Class 08

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1. Preparing the data

```
#import the data to R studio

fna.data <- "WisconsinCancer.csv"

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
```

```
#removing first column

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

```r
# form a new data frame and call it diagnosis

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

Exploring data analysis

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(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

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

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

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

2. Principal Component Analysis

```r
# using colMean and apply for PCA

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(scale(wisc.data))
```

```r
# we get the summery

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
```

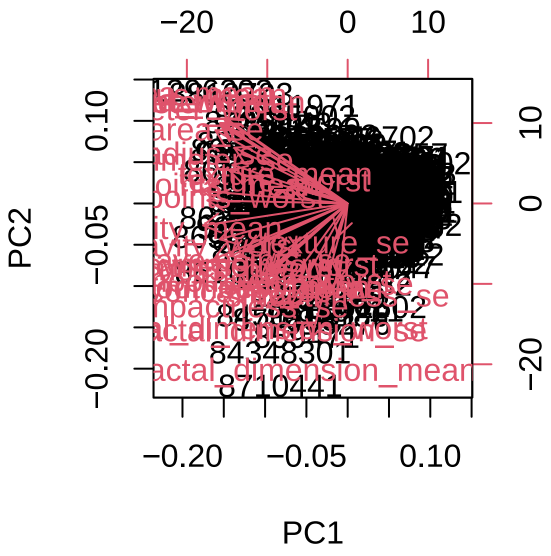
Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)? 0.4427

Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data? at least 3 PCs

Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data? at least 7 PCs

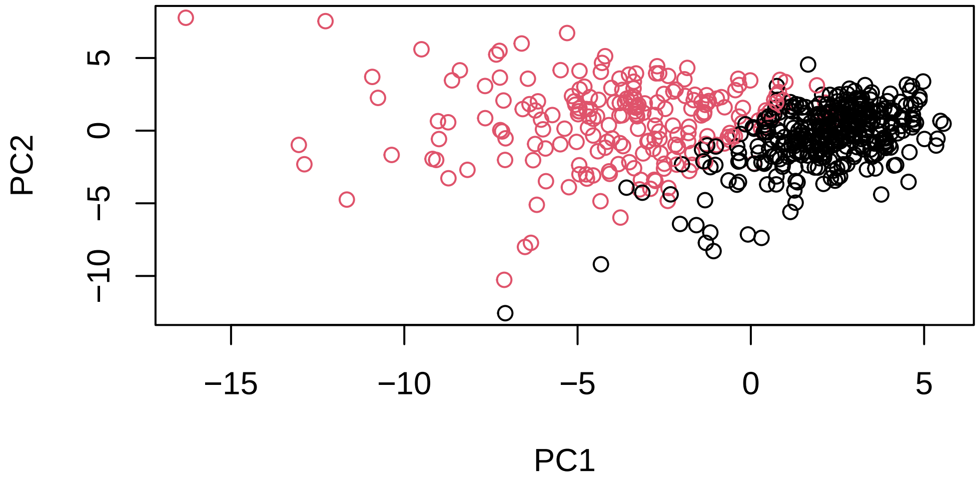
Interpreting PCA results

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



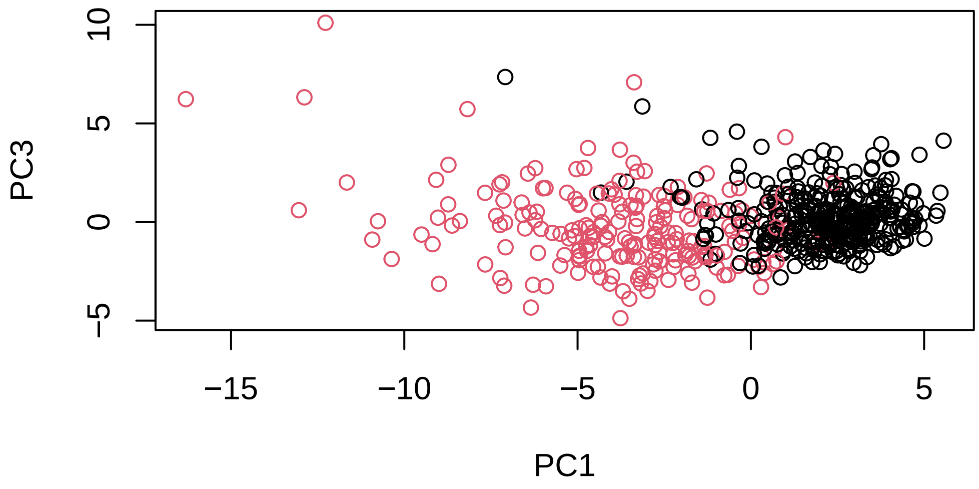
Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why? the plot is very crowded. it is difficult to interpret the data because number of observations are too much.

```r
# we can generate more standard scatter plot
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? There is less separation between malignant and benign.

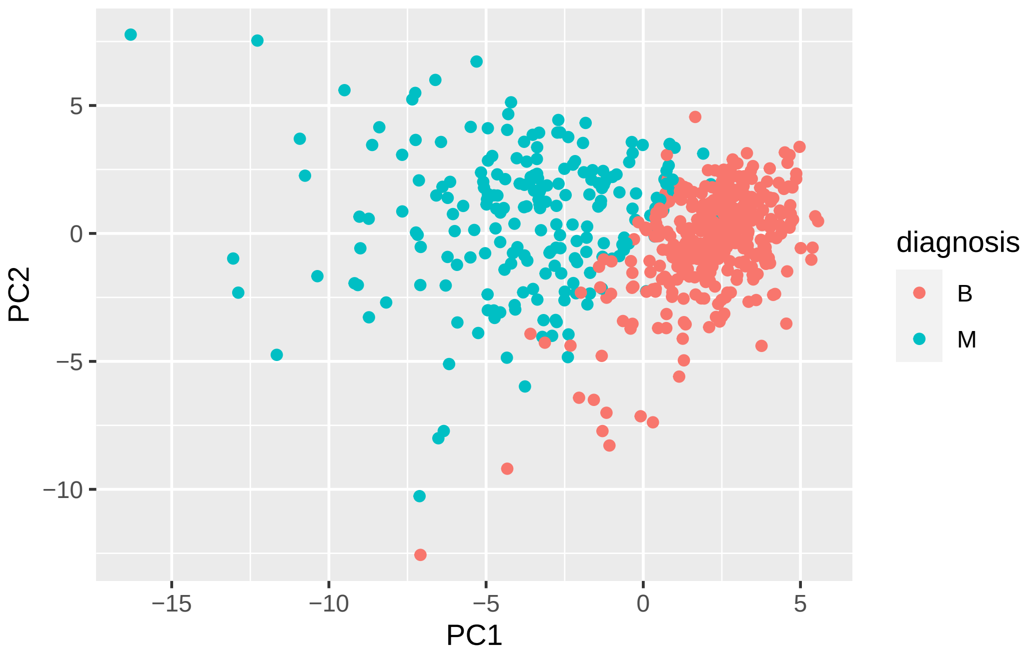
```
plot(wisc.pr$x[,c(1,3)], col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```



```r
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis
```

```r
# We can use ggplot for better visualization

library(ggplot2)
ggplot(df) +
  aes(PC1, PC2, col=diagnosis) +  geom_point()
```



Variance explained

```
# calculate the variance of each PC
pr.var <- wisc.pr$sdev^2
pr.var
```

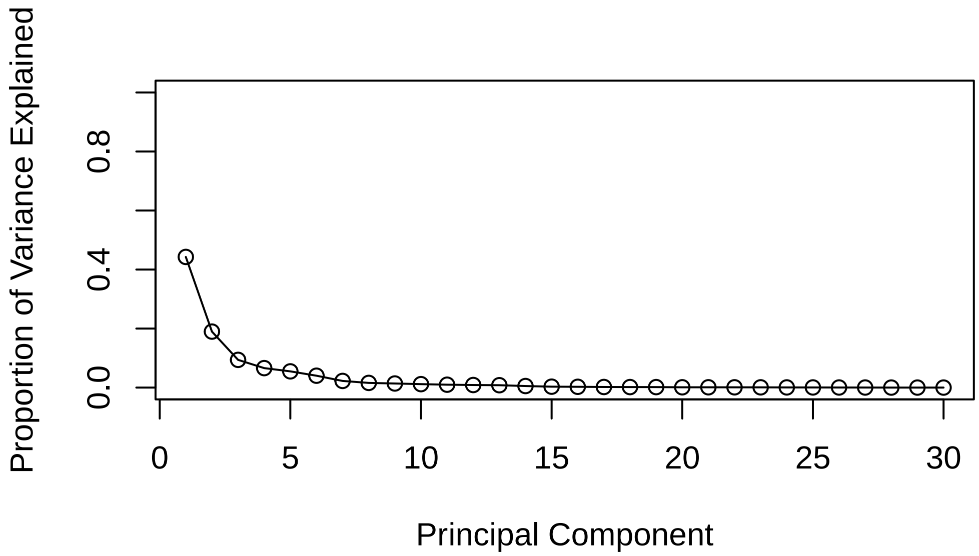
```
 [1] 1.328161e+01 5.691355e+00 2.817949e+00 1.980640e+00 1.648731e+00
 [6] 1.207357e+00 6.752201e-01 4.766171e-01 4.168948e-01 3.506935e-01
[11] 2.939157e-01 2.611614e-01 2.413575e-01 1.570097e-01 9.413497e-02
[16] 7.986280e-02 5.939904e-02 5.261878e-02 4.947759e-02 3.115940e-02
[21] 2.997289e-02 2.743940e-02 2.434084e-02 1.805501e-02 1.548127e-02
[26] 8.177640e-03 6.900464e-03 1.589338e-03 7.488031e-04 1.330448e-04
```

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

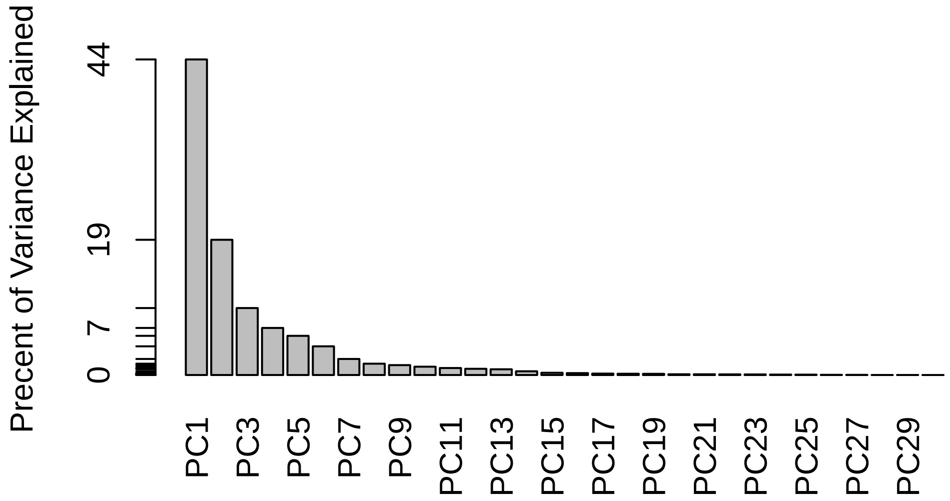
```
 [1] 4.427203e-01 1.897118e-01 9.393163e-02 6.602135e-02 5.495768e-02
 [6] 4.024522e-02 2.250734e-02 1.588724e-02 1.389649e-02 1.168978e-02
[11] 9.797190e-03 8.705379e-03 8.045250e-03 5.233657e-03 3.137832e-03
[16] 2.662093e-03 1.979968e-03 1.753959e-03 1.649253e-03 1.038647e-03
```

```
[21] 9.990965e-04 9.146468e-04 8.113613e-04 6.018336e-04 5.160424e-04
[26] 2.725880e-04 2.300155e-04 5.297793e-05 2.496010e-05 4.434827e-06
```

```
# plotting variance explained for each PC
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



```
# We can plot this data another way
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? contribution of original feature to first PC.

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

```
[1] -0.2608538
```

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

```
    concave.points_mean          concavity_mean    concave.points_worst
            -0.26085376             -0.25840048             -0.25088597
       compactness_mean         perimeter_worst         concavity_worst
            -0.23928535             -0.23663968             -0.22876753
           radius_worst          perimeter_mean              area_worst
            -0.22799663             -0.22753729             -0.22487053
              area_mean             radius_mean            perimeter_se
            -0.22099499             -0.21890244             -0.21132592
      compactness_worst               radius_se                 area_se
```

```
            -0.21009588             -0.20597878             -0.20286964
      concave.points_se          compactness_se            concavity_se
            -0.18341740             -0.17039345             -0.15358979
        smoothness_mean           symmetry_mean fractal_dimension_worst
            -0.14258969             -0.13816696             -0.13178394
       smoothness_worst          symmetry_worst           texture_worst
            -0.12795256             -0.12290456             -0.10446933
           texture_mean    fractal_dimension_se  fractal_dimension_mean
            -0.10372458             -0.10256832             -0.06436335
            symmetry_se              texture_se           smoothness_se
            -0.04249842             -0.01742803             -0.01453145
```

3. Hierarchical clustering

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

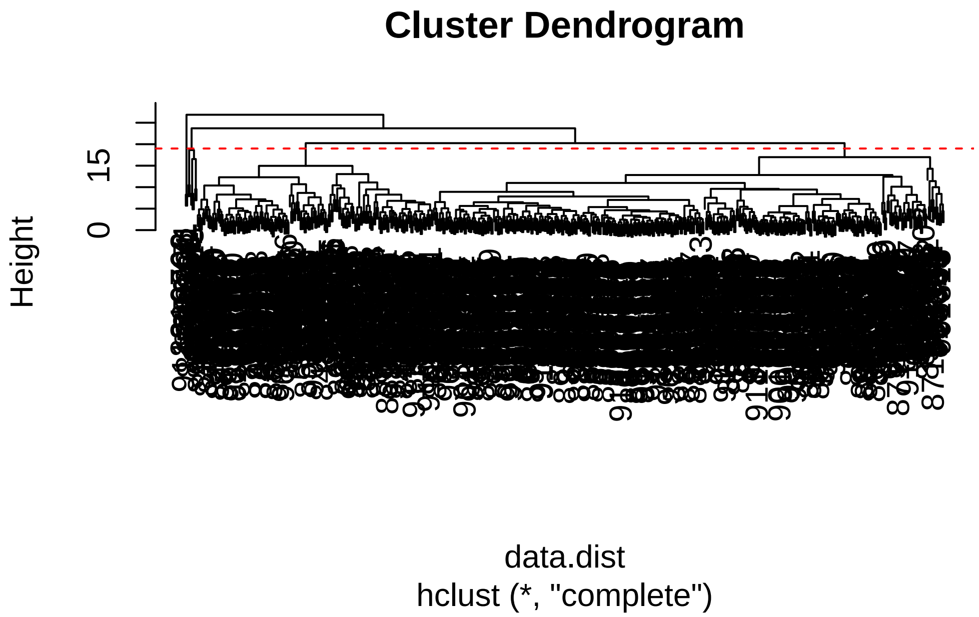
```
# calculate the distance
data.dist <- dist(data.scaled)
```

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

Results of hierarchical clustering

Q10. Using the `plot()` and `abline()` functions, what is the height at which the clustering model has 4 clusters? 19

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



Selecting number of clusters

```
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
```

Using different methods

Q12. Which method gives your favorite results for the same `data.dist` dataset? Explain your reasoning ward.D2 decrease the total variance, that result better clusters.

4. Combining methods

Clustering on PCA results

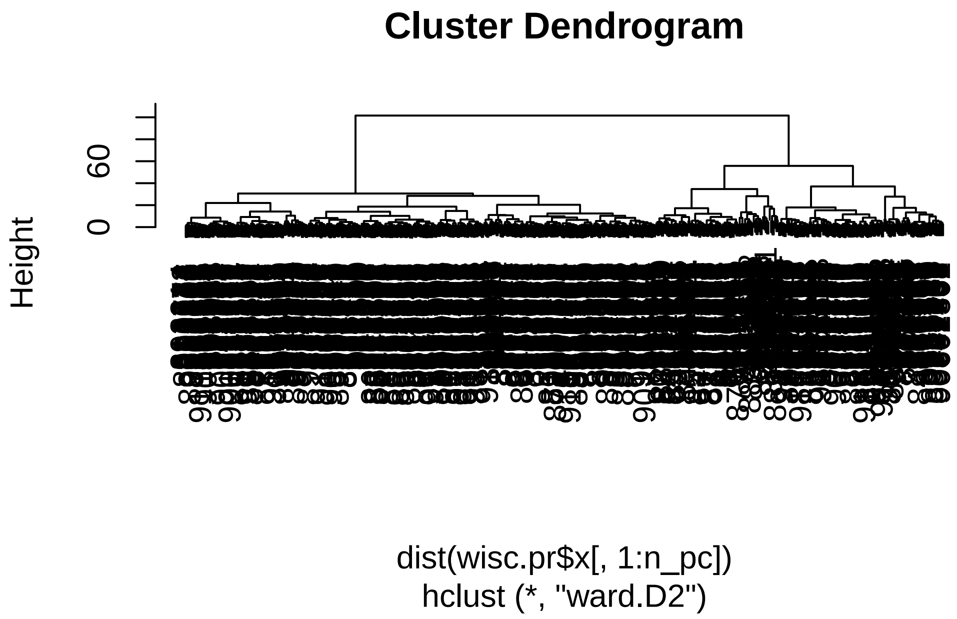
```
cum_var <- cumsum(wisc.pr$sdev^2 / sum(wisc.pr$sdev^2))
```

```
n_pc <- min(which(cum_var >= 0.9))
n_pc
```

```
[1] 7
```

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

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



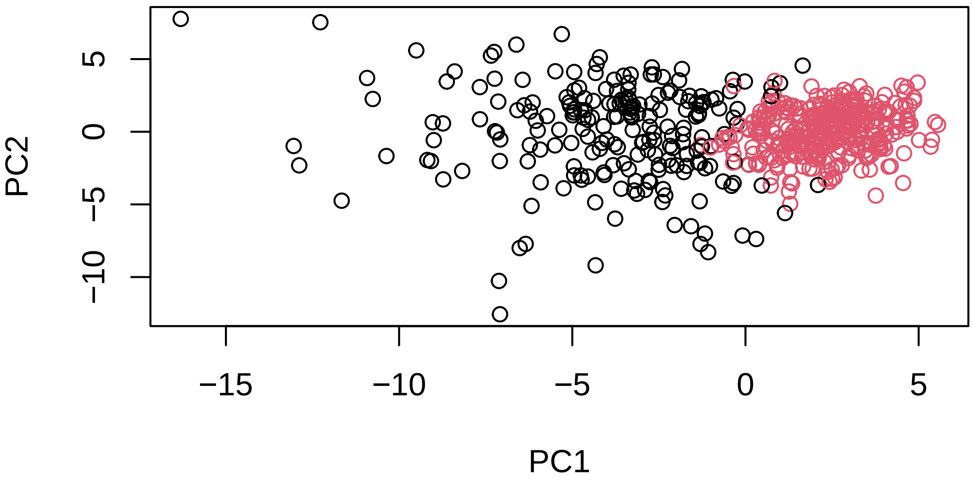
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2 
216 353 
```

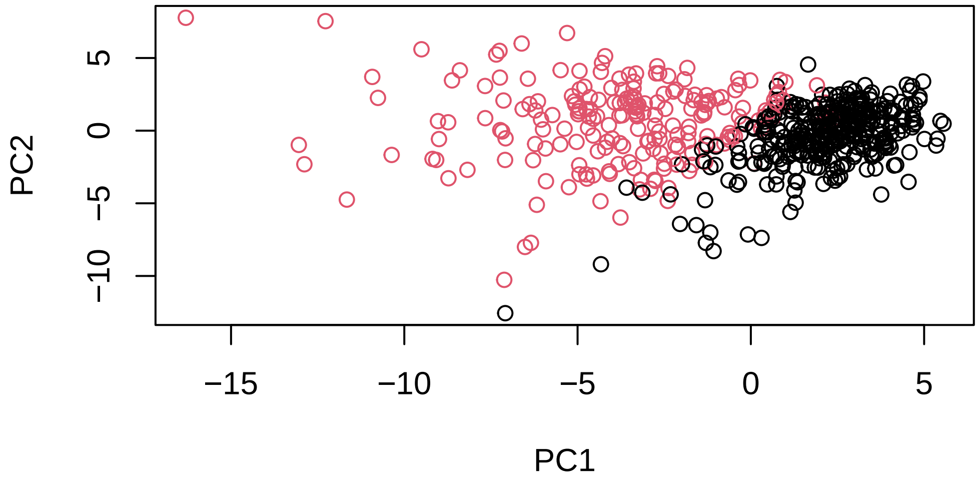
```
table(grps, diagnosis)
```

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

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



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



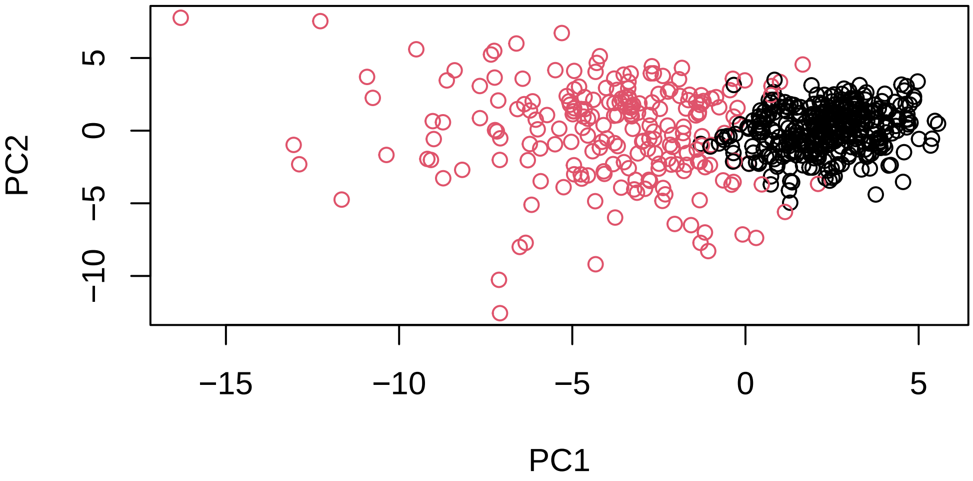
```
g <- as.factor(grps)
levels(g)
```

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

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

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

```
# Plot using our re-ordered factor
plot(wisc.pr$x[,1:2], col=g)
```



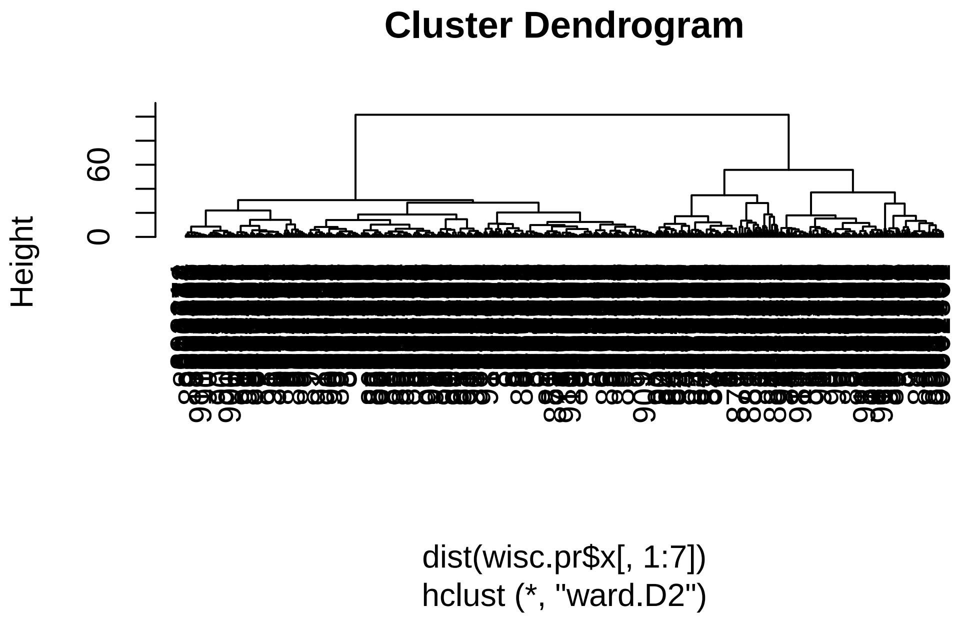
```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method="ward.D2")
wisc.pr.hclust
```

```
Call:
hclust(d = dist(wisc.pr$x[, 1:7]), method = "ward.D2")

Cluster method   : ward.D2
Distance         : euclidean
Number of objects: 569
```

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

```
plot(wisc.pr.hclust, hang = -1)
```



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

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

Q13. How well does the newly created model with four clusters separate out the two diagnoses? separated clusters are looking good.

Q14. How well do the hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses? the wisc.hclust.clusters with 4 clusters should be used due to better separation.

```
wisc.hclust <- hclust(dist(wisc.data[, -1]))
wisc.hclust.clusters <- cutree(wisc.hclust, k=2)
```

```
wisc.data <- read.csv("WisconsinCancer.csv")
wisc.km <- kmeans(wisc.data[,3:32], centers = 2)
wisc.hclust <- hclust(dist(wisc.data[,3:32]), method="ward.D2")
wisc.hclust.clusters <- cutree(wisc.hclust, k=2)
```

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

```
    B   M
1   1 130
2 356  82
```

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

```
wisc.hclust.clusters   B   M
                   1   0  86
                   2 357 126
```

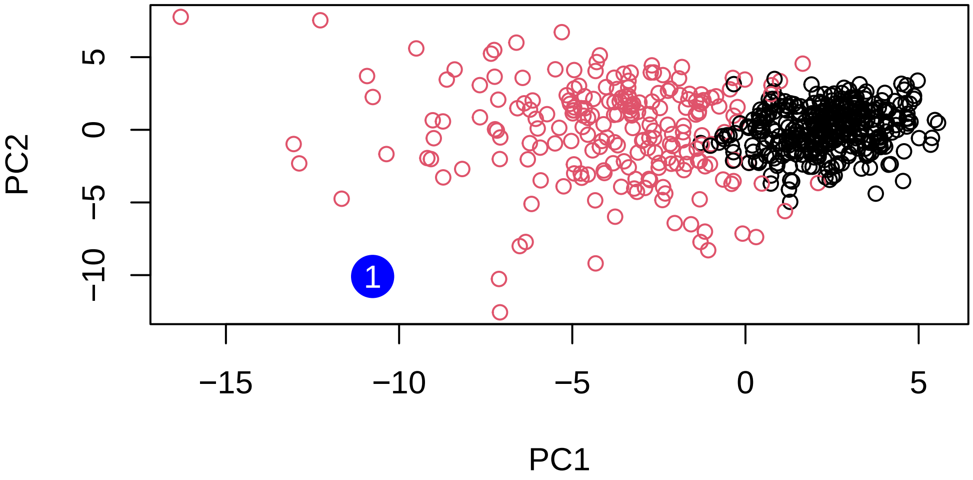
6. Prediction

```
#url <- "new_samples.csv"
newcancer_cell_data <- "new_samples.csv"
new <- read.csv("https://tinyurl.com/new-samples-CSV")
npc <- predict(wisc.pr, newdata=new)
npc
```

```
           PC1        PC2        PC3       PC4      PC5       PC6        PC7
[1,] -10.76452 -10.093978 -0.5897994 -4.164748 10.61922 -1.630738 0.03566861
[2,] -18.09606  -9.967098 -2.1549431 -4.006848  6.69687 -2.034714 1.25088149
           PC8       PC9     PC10       PC11     PC12       PC13      PC14
[1,] 0.7308658 -1.580861 3.166451 -0.7167150 3.850569 -0.8259764 1.0195729
[2,] 0.6308585 -1.155629 3.608207 -0.3405375 2.288732 -0.3976672 0.1347203
         PC15      PC16      PC17      PC18     PC19      PC20      PC21
[1,] 3.735687 -4.068783 1.0877034 0.9985959 1.022760 -2.430215 -1.295749
[2,] 3.543905 -3.749616 0.7613603 1.1763217 1.366702 -2.609643 -1.541050
          PC22       PC23      PC24       PC25      PC26      PC27       PC28
[1,] -1.348026 -0.7388274 -1.083000 -0.4220831 -1.892993 -1.176056 0.05527974
[2,] -1.424290 -0.7591376 -1.439202 -0.6508838 -1.981711 -1.397390 0.18112357
          PC29       PC30
```

```
[1,] 0.2658028 0.05162840
[2,] 0.2842191 0.02734355
```

```
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? The patient closer to the malignant cluster