Class 8: Breast Cancer Analysis Mini Project

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Background

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

{r wisc.df

Remove the diagnosis from dta for subsequent analysis

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

```
 [1]  1  2  3  4  5  6  7  8  9 10
```

Principal Component Analysis (PCA)

The `prcomp()` function to do PCA has a "scale=FALSE" deault. in general we nearly always want to set this to TRUE so our analysis is not dominated by columns/variables in our dataset that have high standard deviation and mean when compared to others just because units of measurement are on different 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
```

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

44.27% of the original variance is captured by the first PC (PC1). >Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

Three PCs are required for atleast 70%. >Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

7 PCS are required for at least 90% of the variance.

```
colMeans(wisc.data)
```

```
            radius_mean            texture_mean          perimeter_mean
           1.412729e+01            1.928965e+01            9.196903e+01
              area_mean         smoothness_mean        compactness_mean
           6.548891e+02            9.636028e-02            1.043410e-01
         concavity_mean     concave.points_mean          symmetry_mean
           8.879932e-02            4.891915e-02            1.811619e-01
  fractal_dimension_mean               radius_se              texture_se
           6.279761e-02            4.051721e-01            1.216853e+00
            perimeter_se                 area_se          smoothness_se
           2.866059e+00            4.033708e+01            7.040979e-03
         compactness_se           concavity_se       concave.points_se
           2.547814e-02            3.189372e-02            1.179614e-02
             symmetry_se    fractal_dimension_se            radius_worst
           2.054230e-02            3.794904e-03            1.626919e+01
          texture_worst         perimeter_worst              area_worst
           2.567722e+01            1.072612e+02            8.805831e+02
       smoothness_worst       compactness_worst         concavity_worst
           1.323686e-01            2.542650e-01            2.721885e-01
    concave.points_worst          symmetry_worst fractal_dimension_worst
           1.146062e-01            2.900756e-01            8.394582e-02
```

```
apply(wisc.data,2,sd)
```

```
            radius_mean            texture_mean          perimeter_mean
           3.524049e+00            4.301036e+00            2.429898e+01
```

```
            area_mean         smoothness_mean        compactness_mean
         3.519141e+02            1.406413e-02            5.281276e-02
       concavity_mean     concave.points_mean          symmetry_mean
         7.971981e-02            3.880284e-02            2.741428e-02
fractal_dimension_mean               radius_se              texture_se
         7.060363e-03            2.773127e-01            5.516484e-01
       perimeter_se                 area_se          smoothness_se
         2.021855e+00            4.549101e+01            3.002518e-03
      compactness_se           concavity_se       concave.points_se
         1.790818e-02            3.018606e-02            6.170285e-03
        symmetry_se    fractal_dimension_se            radius_worst
         8.266372e-03            2.646071e-03            4.833242e+00
       texture_worst         perimeter_worst              area_worst
         6.146258e+00            3.360254e+01            5.693570e+02
     smoothness_worst       compactness_worst         concavity_worst
         2.283243e-02            1.573365e-01            2.086243e-01
  concave.points_worst          symmetry_worst fractal_dimension_worst
         6.573234e-02            6.186747e-02            1.806127e-02
```

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

```
library(ggplot2)
```

```
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
```

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


```
pr.var<- wisc.pr$sdev^2
head(pr.var)
```

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

Variance explained by each principal component: pve

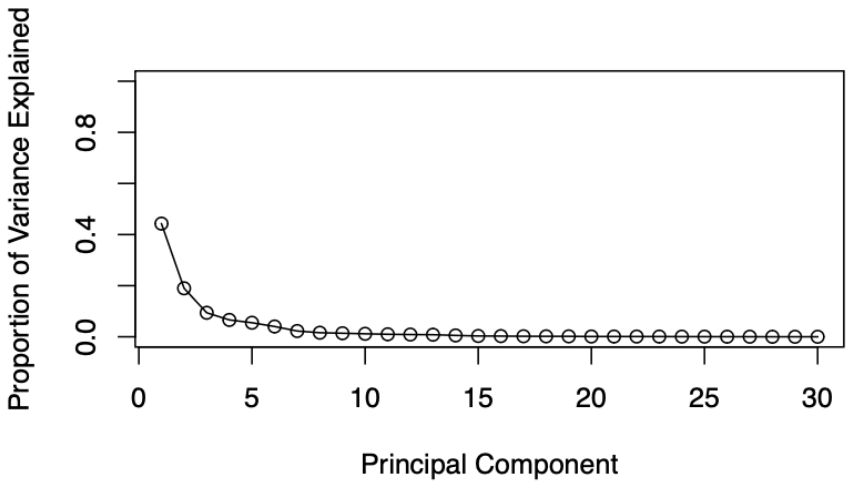
```
pve<- pr.var/sum(pr.var)
```

##PCA Scree-plot

A plot of how much variance each PC captures. We can get this from `wist.` from the output

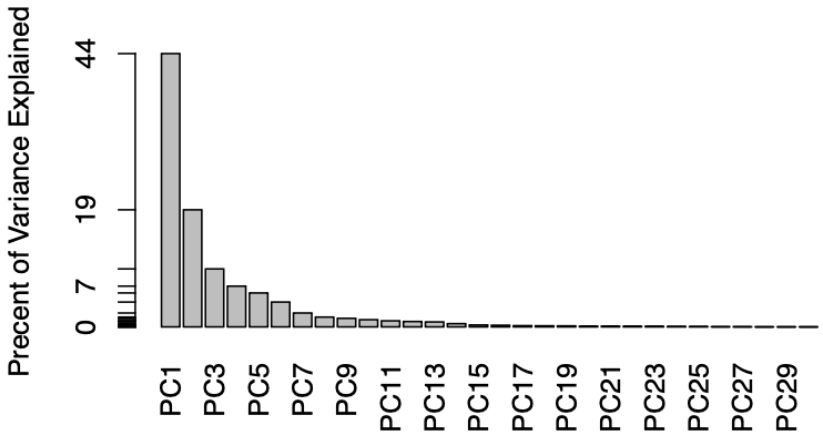
Plot variance explained for each principal component

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



Alternative scree plot of the same data, note data driven y-axis

```
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```



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?

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

```
[1] -0.2608538
```

```
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?

```
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
```

Five minimum components to reach 80% variance.

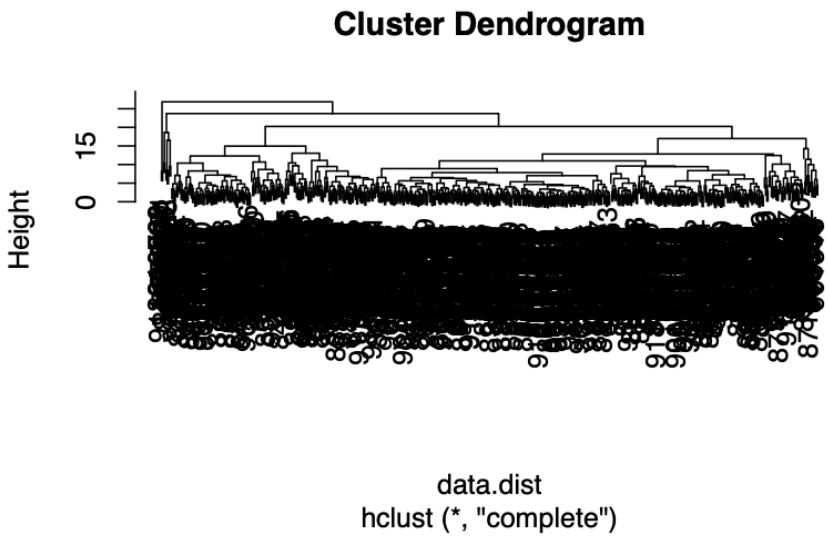
Hierarchical clustering

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

```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
data.dist<-dist(data.scaled)
wisc.hclust<-hclust(data.dist)
```

View the clustering dendogram result

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



Q11. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

There are 4 clusters at h=20

```
wisc.hclust.clusters<-wisc.hclust
```

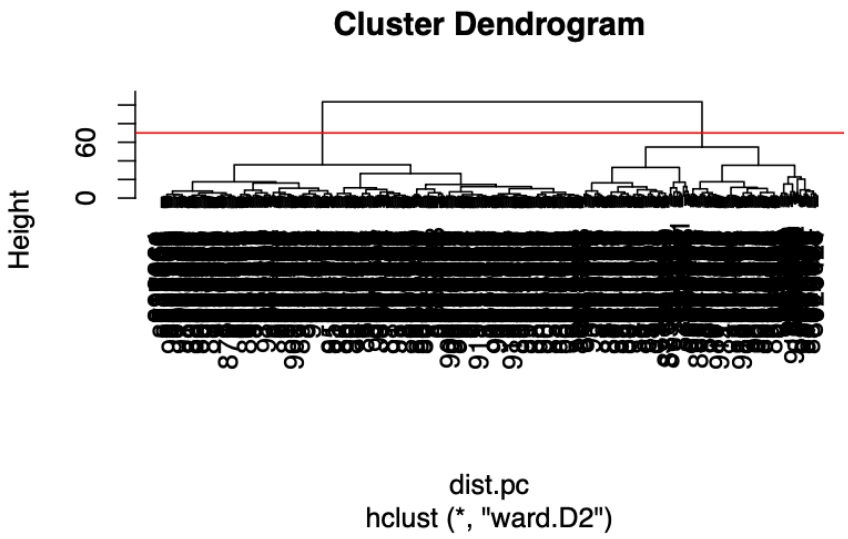
Combing methods (PCA and Clustering)

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

```
## Take the first 3 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... the tree at a desired height or to yield a dsired number of "k" groups

```
cutree(wisc.pr.hclust, k=2)
```

842302	842517	84300903	84348301	84358402	843786	844359	84458202
1	1	1	1	1	1	1	1
844981	84501001	845636	84610002	846226	846381	84667401	84799002
1	1	2	1	1	2	1	1
848406	84862001	849014	8510426	8510653	8510824	8511133	851509
2	1	1	2	2	2	1	1
852552	852631	852763	852781	852973	853201	853401	853612
1	1	1	1	1	2	1	1
85382601	854002	854039	854253	854268	854941	855133	855138
1	1	1	1	1	2	2	1
855167	855563	855625	856106	85638502	857010	85713702	85715
2	1	1	1	2	1	2	1
857155	857156	857343	857373	857374	857392	857438	85759902
2	2	2	2	2	1	2	2
857637	857793	857810	858477	858970	858981	858986	859196
1	1	2	2	2	2	1	2
85922302	859283	859464	859465	859471	859487	859575	859711
1	1	2	2	1	2	1	1

905978	90602302	906024	906290	906539	906564	906616	906878
2	1	2	2	2	1	2	2
907145	907367	907409	90745	90769601	90769602	907914	907915
2	2	2	2	2	2	1	2
908194	908445	908469	908489	908916	909220	909231	909410
1	1	2	1	2	2	2	2
909411	909445	90944601	909777	9110127	9110720	9110732	9110944
2	1	2	2	1	2	1	2
911150	911157302	9111596	9111805	9111843	911201	911202	9112085
2	1	2	1	2	2	2	2
9112366	9112367	9112594	9112712	911296201	911296202	9113156	911320501
2	2	2	2	1	1	2	2
911320502	9113239	9113455	9113514	9113538	911366	9113778	9113816
2	1	2	2	1	2	2	2
911384	9113846	911391	911408	911654	911673	911685	911916
2	2	2	2	2	2	2	1
912193	91227	912519	912558	912600	913063	913102	913505
2	2	2	2	2	1	2	1
913512	913535	91376701	91376702	914062	914101	914102	914333
2	2	2	2	1	2	2	2
914366	914580	914769	91485	914862	91504	91505	915143
1	2	1	1	2	1	2	1
915186	915276	91544001	91544002	915452	915460	91550	915664
1	1	2	2	2	1	2	2
915691	915940	91594602	916221	916799	916838	917062	917080
1	2	2	2	1	1	2	2
917092	91762702	91789	917896	917897	91805	91813701	91813702
2	1	2	2	2	2	2	2
918192	918465	91858	91903901	91903902	91930402	919537	919555
2	2	2	2	2	1	2	1
91979701	919812	921092	921362	921385	921386	921644	922296
1	2	2	2	2	1	2	2
922297	922576	922577	922840	923169	923465	923748	923780
2	2	2	2	2	2	2	2
924084	924342	924632	924934	924964	925236	925277	925291
2	2	2	2	2	2	2	2
925292	925311	925622	926125	926424	926682	926954	927241
2	2	1	1	1	1	2	1
92751							
2							

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

```
grps
  1   2
203 366
```

How does this clustering grps compare ot the expert

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

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

Sensitivity: TP/(TP + FN) 179/(179 + 33) Specificity: TN/(TN + FN) 333/(333+24)

7. Prediction

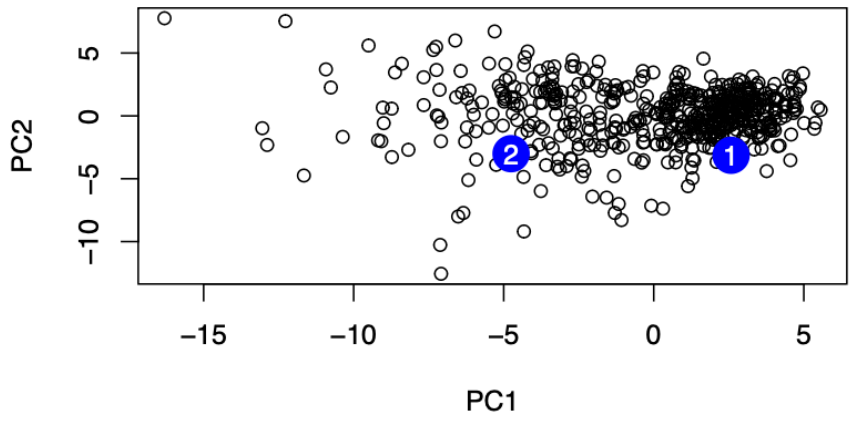
We can use our PCA model for prediction with new input patient samples.

```
#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])
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?

Patient 2