Class08

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Backround

In tosay's ckasss we will apply the moethods and techiques clustering and PCA to help make sense of real world breast cancer data

Data import

we start by importing our data. it is a CSV file so we will use the `read.csv()function`

```
#read.csv("WisconsinCancer.csv")

fna.data <- "WisconsinCancer.csv"


wisc.df <- read.csv(fna.data, row.names=1)
```

Make sure to remove the first `diagnosis` column - I dont want to use this for my machine learning models. We will use it later to compare our results to the expert diagnosis.

```
head(wisc.df, 4)
```

```
         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
         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
         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
         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
         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
         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
         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
         fractal_dimension_worst
842302                   0.11890
842517                   0.08902
84300903                 0.08758
84348301                 0.17300
```

```r
wisc.data <- wisc.df[,-1]

diagnosis <- wisc.df$diagnosis

nrow(wisc.data)
```

```
[1] 569
```

```r
dim(wisc.data)
```

```
[1] 569  30
```

```r
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

```r
coln <-colnames(wisc.data)

length(grep("_mean",coln))
```

```
[1] 10
```

> Q1. How many observations are in this dataset?

569

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

212

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

10

Principal component analysis

The main function is `prcomp()` and we want to make sure we set the ptional argument `Scale=True`

```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 component (PC1)?

44.27%

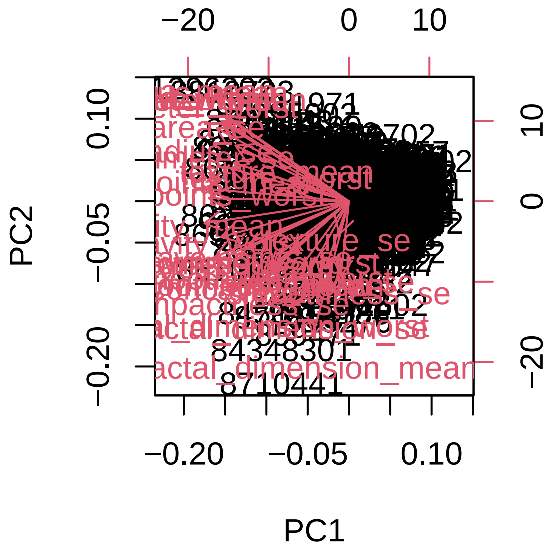
> Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

PC3

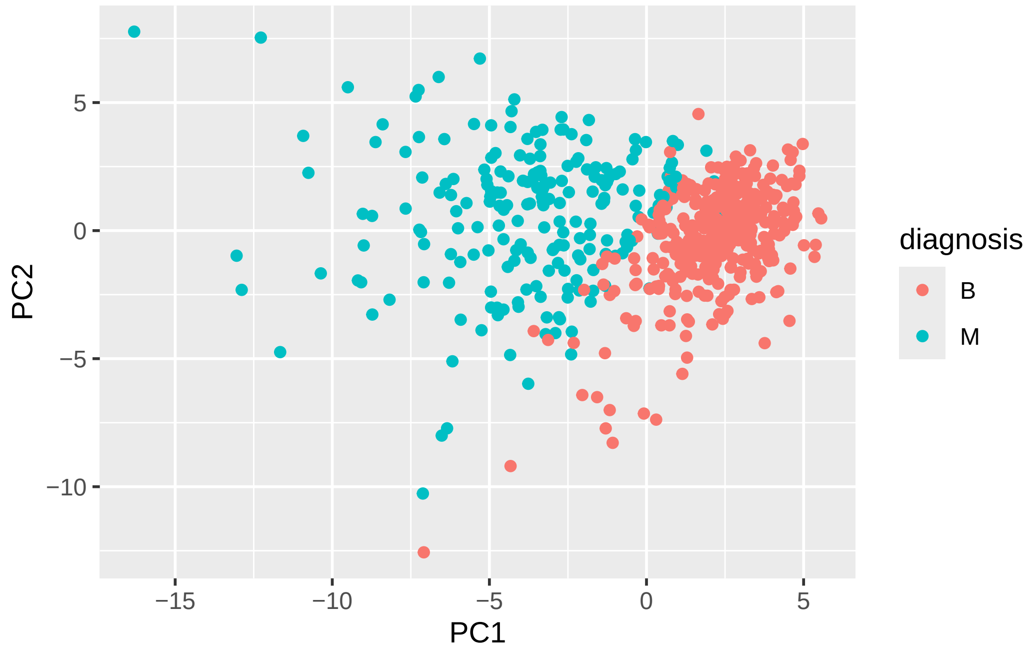
> Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

PC7

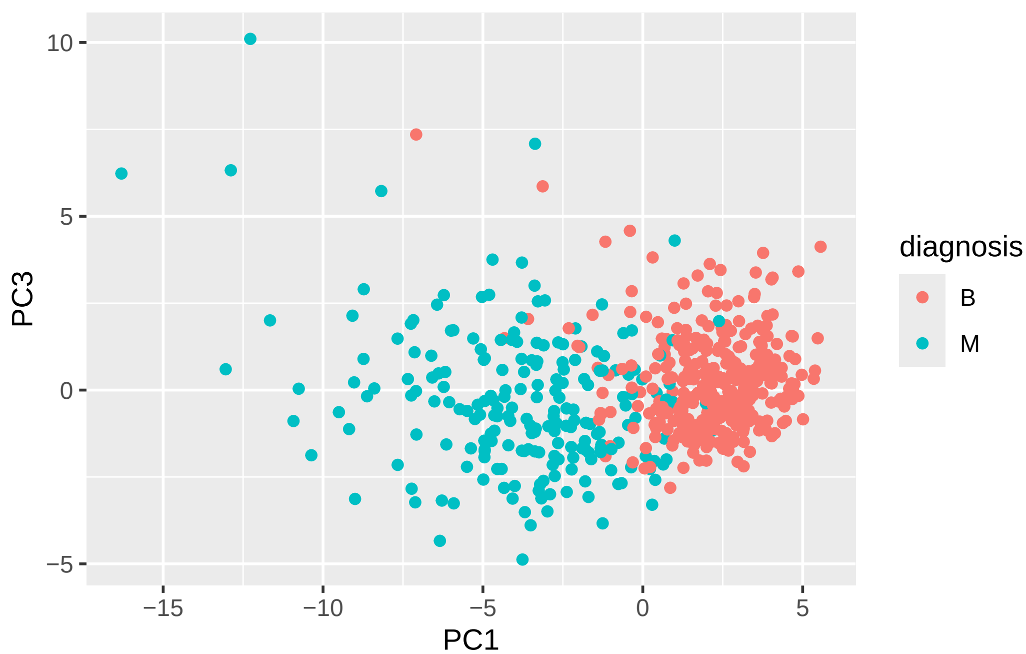
```r
biplot(wisc.pr)
```




```
library(ggplot2)

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




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

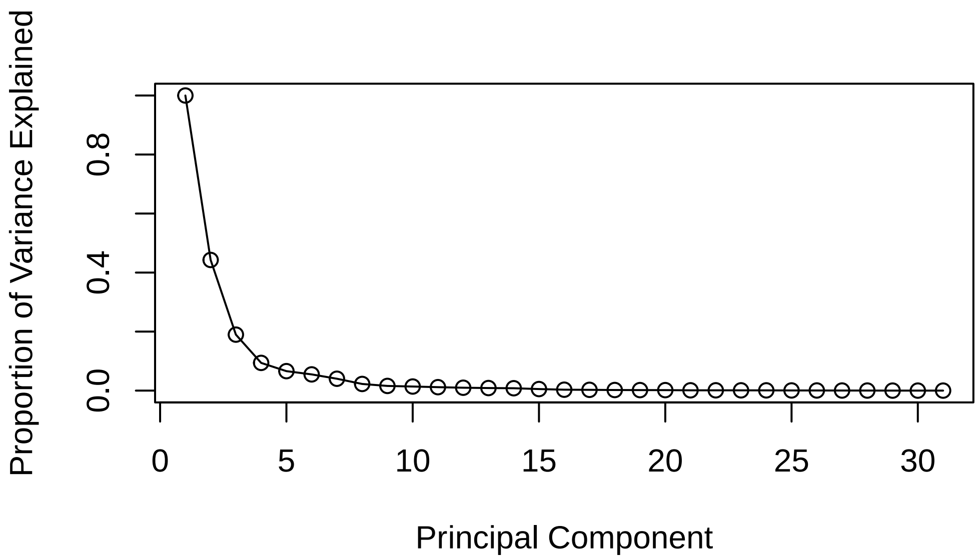


```r
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

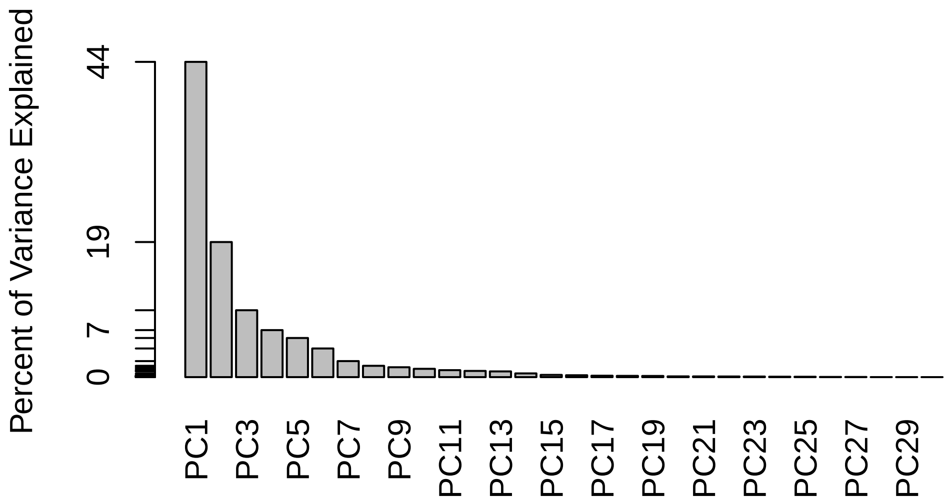
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```r
total.var <- sum(wisc.pr$sdev^2)
```

```r
pve <- pr.var / total.var

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




```r
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? This tells us how much this original feature contributes to the first PC. Are there any features with larger contributions than this one?

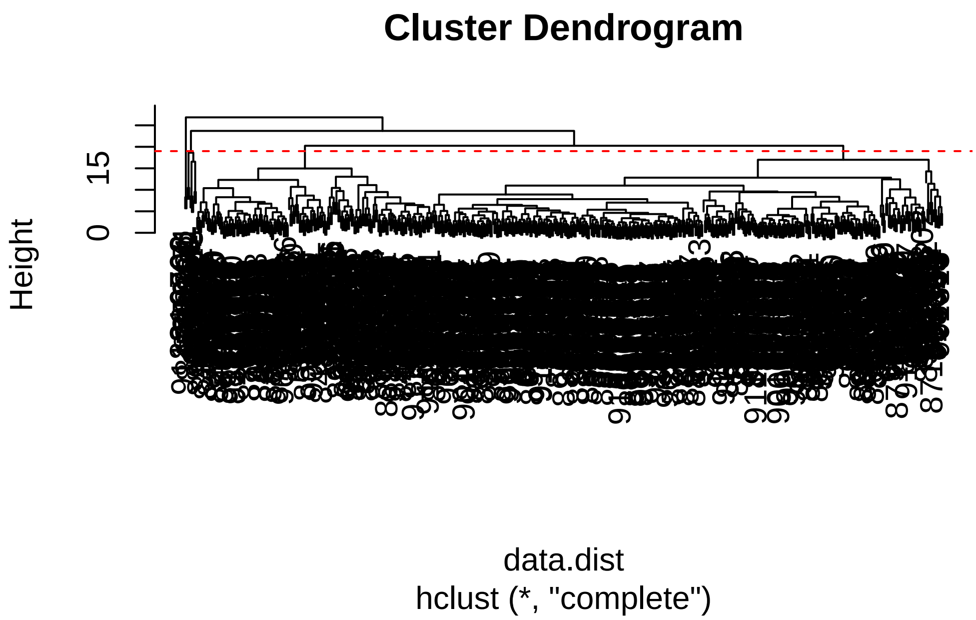
```
wisc.pr$rotation["concave.points_mean",1]
```

```
[1] -0.2608538
```

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

data.dist <-dist(data.scaled)

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




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

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

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

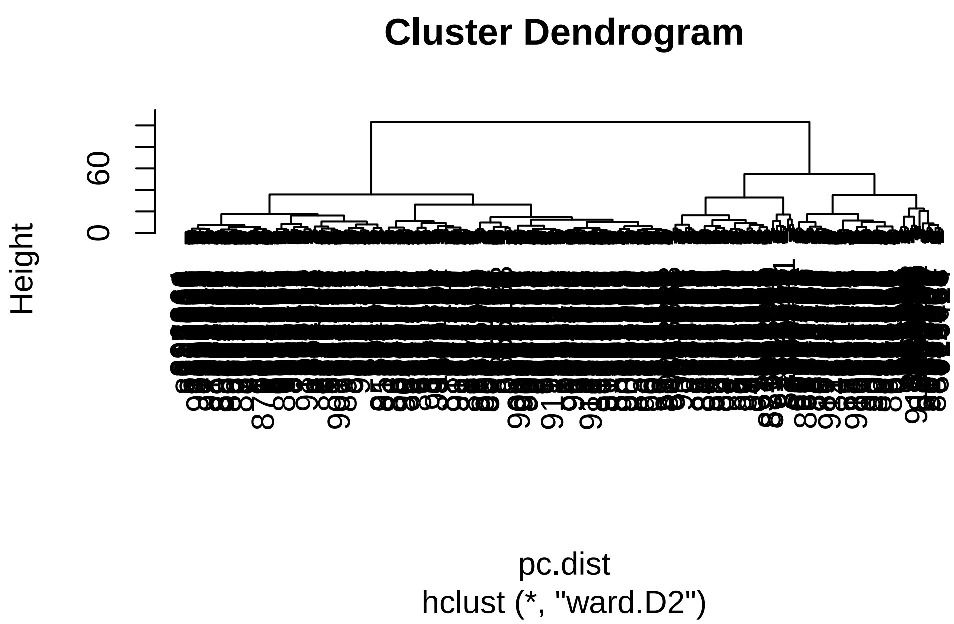
the height is 19 to give us 4 clusters.

You can also use the argument k=4 in cutree() function instead of h.

Combining Methods

Here we will take our PCA results and use those as input for clustering. in other words our `wisc.pr$x` scores that we plotted above (the main output from PCA - How the data lie in our new principal component axis/variables) and use a subset of these PCs that capture the most variance as input for `hclust()`

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



I want to know how clustering into groups with values of 1 or 2 coorespond to the diagnosis

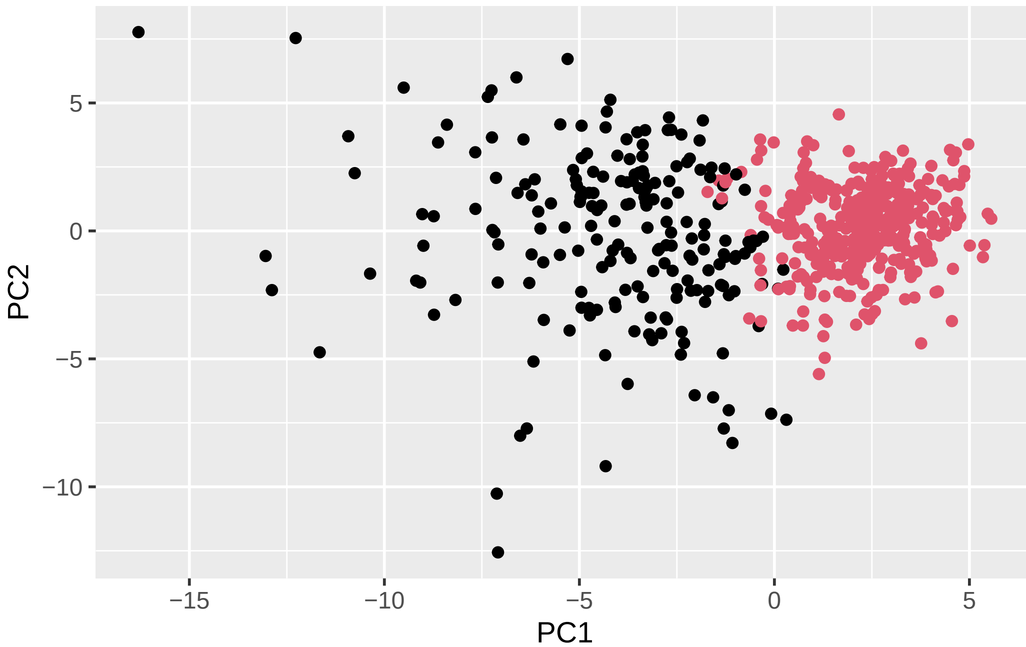
```r
wisc.pr.hclust<-hclust(pc.dist,"ward.D2")

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

```
grps
  1   2 
203 366 
```

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

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

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



My clustering **groups 1** of M diagnosis (179) and my clustering **group 2** are mostly "B" diagnosis

24 False positives 179 true positives

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

the "ward.D2" method

> Q13. How well does the newly created hclust model with two clusters separate out the two "M" and "B" diagnoses?

```r
dist7<-dist(wisc.pr$x[,1:7])
wisc.pr.hclust <- hclust(dist7, 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
```

the new hclust model with two clusters appear to seperate them out similar to the previouse one despite considering up to PC7

> Q14. How well do the hierarchical clustering models you created in the previous sections (i.e. without first doing PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.hclust.clusters and wisc.pr.hclust.clusters) with the vector containing the actual diagnoses.

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

```
wisc.hclust.clusters
  1   2   3   4 
177   7 383   2 
```

```
table(wisc.pr.hclust.clusters)
```

```
wisc.pr.hclust.clusters
  1   2 
216 353 
```

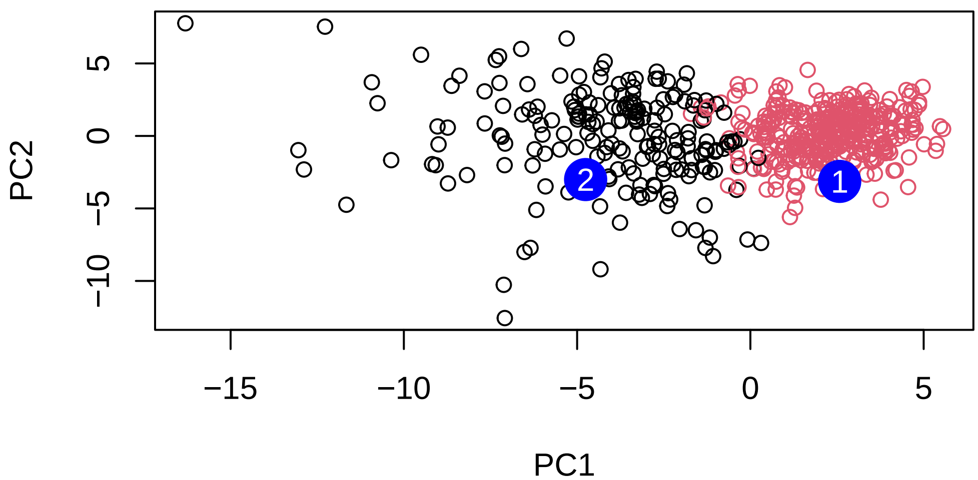
Sensitivity/Specificity - Prediction

```
new <- read.csv("new_samples.csv")
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=grps)
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?

Patients cluster under 2 we should prioritize for follow up based on results.