Class8

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Table of contents

Background

The goal of this mini-project is for you to explore a complete analysis using the unsupervised learning techniques covered in class. You'll extend what you've learned by combining PCA as a preprocessing step to clustering using data that consist of measurements of cell nuclei of human breast masses. This expands on our RNA-Seq analysis from last day.

The data itself comes from the Wisconsin Breast Cancer Diagnostic Data Set first reported by K. P. Benne and O. L. Mangasarian: "Robust Linear Programming Discrimination of Two Linearly Inseparable Sets".

Data Import

Here we downloaded the file to our laptops then added it to our BIMM 143 folder. Then it will appear in the "Files" on the right and can be added into wisc.df.

```
wisc.df <- read.csv("WisconsinCancer.csv", row.names=1)
```

Now let's view some of our data.

```
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
```

Let's remove the first column from the data.

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

Let's create a vector for later that contains the diagnosis column data.

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

Q1. How many observations are in the diagnosis dataset?

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

```
[1] 569
```

Q2. How many observations are malignant?

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

```
  B   M
357 212
```

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

```
allcolnames<-colnames(wisc.data)
grep("_mean",allcolnames,value=TRUE)
```

```
 [1] "radius_mean"            "texture_mean"           "perimeter_mean"
 [4] "area_mean"              "smoothness_mean"        "compactness_mean"
 [7] "concavity_mean"         "concave.points_mean"    "symmetry_mean"
[10] "fractal_dimension_mean"
```

Principal Component Analysis (PCA)

We need to determine if we should perform a PCA on the data. If units are different across the data it will likely be beneficial to scale the data.

```
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
```

```
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
```

As we can see it is worth performing a PCA.

```
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. What proportion of the orginial variance is captured by the first principal components?

Answer: 0.4427

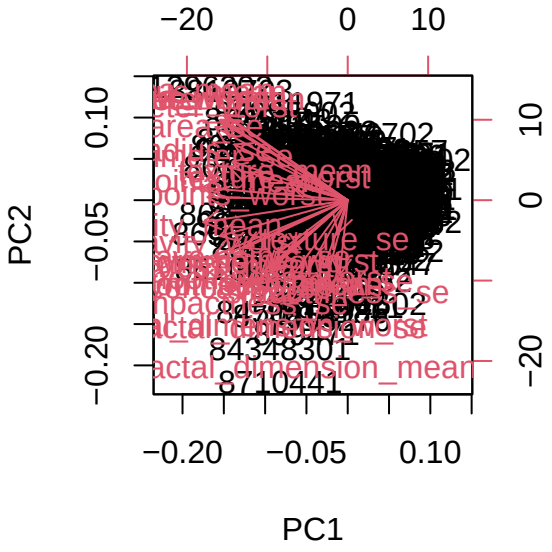
Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

Answer: For this we look at cumulative proportion. PC3 contains 0.72636 of the original variance.

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

Answer: PC7.

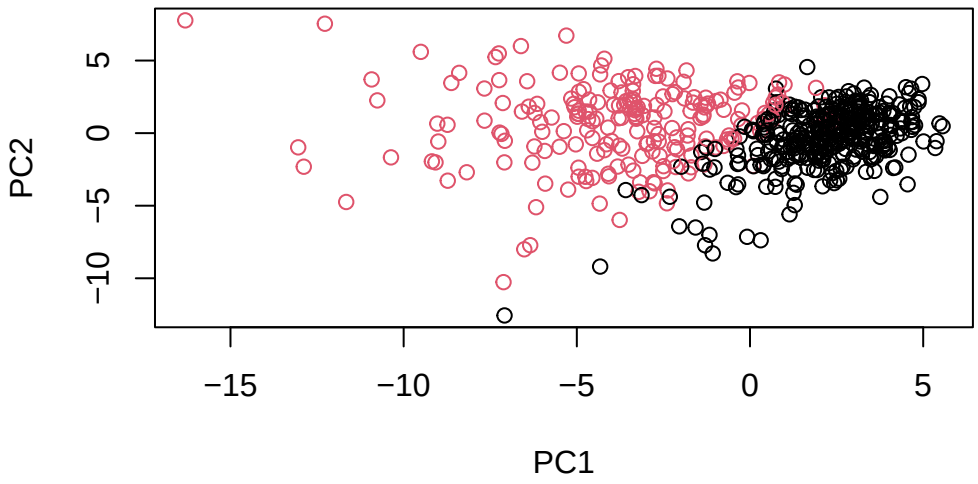
```
biplot(wisc.pr)
```



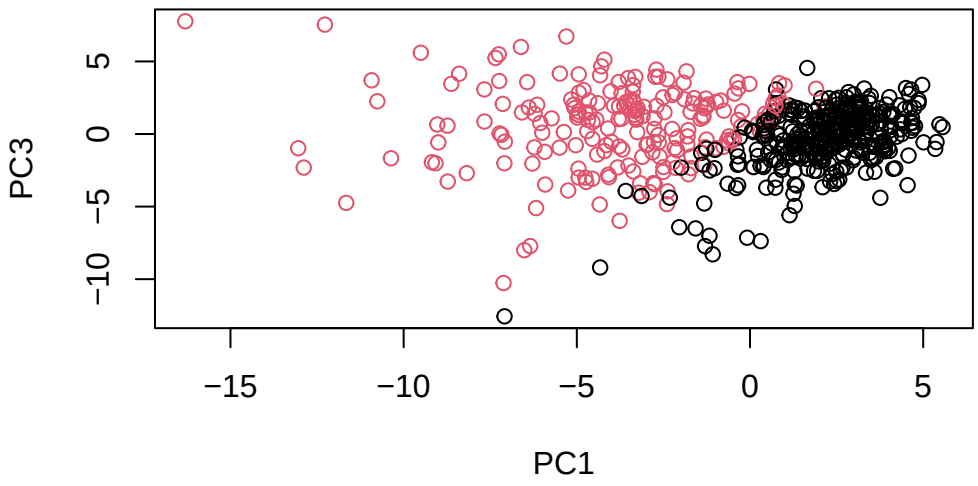
Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

Answer: What stands out is how much information is shown at once making it hard for me to understand. There are numbers on all four sides of the graph and too much overlap at data at once.

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




```
plot(wisc.pr$x[, 1:2 ], col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```



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

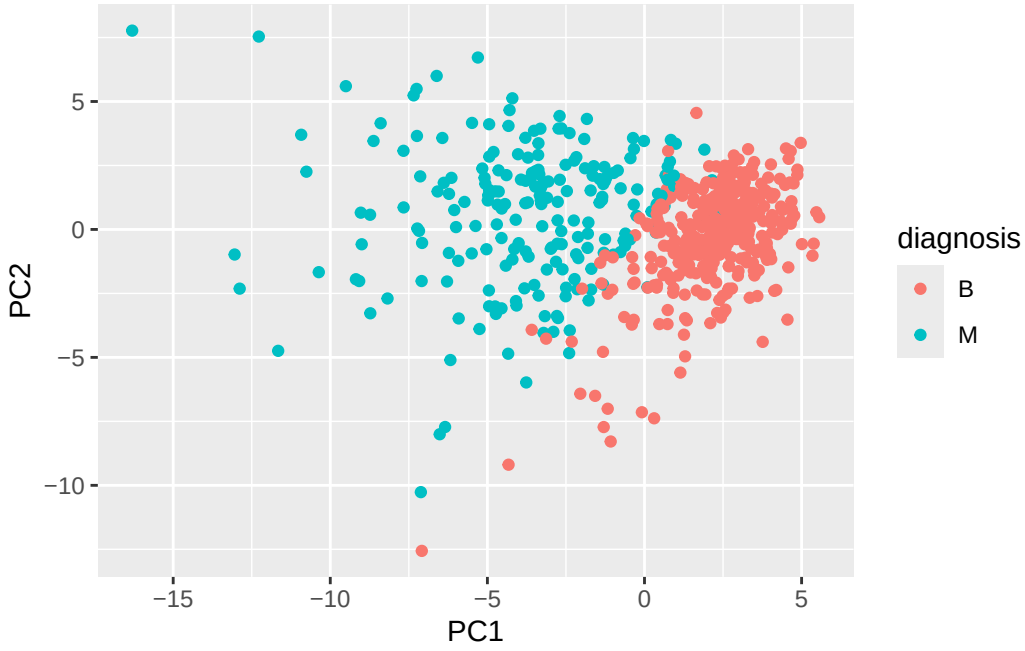
Answer: They are seperating the spread between malignant and benign tumors.

The main PCA result figure is called a "score plot" or "PC plot" or "ordination plot"...

```
library(ggplot2)
```

Lets plot PC1 vs PC2.

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



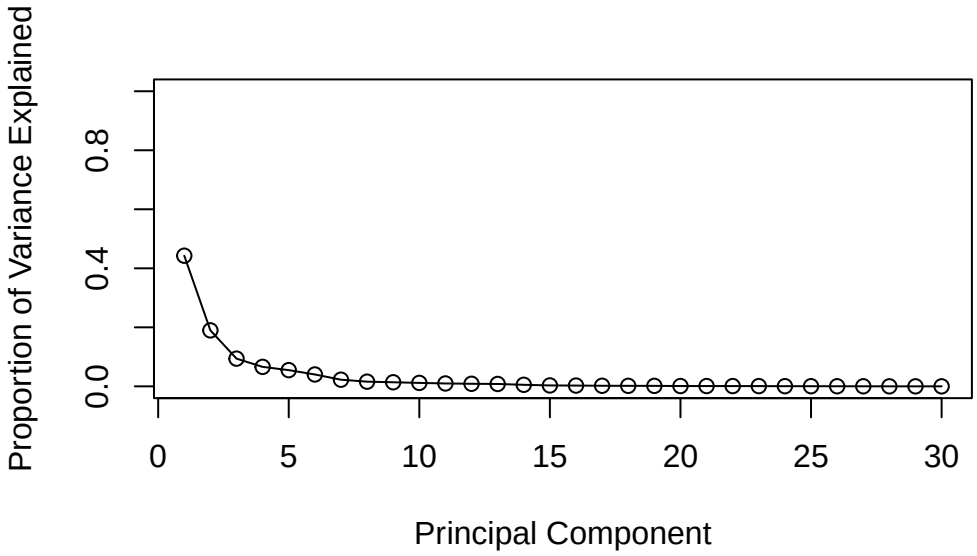
Let's calculate the variance of each component in wisc.pr.

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

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

```
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")
```



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?

Answer: -0.2609

```
summary(wisc.pr$rotation["concave.points_mean","PC1"])
```

```
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max. 
-0.2609 -0.2609 -0.2609 -0.2609 -0.2609 -0.2609 
```

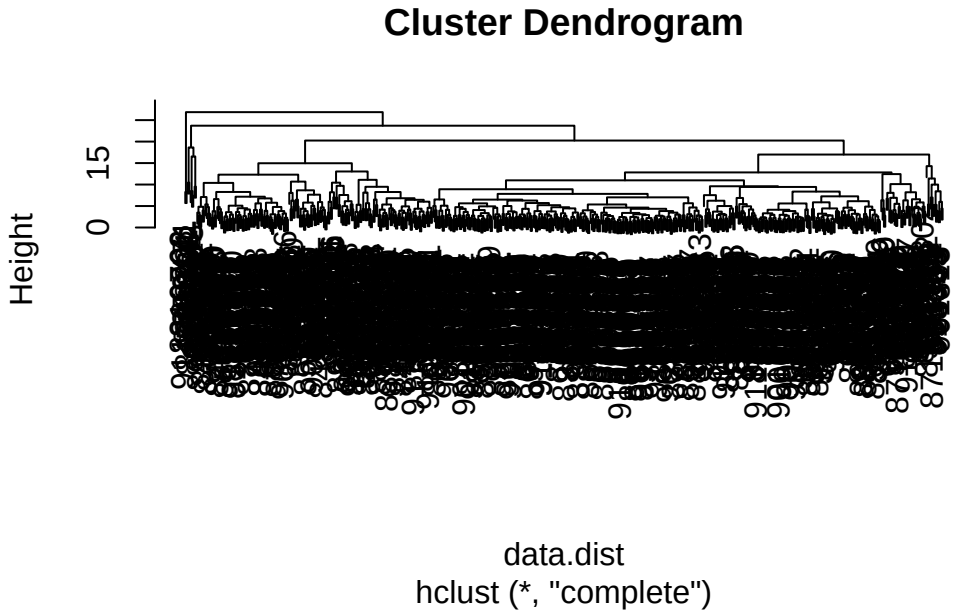
Q10. What is the minimum number of principal components required to explain 80% of the variance of the data?

Answer: PC5

Hierarchical clustering

Just clustering the original data is not very informative or helpful.

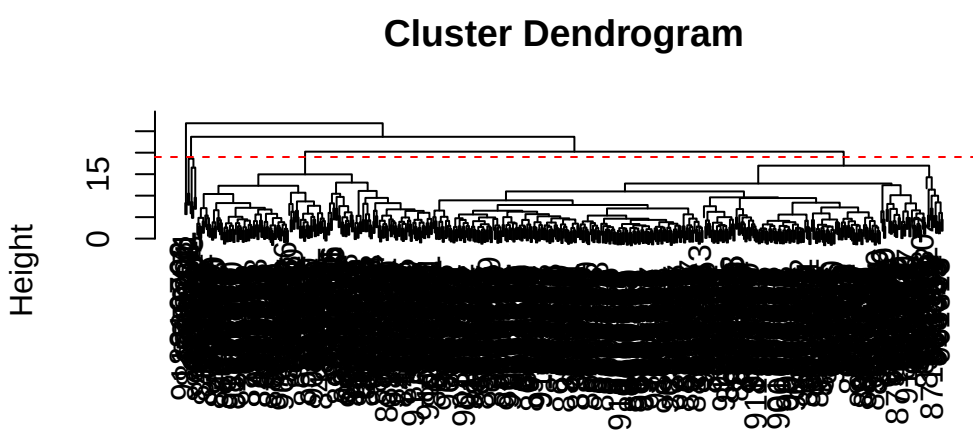
```
data.scaled<-scale(wisc.data)
data.dist<-dist(data.scaled)
wisc.hclust<-hclust(data.dist)
plot(wisc.hclust)
```



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

Answer: h=19

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




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

```
  1   2
567   2
```

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

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1 357 210
                   2   0   2
```

Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

Answer: Two clusters provides a more even distribution between benign and malignant.

Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

Answer: I prefer ward.D2 the most because the plots themselves are very busy with data and this method most clearly conveys the high amount of information.

```
wisc.km <- kmeans(wisc.data, centers= 2, nstart= 20)
```

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

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

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

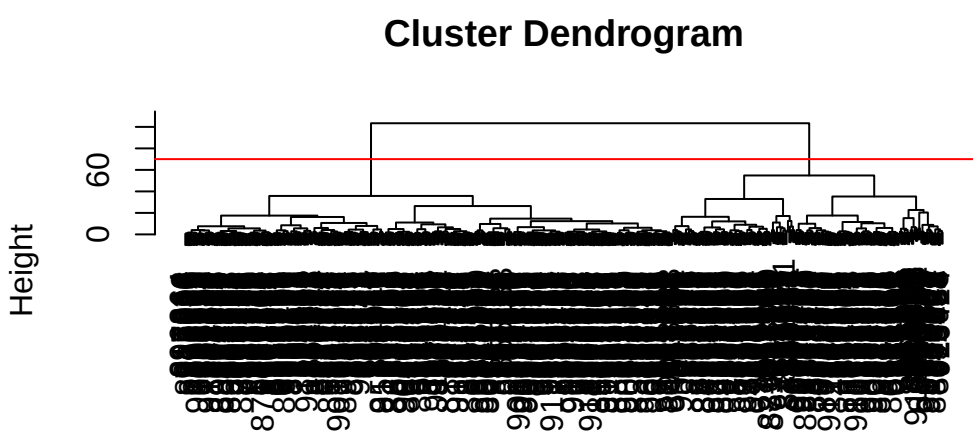
Answer: HClust once adjusted to two clusters does a slightly better job in my opinion of seperating the results into a more even distribution while k-means does a decent job but not as well. HClust seperated benign and malignant into roughly 350 and 200 while the distribution for k-means is about 350 to 130.

Combining methods (PCA and Clustering)

Clustering the original data was not productive. The PCA results looked promising. Here we combine these methods by clustering from our PCA results. In other words "clustering in PC space".

```
## Take the first 3 PCs
dist.pc<-dist(wisc.pr$x[,1:3])
wisc.pr.hclust<-hclust(dist.pc,method="ward.D2")
```

```
plot(wisc.pr.hclust)
abline(h=70,col="red")
```



To get our clustering membership vector (i.e. our main clustering result) we "cut" the tree at a desired height or to yield a desired number of "k" groups.

This is the code being used but for the sake of not adding 5 pages it will not be executed.

cutree(wisc.pr.hclust,k=2)

```
grps<-cutree(wisc.pr.hclust,h=70)
table(grps)
```

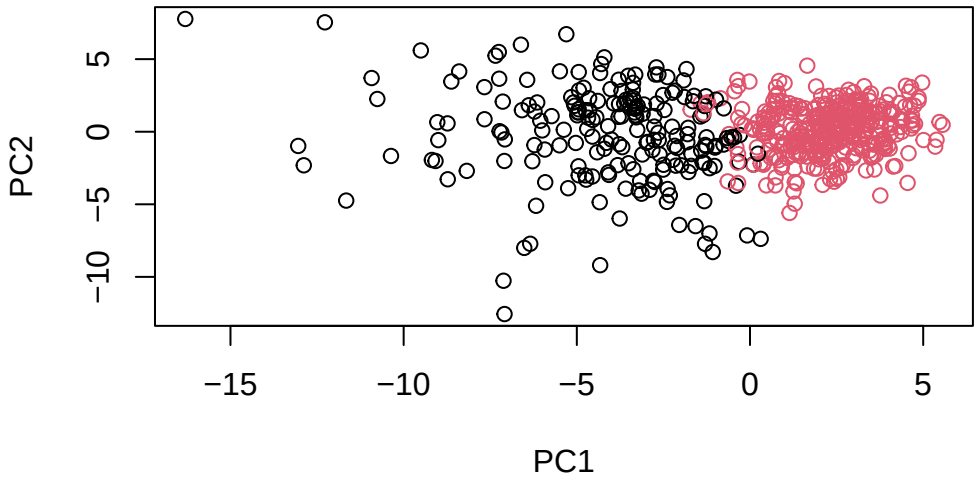
```
grps
  1   2
203 366
```

How does this clustering grps compare to the expert?

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

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

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




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

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

Answer: The new model doesn't do the best job of separating the two diagnoses with four clusters as they are very skewed.

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.

Answer: In this case the k-means method provides a better seperation of the data because the data is more evenly distributed between the clusters.

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

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

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

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1 357 210
                   2   0   2
```

##Sensitivity

Sensitivity: TP/(TP+FN) Specificity: TN/(TN+FN)

K-means: Sensitivity: 175/(175+37)=0.825 Specificity: 343/(343+357)=0.961

Hierarchical: Sensitivity: 172/(172+40)=0.811 Specificity: 343/(343+14)=0.961

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

Answer: The K-means has slightly higher sensitivity but both have equal specificity.

7. Prediction

We can use our PCA model for prediction with new input patient samples.

```
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
```

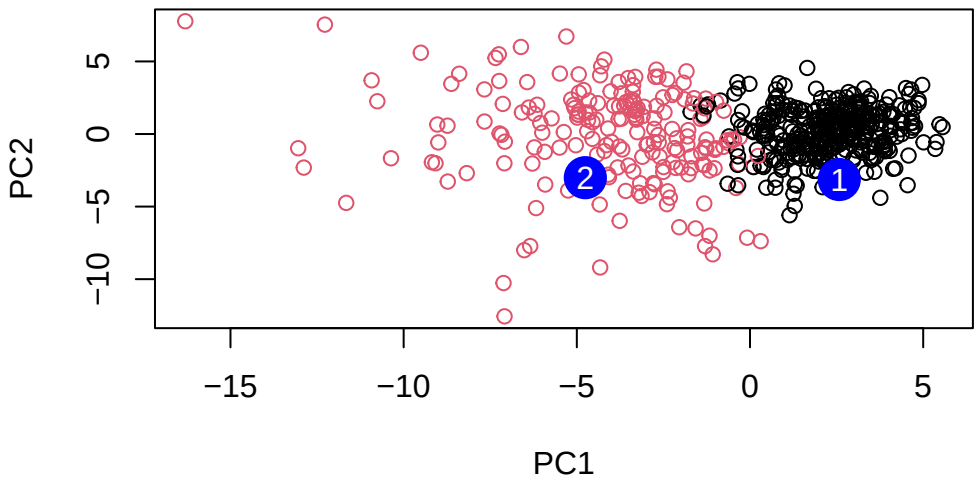
```
g <- as.factor(grps)
levels(g)
```

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

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

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

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

Answer: Patient 2 should be followed up with because malignent tumors have been seen on the lower end of PC1.

```
sessionInfo()
```

```
R version 4.5.1 (2025-06-13)
Platform: aarch64-apple-darwin20
Running under: macOS Tahoe 26.0.1

Matrix products: default
BLAS:   /Library/Frameworks/R.framework/Versions/4.5-arm64/Resources/lib/libRblas.0.dylib
LAPACK: /Library/Frameworks/R.framework/Versions/4.5-arm64/Resources/lib/libRlapack.dylib;  L

locale:
[1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8

time zone: America/Los_Angeles
tzcode source: internal

attached base packages:
```

```
[1] stats     graphics  grDevices utils     datasets  methods   base

other attached packages:
[1] ggplot2_4.0.0

loaded via a namespace (and not attached):
 [1] digest_0.6.37      labeling_0.4.3     RColorBrewer_1.1-3 R6_2.6.1
 [5] fastmap_1.2.0      xfun_0.53          farver_2.1.2       gtable_0.3.6
 [9] glue_1.8.0         knitr_1.50         htmltools_0.5.8.1  rmarkdown_2.30
[13] lifecycle_1.0.4    cli_3.6.5          S7_0.2.0           scales_1.4.0
[17] vctrs_0.6.5        grid_4.5.1         withr_3.0.2        compiler_4.5.1
[21] tools_4.5.1        evaluate_1.0.5     yaml_2.3.10        rlang_1.1.6
[25] jsonlite_2.0.0
```