC1"]

pc1_loading_concave
```

```
[1] -0.2608538
```

```
pc1_loadings <- wisc.pr$rotation[, "PC1"]


ordered_loadings <- sort(abs(pc1_loadings), decreasing = TRUE)


head(ordered_loadings, 10)
```

```
 concave.points_mean       concavity_mean concave.points_worst
           0.2608538            0.2584005            0.2508860
    compactness_mean      perimeter_worst      concavity_worst
```

```
   0.2392854        0.2366397        0.2287675
radius_worst   perimeter_mean       area_worst
   0.2279966        0.2275373        0.2248705
   area_mean
   0.2209950
```

```
abs(pc1_loading_concave)
```

```
[1] 0.2608538
```

```
ordered_loadings["concave.points_mean"]
```

```
concave.points_mean
          0.2608538
```

concave.points_mean is the largest contributor, ever other contributor is smaller than concave.points_mean

4. 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

In short, these results are not good!

First we will scale our `wisc.data` then calculate a distance matrix

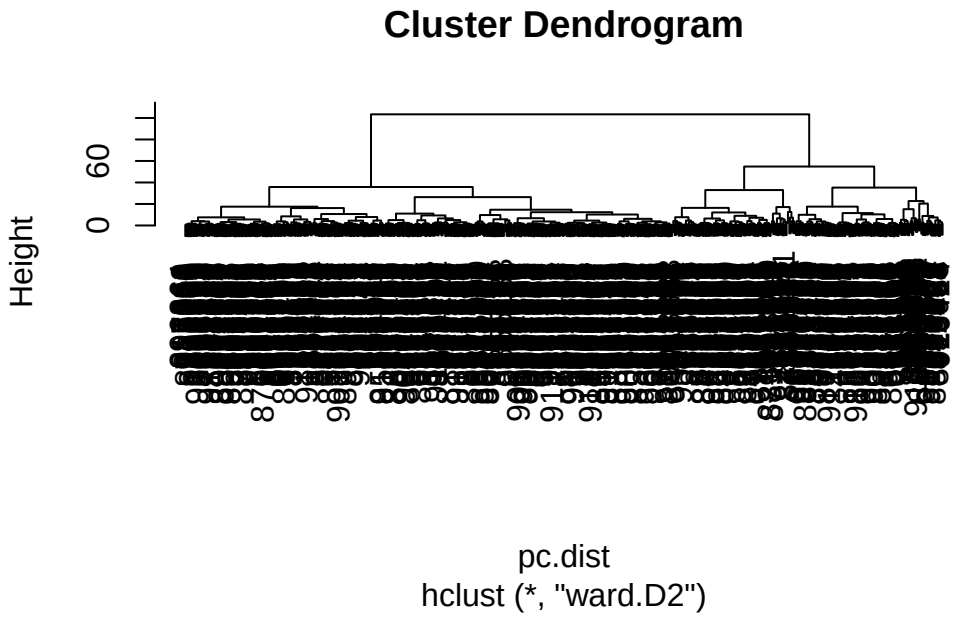
```
wisc.hclust <- hclust( dist( scale(wisc.data)))
wisc.hclust.clusters <- cutree(wisc.hclust, k=2)
table(wisc.hclust.clusters)
```

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

Combining methods

The idea here is that I can take my new variables (i.e. the scores on the 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 clustering.

```
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
```

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

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

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

Our cluster "1" has 179 "M" diagnosis or cluster "2" has 333 "B" diagnosis

179 TP 24 FP 333 TN 33 FN

Sensitivity: TP/(TP+FN)

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

```
[1] 0.8443396
```

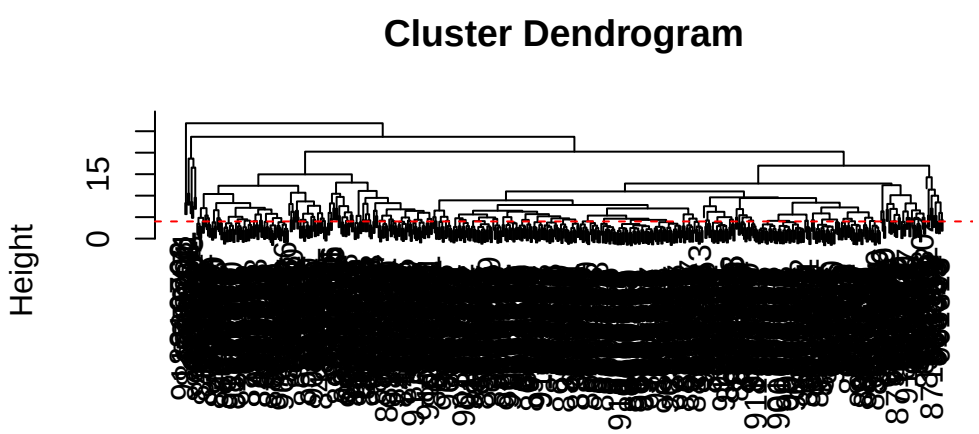
Specificity: TN/(TN+FP)

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

```
[1] 0.9327731
```

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

```
wisc.hclust <- hclust(dist(scale(wisc.data)))
plot(wisc.hclust)
abline(h = 4, col="red", lty=2)
```



at around a height of 15 is when the cluster model has 4 clusters.

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

I prefer ward.d2 because in my opinion it organizes the clusters the best out of all the methods which makes interpreting the cluster model not too difficult compared to other methods as the other methods make the clusters look too cluttered.

> 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
```

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

```
                        diagnosis
wisc.pr.hclust.clusters   B   M
                      1  24 179
                      2 333  33
```

The "PR" cluster seperates better than the other cluster model as the ratios of Benign and Malignant for the "PR" cluster model are larger then the other cluster model.

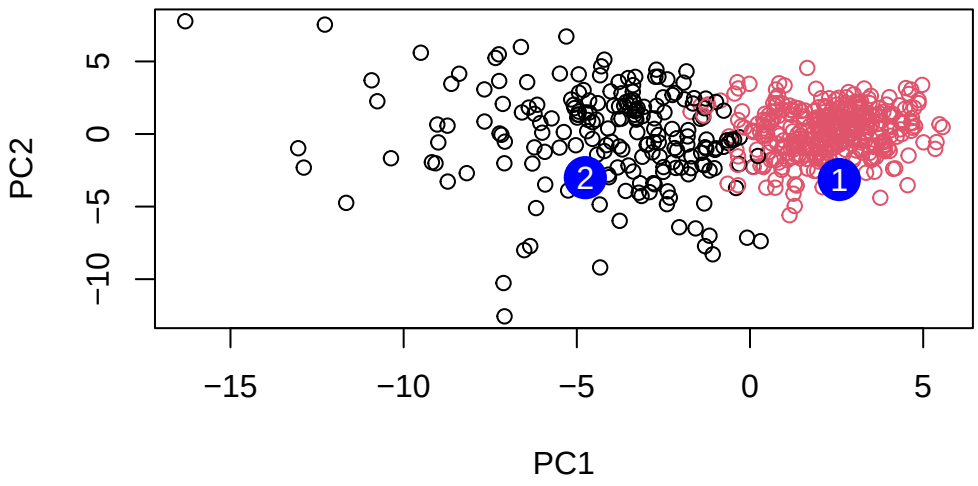
Prediction

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

```
#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 the graph the 2nd group of patients (2 on graph) should be prioritized due to the high amount of patients that have malignant cancer.