Class 8: Machine Learning Mini Project

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In today's mini-project we will explore a complete analysis using the unsupervised learning techniques covered in class (clustering and PCA for now).

The data itself comes from the Wisconsin Breast Cancer Diagnostic Data Set FNA breast biopsy data.

##Data import

```r
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
```

Remove the diagnosis column and keep it in a seperate vector for later.

```r
diagnosis <-  as.factor(wisc.df$diagnosis)
wisc.data <- wisc.df[,-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
```

##Exploratory data analysis

The first step of any data analysis, unsupervised or supervised, is to familiarize yourself with the data

> Q1. How many observations are in this dataset?

```r
nrow(wisc.data)
```

```
[1] 569
```

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

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

```

  B   M 
357 212 
```

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

First find the column names

```r
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"
```

Next I need to search within the column names for "_mean" pattern. The `grep()` function might help here.

```r
inds <- grep("_mean", colnames(wisc.data))
length(inds)
```

```
[1] 10
```

> Q4. How many dinmensions are in this dataset?

```r
ncol(wisc.data)
```

```
[1] 30
```

Principal Componenet Analysis

First do we need to scale the data before PCA or not.

```r
round(apply(wisc.data, 2, sd), 3)
```

```
            radius_mean            texture_mean          perimeter_mean
                  3.524                   4.301                  24.299
              area_mean         smoothness_mean        compactness_mean
```

```
                351.914                  0.014                    0.053
         concavity_mean     concave.points_mean            symmetry_mean
                  0.080                  0.039                    0.027
 fractal_dimension_mean              radius_se               texture_se
                  0.007                  0.277                    0.552
            perimeter_se                 area_se           smoothness_se
                  2.022                 45.491                    0.003
         compactness_se            concavity_se        concave.points_se
                  0.018                  0.030                    0.006
            symmetry_se    fractal_dimension_se             radius_worst
                  0.008                  0.003                    4.833
          texture_worst         perimeter_worst               area_worst
                  6.146                 33.603                  569.357
       smoothness_worst       compactness_worst          concavity_worst
                  0.023                  0.157                    0.209
   concave.points_worst          symmetry_worst  fractal_dimension_worst
                  0.066                  0.062                    0.018
```

Looks like we need to scale.

```r
# Perform PCA on wisc.data by completing the following code
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%

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

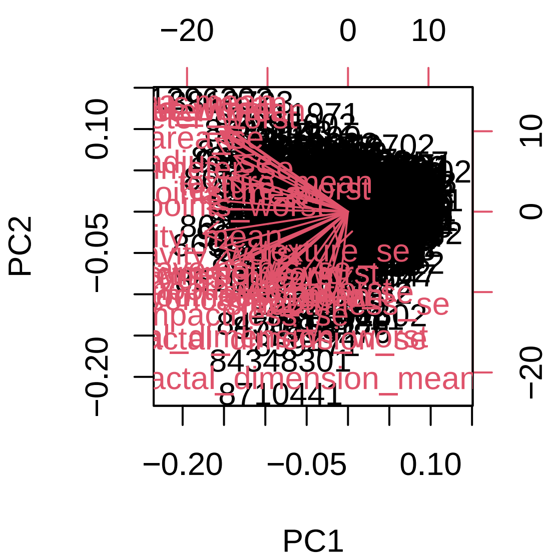
3 PCs capture 72%

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

7 PCs capture 91%

PC plot

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

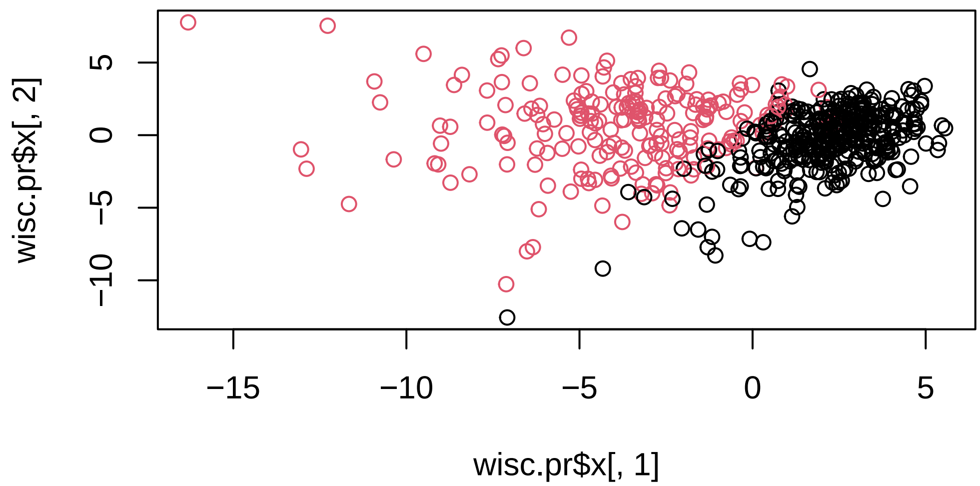


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

There are too many characters on the plot and they are overlapping each other. This makes it difficult to understand. The x and y axes are difficult to interpret. The plot is too confusing.

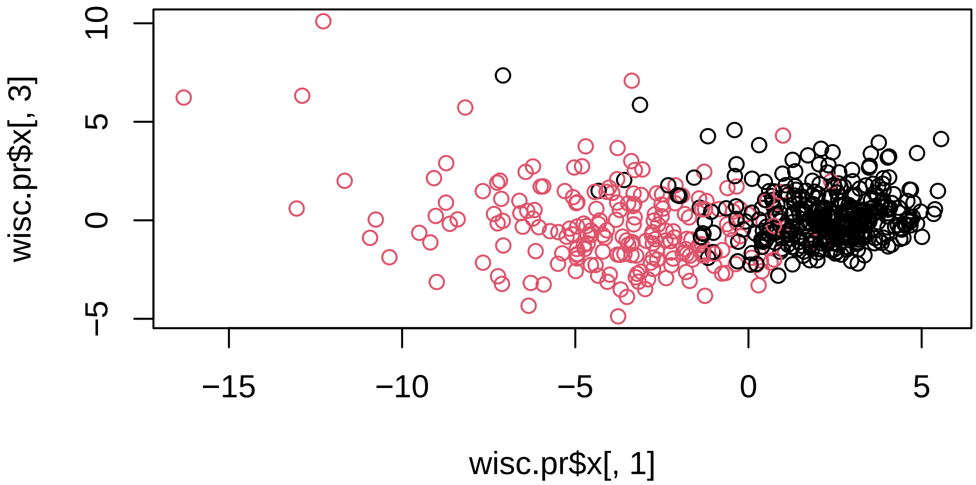
We need to make our plot of PC1 vs PC2 (a.k.a score plot, PC-plot, etc.) The main result of PCA…

```
plot(wisc.pr$x[,1], wisc.pr$x[,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)
```

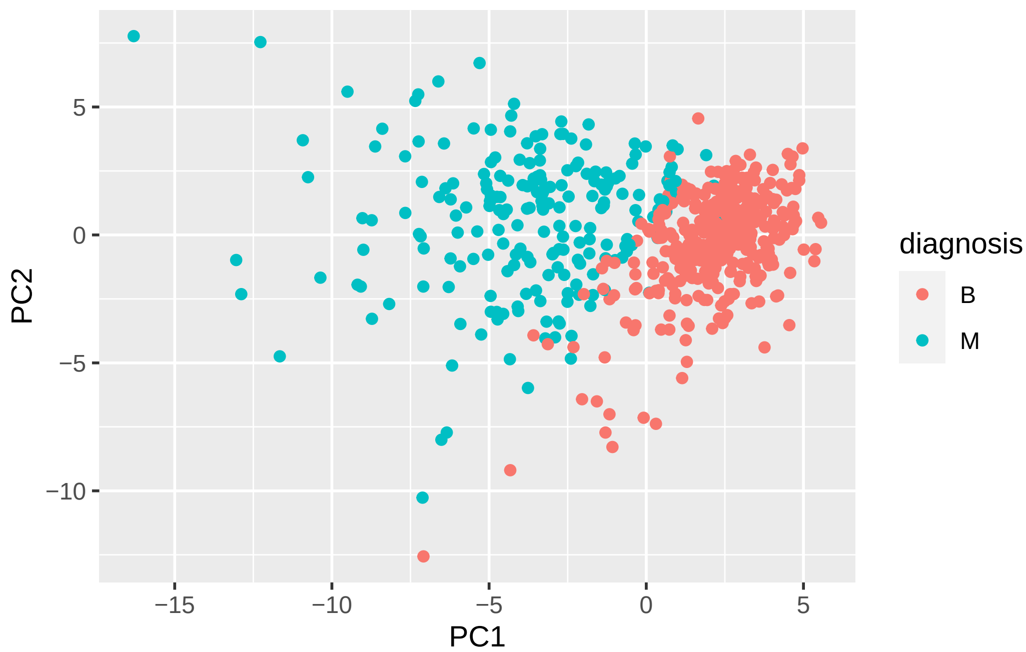


The y-values on the y-axis for this plot has increased compared to the previous plot. PC2 shows more variance compared to PC3.

```
library(ggplot2)

pc <- as.data.frame(wisc.pr$x)
pc$diagnosis <-  diagnosis

ggplot(pc)+
  aes(PC1, PC2, col=diagnosis) +
  geom_point()
```



Variance explained

We can get this from the output of the `summary()` function.

```
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
```

Calculate the variance of each principal component by squaring the sdev component of wisc.pr (i.e. wisc.pr$sdev^2).

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

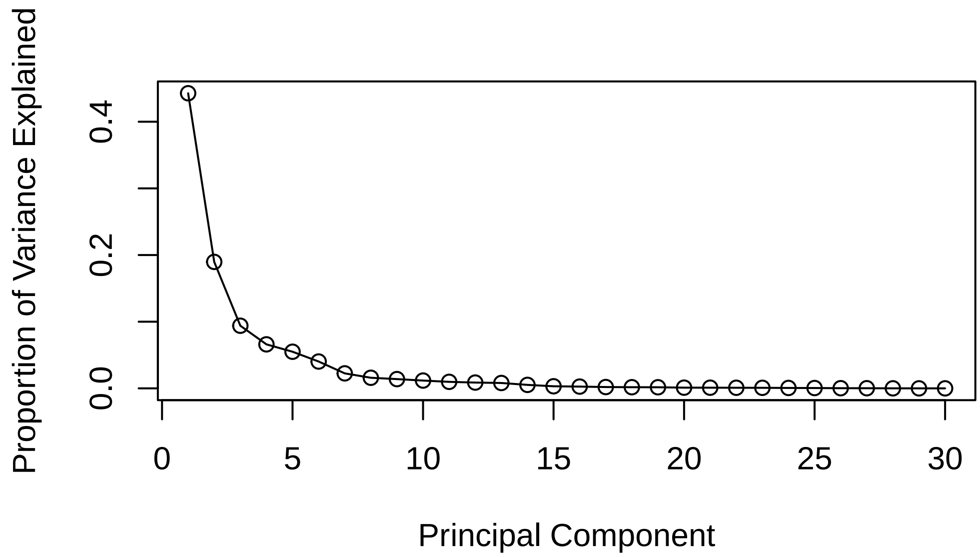
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

Calculate the variance explained by each principal component by dividing the total variance explained of all principal components

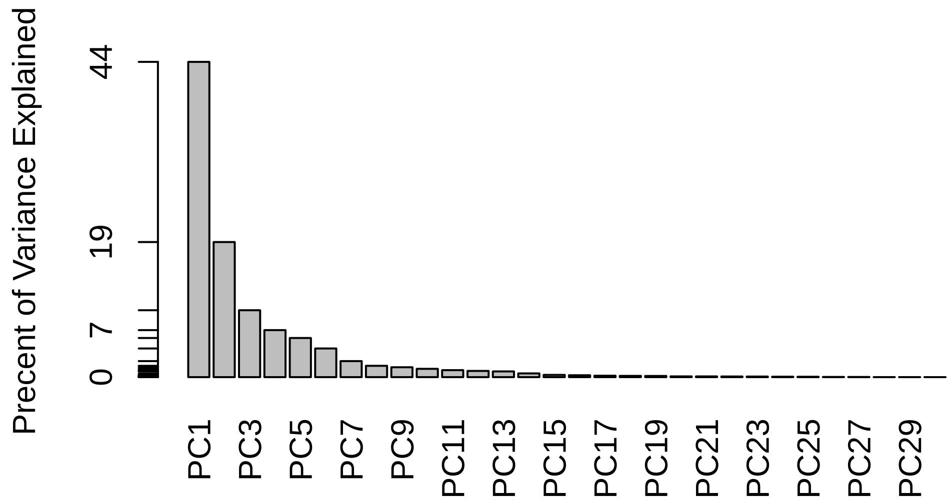
```
pve <- pr.var/ sum(pr.var)
head(pve)
```

```
[1] 0.44272026 0.18971182 0.09393163 0.06602135 0.05495768 0.04024522
```

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




```
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 )
```



Examine the PC loadings

How much do the original variables contribute to the new PCs that we have calculated? To get at this data we can look at the `$rotation` component of the returned PCA object.

```
head(wisc.pr$rotation[,1:3])
```

```
                         PC1         PC2          PC3
radius_mean       -0.2189024  0.23385713 -0.008531243
texture_mean      -0.1037246  0.05970609  0.064549903
perimeter_mean    -0.2275373  0.21518136 -0.009314220
area_mean         -0.2209950  0.23107671  0.028699526
smoothness_mean   -0.1425897 -0.18611302 -0.104291904
compactness_mean  -0.2392854 -0.15189161 -0.074091571
```

Focus in on PC1

```
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
```

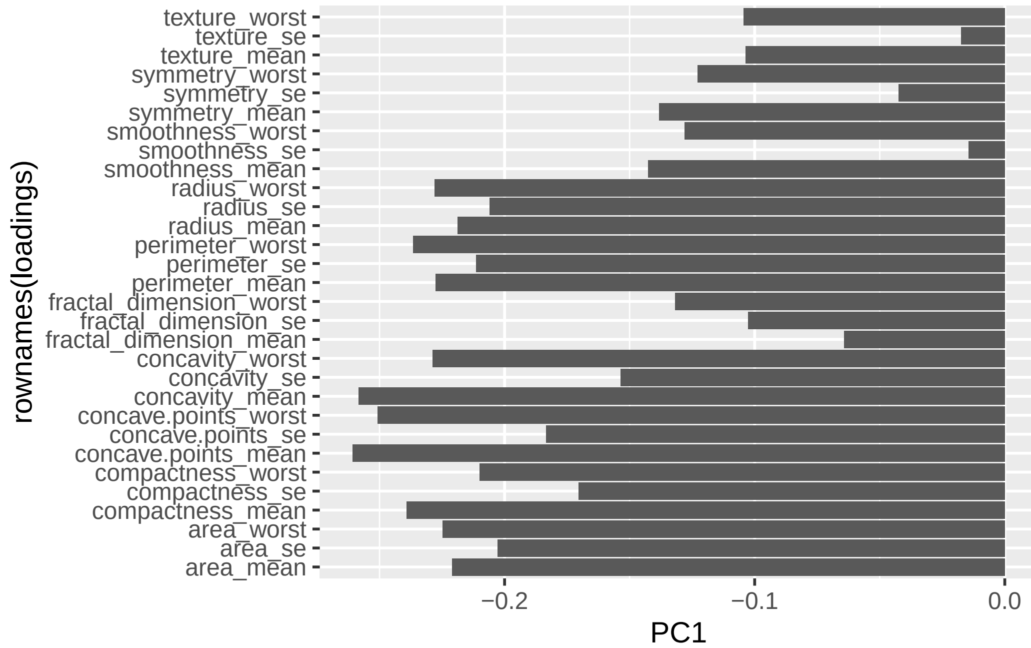
Q9. For the first principal component, what is the component of the loading vector (i.e. wisc.pr$rotation[,1]) for the feature concave.points_mean?

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

```
[1] -0.2608538
```

There is a complicated mix of variables that go together to make up PC1 - i.e. there are many of the original variables that together contribute highly to PC1.

```r
loadings <- as.data.frame(wisc.pr$rotation)
library(ggplot2)
ggplot(loadings) +
  aes(PC1, rownames(loadings)) +
  geom_col()
```



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

5 PCs capture 84.7%.

Hierarchial Clustering

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

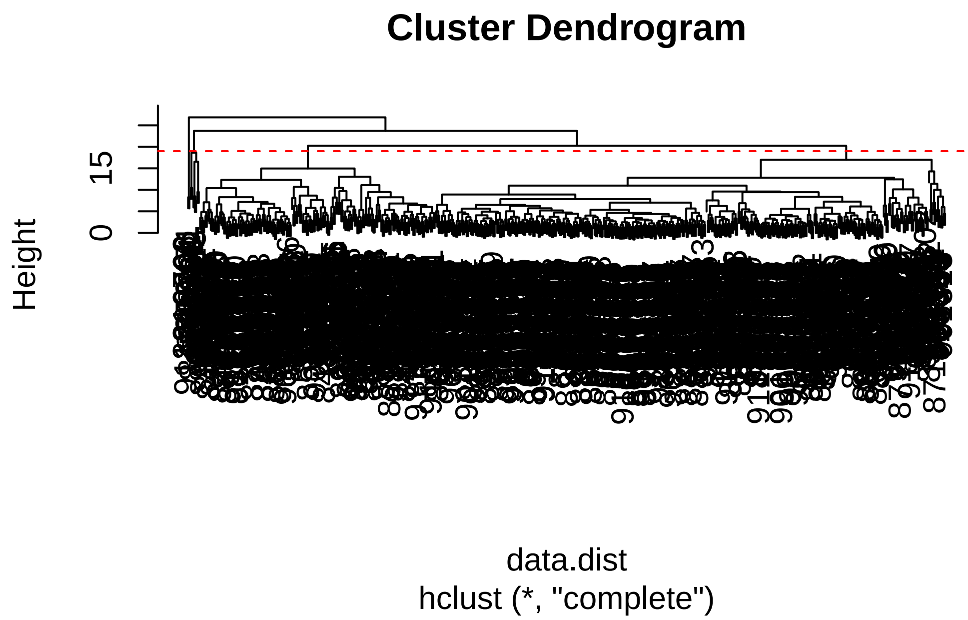
```
data.scaled <- scale(wisc.data)
```

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)
```

```
wisc.hclust <- hclust(data.dist)
```

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



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

At height 19.

```
wisc.hclust.clusters <- cutree(wisc.hclust, k=4)
```

Cut this tree to yield cluster membership

```
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?

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

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

```
table(cutree(wisc.hclust, k=10), diagnosis)
```

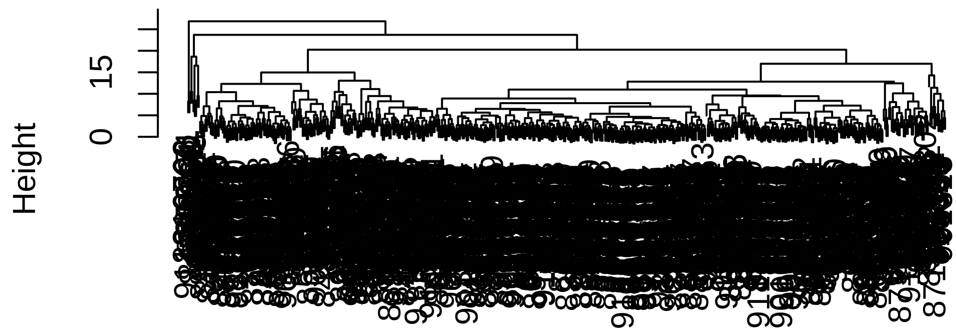
```
    diagnosis
       B   M
  1   12  86
  2    0  59
  3    0   3
  4  331  39
  5    0  20
  6    2   0
  7   12   0
  8    0   2
  9    0   2
  10   0   1
```

The smaller amount of clusters is better to find simpler similarities. The greater the size of the cluster, the more difficult it is to interpret.

> Q13. What is your favorite results for the same data.dist dataset? Explain your reasoning.

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

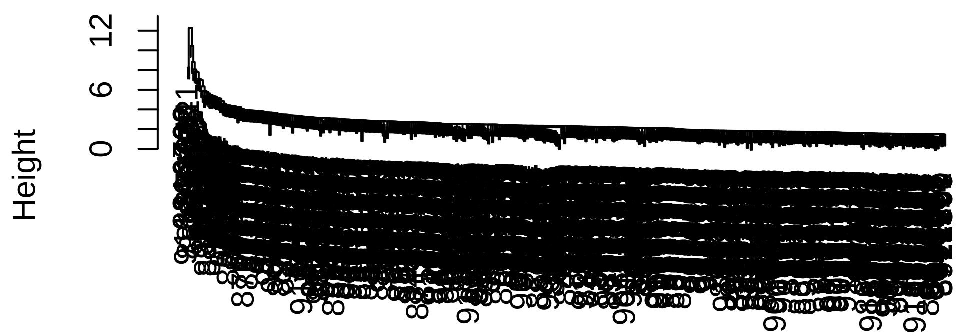
Cluster Dendrogram



dist(scale(wisc.data))
hclust (*, "complete")

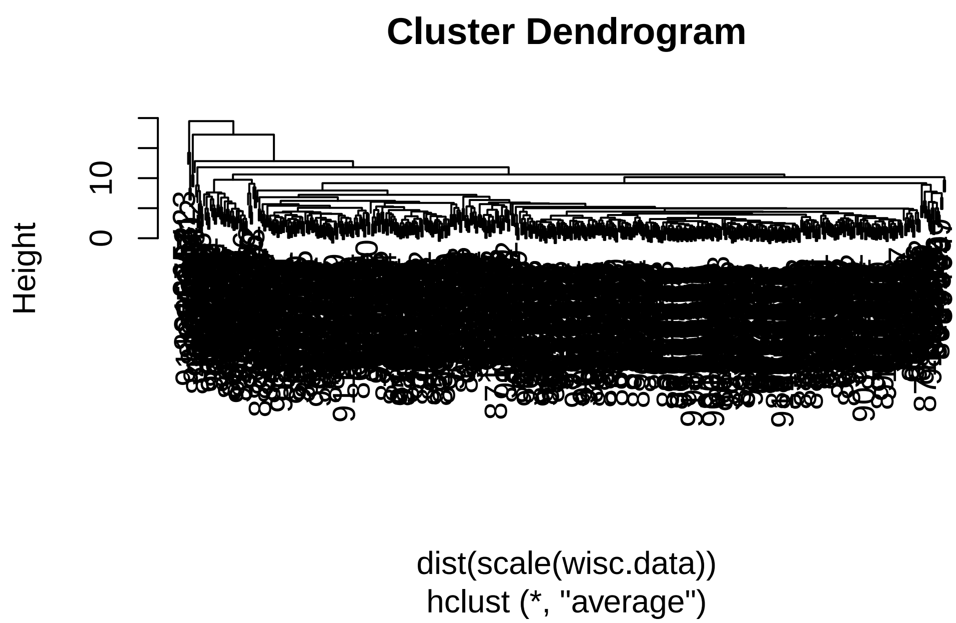
```r
hc.single <- hclust(dist(scale(wisc.data)), method="single")
plot(hc.single)
```

Cluster Dendrogram

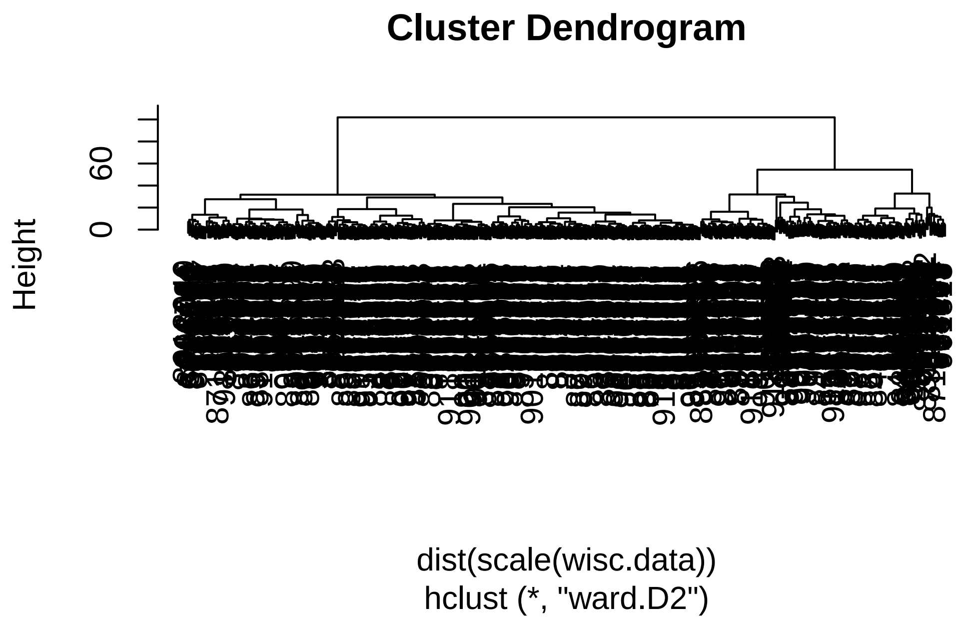


dist(scale(wisc.data))
hclust (*, "single")

```r
hc.average <- hclust(dist(scale(wisc.data)), method="average")
plot(hc.average)
```




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



I prefer the ward.D2 clustering method because the resulting dendrogram appears the clearest to understand.

Combine methods: PCA and HCLUST

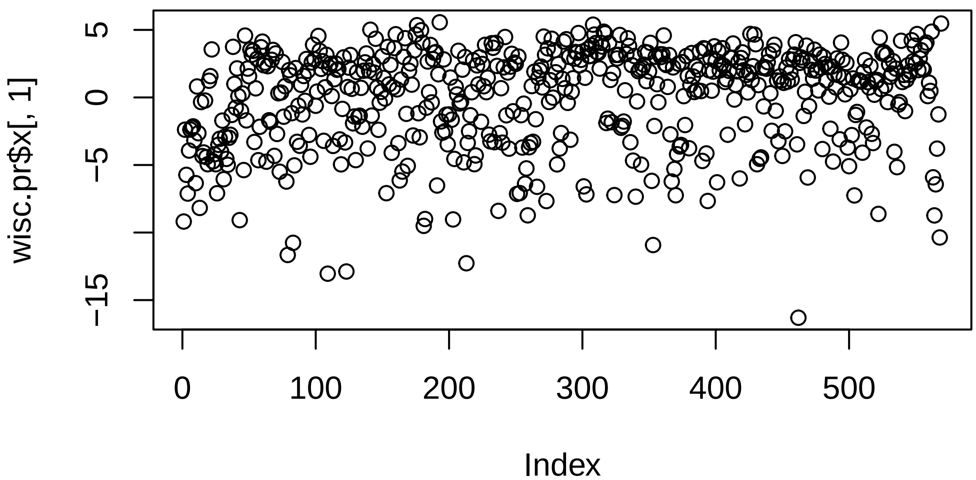
```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]), method="ward.D2")
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
216 353
```

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

```
    diagnosis
grps   B   M
   1  28 188
   2 329  24
```

```r
plot(wisc.pr$x[,1])
```



I want to cluster my PCA results - that is use `wisc.pr$x` as input to `hclust()`

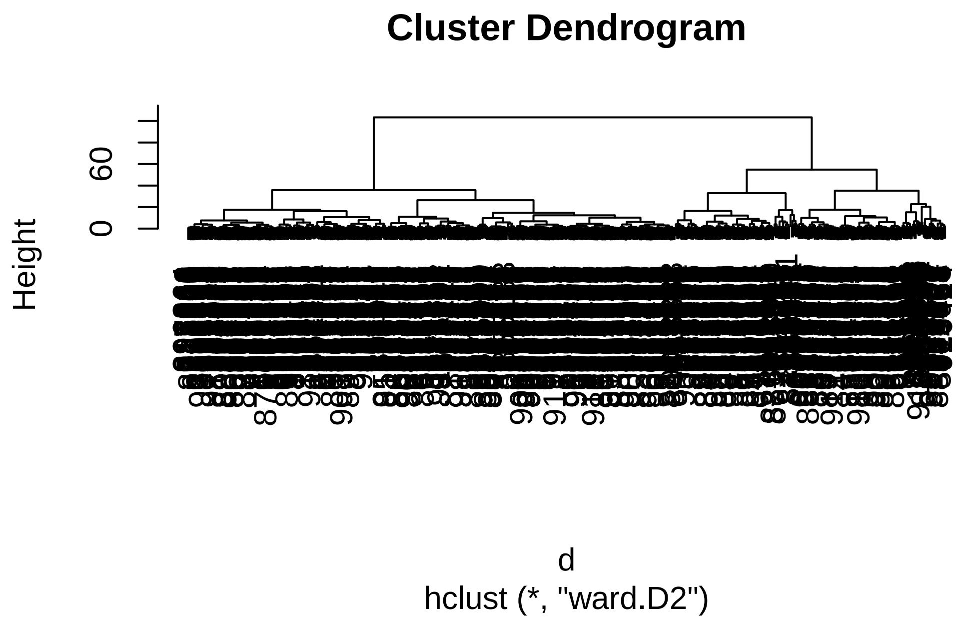
Try clustering in 3 PCs, that is PC1, PC2 and PC3 as input

```r
d <- dist(wisc.pr$x[,1:3])

wisc.pr.hclust <- hclust(d, method="ward.D2")
```

And my tree result figure

```r
plot(wisc.pr.hclust)
```

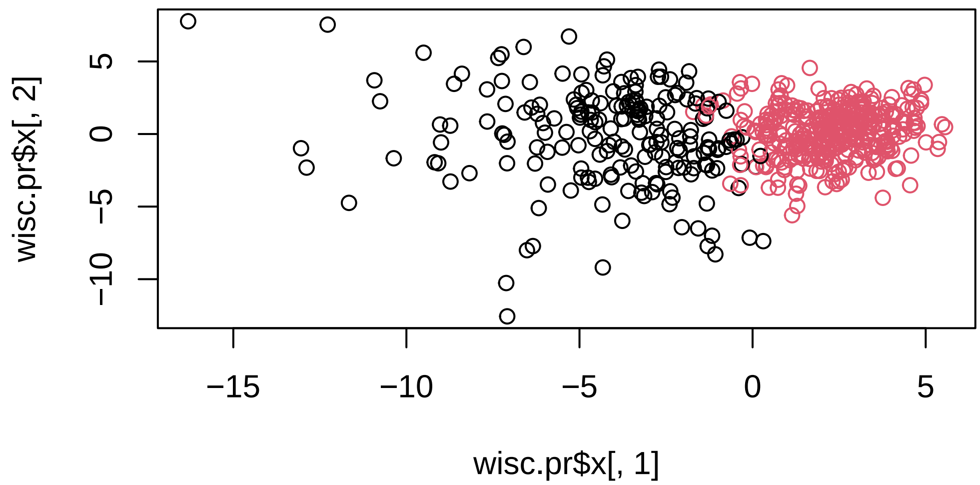


Let's cut this tree into two groups/clusters

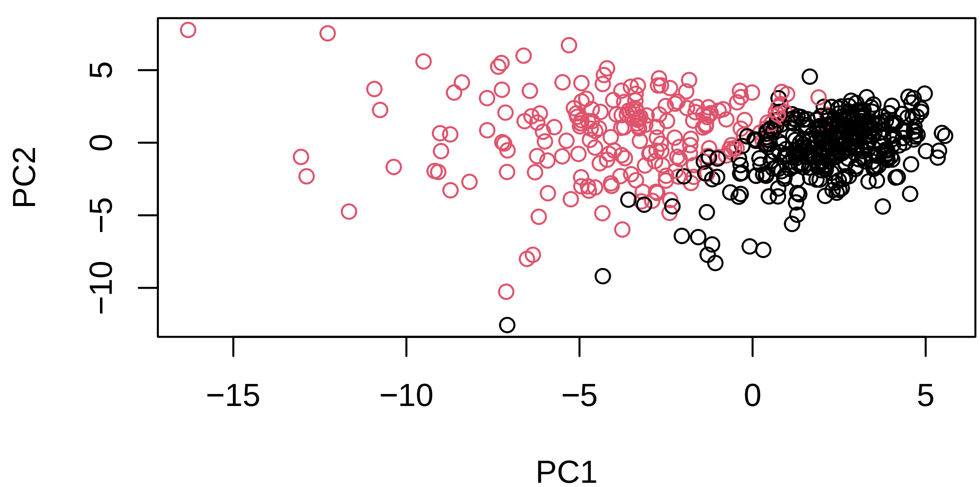
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
203 366
```

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




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



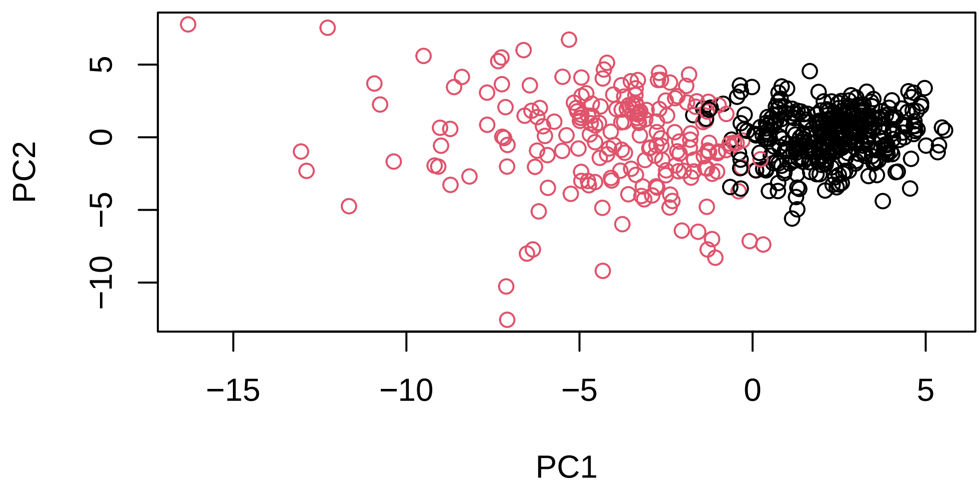
```r
g <- as.factor(grps)
levels(g)
```

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

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

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

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



How well do the two clusters separate the M and B diagnosis?

```r
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]), method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
table(wisc.pr.hclust.clusters, diagnosis)
```

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

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

```r
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]), method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=4)
table(wisc.pr.hclust.clusters, diagnosis)
```

```
                         diagnosis
wisc.pr.hclust.clusters   B   M
                      1   0  45
                      2   2  77
                      3  26  66
                      4 329  24
```

The newly created model with four clusters separates the two diagnoses. However, with two clusters, the seperation is more clear.

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

```
[1] 0.8998243
```