class08: Mini Project

Laura Sun (PID: A17923552)

Background

The goal of this mini-project is for you to explore a complete analysis using the unsupervised learning techniques covered in class.

The data itself comes from the Wisconsin Breast Cancer Diagnostic Data Set first reported by K. P. Benne and O. L. Mangasarian: "Robust Linear Programming Discrimination of Two Linearly Inseparable Sets".

Values in this data set describe characteristics of the cell nuclei present in digitized images of a fine needle aspiration (FNA) of a breast mass.

Data Import

```
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

The first column `diagnosis` is the expert opinion on the sample (i.e. patient FNA)

```
wisc.data <- wisc.df[,-1]
dim(wisc.data)
```

```
[1] 569  30
```

Store the diagnosis as a vector for use later when we compare our results to those from experts in the field.

```
diagnosis <- factor(wisc.df$diagnosis)
```

Q1: How many observations are in this dataset?

There are 569 observations/patients in the dataset.

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

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

```
  B   M
357 212
```

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

```
#colnames(wisc.data), if you want to check the names by eye.
length( grep("_mean", colnames(wisc.data)) )
```

```
[1] 10
```

Principal Component Analysis (PCA)

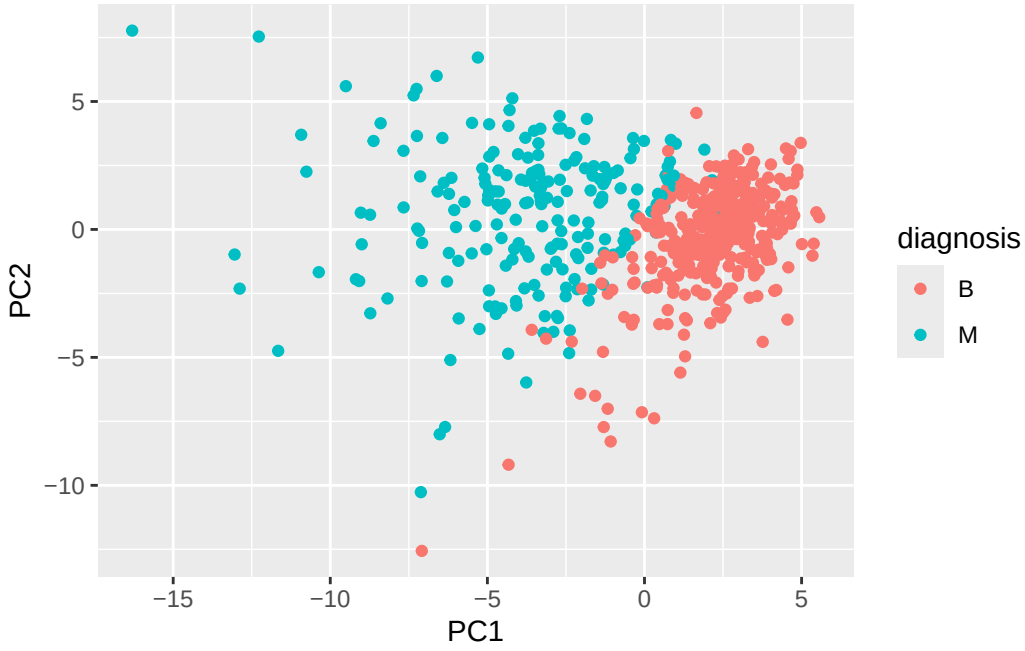
The `prcomp()` function to PCA. prcomp(x, scale=F, center=F), scale and center are optional arguments, default is false. We want to scale and center prior to PCA so each feature contributes equally to the analysis, not dominated by columns/variables in dataset that have high standard deviation and mean when compared to others just because the units of measurements are on different units/scales.

```
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
```

The main PC result figure is called a "score plot" or "PC plot" or "ordination plot"...

```
library(ggplot2)
ggplot(wisc.pr$x, aes(PC1, PC2, col=diagnosis)) + geom_point()
```



PC1 captures the direction of most variations. We cab score genes based on how much they influence PC1. PC2 captures the direction with the second most variations.

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

44.27% portion of the original variance is captured by PC1.

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

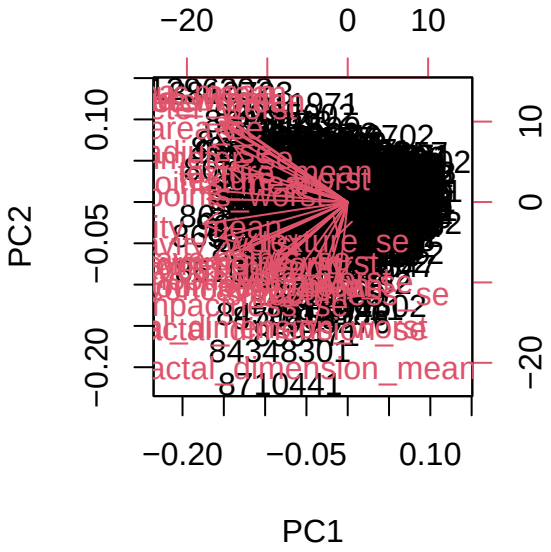
3 PCs are required to describe at least 70% of the variance. (0.72636)

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

7 PCs are required (0.91010).

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

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

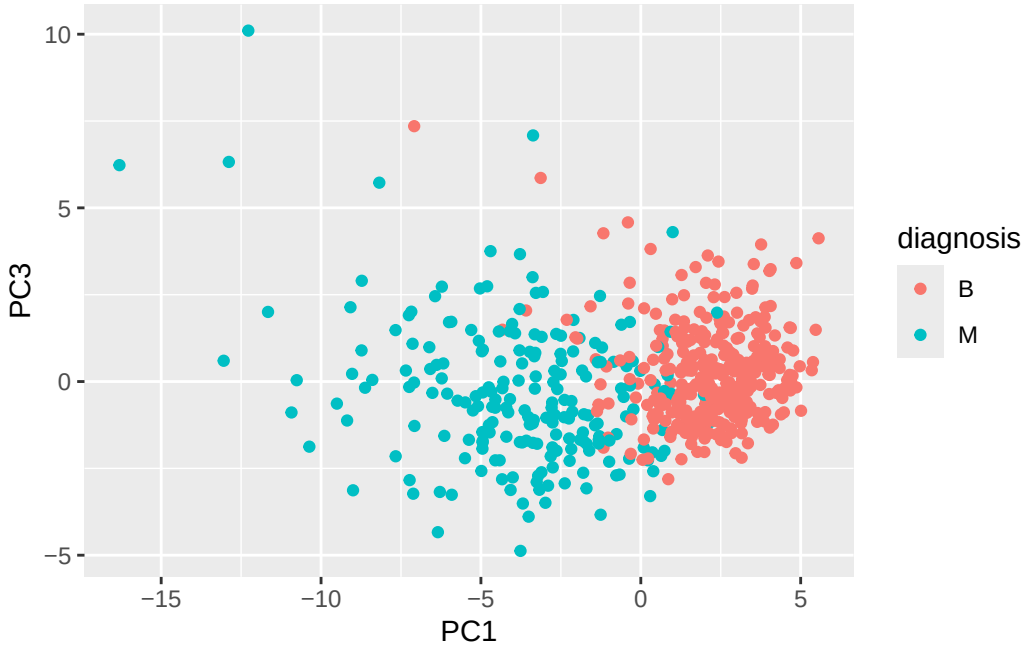


The points and names overlap each other. This plot is very hard to understand.

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

This is much more easier to understand. The groups are separated by colors and easier to read.

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



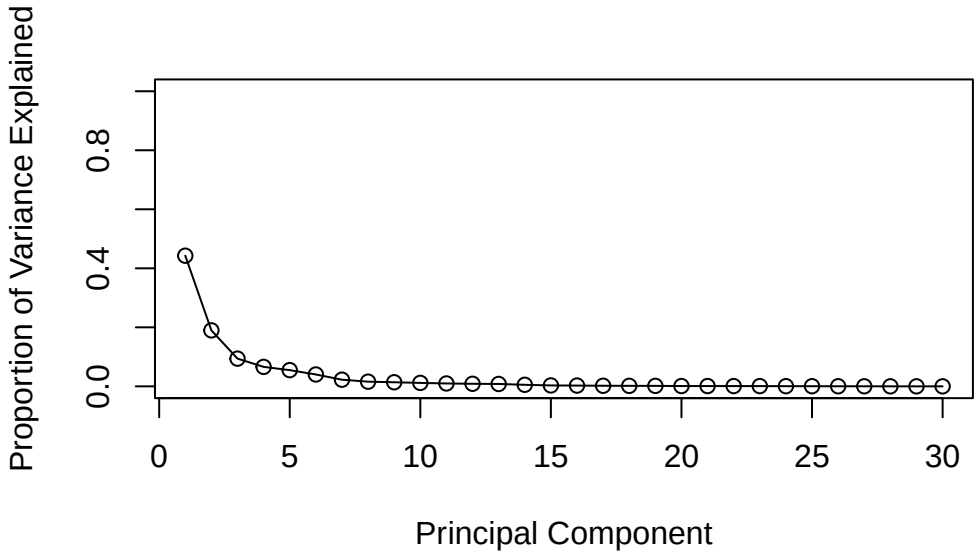
Variance

```
# 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
```

```
pve <- pr.var/ sum(pr.var)

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



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?

The concave.points_mean is row, and PC1 is column for the first principal component.

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

```
[1] -0.2608538
```

Q10. What is the minimum number of principal components required to explain 80% of the variance of the data?

We need 5 PCs to capture more than 80% variance.

```
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
```

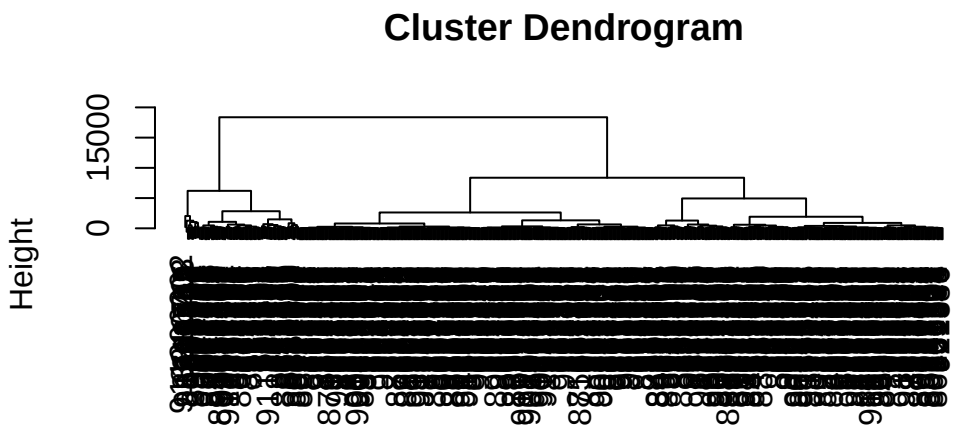
Hierarchical Clustering

Just clustering the original data is not very informative or helpful.

```
data.scaled <- scale(wisc.data)
data.dist <- dist(wisc.data)
wisc.hclust <- hclust(data.dist, method="ward.D2")
```

View the clustering

```
plot(wisc.hclust)
```




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

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1   0  86
                   2 357 126
```

```
wisc.hclust.clusters2 <- cutree(wisc.hclust, k=4)
table(wisc.hclust.clusters2, diagnosis)
```

```
                     diagnosis
wisc.hclust.clusters2   B   M
                    1   0  75
                    2 260   6
                    3  97 120
                    4   0  11
```

Combining Methods (PCA and Clustering)

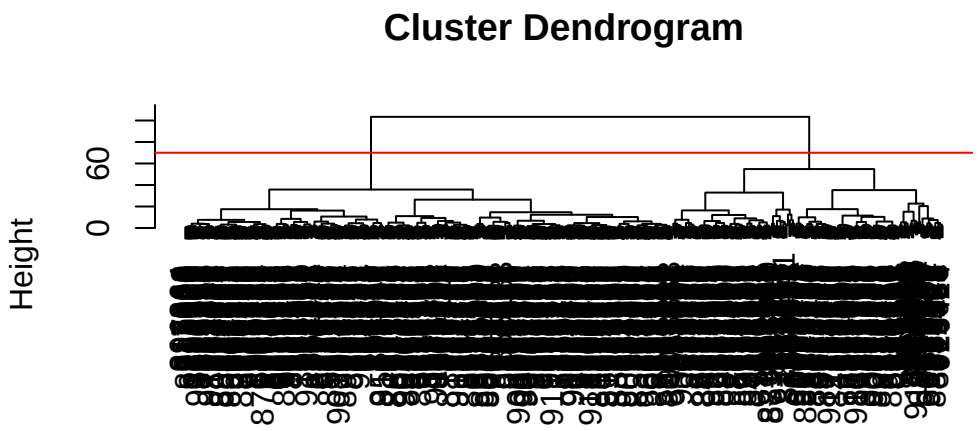
Clustering the original data was not very productive. The PCA results looked promising. Here we combine these methods by clustering from our PCA results. In other words, "clustering in

PC space" ...

```
## Take the first three PCs.
dist.pc <- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <- hclust(dist.pc, method="ward.D2")
```

View the tree!

```
plot(wisc.pr.hclust)
abline(h=70, col="red")
```



To get our clustering membership vector (i.e. our main clustering result) we "cut" the tree at a desired height or to yield a desired number of "k" groups.

```
grps <- cutree(wisc.pr.hclust, h=70)
table(grps)
```

```
grps
  1   2
203 366
```

How does this clustering grps compare to the expert?

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

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

Sensitivity/ Specificity

True positive, False negative Sensitivity: TP/(TP+FN) Specificity: TN/(TN+FN)

> Q15. How well does the newly created model with four clusters separate out the two diagnoses?

The newly created model with four clusters separated the two diagnoses are better. The results are more "pure" with mostly one diagnosis in one cluster, except for cluster 3.

> Q16. How well do the k-means and 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.

```
wisc.km <- kmeans(wisc.data, centers = 2, nstart = 20)
table(wisc.km$cluster, diagnosis)
```

```
   diagnosis
      B   M
  1   1 130
  2 356  82
```

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

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1   0  86
                   2 357 126
```

Kmeans are doing better than hierarchical clustering because k-means form cluster that successfully separate most of the diagnosis, only mismatched a small number. Cluster 1 has mostly benign and cluster 2 is almost all malignant. Hierarchical clustering has more mixing, so less clearly separated.

Prediction

```
#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
```

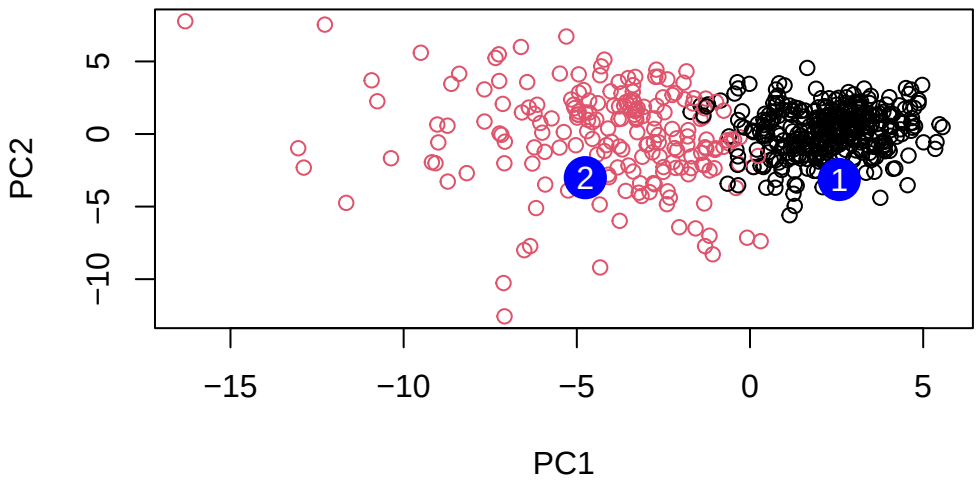
```
g <- as.factor(grps)
levels(g)
```

```
[1] "1" "2"
```

```
g <- relevel(g, 2)
levels(g)
```

```
[1] "2" "1"
```

```
plot(wisc.pr$x[,1:2], col=g)
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



Q18. Which of these new patients should we prioritize for follow up based on your results?

We should prioritize for follow up for patient 1. This patient's data point locates closer to the black, or malignant cluster, so this new patient is likely malignant.