# Class 8 Mini-Project

4/28/23

## Preparing the data

```
#assigning the .csv file to an object
fna.data <- "WisconsinCancer.csv"
#reading the csv and assigning it to a new object
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 |

#### Setting up the data

```
#removing the first column of the dataset
wisc.data <- wisc.df[,-1]

#making a new vector for the diagnosis column
diagnosis <- factor(wisc.df$diagnosis)
```

## Exploratory Data Analysis

#### Q1. How many observations are in this dataset?

```
#using dim() to see the rows and columns of the dataset
dim(wisc.df)
```

```
[1] 569  31
```

There are 569 observations in this dataset.

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

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

```

  B   M 
357 212 
```

There are 212 observations that have a malignant diagnosis.

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

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

```
[1] 10
```

There are 10.

# 2. Principal Component Analysis

## Performing PCA

```r
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 
```

```r
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
```

```r
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)?**

.4427 (44.27%) is the proportion of the original variance captured by the PC1.

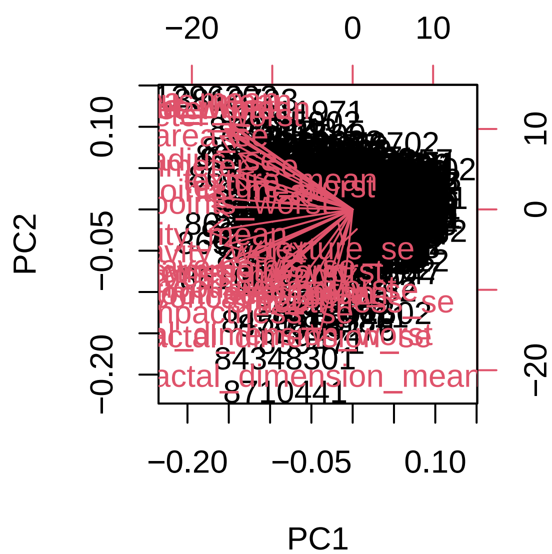
**Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?**

3 PCs are required.

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

7 PCs are required.

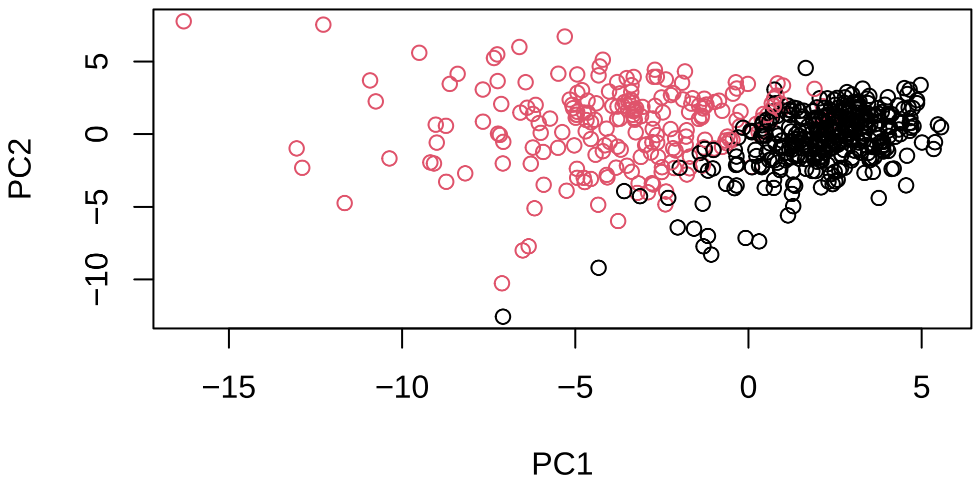
```r
biplot(wisc.pr)
```




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

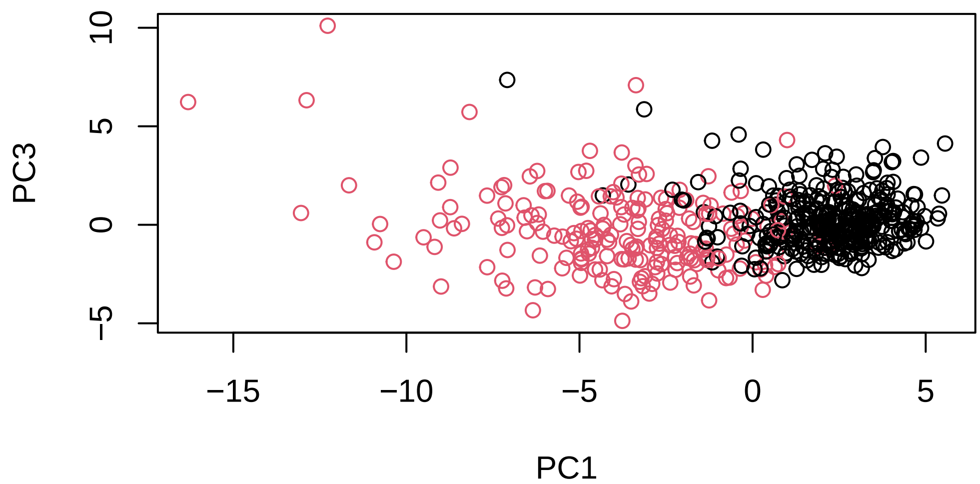
This plot is incredibly cluttered and hard to read, making it difficult to understand as there is no general trend that is really visible to someone trying to pull information from the plot.

```r
plot( wisc.pr$x[,1:2] , col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



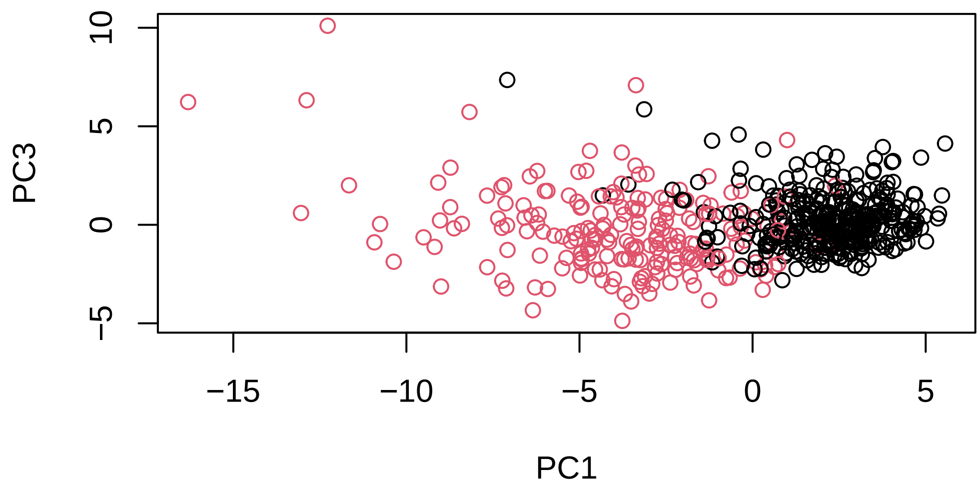

**Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?**

```
plot(wisc.pr$x[, -2], col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```




```
#or

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

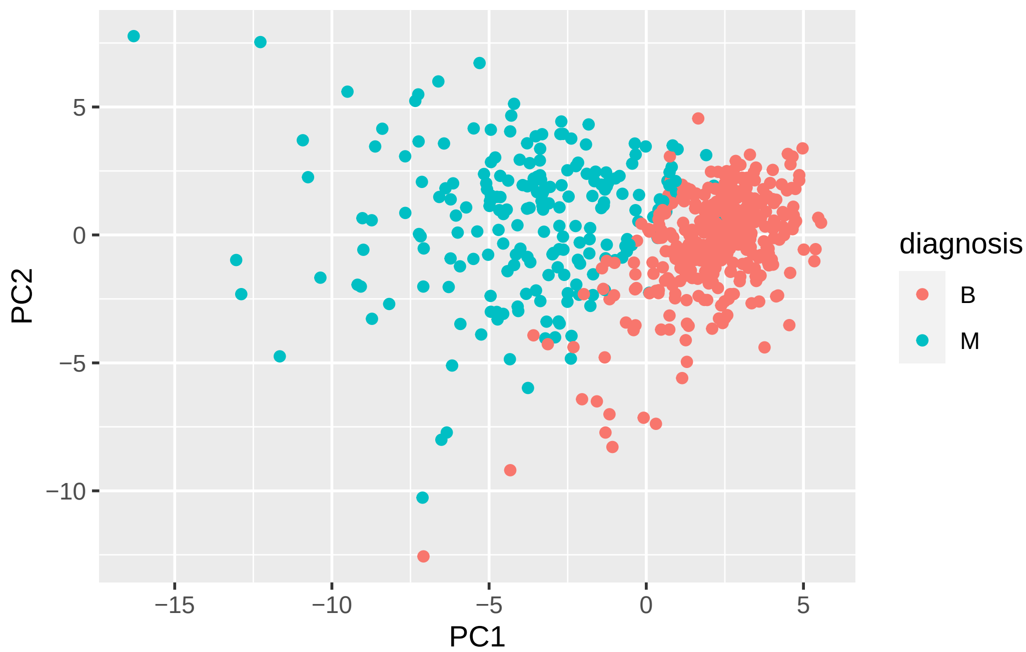



As PC2 explains more variance in the original data than PC3, the first plot generated has a cleaner separation between the two subgroups. The plots overall show that PC1 is capturing a difference between malignant (red) and benign (black) samples.

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

# Load the ggplot2 package
library(ggplot2)

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



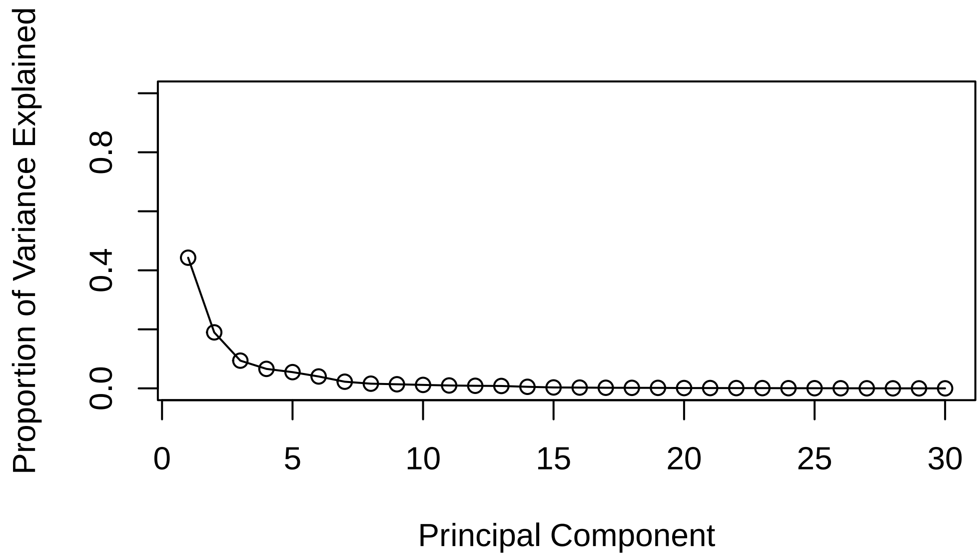

## Variance explained

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

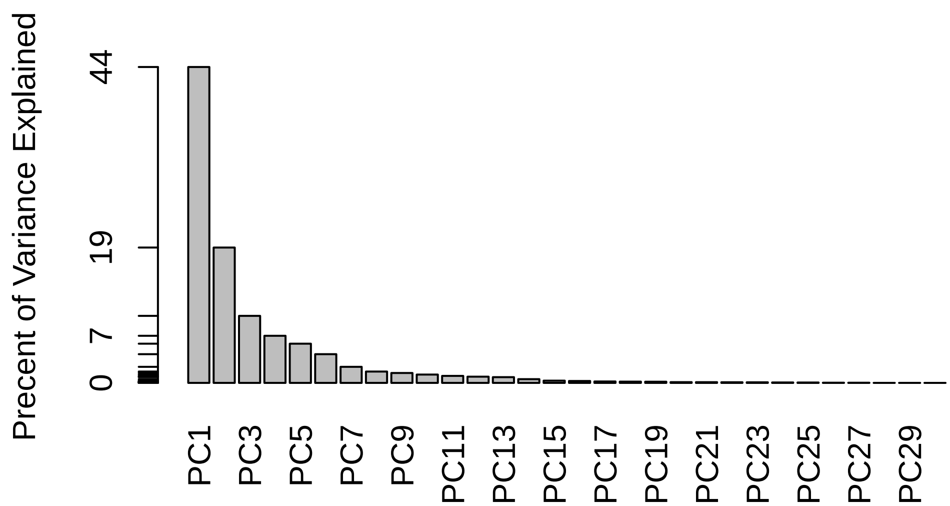
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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 )
```




## 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`? This tells us how much this original feature contributes to the first PC.**

```
(wisc.pr$rotation[,1])
```

```
           radius_mean            texture_mean          perimeter_mean 
           -0.21890244             -0.10372458             -0.22753729 
             area_mean         smoothness_mean        compactness_mean 
           -0.22099499             -0.14258969             -0.23928535 
        concavity_mean     concave.points_mean           symmetry_mean 
           -0.25840048             -0.26085376             -0.13816696 
fractal_dimension_mean               radius_se              texture_se 
           -0.06436335             -0.20597878             -0.01742803 
          perimeter_se                 area_se           smoothness_se 
           -0.21132592             -0.20286964             -0.01453145 
        compactness_se            concavity_se       concave.points_se 
           -0.17039345             -0.15358979             -0.18341740 
```

```
         symmetry_se    fractal_dimension_se             radius_worst
         -0.04249842             -0.10256832              -0.22799663
       texture_worst         perimeter_worst               area_worst
         -0.10446933             -0.23663968              -0.22487053
    smoothness_worst       compactness_worst          concavity_worst
         -0.12795256             -0.21009588              -0.22876753
concave.points_worst          symmetry_worst  fractal_dimension_worst
         -0.25088597             -0.12290456              -0.13178394
```

-0.26085376

## 3. Hierarchical clustering

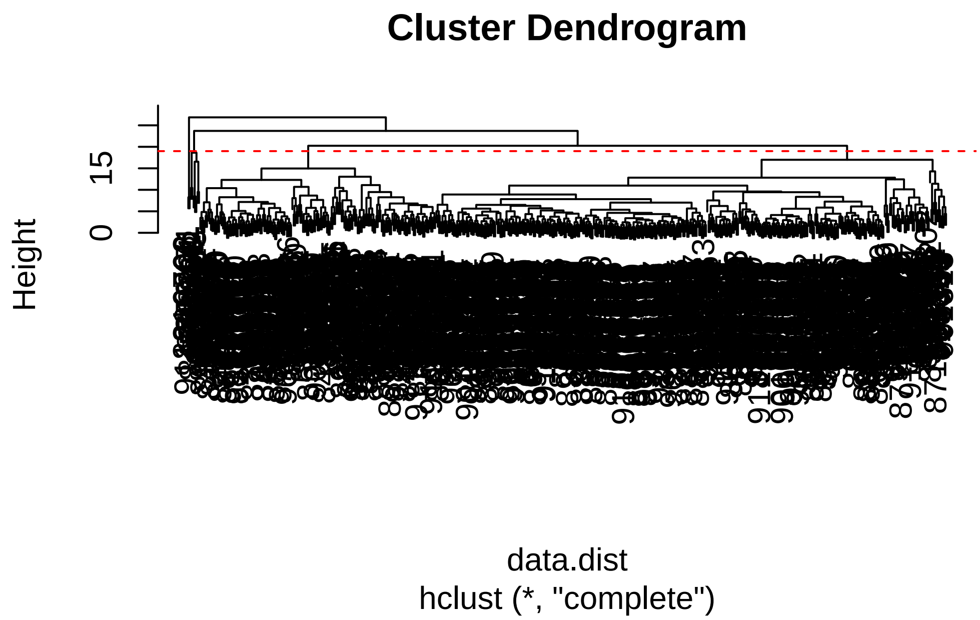
```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)

#Euclidean distnaces between pairs of observations
data.dist <- dist(data.scaled)

#creation of a hierarchical clustering model
wisc.hclust <- hclust(data.dist, method = "complete")
```

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

```
plot(wisc.hclust)
abline(h=19, col="red", lty=2)
```



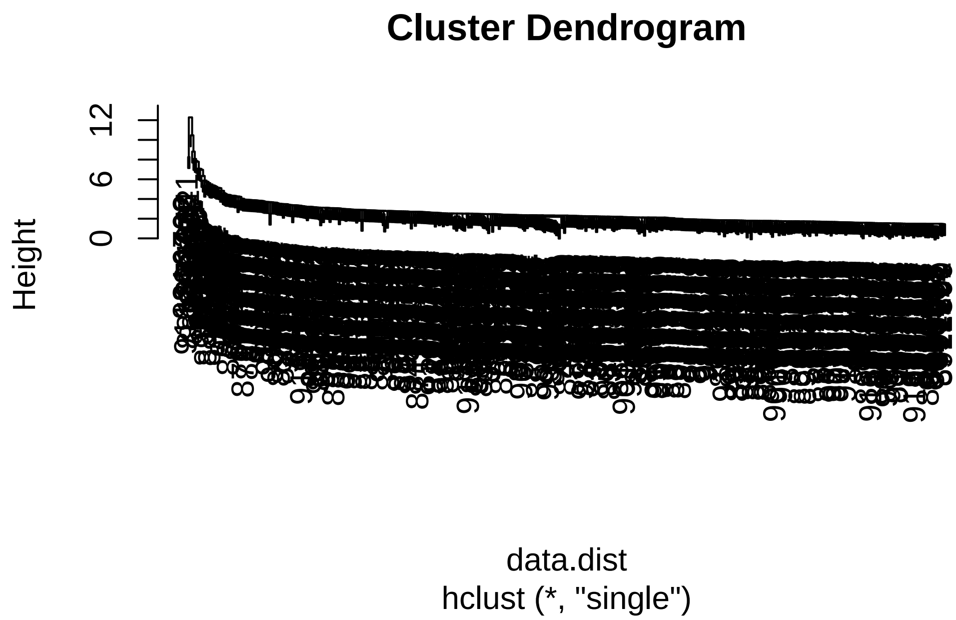

The height is 19.

```
wisc.hclust.clusters <- cutree(wisc.hclust, h= 19)
table(wisc.hclust.clusters, diagnosis)
```

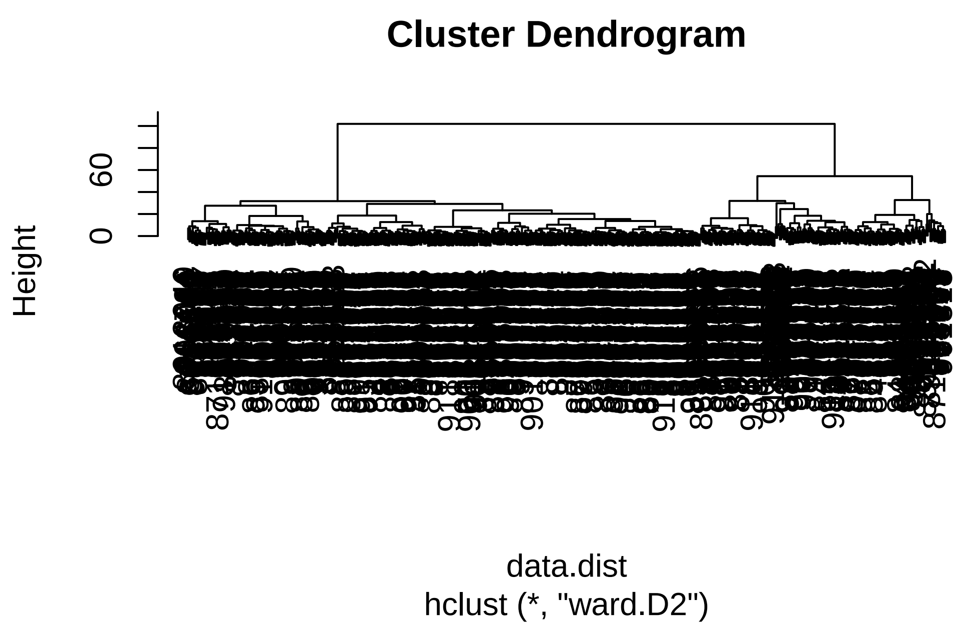
```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   2   5
                   3 343  40
                   4   0   2
```

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

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



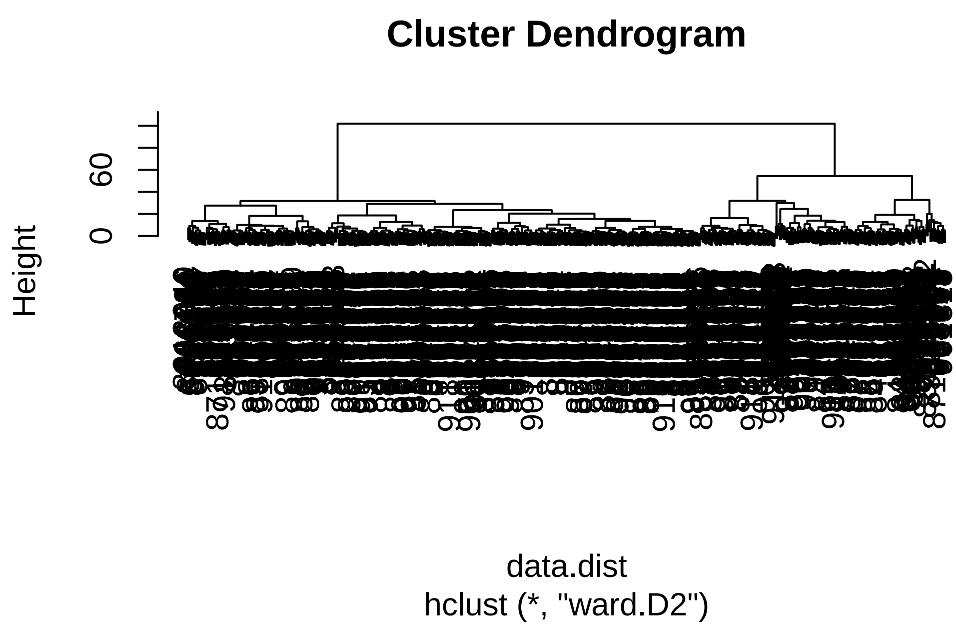

```r
wisc.pr.hclust <- hclust(data.dist, method = "ward.D2")
plot(wisc.pr.hclust)
```



The "ward.D2" method gives my favorite results, as the clustering is incredibly clear and easier to interpret compared to the other methods. It is also more visually appealing in my opinion.

## 4. Combining methods

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



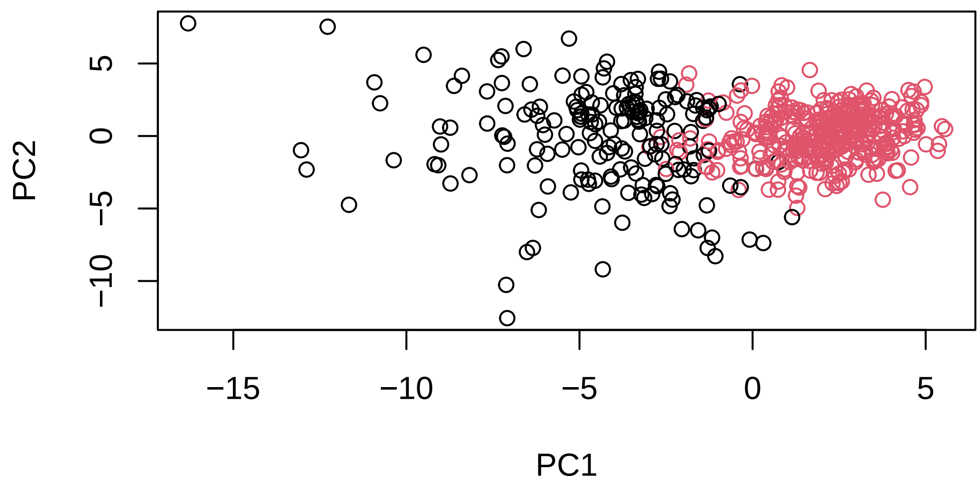

```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
184 385
```

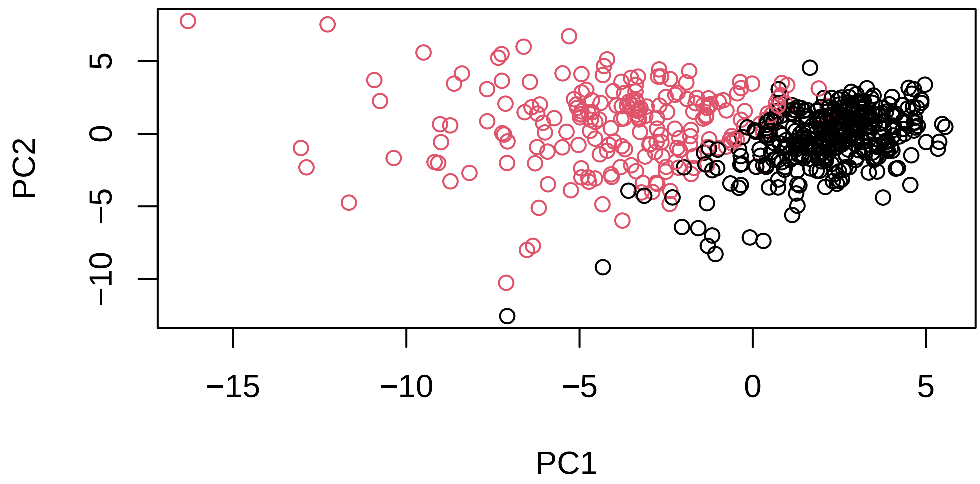
```
table(grps,diagnosis)
```

```
     diagnosis
grps   B   M
   1  20 164
   2 337  48
```

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




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



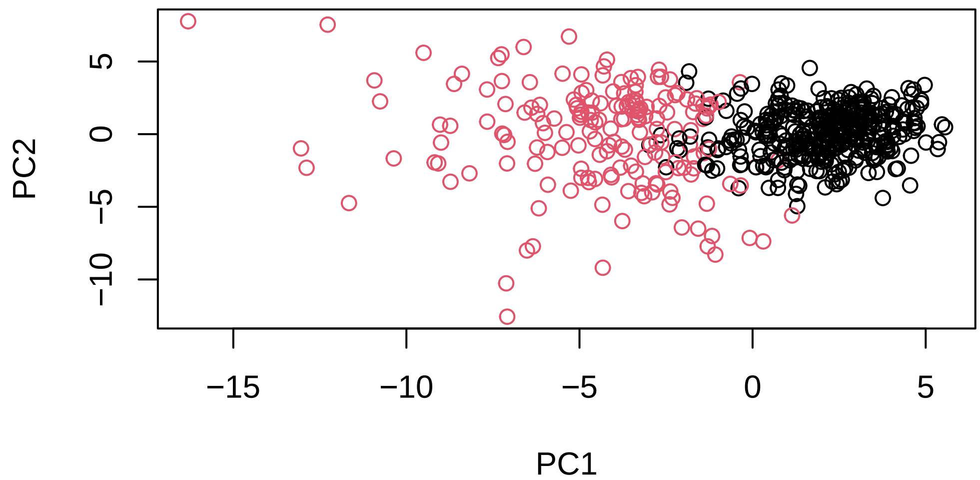

```
g <- as.factor(grps)
levels(g)
```

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

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

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

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




```
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]), method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
```

**Q13. How well does the newly created model with four clusters separate out the two diagnoses?**

```
# Compare to actual diagnoses
table(wisc.pr.hclust.clusters, diagnosis)
```

```
                       diagnosis
wisc.pr.hclust.clusters   B   M
                      1  28 188
                      2 329  24
```

The newly created model separates out the two diagnoses well, creating compacted clusters in four groups that more clearly define the diagnoses. The clustering yields a more digestible/easy to understand idea of how the data is spread.

**Q14. How well do the 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(wisc.hclust.clusters, diagnosis)
```

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

Prior to PCA, the hierarchical clustering models feature more spread and are less compact. It is harder to interpret what the data is actually trying to show, and the difference in clustering between diagnoses is not as clear.

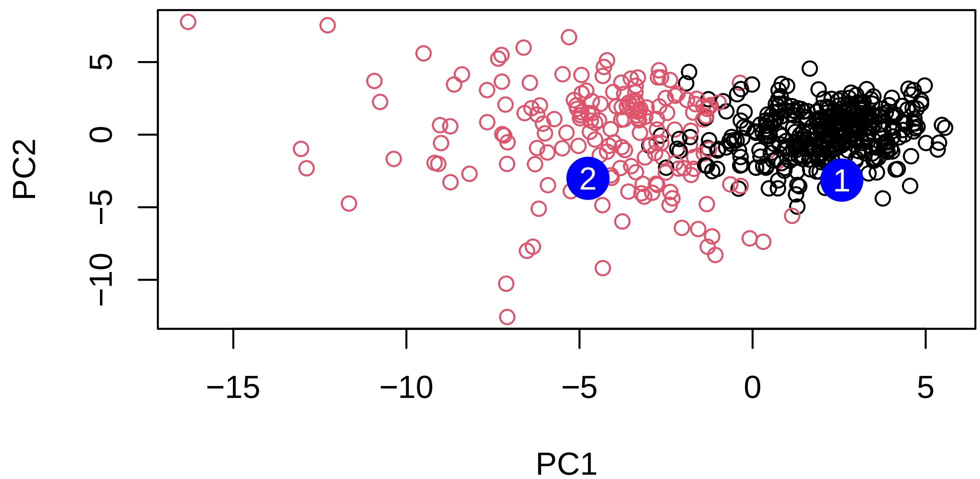
## 6. Prediction

```
#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
```

```r
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")
```




**Q16. Which of these new patients should we prioritize for follow up based on your results?**

```r
g
```

```
  842302   842517 84300903 84348301 84358402   843786   844359 84458202
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  844981 84501001   845636 84610002   846226   846381 84667401 84799002
       1        1        2        2        1        2        1        1
  848406 84862001   849014  8510426  8510653  8510824  8511133   851509
       2        1        1        2        2        2        1        1
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       1        1        1        1        1        1        1        1
```

| | | | | | | | |
|---|---|---|---|---|---|---|---|
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| 857155 | 857156 | 857343 | 857373 | 857374 | 857392 | 857438 | 85759902 |
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| 86211 | 862261 | 862485 | 862548 | 862717 | 862722 | 862965 | 862980 |
| 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| 862989 | 863030 | 863031 | 863270 | 86355 | 864018 | 864033 | 86408 |
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| 865137 | 86517 | 865423 | 865432 | 865468 | 86561 | 866083 | 866203 |
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| 866458 | 866674 | 866714 | 8670 | 86730502 | 867387 | 867739 | 868202 |
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| 868223 | 868682 | 868826 | 868871 | 868999 | 869104 | 869218 | 869224 |
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| 2 | 2 | 1 | 2 | 2 | 2 | 2 | 1 |
| 8710441 | 87106 | 8711002 | 8711003 | 8711202 | 8711216 | 871122 | 871149 |
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| 875099 | 875263 | 87556202 | 875878 | 875938 | 877159 | 877486 | 877500 |
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| 877501 | 877989 | 878796 | 87880 | 87930 | 879523 | 879804 | 879830 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 1 | 1 | 2 | 2 | 2 | 2 |
| 8810158 | 8810436 | 881046502 | 8810528 | 8810703 | 881094802 | 8810955 | 8810987 |
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| 2 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| 899987 | 9010018 | 901011 | 9010258 | 9010259 | 901028 | 9010333 | 901034301 |
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| 2 | 2 | 2 | 2 | 2 | 1 | 1 | 2 |
| 9011971 | 9012000 | 9012315 | 9012568 | 9012795 | 901288 | 9013005 | 901303 |
| 1 | 1 | 1 | 2 | 1 | 1 | 2 | 2 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 901315 | 9013579 | 9013594 | 9013838 | 901549 | 901836 | 90250 | 90251 |
| 1 | 2 | 2 | 1 | 2 | 2 | 2 | 2 |
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| 2 | 2 | 2 | 2 | 2 | 1 | 2 | 2 |
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| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
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| 1 | 1 | 2 | 2 | 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 | 2 | 2 | 2 | 1 | 1 | 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 |
| 2 | 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 |
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| 2 | 2 | 2 | 2 | 2 | 1 | 2 | 1 |
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| 2 | 1 | 2 | 1 | 2 | 2 | 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       1       1
  92751
      2
Levels: 2 1
```

In the generated chart, the black clustering indicates 'benign' and the red clustering indicates 'metastatic' tumors. The normal cells (benign) tend to cluster, whereas there is more spread in the metastatic cells.

As such, we should prioritize patient 2 because they are more likely to have a metastatic tumor, as patient 2 falls within the metastatic clustering whereas patient 1 falls within the benign clustering.