Class08_Mini_Project

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Exploratory data analysis

Data import

Data was downloaded from class website as a .csv file. The csv file is imported into R as a data frame.

Note that the first column here wisc.df$diagnosis is a pathologist provided expert diagnosis. We will not be using this for our unsupervised analysis as it is essentially the "answer" to the question which cell samples are malignant or benign.

```
# Save your input data file into your Project directory
fna.data <- read.csv("WisconsinCancer.csv")

# Complete the following code to input the data and store as wisc.df
wisc.df <- read.csv("WisconsinCancer.csv", row.names=1)

# We can use -1 here to remove the first column
wisc.data <- wisc.df[,-1]
head(wisc.data)
```

```
         radius_mean texture_mean perimeter_mean area_mean smoothness_mean
842302         17.99        10.38         122.80    1001.0         0.11840
842517         20.57        17.77         132.90    1326.0         0.08474
84300903       19.69        21.25         130.00    1203.0         0.10960
84348301       11.42        20.38          77.58     386.1         0.14250
84358402       20.29        14.34         135.10    1297.0         0.10030
843786         12.45        15.70          82.57     477.1         0.12780
         compactness_mean concavity_mean concave.points_mean symmetry_mean
842302            0.27760         0.3001             0.14710        0.2419
842517            0.07864         0.0869             0.07017        0.1812
84300903          0.15990         0.1974             0.12790        0.2069
84348301          0.28390         0.2414             0.10520        0.2597
84358402          0.13280         0.1980             0.10430        0.1809
843786            0.17000         0.1578             0.08089        0.2087
         fractal_dimension_mean radius_se texture_se perimeter_se area_se
842302                  0.07871    1.0950     0.9053        8.589  153.40
842517                  0.05667    0.5435     0.7339        3.398   74.08
84300903                0.05999    0.7456     0.7869        4.585   94.03
84348301                0.09744    0.4956     1.1560        3.445   27.23
84358402                0.05883    0.7572     0.7813        5.438   94.44
843786                  0.07613    0.3345     0.8902        2.217   27.19
```

```
         smoothness_se compactness_se concavity_se concave.points_se
842302         0.006399        0.04904      0.05373           0.01587
842517         0.005225        0.01308      0.01860           0.01340
84300903       0.006150        0.04006      0.03832           0.02058
84348301       0.009110        0.07458      0.05661           0.01867
84358402       0.011490        0.02461      0.05688           0.01885
843786         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
```

Setup a separate new vector called diagnosis that contains the data from the diagnosis column of the original dataset. We will store this as a factor (useful for plotting) and use this later to check our results. (we want to test clustering to see if it partitions the data correctly, having this would be cheating)

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

```
[1] M M M M M M
Levels: B M
```

Exploratory data analysis

Q1. How many observations are in this dataset?

There are 569 observations in this datase

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

There are 212 malignant diagnosis

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

```
  B   M
357 212
```

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

There are 10 variables/features in the data are suffixed with "_mean"

```
colnames(wisc.df)
```

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

```
[27] "compactness_worst"       "concavity_worst"
[29] "concave.points_worst"    "symmetry_worst"
[31] "fractal_dimension_worst"
```

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

```
 [1]  2  3  4  5  6  7  8  9 10 11
```

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

```
[1] 10
```

Principal Component Analysis

Performing PCA

Note: use the `prcomp()`function to do PCA

- If we look at the argument in `prcomp()`, we can see that `scale. = FALSE` by default. However, if a column has a high value of variance, and `scale. = FALSE`, PCA will be dominated by columns with large variance (*not a feature, just the nature of numbers for certain parameter, i.e.speed of walking for different people is give or take ~4-5m/s, but the number of hairs is ~90k-150k. Number of hair would have a much larger variance, which will dominate PCA, but it doesn't necessarily makes it a more meaningful way to cluster different groups of people*). That's why **in general we should use `scale. = TRUE`**

Check the mean and standard deviation of the features (i.e. columns) of the wisc.data to determine if the data should be scaled. Use the colMeans() and apply() functions like you've done before.

```
# 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
```

We can see that there's large difference between the standard deviations of different variables, so we should use scaling

Next, we do our PCA

```r
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp(wisc.data,scale. = TRUE)

# Look at summary of results
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 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, because the Cumulative Proportion for PC3 is 72.636%

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

7 PCs are required

Interpreting PCA results

Now you will use some visualizations to better understand your PCA model.

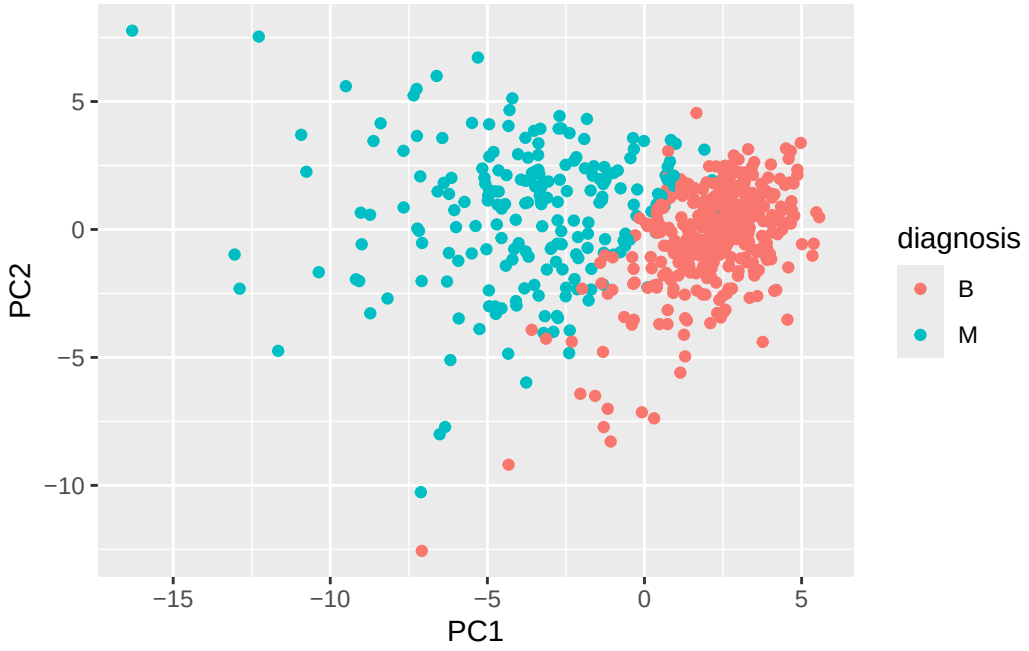
First, we use gg plot to make scatter plot

```
library(ggplot2)
head(wisc.pr$x)
```

```
              PC1        PC2        PC3       PC4        PC5         PC6
842302   -9.184755  -1.946870 -1.1221788 3.6305364  1.1940595  1.41018364
842517   -2.385703   3.764859 -0.5288274 1.1172808 -0.6212284  0.02863116
84300903 -5.728855   1.074229 -0.5512625 0.9112808  0.1769302  0.54097615
84348301 -7.116691 -10.266556 -3.2299475 0.1524129  2.9582754  3.05073750
84358402 -3.931842   1.946359  1.3885450 2.9380542 -0.5462667 -1.22541641
843786   -2.378155  -3.946456 -2.9322967 0.9402096  1.0551135 -0.45064213
                PC7         PC8         PC9        PC10        PC11        PC12
842302    2.15747152  0.39805698 -0.15698023 -0.8766305 -0.2627243 -0.8582593
842517    0.01334635 -0.24077660 -0.71127897  1.1060218 -0.8124048  0.1577838
84300903 -0.66757908 -0.09728813  0.02404449  0.4538760  0.6050715  0.1242777
84348301  1.42865363 -1.05863376 -1.40420412 -1.1159933  1.1505012  1.0104267
84358402 -0.93538950 -0.63581661 -0.26357355  0.3773724 -0.6507870 -0.1104183
843786    0.49001396  0.16529843 -0.13335576 -0.5299649 -0.1096698  0.0813699
                PC13         PC14         PC15        PC16        PC17
842302    0.10329677 -0.690196797  0.601264078  0.74446075 -0.26523740
842517   -0.94269981 -0.652900844 -0.008966977 -0.64823831 -0.01719707
84300903 -0.41026561  0.016665095 -0.482994760  0.32482472  0.19075064
84348301 -0.93245070 -0.486988399  0.168699395  0.05132509  0.48220960
84358402  0.38760691 -0.538706543 -0.310046684 -0.15247165  0.13302526
843786   -0.02625135  0.003133944 -0.178447576 -0.01270566  0.19671335
                PC18        PC19        PC20         PC21        PC22
842302   -0.54907956  0.1336499  0.34526111  0.096430045 -0.06878939
842517    0.31801756 -0.2473470 -0.11403274 -0.077259494  0.09449530
84300903 -0.08789759 -0.3922812 -0.20435242  0.310793246  0.06025601
84348301 -0.03584323 -0.0267241 -0.46432511  0.433811661  0.20308706
84358402 -0.01869779  0.4610302  0.06543782 -0.116442469  0.01763433
843786   -0.29727706 -0.1297265 -0.07117453 -0.002400178  0.10108043
                PC23         PC24         PC25         PC26        PC27
842302    0.08444429  0.175102213  0.150887294 -0.201326305 -0.25236294
842517   -0.21752666 -0.011280193  0.170360355 -0.041092627  0.18111081
84300903 -0.07422581 -0.102671419 -0.171007656  0.004731249  0.04952586
84348301 -0.12399554 -0.153294780 -0.077427574 -0.274982822  0.18330078
```

```
84358402  0.13933105  0.005327110 -0.003059371  0.039219780  0.03213957
843786    0.03344819 -0.002837749 -0.122282765 -0.030272333 -0.08438081
                 PC28          PC29          PC30
842302   -0.0338846387  0.045607590  0.0471277407
842517    0.0325955021 -0.005682424  0.0018662342
84300903  0.0469844833  0.003143131 -0.0007498749
84348301  0.0424469831 -0.069233868  0.0199198881
84358402 -0.0347556386  0.005033481 -0.0211951203
843786    0.0007296587 -0.019703996 -0.0034564331
```

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

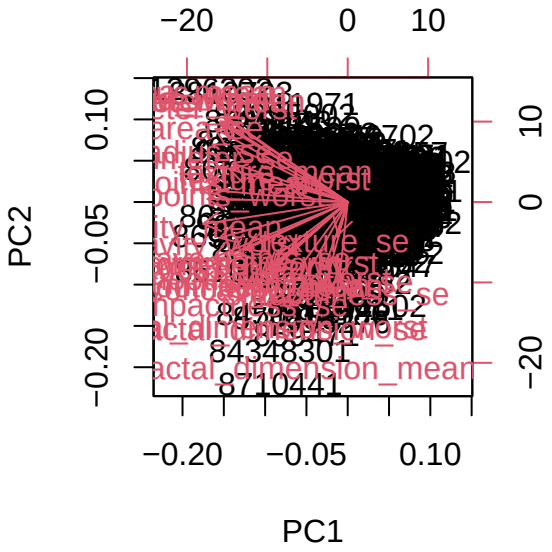


This plot clearly shows two distinct population of patients within our data set. We are going to compare this plot with some other plots.

A common visualization for PCA results is the so-called biplot.

Create a biplot of the wisc.pr using the biplot() function.

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



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

No thing really stands out about this plot. It is very messy and difficult to understand because the text labels are all clumpped together

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

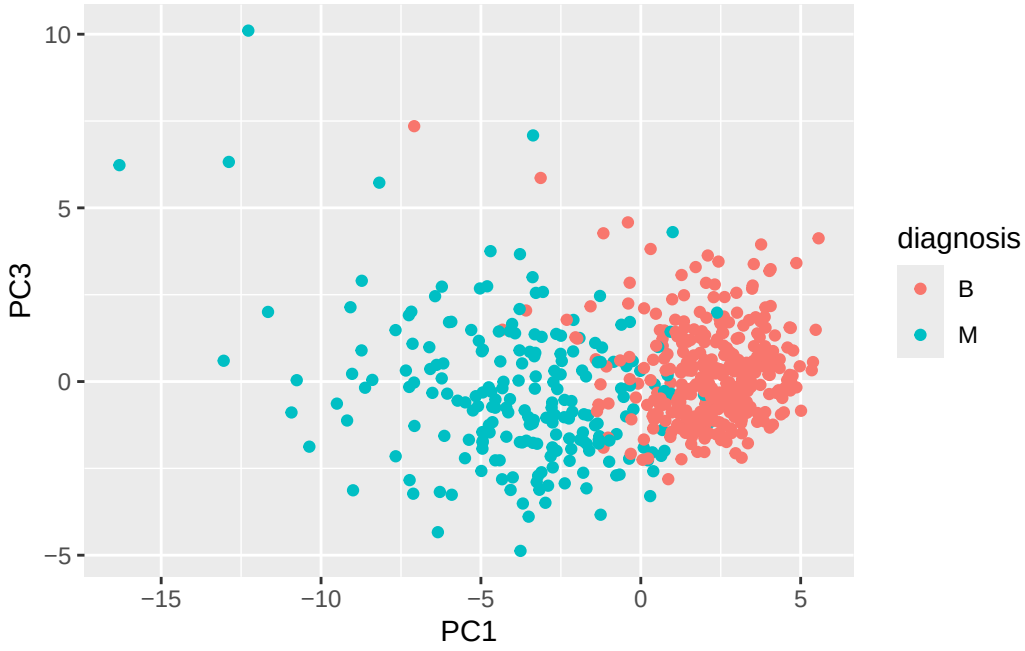
I noticed that from these scatter plot that the there are clearly two distinct patient population with in the dataset, and these groups can be separated by the diagnosis. Compare PC1 vs PC2 and PC1 vs PC3, we can see that PC1 vs PC2 gives a clearer separation (makes sense because PC1 and PC2 collectively captures more variance)

```
library(ggplot2)
head(wisc.pr$x)
```

```
               PC1        PC2        PC3       PC4        PC5         PC6
842302   -9.184755  -1.946870 -1.1221788 3.6305364  1.1940595  1.41018364
842517   -2.385703   3.764859 -0.5288274 1.1172808 -0.6212284  0.02863116
84300903 -5.728855   1.074229 -0.5512625 0.9112808  0.1769302  0.54097615
84348301 -7.116691 -10.266556 -3.2299475 0.1524129  2.9582754  3.05073750
84358402 -3.931842   1.946359  1.3885450 2.9380542 -0.5462667 -1.22541641
```

```
843786   -2.378155  -3.946456 -2.9322967 0.9402096  1.0551135 -0.45064213
                PC7         PC8         PC9       PC10       PC11       PC12
842302    2.15747152  0.39805698 -0.15698023 -0.8766305 -0.2627243 -0.8582593
842517    0.01334635 -0.24077660 -0.71127897  1.1060218 -0.8124048  0.1577838
84300903 -0.66757908 -0.09728813  0.02404449  0.4538760  0.6050715  0.1242777
84348301  1.42865363 -1.05863376 -1.40420412 -1.1159933  1.1505012  1.0104267
84358402 -0.93538950 -0.63581661 -0.26357355  0.3773724 -0.6507870 -0.1104183
843786    0.49001396  0.16529843 -0.13335576 -0.5299649 -0.1096698  0.0813699
               PC13         PC14         PC15        PC16        PC17
842302    0.10329677 -0.690196797  0.601264078  0.74446075 -0.26523740
842517   -0.94269981 -0.652900844 -0.008966977 -0.64823831 -0.01719707
84300903 -0.41026561  0.016665095 -0.482994760  0.32482472  0.19075064
84348301 -0.93245070 -0.486988399  0.168699395  0.05132509  0.48220960
84358402  0.38760691 -0.538706543 -0.310046684 -0.15247165  0.13302526
843786   -0.02625135  0.003133944 -0.178447576 -0.01270566  0.19671335
               PC18       PC19        PC20         PC21        PC22
842302   -0.54907956  0.1336499  0.34526111  0.096430045 -0.06878939
842517    0.31801756 -0.2473470 -0.11403274 -0.077259494  0.09449530
84300903 -0.08789759 -0.3922812 -0.20435242  0.310793246  0.06025601
84348301 -0.03584323 -0.0267241 -0.46432511  0.433811661  0.20308706
84358402 -0.01869779  0.4610302  0.06543782 -0.116442469  0.01763433
843786   -0.29727706 -0.1297265 -0.07117453 -0.002400178  0.10108043
               PC23         PC24         PC25         PC26        PC27
842302    0.08444429  0.175102213  0.150887294 -0.201326305 -0.25236294
842517   -0.21752666 -0.011280193  0.170360355 -0.041092627  0.18111081
84300903 -0.07422581 -0.102671419 -0.171007656  0.004731249  0.04952586
84348301 -0.12399554 -0.153294780 -0.077427574 -0.274982822  0.18330078
84358402  0.13933105  0.005327110 -0.003059371  0.039219780  0.03213957
843786    0.03344819 -0.002837749 -0.122282765 -0.030272333 -0.08438081
                PC28         PC29          PC30
842302   -0.0338846387  0.045607590  0.0471277407
842517    0.0325955021 -0.005682424  0.0018662342
84300903  0.0469844833  0.003143131 -0.0007498749
84348301  0.0424469831 -0.069233868  0.0199198881
84358402 -0.0347556386  0.005033481 -0.0211951203
843786    0.0007296587 -0.019703996 -0.0034564331
```

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



Variance Explained

Calculate the variance of each principal component by squaring the sdev component of wisc.pr (i.e. wisc.pr$sdev^2). Save the result as an object called pr.var.

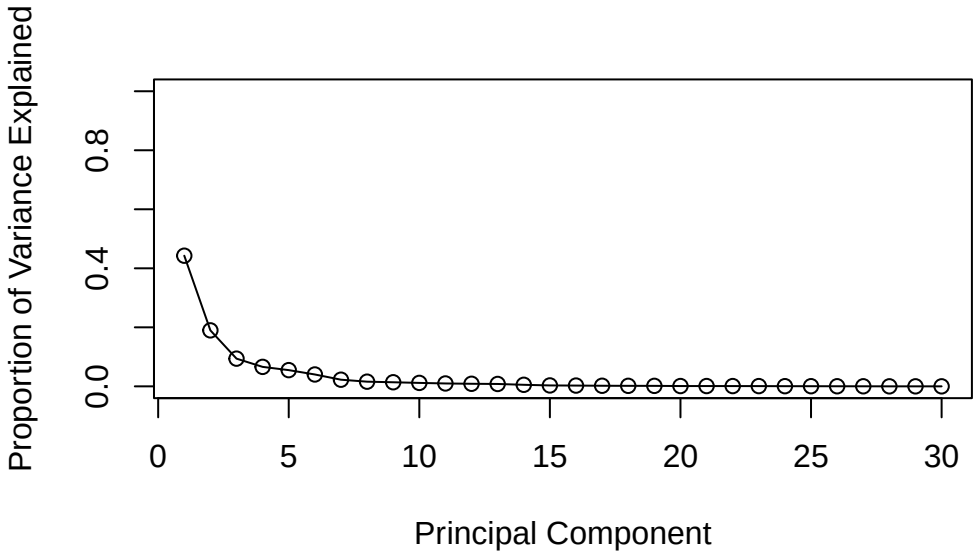
```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

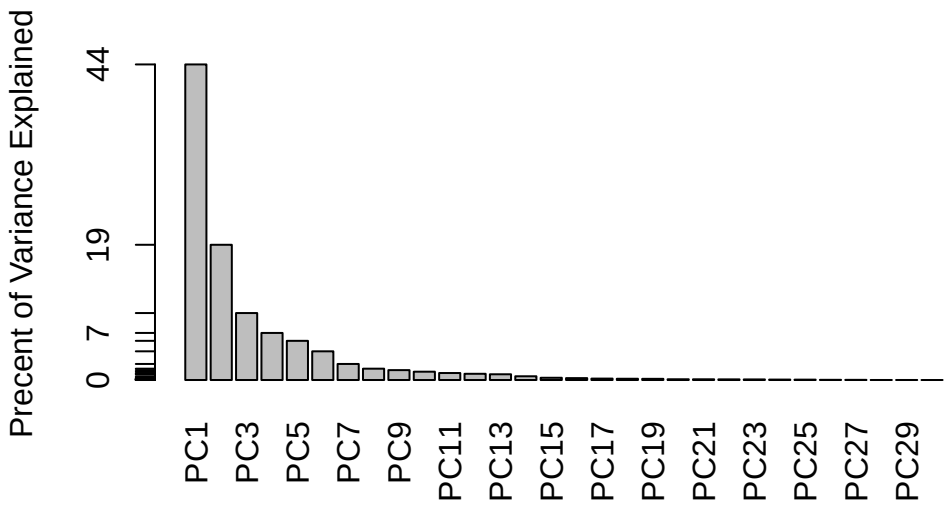
Calculate the variance explained by each principal component by dividing by the total variance explained of all principal components. Assign this to a variable called pve and create a plot of variance explained for each principal component.

```
# Variance explained by each principal component: pve
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")
```




```
# 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 )
```

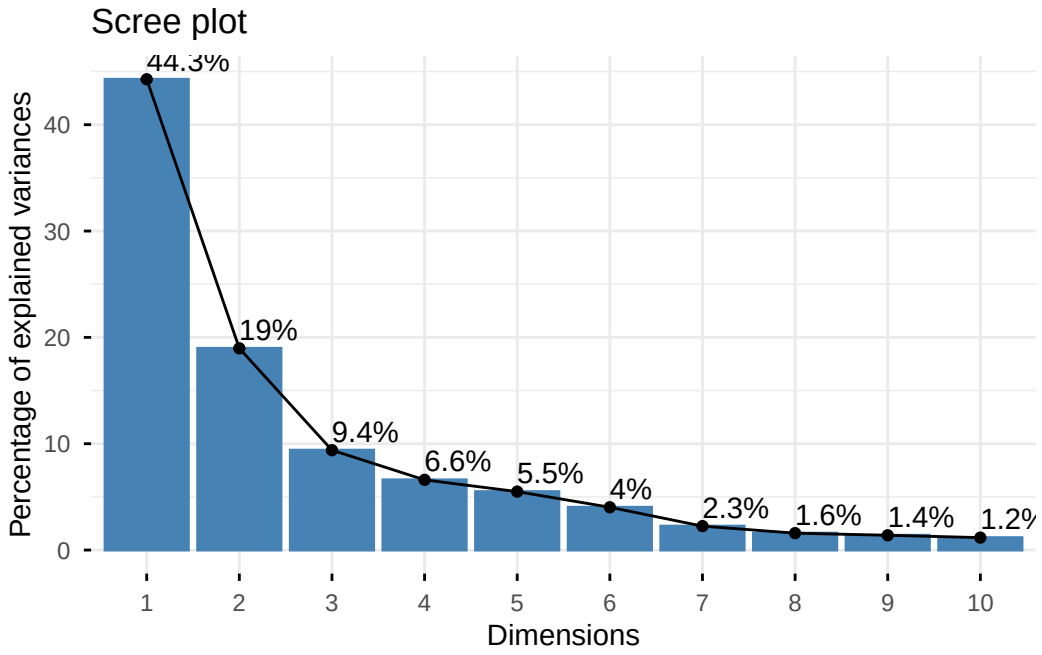



```
## ggplot based graph
#install.packages("factoextra")
library(factoextra)
```

```
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`.
```



Communicating PCA results

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 loading vector of the first PC for the feature concave.point_mean is -0.2608538

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

5

```
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 helpful, so...

First scale the wisc.data data and assign the result to data.scaled.

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

Calculate the (Euclidean) distances between all pairs of observations in the new scaled dataset and assign the result to data.dist.

```
data.dist <- dist(data.scaled)
```

Create a hierarchical clustering model using complete linkage. Manually specify the method argument to hclust() and assign the results to wisc.hclust.

```
wisc.hclust <- hclust(data.dist,method = "complete")
```

Results of hierarchical clustering

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

At height = 19, we can get 4 clusters

- Note: But this is not very helpful because it really doesnt relay any insight/information about the dataset to us. So we give up on this approach

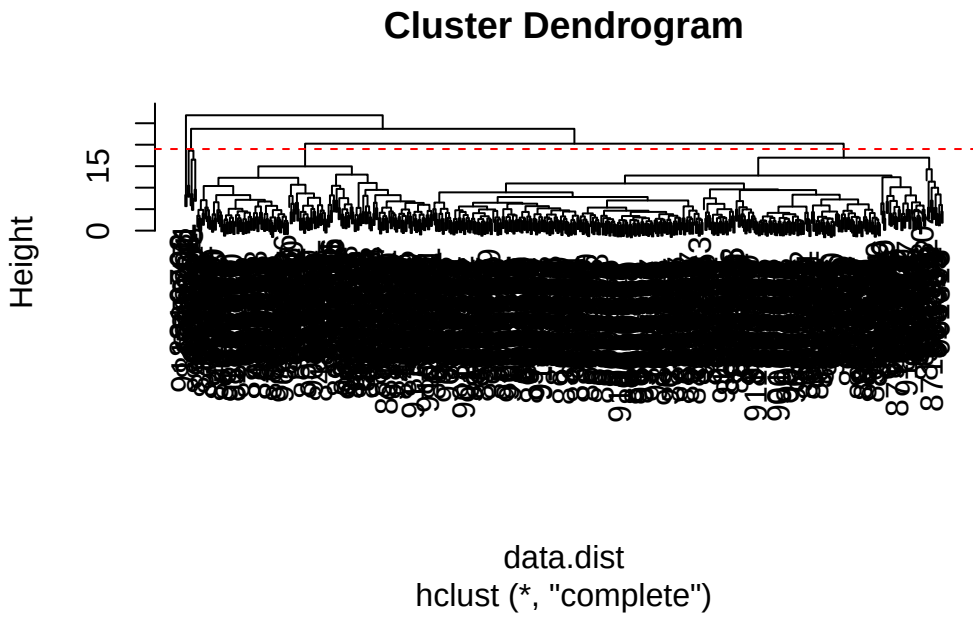
```
plot(wisc.hclust)
head(cutree(wisc.hclust, k=4))
```

```
  842302   842517 84300903 84348301 84358402   843786
       1        1        1        2        1        1
```

```
table(cutree(wisc.hclust,k=4))
```

```
  1   2   3   4
177   7 383   2
```

```
abline(h=19, col="red", lty=2)
```



Selecting number of clusters

Next we are going to compare the outputs from the hierarchical clustering model to the actual diagnosis.

Recall, we have the diagnosis factor, maybe it will help if we see where the malignent and benign diagnosis are in the h-clustering?

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

```
   diagnosis
      B   M
  1  12 165
  2   2   5
  3 343  40
  4   0   2
```

Next, we are gonna explore how different number of clusters affect the ability of the hierarchical clustering to separate the different diagnosis

> Q12. Can you fin d abetter cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

It is difficulty to find a cluster vs diagnoses match that is meaningful. In comparison, it is slightly better when we cluster the data in 4,5, 6, or 7 clusters as in these cases, most malignent diagnosis is clustered under cluster 1 and most benign diagnosis is clustered under cluster 3, but these clustering methods also generates a number of cluster that is meaningless (can be interpreted as another cluster's equivalent), so without prior knowledge of the diagnosis, they would not be meaningful to us.

```
test_cluster <- function(x){
  table((cutree(wisc.hclust,k=x)), diagnosis)
}
test_cluster(2)
```

```
   diagnosis
      B   M
  1 357 210
  2   0   2
```

```
test_cluster(3)
```

```
   diagnosis
      B   M
  1 355 205
  2   2   5
  3   0   2
```

```
test_cluster(5)
```

```
   diagnosis
      B   M
  1  12 165
  2   0   5
  3 343  40
  4   2   0
  5   0   2
```

```
test_cluster(6)
```

```
   diagnosis
      B   M
  1  12 165
  2   0   5
  3 331  39
  4   2   0
  5  12   1
  6   0   2
```

```
test_cluster(7)
```

```
   diagnosis
      B   M
  1  12 165
  2   0   3
  3 331  39
  4   2   0
  5  12   1
  6   0   2
  7   0   2
```

```
test_cluster(8)
```

```
   diagnosis
      B   M
  1  12  86
  2   0  79
  3   0   3
  4 331  39
  5   2   0
  6  12   1
  7   0   2
  8   0   2
```

```
test_cluster(9)
```

```
   diagnosis
      B   M
  1  12  86
  2   0  79
  3   0   3
  4 331  39
  5   2   0
  6  12   0
  7   0   2
  8   0   2
  9   0   1
```

```
test_cluster(10)
```

```
    diagnosis
       B   M
  1   12  86
  2    0  59
  3    0   3
  4  331  39
  5    0  20
  6    2   0
  7   12   0
  8    0   2
  9    0   2
  10   0   1
```

This confirms that this clustering is useless.

Using different methods

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

the complete linkage method usually gives me my favorite results for the same data.dist dataset because it always give me distinct populations/clustering by using the largest of all pair-wise similarity to determine the clustering.

Optional: K-means Clustering

k-means clustering and comparing results

We will next try create a k-means clustering model on the Wisconsin breat cancer data and compare the results to the acutual diagnosis

First, we will create a k-means model on `wisc.data`

```
wisc.km <- kmeans(data.scaled,centers=2,nstart=3)
table(wisc.km$cluster, diagnosis)
```

```
   diagnosis
      B   M
  1 343  37
  2  14 175
```

> Q14. How well does k-means separate the two diagnoses?How does it compare to your hclust results?

The k-means separate the two diagnoses fairlyl well, with the malignent and benign diagnoses in cluster 1 and 2 respectively. It is does do a better job compare to the hclust we performed earlier.

```
test_cluster(4)
```

```
  diagnosis
     B   M
1   12 165
2    2   5
3  343  40
4    0   2
```

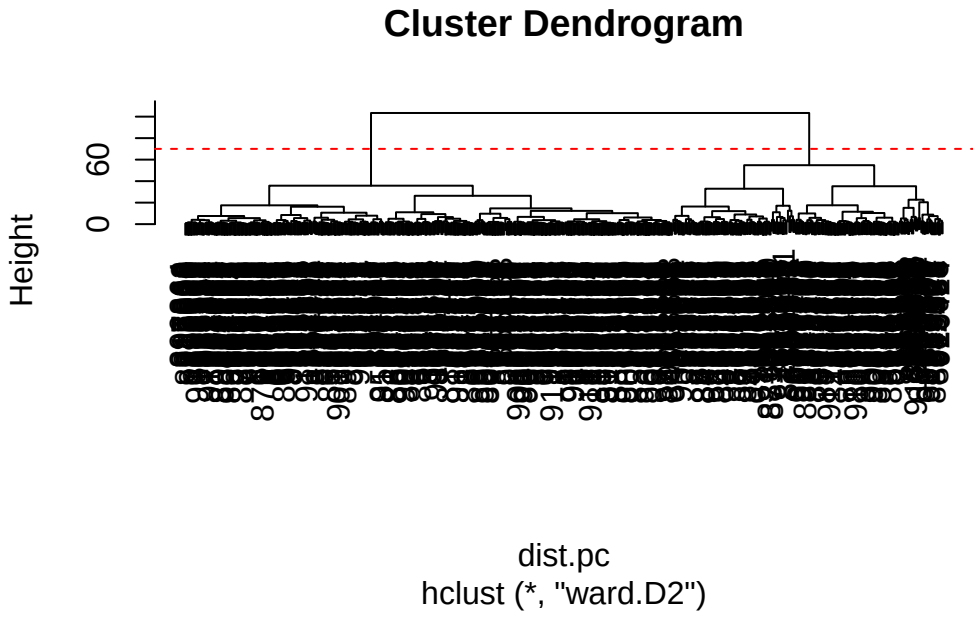
Combining methods

So let's try combine PCA with h-clustering since clustering of the origianl data is not productive, PCA is promising, so maybe we can cluster from PCA results (clustering in PC space)

Clustering on PCA results

Since the first 3 PCs can capture 70% of variance, we can try to cluster them first

```
# First we get the frist 3 PCs, pastt it through a dist matrix function, call it dist.pc
dist.pc <- dist(wisc.pr$x[, 1:3])
wisc.pr.hclust <- hclust(dist.pc, method="ward.D2")
plot(wisc.pr.hclust)
abline(h=70, col="red", lty=2)
```



It is good that we can see there's two main clusters. Now we are gonna try to see if this clustering is good by comparing it with the diagnosis results.

To get our clustering membership vector, we cut the tree at a desired height to yeild 2 cluster (with `cuttree()` at either h=70, or k=2) We can the use `table()` to compare the clustering results with the diagnosis results. This clustering groups is fairly accurate when compare to expert diagnosis. (For Diagnosis purpose, for malignent, we have 24 false positives out of 203 cases.)

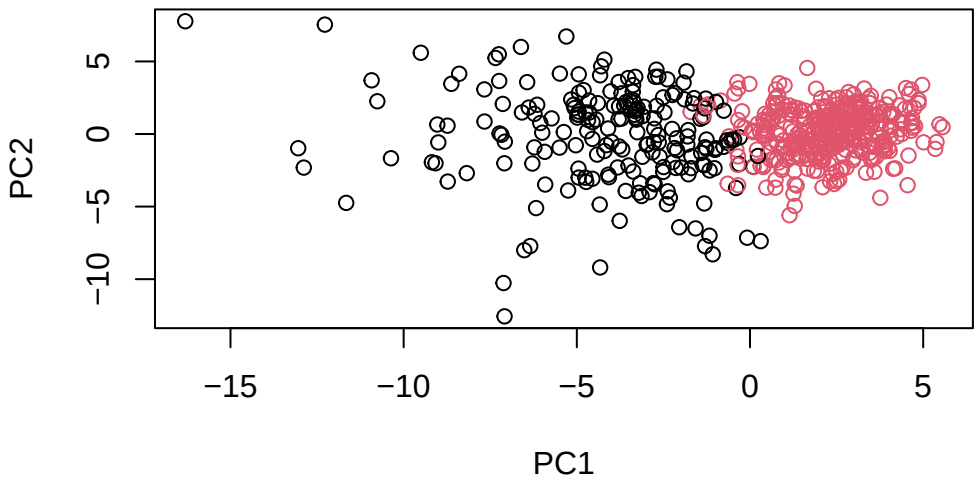
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
203 366
```

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

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

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



Sensitivity & Specificity

> Q15. How well does the newly created model with four clusters separates out the two diagnosis

The newly created model with 2 clusters separates out eh two diagnosis pretty neatly, as most of the malignent diagnosis is in cluster 1 while most of the benign diagnosis is in cluster 2

> Q16. How well do the k-means and hierarchical clustering you created in previous section do in terms of separating the diagnoses?

The k-means clustering does a decent job separating the diagnoses (not as well as PCA); the hierarchical clustering does not do a goo job separating the diagnosis.

```
table(wisc.km$cluster,diagnosis)
```

```
   diagnosis
      B   M
  1 343  37
  2  14 175
```

```
test_cluster(4)
```

```
   diagnosis
      B   M
  1  12 165
  2   2   5
  3 343  40
  4   0   2
```

Sensitivity refers to a test's ability to correctly detect ill patients who do have the condition. In our example here the sensitivity is the total number of samples in the cluster identified as predominantly malignant (cancerous) divided by the total number of known malignant samples. In other words: TP/(TP+FN).

Specificity relates to a test's ability to correctly reject healthy patients without a condition. In our example specificity is the proportion of benign (not cancerous) samples in the cluster identified as predominantly benign that are known to be benign. In other words: TN/(TN+FN).

Now let's try calculate these numbers from the matrix

```
N <- table(grps, diagnosis)
N
```

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

```
Sensitivity <- N[1,2]/sum(N[1,])
Sensitivity
```

```
[1] 0.8817734
```

```
Specificity <- N[2,1]/sum(N[2,])
Specificity
```

```
[1] 0.9098361
```

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

Both K-means and PCA-hclust combined clustering both results in the highest specificity. The hierarchical clustering with k=2 has the highest sensitivity, but this is because almost all patients are grouped under cluster 1, so it has good ability to correctly detect ill patients who do have the condition. Otherwise, the sensitivities of the k-means method and the combined method are the same.

```
N <- table(grps, diagnosis)
N
```

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

```
Sensitivity <- N[1,2]/sum(N[1,])
Sensitivity
```

```
[1] 0.8817734
```

```
Specificity <- N[2,1]/sum(N[2,])
Specificity
```

```
[1] 0.9098361
```

```
M <- table(wisc.km$cluster, diagnosis)
M
```

```
   diagnosis
      B   M
  1 343  37
  2  14 175
```

```
Sensitivity <- N[1,2]/sum(N[1,])
Sensitivity
```

```
[1] 0.8817734
```

```
Specificity <- N[2,1]/sum(N[2,])
Specificity
```

```
[1] 0.9098361
```

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

```
   diagnosis
      B   M
  1 357 210
  2   0   2
```

```
Sensitivity <- O[1,2]/sum(N[1,])
Sensitivity
```

```
[1] 1.034483
```

```
Specificity <- O[2,1]/sum(N[2,])
Specificity
```

```
[1] 0
```

Prediction

We can use our PCA model for predicting 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
```

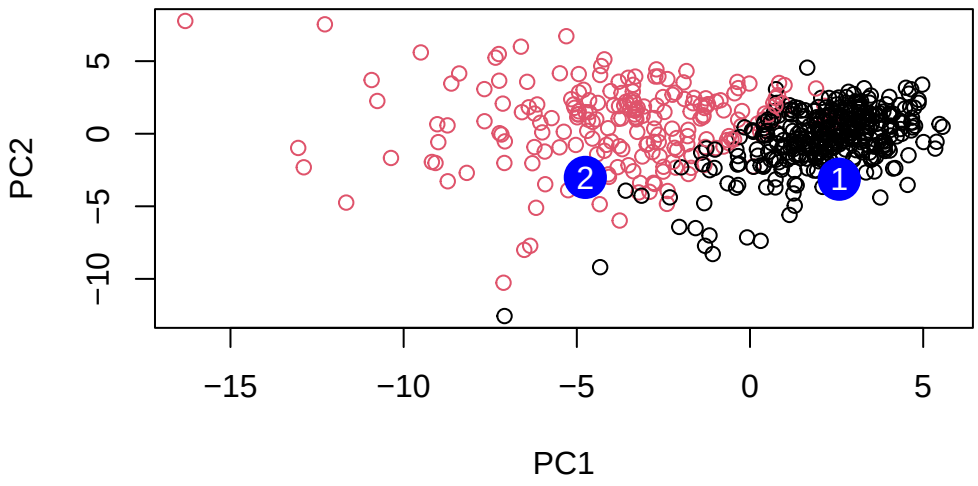
```
          PC1       PC2        PC3        PC4       PC5        PC6        PC7
[1,]  2.576616 -3.135913  1.3990492 -0.7631950  2.781648 -0.8150185 -0.3959098
[2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698 -1.2189945  0.8193031
           PC8       PC9       PC10      PC11      PC12      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],col=diagnosis)
cat(paste(levels(diagnosis),"=",palette()[seq_along(levels(diagnosis))],collapse = ","))
```

```
B = black,M = #DF536B
```

```
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 patient 2 based on the results since patient 2 is placed in the cluster with malignent diagnosis.