Class 8

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> **Take-home**: Generally we always want to set `scale=TRUE` when we do this type of analysis to avoid our analysis being dominated by individual variables with the largest variance just due to their unit of measurement.

##FNA breast cancer data

Load the data into 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
```

Q1. How many observations are in this dataset?

```
nrow(wisc.df)
```

```
[1] 569
```

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

```
sum(wisc.df$diagnosis == "M")
```

```
[1] 212
```

The `table()` function is super useful here:

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

```
  B   M
357 212
```

Q3. How many 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"
```

A useful function for this is `grep()`

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

```
[1] 10
```

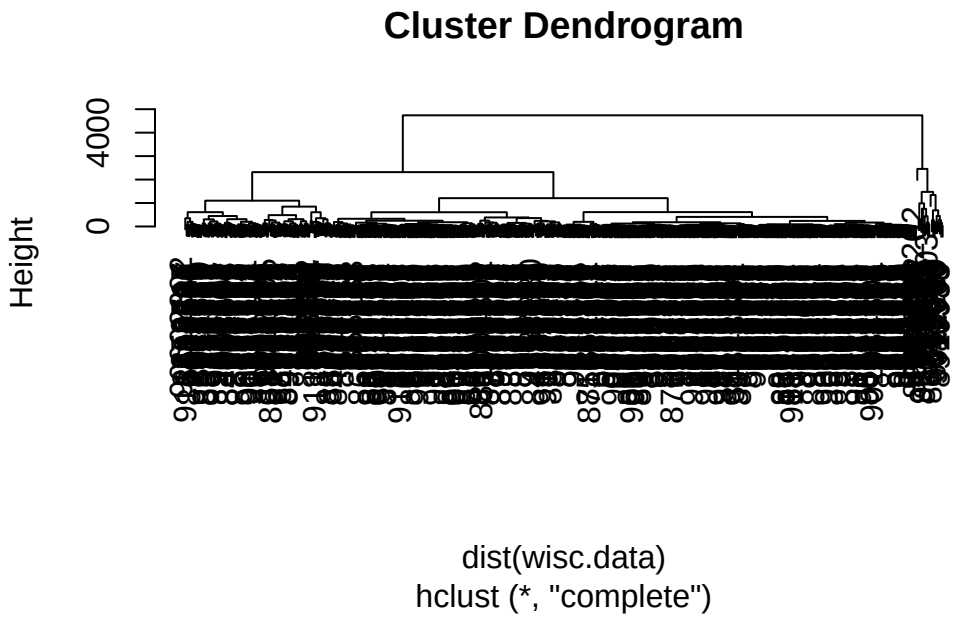
Before we go any further we need to exclude the diagnosis column from any future analysis - this tells us whether a sample to cancer or non-cancer.

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

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

Lets see if we can cluster the `wisc.data` to find some structure in the data set.

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



Principal Component Analysis (PCA)

```
wisc.pr<-prcomp(wisc.data,scale = T)
summary(wisc.pr)
```

```
Importance of components:
                          PC1     PC2      PC3      PC4      PC5      PC6      PC7
```

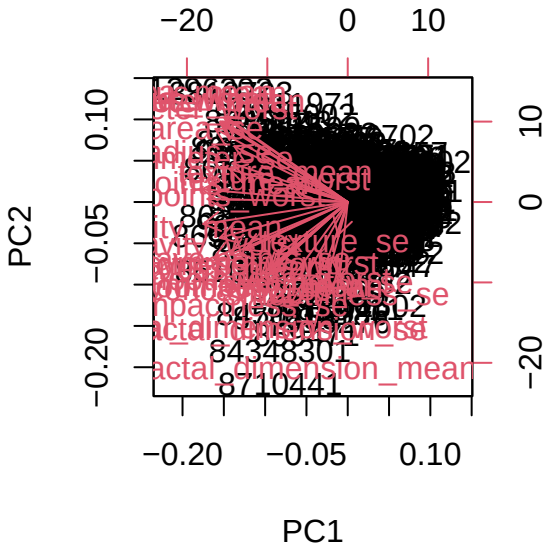
```
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
                           PC8    PC9    PC10   PC11    PC12    PC13    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 of the original variance is captured by the first principal components.

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

Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data? 9 principal components are required to describe at least 90% of the original variance in the data.

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



Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why? This plot has a lot of dots and lines that make the plot difficult to understand.

This biplot sucks! We need to build our own PCA score plot of PC1 vs PC2

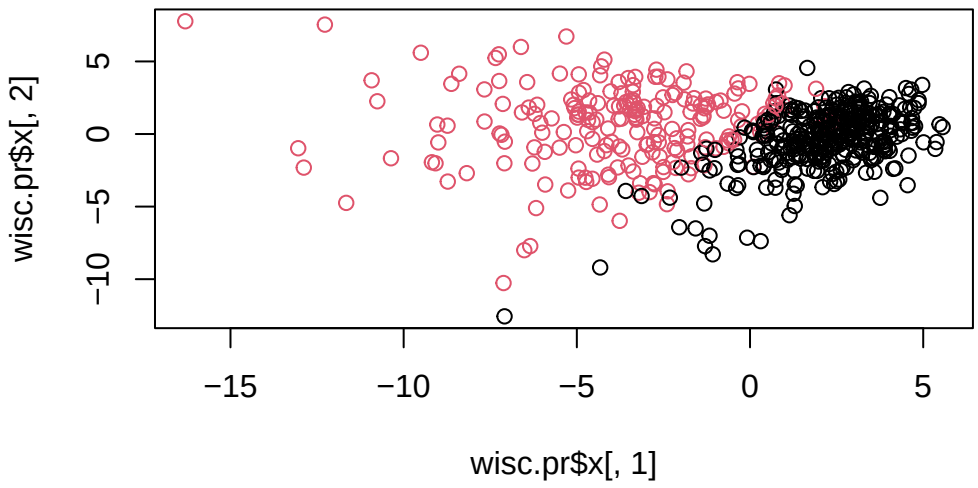
```
head(wisc.pr$x)
```

```
               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
```

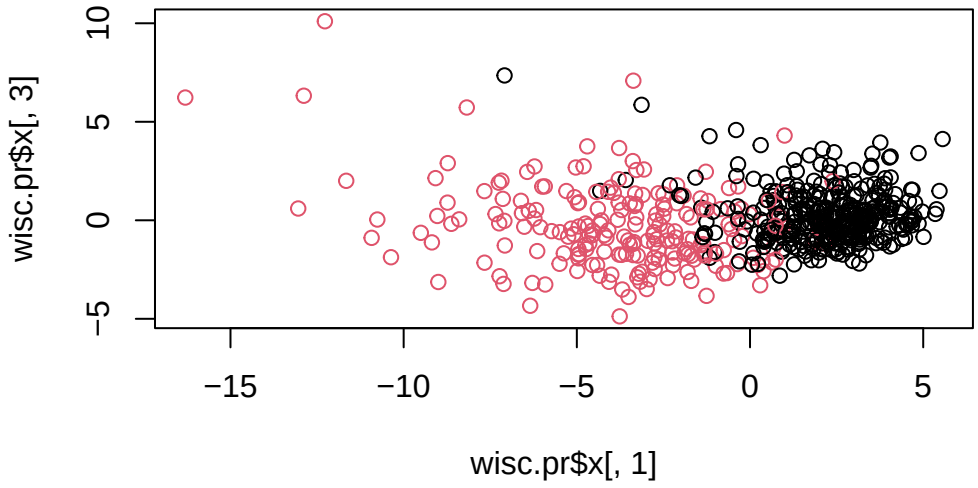
Plot of PC1 vs PC2 the first two columns

```
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? These plots are similar but there are more overlaps between the malignant and benign diagnosis.

```
plot(wisc.pr$x[,1], wisc.pr$x[,3], col = diagnosis)
```



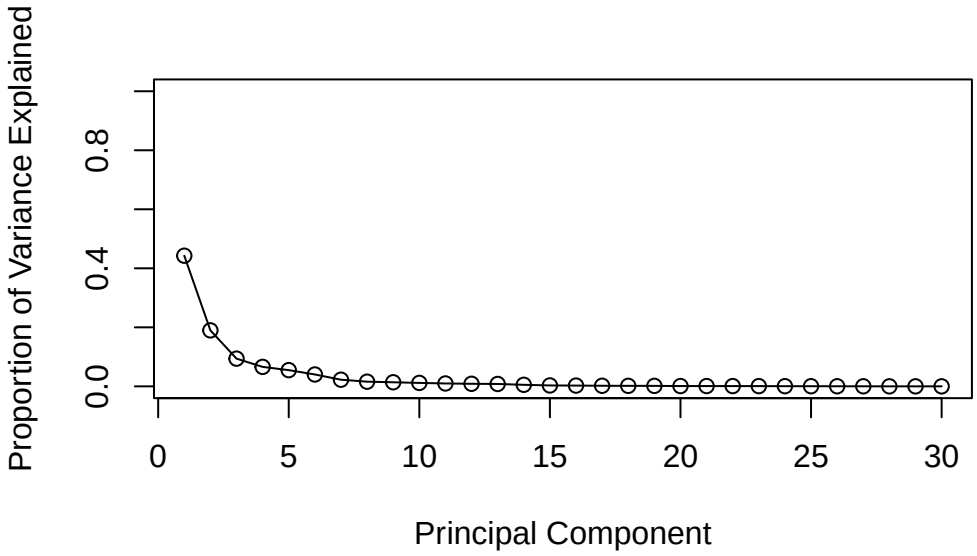
Calculating the variance of each component

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

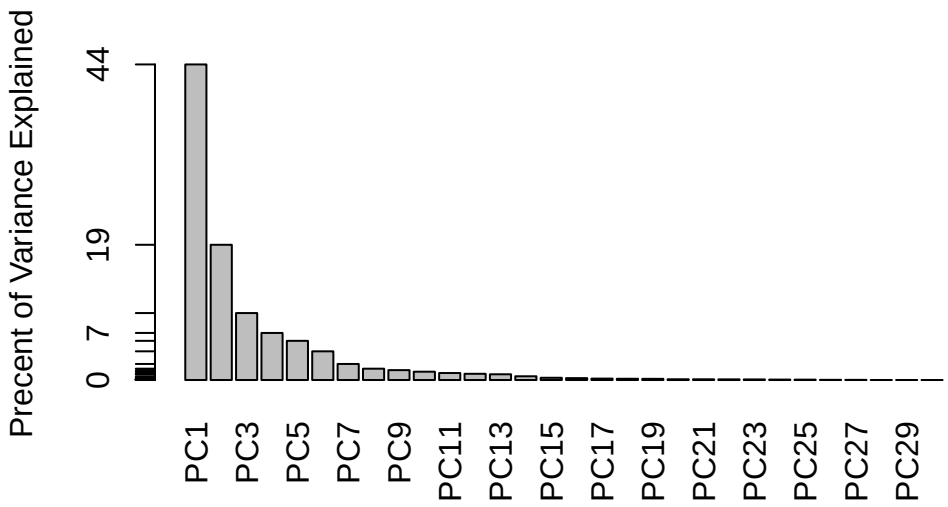
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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? concave.points_mean is -0.26085376

```
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
```

Q10. What is the minimum number of principal components required to explain 80% of the variance of the data? 5 principal components

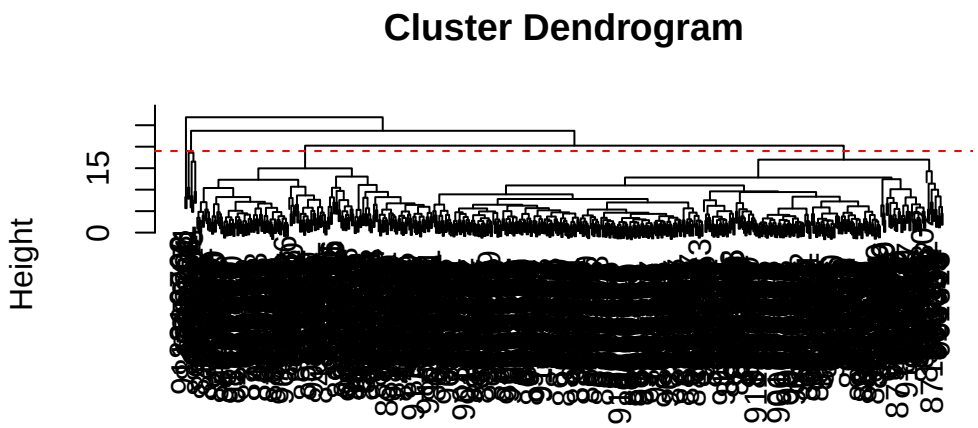
Hierarchical clustering

```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
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, the clustering model has 4 clusters.

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




```
unique(cutree(wisc.hclust,h=19))
```

```
[1] 1 2 3 4
```

Selecting number of clusters

```
wisc.hclust.clusters <- cutree(wisc.hclust,k=6)
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   0   5
                   3 331  39
                   4   2   0
                   5  12   1
                   6   0   2
```

Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10? Dividing the clusters into k=4 will result in a better cluster vs diagnoses match.

```
wisc.hclust.clusters <- cutree(wisc.hclust,k=3)
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1 355 205
                   2   2   5
                   3   0   2
```

```
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
```

```
wisc.hclust.clusters <- cutree(wisc.hclust,k=5)
table(wisc.hclust.clusters, diagnosis)
```

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

```
wisc.hclust.clusters <- cutree(wisc.hclust,k=7)
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   0   3
                   3 331  39
                   4   2   0
```

```
  5  12   1
  6   0   2
  7   0   2
```

```
wisc.hclust.clusters <- cutree(wisc.hclust,k=8)
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   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
```

```
wisc.hclust.clusters <- cutree(wisc.hclust,k=9)
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   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
```

Using different methods

Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning. The "complete" method gives my favorite results for the same data.dist dataset because it provides all the data for clustering and adjustments can be made after to separate the clusters.

K-means clustering and comparing results

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

```
wisc.km <- kmeans(scale(wisc.data), centers= 2, nstart= 20)
table(wisc.hclust.clusters, wisc.km$cluster)
```

```
wisc.hclust.clusters   1   2
                   1  17  81
                   2   0  79
                   3   0   3
                   4 358  12
                   5   0   2
                   6   5   7
                   7   0   2
                   8   0   2
                   9   0   1
```

Clustering on PCA results

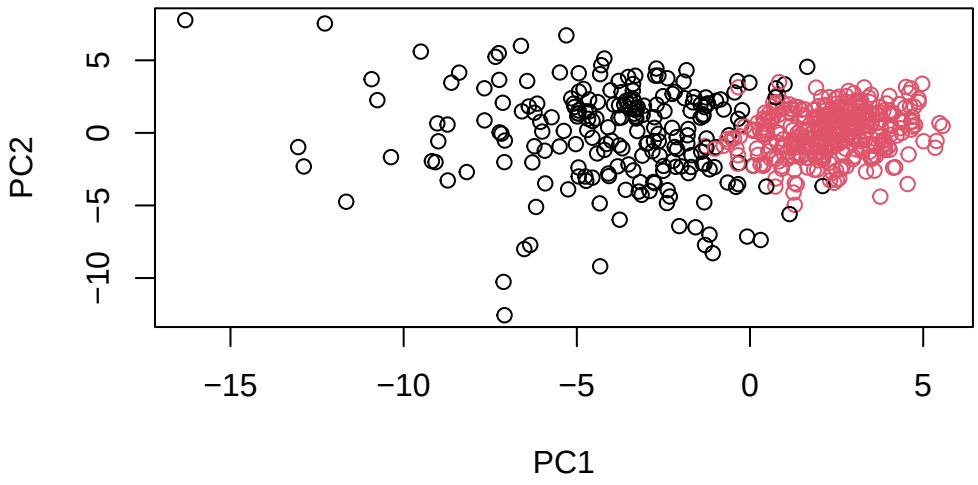
```
wisc.pr.hclust<-hclust(dist(wisc.pr$x[,1:7]),method="ward.D2")
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
216 353
```

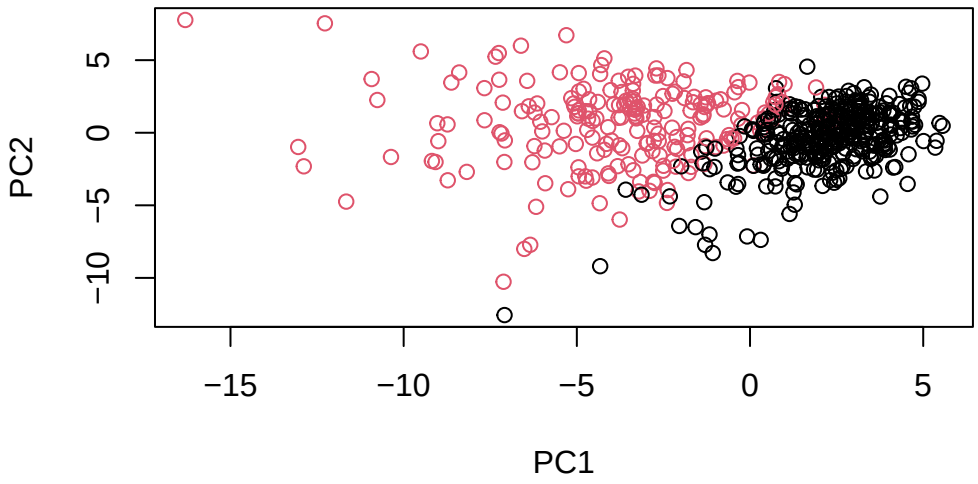
```
table(grps, diagnosis)
```

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

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




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



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

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

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

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

Q16. How well do the k-means and 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.km$cluster, diagnosis)
```

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

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

```
                    diagnosis
wisc.hclust.clusters   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
```

Sensitivity/Specificity

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

Sensitivity

```
#wisc.km$cluster
175/(175+14)
```

```
[1] 0.9259259
```

```
#wisc.hclust.clusters
86/(86+12)
```

```
[1] 0.877551
```

Specificity

```
#wisc.km$cluster
343/(343+37)
```

```
[1] 0.9026316
```

```
#wisc.hclust.clusters
331/(331+39)
```

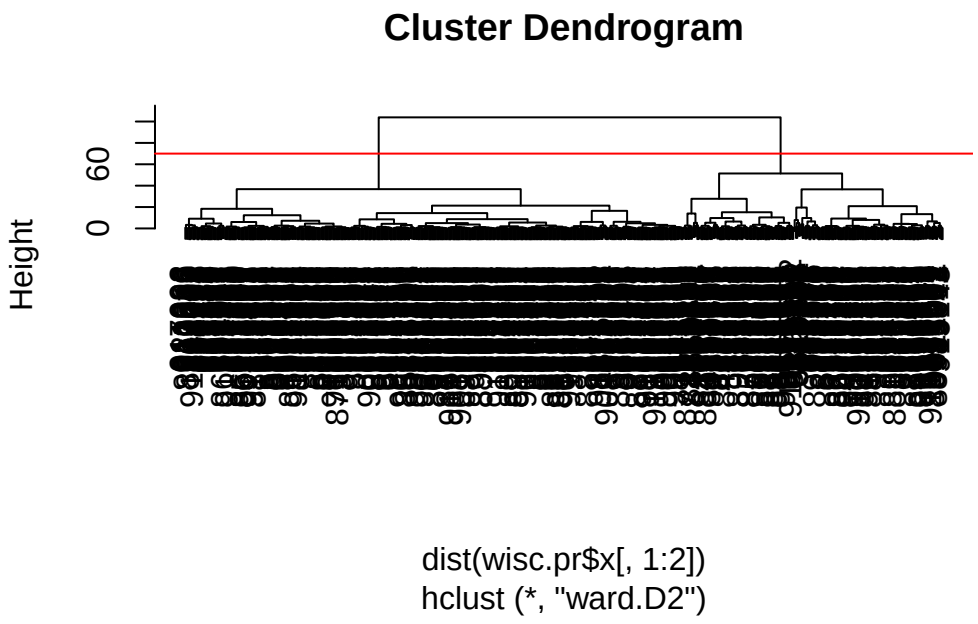
```
[1] 0.8945946
```

The wisc.km$cluster had a better specificity and sensitivity.

Clustering in PC space

```
hc<-hclust(dist(wisc.pr$x[,1:2]), method="ward.D2")

plot(hc)
abline(h=70, col="red")
```



Cluster membership vector

```
grps<-cutree(hc, h=70)
table(grps)
```

```
grps
  1   2
195 374
```

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

Cross-table to see how my clustering groups correspond to the expert diagnosis vector of M and B values

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

```
    diagnosis
grps   B   M
   1  18 177
   2 339  35
```

Positive => cancer M Negative => non-cancer B

True = cluster/group 1 False = group 2

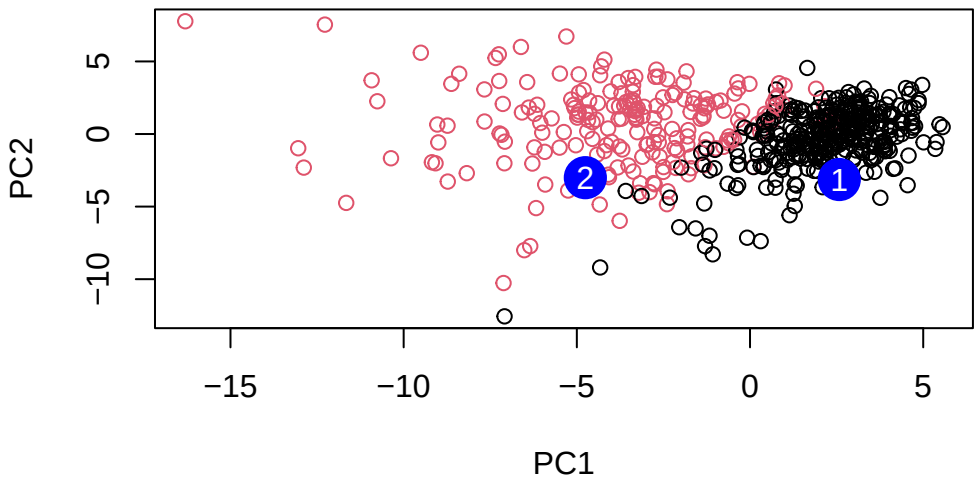
True Positive = 177 False Positive = 18 True Negative = 339 False Negative = 35

Predictions

We can use our PCA results (wisc.pr) to make predictions on new unseen data.

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

```
plot(wisc.pr$x[,1:2],col=diagnosis)
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 patients who are truly ill and have tested positive for the condition.