

classs099miniproject

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Mini Project

Exploratory Data Analysis

```
wisc.df <- read.csv("https://bioboot.github.io/bimm143_S20/class-material/WisconsinCancer.csv")
```

```
#save input data file into project directory
```

```
fna.data <- "WisconsinCancer.csv"
```

```
#input data and store as wisc.df
```

```
wisc.df <- read.csv(fna.data, 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
```

```
# omit first column
wisc.data <- wisc.df[,-1]
```

```
# create vector for diagnosis
diagnosis <- as.factor(wisc.df$diagnosis)
```

Q1. Ho many observations are in this dataset?

569 observations

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

```
table(diagnosis)
```

```
## diagnosis
## B M
## 357 212
```

There are 212 observations with malignant diagnosis.

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

```
library(stringr)
colnames(wisc.data)
```

```
## [1] "radius_mean"      "texture_mean"
## [3] "perimeter_mean"   "area_mean"
## [5] "smoothness_mean"  "compactness_mean"
## [7] "concavity_mean"    "concave.points_mean"
## [9] "symmetry_mean"     "fractal_dimension_mean"
## [11] "radius_se"         "texture_se"
## [13] "perimeter_se"      "area_se"
## [15] "smoothness_se"     "compactness_se"
## [17] "concavity_se"      "concave.points_se"
## [19] "symmetry_se"       "fractal_dimension_se"
## [21] "radius_worst"      "texture_worst"
## [23] "perimeter_worst"   "area_worst"
## [25] "smoothness_worst"  "compactness_worst"
## [27] "concavity_worst"   "concave.points_worst"
## [29] "symmetry_worst"    "fractal_dimension_worst"
```

```
sum(str_count(colnames(wisc.data), "_mean"))
```

```
## [1] 10
```

There are 10 variables with `"_mean"`.

```
#can also use grep() to find the number of variables with suffix "mean"
length(grep("mean", colnames(wisc.df)))
```

```
## [1] 10
```

Principal Component Analysis

```
#check column means and standard deviations
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
```

```
#perform PCA on wisc.data
wisc.pr <- prcomp(wisc.data)
```

```
#summary of results
summary(wisc.pr)
```

```
## Importance of components:
##          PC1    PC2    PC3    PC4    PC5    PC6    PC7
## Standard deviation    666.170 85.49912 26.52987 7.39248 6.31585 1.73337 1.347
## Proportion of Variance    0.982 0.01618 0.00156 0.00012 0.00009 0.00001 0.000
## Cumulative Proportion    0.982 0.99822 0.99978 0.99990 0.99999 0.99999 1.000
##          PC8    PC9    PC10    PC11    PC12    PC13    PC14
## Standard deviation    0.6095 0.3944 0.2899 0.1778 0.08659 0.05623 0.04649
## Proportion of Variance    0.0000 0.0000 0.0000 0.0000 0.00000 0.00000 0.00000
## Cumulative Proportion    1.0000 1.0000 1.0000 1.0000 1.00000 1.00000 1.00000
##          PC15    PC16    PC17    PC18    PC19    PC20    PC21
## Standard deviation    0.03642 0.0253 0.01936 0.01534 0.01359 0.01281 0.008838
## Proportion of Variance    0.00000 0.0000 0.00000 0.00000 0.00000 0.00000 0.000000
## Cumulative Proportion    1.00000 1.0000 1.00000 1.00000 1.00000 1.00000 1.000000
##          PC22    PC23    PC24    PC25    PC26    PC27
```

```
## Standard deviation      0.00759 0.005909 0.005329 0.004018 0.003534 0.001918
## Proportion of Variance 0.00000 0.000000 0.000000 0.000000 0.000000 0.000000
## Cumulative Proportion  1.00000 1.000000 1.000000 1.000000 1.000000 1.000000
##
##           PC28      PC29      PC30
## Standard deviation  0.001688 0.001416 0.0008379
## Proportion of Variance 0.000000 0.000000 0.0000000
## Cumulative Proportion 1.000000 1.000000 1.0000000
```

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

98.2%

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

```
# need to scale because data is on different scales, we will use scale = TRUE
summary(prcomp(wisc.data, scale = TRUE))
```

```
## 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
```

At PC3

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

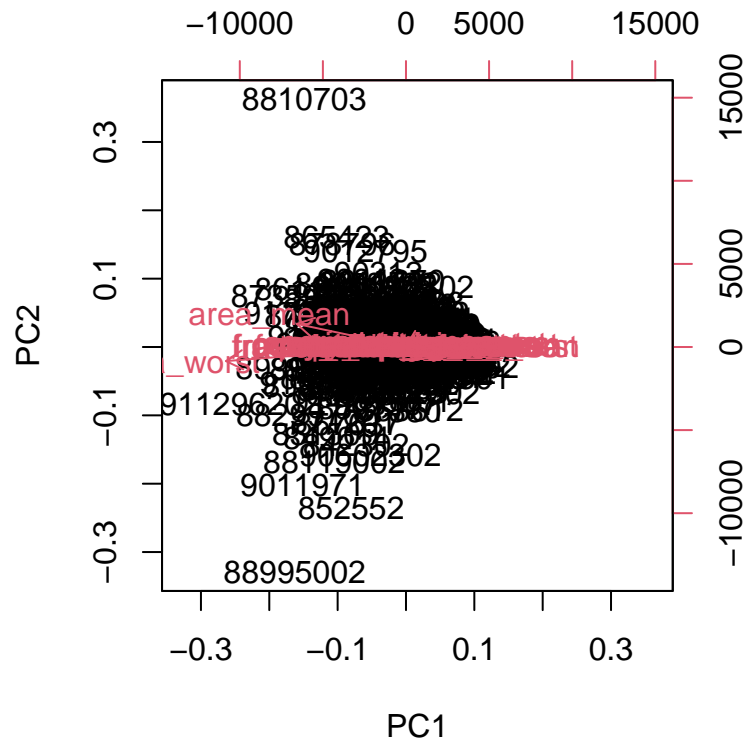
At PC7

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


```
## Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length =
## arrow.len): zero-length arrow is of indeterminate angle and so skipped

## Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length =
## arrow.len): zero-length arrow is of indeterminate angle and so skipped

## Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length =
## arrow.len): zero-length arrow is of indeterminate angle and so skipped
```

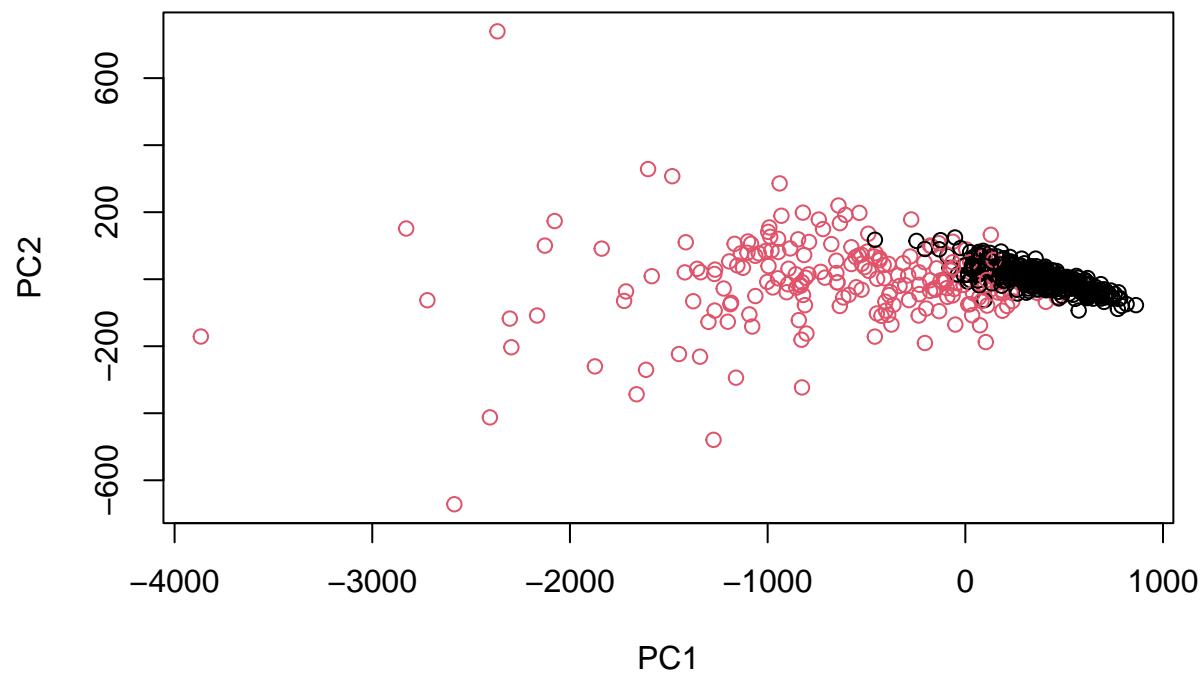


Two sections stand out to me, which are colored into a red and black section. As of right now the plot is difficult to understand. It looks like the red data from PC2 is coming out of PC1.

To make this plot ourselves we need access the PCA scores data.

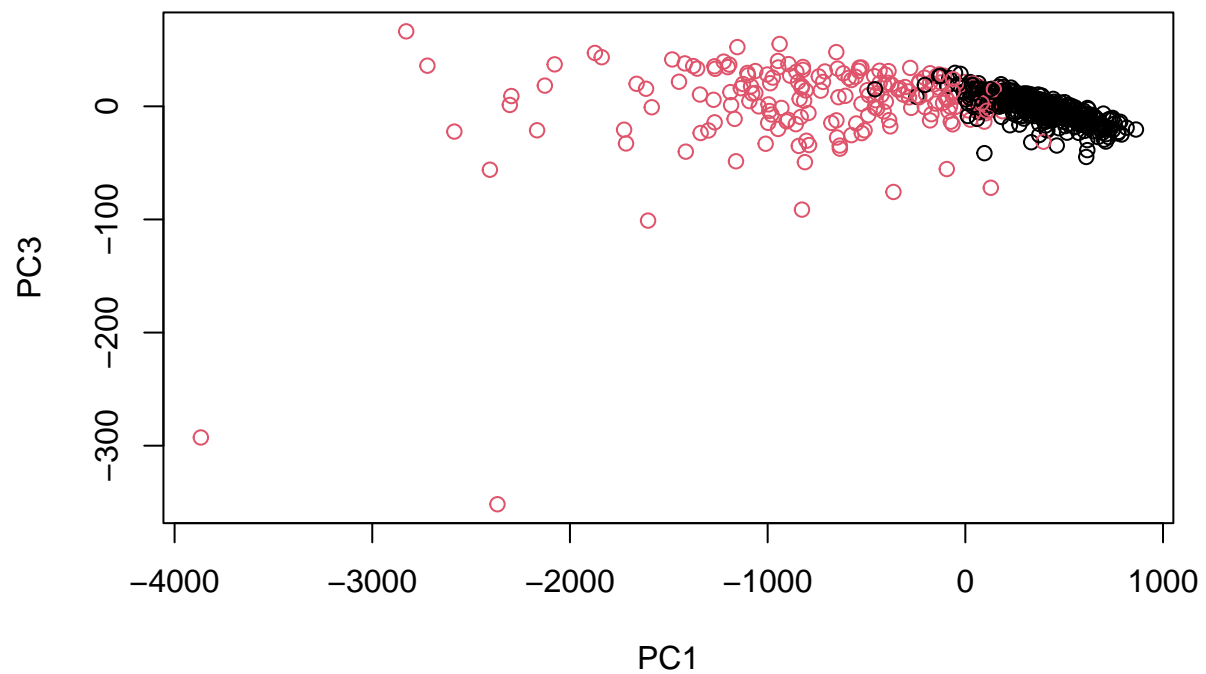
```
# lets make a better plot
# scatter plot observations by components 1 and 2.
```

```
plot(wisc.pr$x[,1:2], col=diagnosis)
```



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

```
plot(wisc.pr$x[,1], wisc.pr$x[,3], col=diagnosis,  
     xlab = "PC1", ylab = "PC3")
```

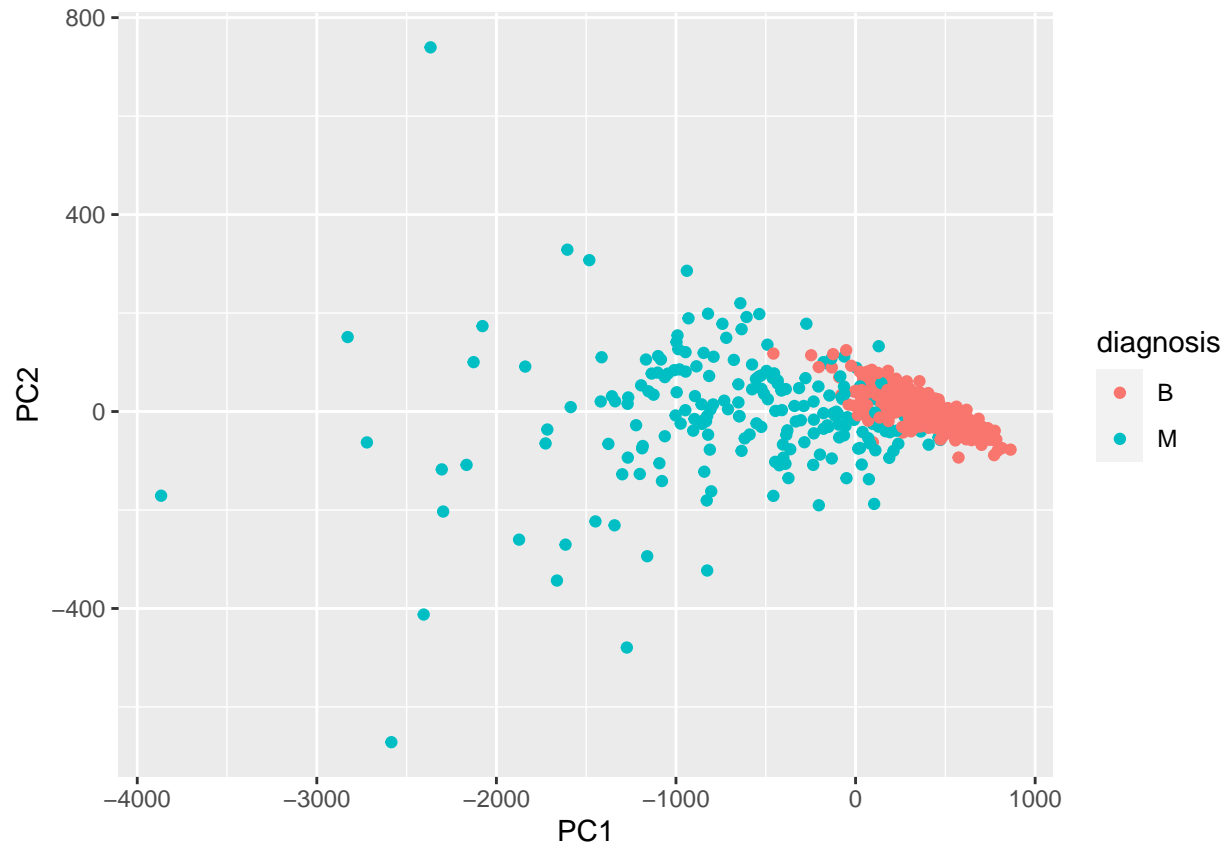



Let's see a ggplot

```
#create a data.frame for ggplot  
df <- as.data.frame(wisc.pr$x)  
df$diagnosis <- diagnosis
```

```
#load ggplot package  
library(ggplot2)
```

```
#make a scatter plot by diagnosis  
ggplot(df) + aes(PC1, PC2, col = diagnosis) + geom_point()
```



```
# calculate variance of each component
```

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

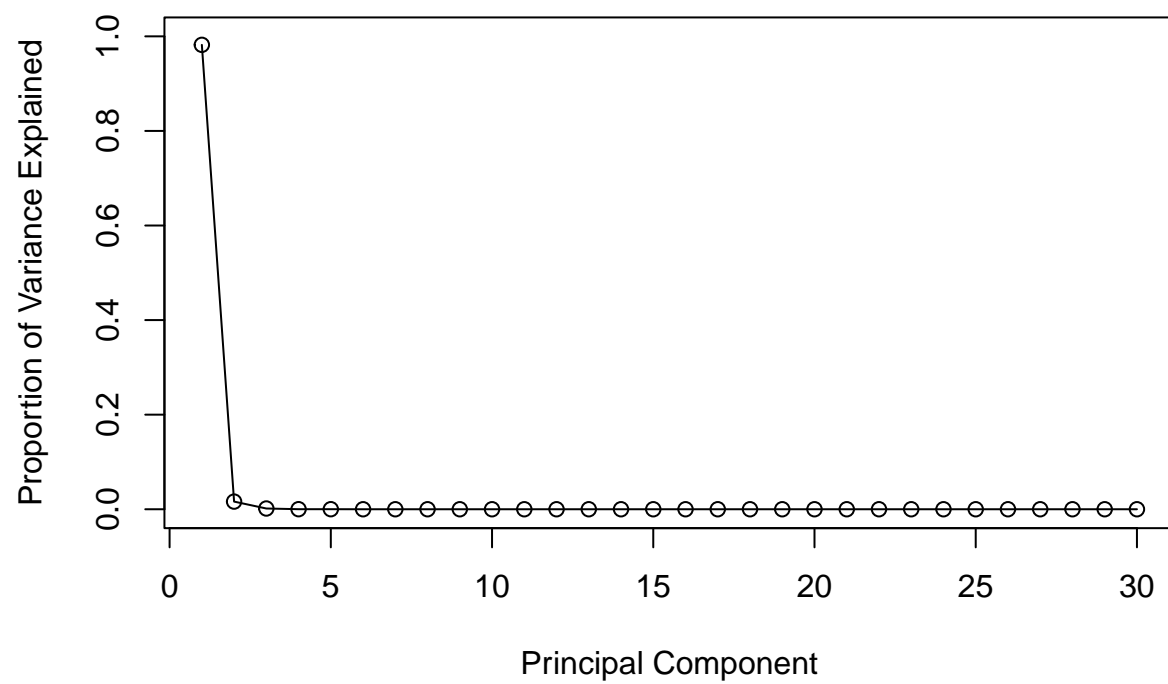
```
## [1] 4.437826e+05 7.310100e+03 7.038337e+02 5.464874e+01 3.989002e+01
## [6] 3.004588e+00
```

```
# variance explained by each principal component
```

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

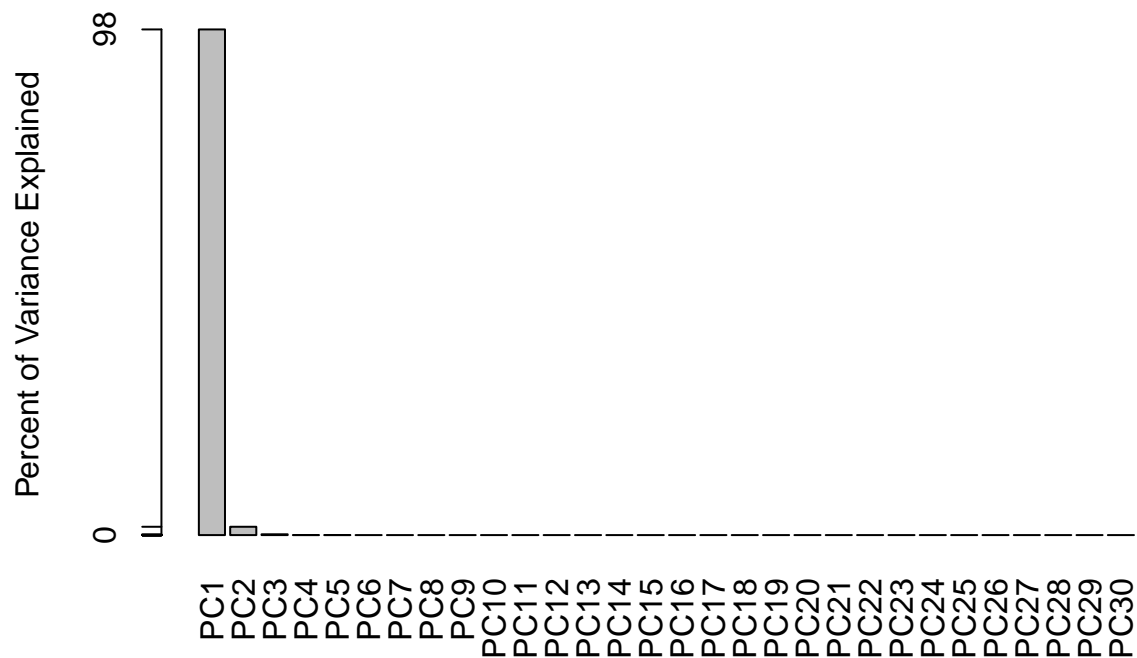
```
#plot variance explained by each principal component
```

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



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

```
barplot(pve, ylab = "Percent 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] -4.778078e-05
```

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

```
var <-summary(wisc.pr)
sum(var$importance[3,]< 0.8)
```

```
## [1] 0
```

```
summary(wisc.pr)
```

```
## Importance of components:
##          PC1          PC2          PC3          PC4          PC5          PC6          PC7
## Standard deviation  666.170  85.49912  26.52987  7.39248  6.31585  1.73337  1.347
## Proportion of Variance  0.982  0.01618  0.00156  0.00012  0.00009  0.00001  0.000
## Cumulative Proportion  0.982  0.99822  0.99978  0.99990  0.99999  0.99999  1.000
##          PC8          PC9          PC10          PC11          PC12          PC13          PC14
```

```
## Standard deviation      0.6095 0.3944 0.2899 0.1778 0.08659 0.05623 0.04649
## Proportion of Variance 0.0000 0.0000 0.0000 0.0000 0.00000 0.00000 0.00000
## Cumulative Proportion 1.0000 1.0000 1.0000 1.0000 1.00000 1.00000 1.00000
##          PC15   PC16   PC17   PC18   PC19   PC20   PC21
## Standard deviation      0.03642 0.0253 0.01936 0.01534 0.01359 0.01281 0.008838
## Proportion of Variance 0.00000 0.0000 0.00000 0.00000 0.00000 0.00000 0.000000
## Cumulative Proportion 1.00000 1.0000 1.00000 1.00000 1.00000 1.00000 1.000000
##          PC22   PC23   PC24   PC25   PC26   PC27
## Standard deviation      0.00759 0.005909 0.005329 0.004018 0.003534 0.001918
## Proportion of Variance 0.00000 0.000000 0.000000 0.000000 0.000000 0.000000
## Cumulative Proportion 1.00000 1.000000 1.000000 1.000000 1.000000 1.000000
##          PC28   PC29   PC30
## Standard deviation      0.001688 0.001416 0.0008379
## Proportion of Variance 0.000000 0.000000 0.0000000
## Cumulative Proportion 1.000000 1.000000 1.0000000
```

Need at least 5 components (until PC5)

#Hierarchal clustering

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

```
#calculate Euclidean distances
data.dist <- dist(data.scaled)
```

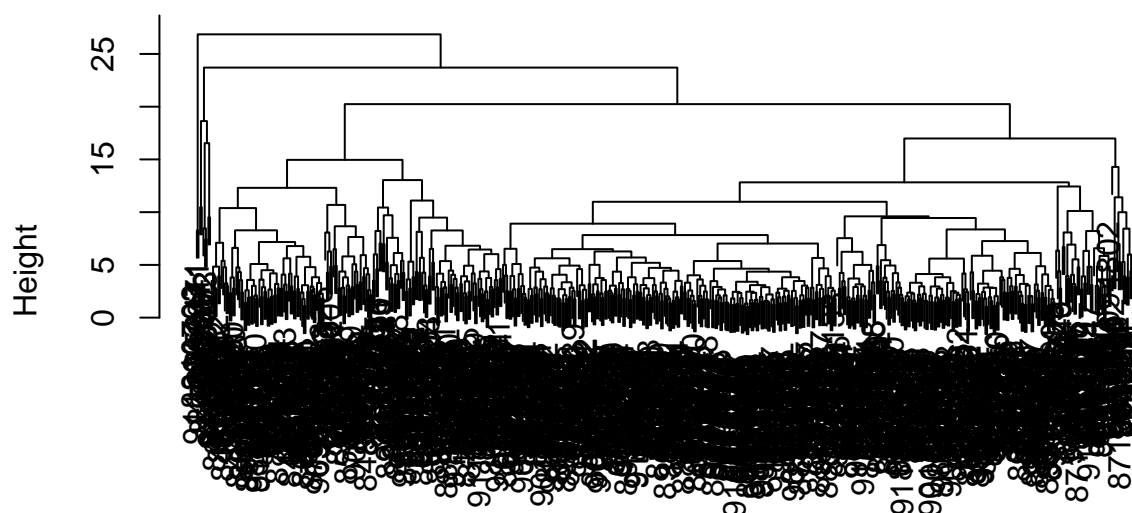
```
#create hierarchal clustering model
wisc.hclust <- hclust(data.dist)
```

#results of hierarchal clustering

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

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

Cluster Dendrogram



```
data.dist
hclust (*, "complete")
```

```
#cut the tree into 4 groups
wisc.hclust.clusters <- cutree(wisc.hclust, k =4)
```

Compare to diagnosis results

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

```
##           diagnosis
## wisc.hclust.clusters  B  M
##           1  12 165
##           2   2   5
##           3 343  40
##           4   0   2
```

Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

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

k = 4 still works the best

5. COmbining Methods

We take the results of our PCA analysis and cluster in this space 'wisc.pr\$x'

```
summary(wisc.pr)
```

```
## Importance of components:
##           PC1      PC2      PC3      PC4      PC5      PC6      PC7
## Standard deviation 666.170 85.49912 26.52987 7.39248 6.31585 1.73337 1.347
## Proportion of Variance 0.982 0.01618 0.00156 0.00012 0.00009 0.00001 0.000
## Cumulative Proportion 0.982 0.99822 0.99978 0.99990 0.99999 0.99999 1.000
##           PC8      PC9      PC10      PC11      PC12      PC13      PC14
## Standard deviation 0.6095 0.3944 0.2899 0.1778 0.08659 0.05623 0.04649
## Proportion of Variance 0.0000 0.0000 0.0000 0.0000 0.00000 0.00000 0.00000
## Cumulative Proportion 1.0000 1.0000 1.0000 1.0000 1.00000 1.00000 1.00000
##           PC15      PC16      PC17      PC18      PC19      PC20      PC21
## Standard deviation 0.03642 0.0253 0.01936 0.01534 0.01359 0.01281 0.008838
## Proportion of Variance 0.00000 0.0000 0.00000 0.00000 0.00000 0.00000 0.000000
## Cumulative Proportion 1.00000 1.0000 1.00000 1.00000 1.00000 1.00000 1.000000
##           PC22      PC23      PC24      PC25      PC26      PC27
## Standard deviation 0.00759 0.005909 0.005329 0.004018 0.003534 0.001918
## Proportion of Variance 0.00000 0.000000 0.000000 0.000000 0.000000 0.000000
## Cumulative Proportion 1.00000 1.000000 1.000000 1.000000 1.000000 1.000000
##           PC28      PC29      PC30
## Standard deviation 0.001688 0.001416 0.0008379
## Proportion of Variance 0.000000 0.000000 0.0000000
## Cumulative Proportion 1.000000 1.000000 1.0000000
```

Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

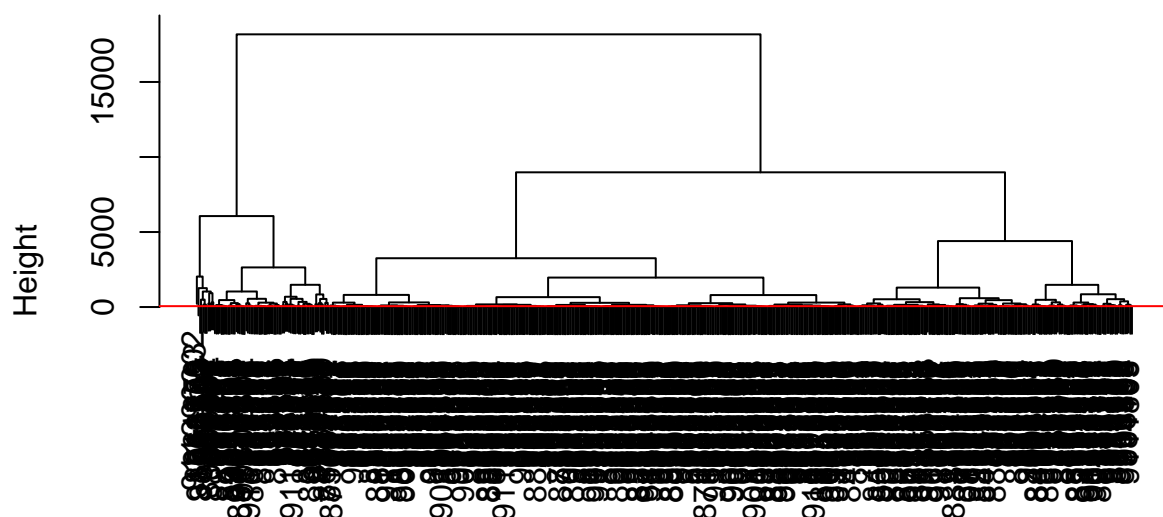
```
wisc.pc.hclust <- hclust(dist(wisc.pr$x[,1:3]), method = "ward.D2")
```

“ward.D2” is able to create groups that have variance minimized within clusters

Plot my dendrogram

```
plot(wisc.pc.hclust )
abline (h=60, col = "red")
```

Cluster Dendrogram



```
dist(wisc.pr$x[, 1:3])
hclust (*, "ward.D2")
```

Cut the tree into k=2 groups

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

```
##      grps
##      1   2
##      81 488
```

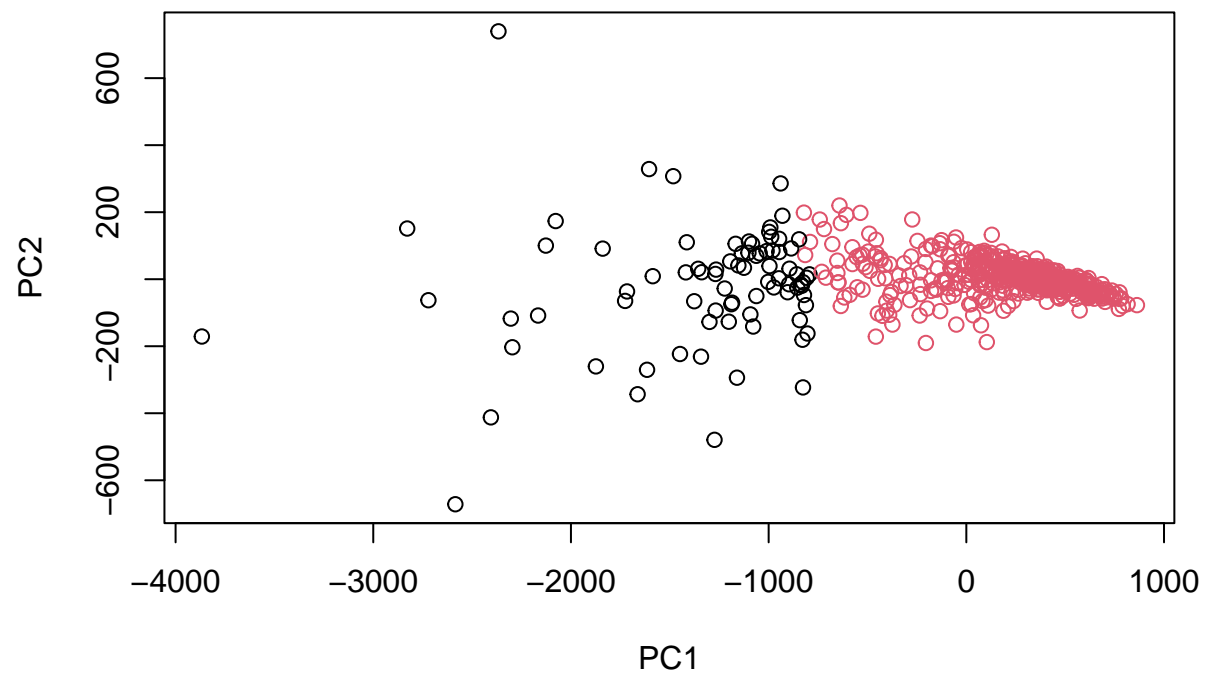
Cross table compare of diagnosis and my cluster groups

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

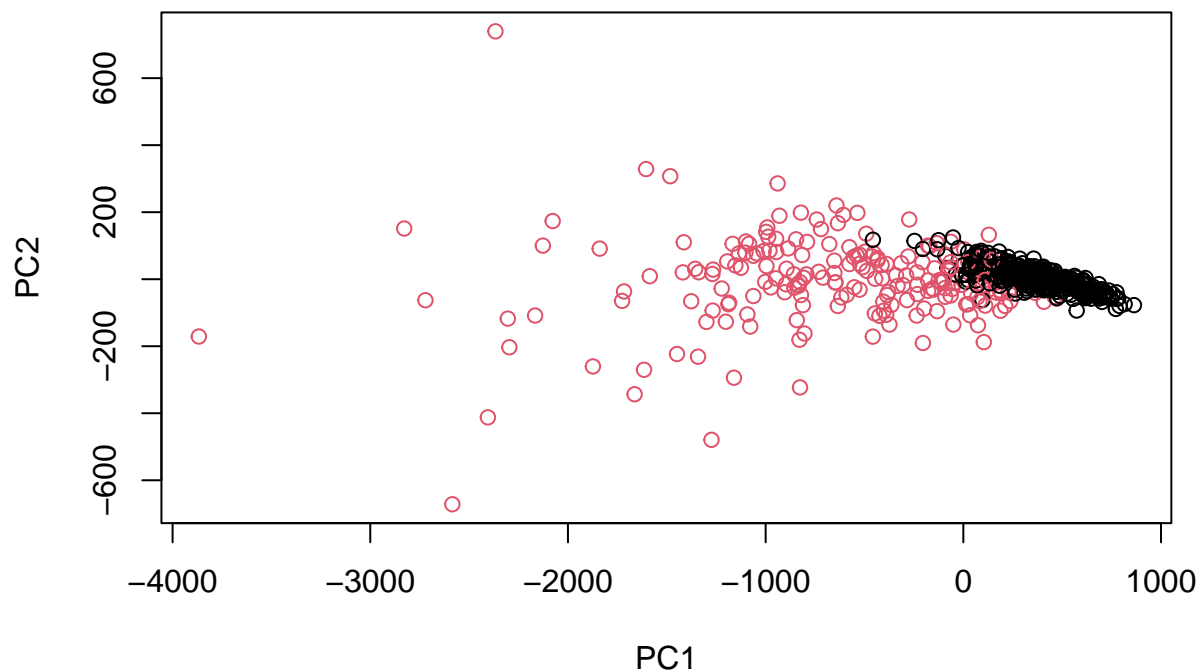
```
table(grps, diagnosis)
```

```
##      diagnosis
## grps    B    M
##    1    0   81
##    2  357  131
```

```
plot(wisc.pr$x[,1:2], col = grps)
```

```
plot(wisc.pr$x[,1:2], col = diagnosis)
```



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.

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

```
##      diagnosis
## grps    B    M
##    1    0   81
##    2  357  131
```

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

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

Sensitivity/ Specificity

Accuracy What proportion did we get correct if we call cluster 1 M and cluster 2 B

```
(333+ 179)/nrow(wisc.data)
```

```
## [1] 0.8998243
```

Sensitivity

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

```
## [1] 0.8443396
```

Specificity

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

```
## [1] 0.9327731
```

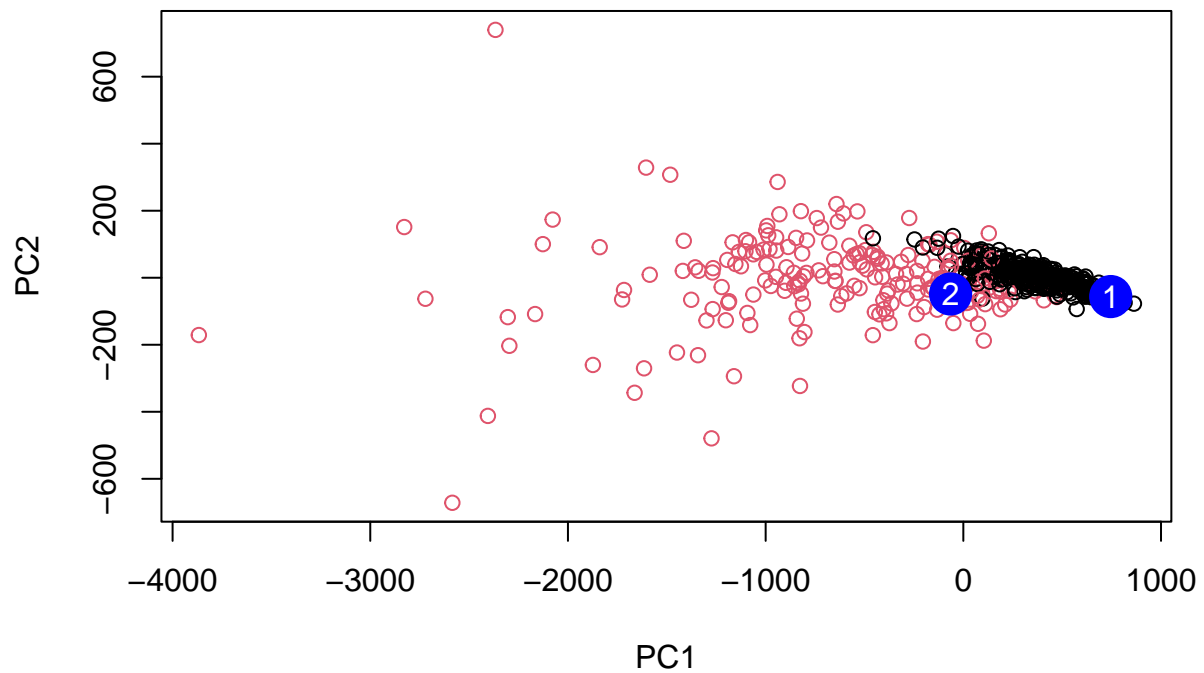
Q17. Which of your analysis procedures resulted in a clustering model with the best specificity?
How about sensitivity?

7. 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,] 745.60081 -56.16454 -21.15609 -3.330663  9.355518  2.317462 -1.147268
## [2,] -64.40839 -48.46996 -15.93413 12.089591 -4.636008 -1.045210 -0.295228
##          PC8          PC9          PC10          PC11          PC12          PC13
## [1,] -0.7644759  0.11704582  0.06401851  0.1191717 -0.05611973 -0.040020096
## [2,] -0.7454142 -0.09167106 -0.76173550  0.3206674  0.02602751  0.005023528
##          PC14          PC15          PC16          PC17          PC18          PC19
## [1,]  0.01354667 -0.018755904 -0.01050870 -0.01183961  0.020946097  0.030567858
## [2,] -0.11943490  0.008958015  0.03391077 -0.02468455  0.008002482 -0.006896744
##          PC20          PC21          PC22          PC23          PC24
## [1,] -0.007960122 -0.003773165  0.018561168  0.0001875602 -0.005463212
## [2,]  0.007001178 -0.022182056  0.008725155  0.0075849336  0.004619616
##          PC25          PC26          PC27          PC28          PC29
## [1,] -0.005992320  0.005357732  4.550233e-05  0.003252776  0.0012510265
## [2,]  0.002804663  0.003229335  1.977351e-03 -0.002261832  0.0009130702
##          PC30
## [1,] -0.0009794321
## [2,] -0.0009078383
```

```
plot(wisc.pr$x[,1:2], col = diagnosis)
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 patients 2 because the red cluster signifies malignant.