Class 8: Mini Project

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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".

Values in this data set describe characteristics of the cell nuclei present in digitized images of a fine needle aspiration (FNA) of a breast mass.

Data input

Data was downloaded from the class website as a CSV file.

```
# Save your input data file into your Project directory
fna.data <- "WisconsinCancer.csv"

# Complete the following code to input the data and store as wisc.df
wisc.df <- read.csv(fna.data, row.names=1)

# First 6 rows of data.frame
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
```

```
# We can use -1 here to remove the first column (remove patient ID)
wisc.data <- wisc.df[,-1]
```

We will create a diagnosis vector for use later when we compare information.

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

Exploratory data analysis

Q1. How many observations are in this dataset?

There are 569 observations/patients in data set.

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

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

```
  B   M
357 212
```

212 malignant diagnoses, and 357 benign diagnoses.

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

```
length(grep("_mean$", colnames(wisc.data)))
```

```
[1] 10
```

Principal Component Analysis (PCA)

The `prcomp()` function to do PCA has a `scale=FALSE` default. We want scale=TRUE so our analysis is not dominated by columns/variables in our dataset that have high standard deviation and mean when compared to others just because the units of measurement are different.

```
# Check column means and standard deviations
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
```

```
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp(wisc.data, scale = T)
```

```
# Look at summary of results
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)?

Proportion of Variance for PC1 is 0.4427.

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

3 PCs

```
which(summary(wisc.pr)$importance["Cumulative Proportion", ] >= 0.70)[1]
```

```
PC3
  3
```

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

7 PCs.

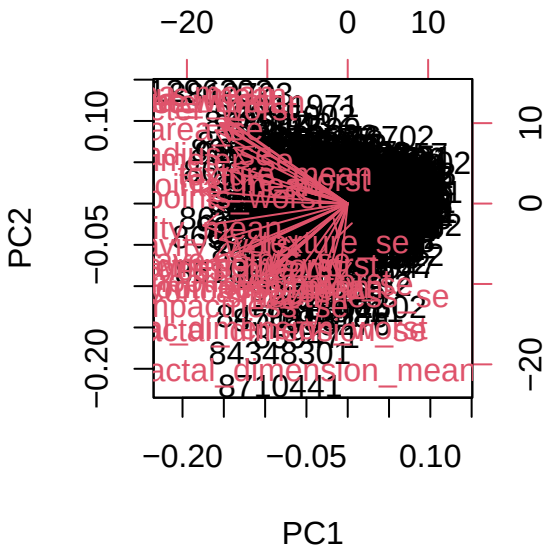
```
which(summary(wisc.pr)$importance["Cumulative Proportion", ] >= 0.90)[1]
```

```
PC7
  7
```

Interpreting PCA results

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

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

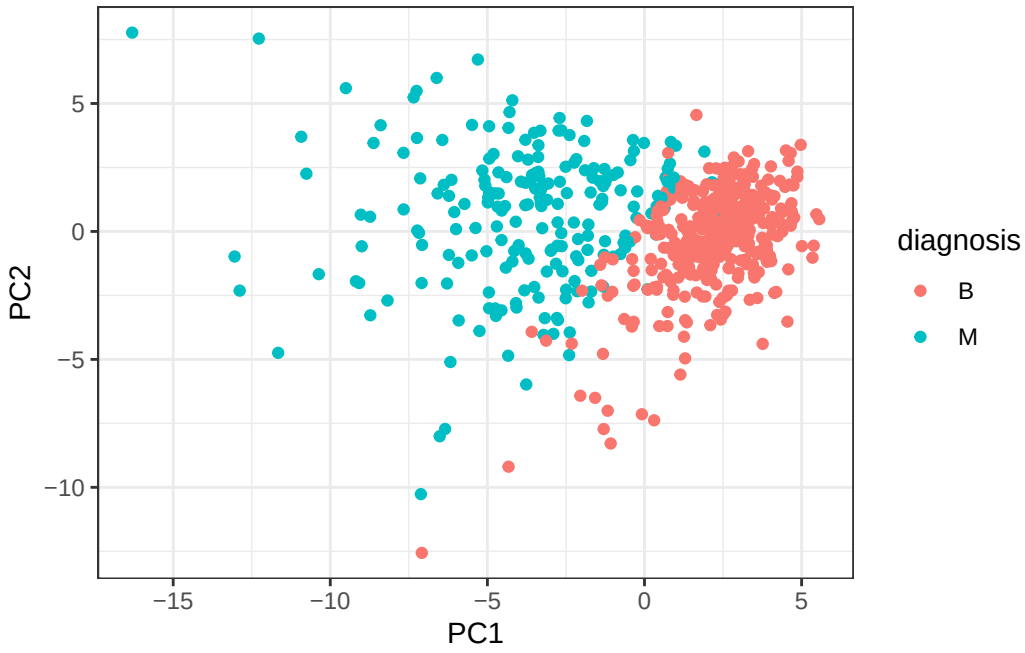


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

`biplot(wisc.pr)` is very difficult to read/understand. Too many points.

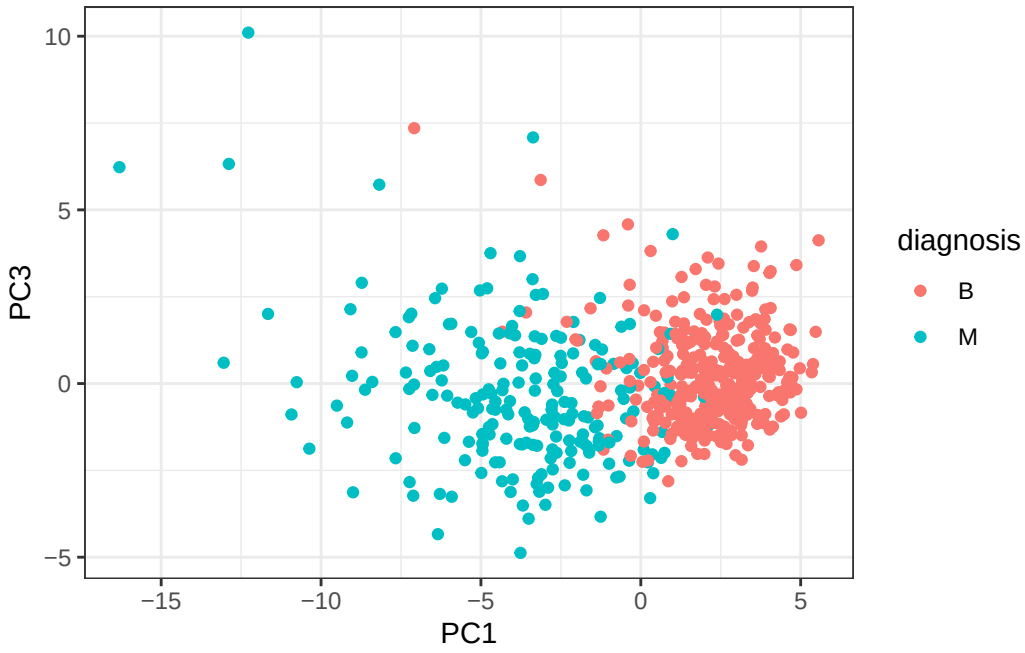
```
library(ggplot2)

#Scatter plot observations by components 1 and 2
ggplot(wisc.pr$x) +
  aes(PC1, PC2, col = diagnosis) +
  geom_point() +
  theme_bw()
```



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

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



The values in the PC1 and PC3 plots tend to be more negative than the PC1 and PC2 plot (therefore, PC1 and PC2 plot have more positive values than the PC1 and PC3 plot). There is more overlap between PC1 and PC3 than PC1 and PC2.

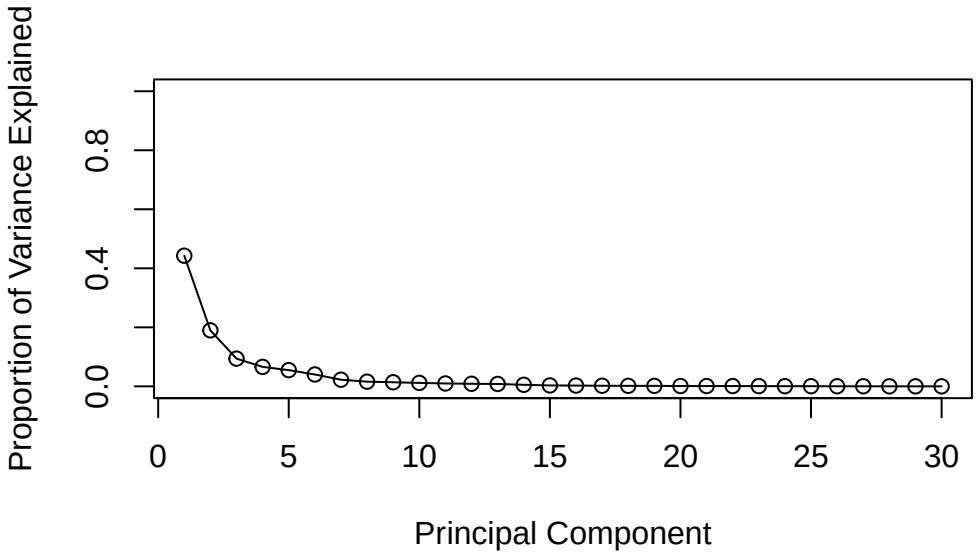
Variance explained

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

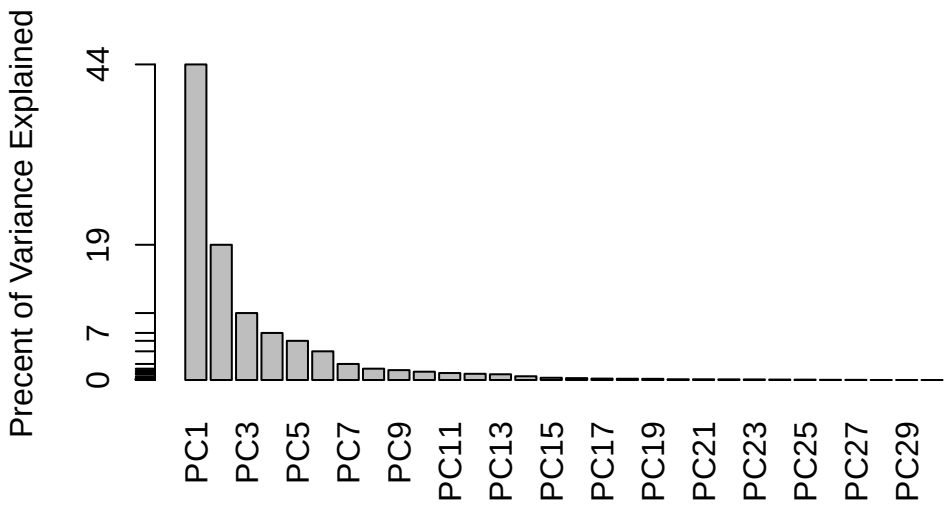
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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 )
```

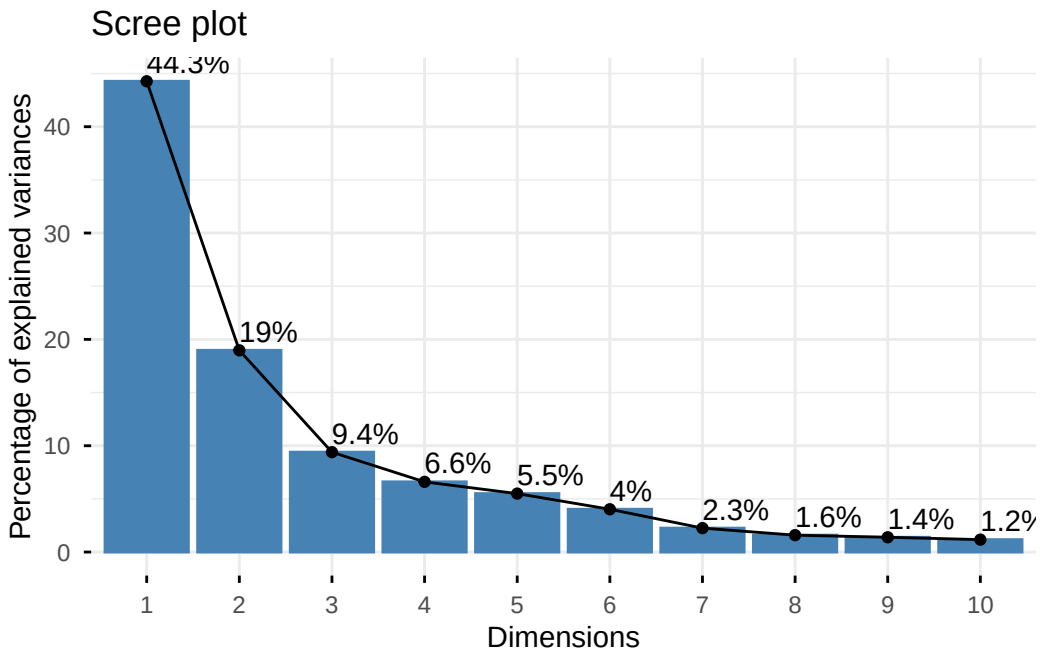



```
## ggplot based graph
#install.packages("factoextra")
library(factoextra)
```

```
Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
```

```
fviz_eig(wisc.pr, addlabels = TRUE)
```

```
Warning in geom_bar(stat = "identity", fill = barfill, color = barcolor, :
Ignoring empty aesthetic: `width`.
```



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?

```
# Loading of 'concave.points_mean' on PC1
wisc.pr$rotation["concave.points_mean", "PC1"]
```

```
[1] -0.2608538
```

The feature concave.points_mean has a loading of −0.2608538 on the first principal component (PC1), indicating it has low influence on PC1. The negative sign means that higher values of concave.points_mean tend to decrease the PC1 score for an observation. Since the loading of concave.points_mean on PC1 is −0.2608538, higher values of this feature push PC1 toward the negative direction, which corresponds to malignant cases.

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

```r
# Cumulative proportion
cum.pve <- cumsum(pve)

# Find minimum number of PCs to reach 80%
which(cum.pve >= 0.80)[1]
```

```
[1] 5
```

5 PCs are needed to explain 80% of the variance of the data.

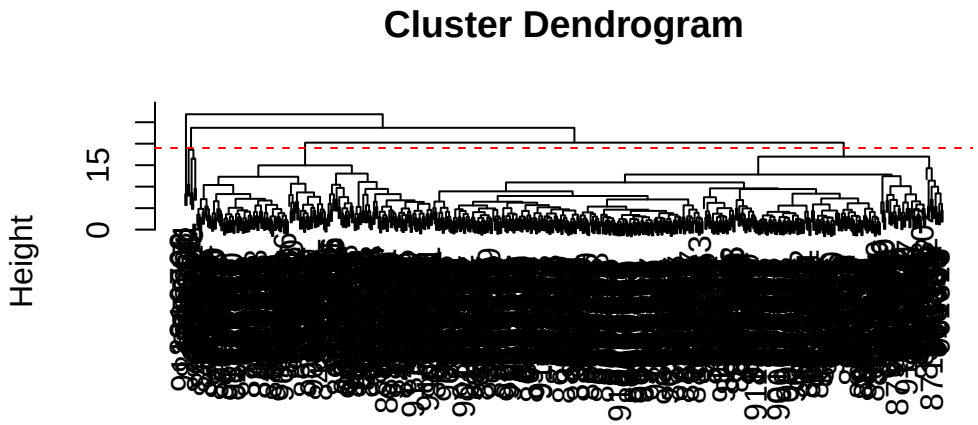
Hierarchical clustering

```r
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)

# Hierarchical clustering using complete linkage
wisc.hclust <- hclust(data.dist, method = "complete")
```

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

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



Height = 19 for when the clustering model has 4 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
```

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

```
best_k <- 0
best_match <- 0

for(k in 2:10){
  clusters <- cutree(wisc.hclust, k = k)
  tbl <- table(clusters, diagnosis)
  match <- sum(apply(tbl, 1, max)) / length(diagnosis)
```

```
  if(match > best_match){
    best_match <- match
    best_k <- k
  }
}

cat("Best number of clusters:", best_k, "\n")
```

```
Best number of clusters: 9
```

```
cat("Matching proportion:", best_match, "\n")
```

```
Matching proportion: 0.9103691
```

```
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
```

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

```
# Hierarchical clustering using ward.D2
wisc.hclust.ward <- hclust(data.dist, method = "ward.D2")

# Cut tree into 2 clusters (since we have benign vs malignant)
ward.clusters <- cutree(wisc.hclust.ward, k = 2)

# Compare to actual diagnosis
table(ward.clusters, diagnosis)
```

```
             diagnosis
ward.clusters   B   M
            1  20 164
            2 337  48
```

```
# Optionally, compute proportion of correct matches
match_proportion <- sum(apply(table(ward.clusters, diagnosis), 1, max)) / length(diagnosis)
match_proportion
```

```
[1] 0.8804921
```

- The ward.D2 method minimizes the variance within clusters at each step, which tends to produce tight, spherical clusters that are more balanced in size. Complete linkage produces compact clusters but can overemphasize outliers, so ward.D2 is preferred.

K-means clustering

```
wisc.km <- kmeans(data.dist, centers = 2, nstart = 20)
table(wisc.km$cluster, diagnosis)
```

```
   diagnosis
      B   M
  1 337  78
  2  20 134
```

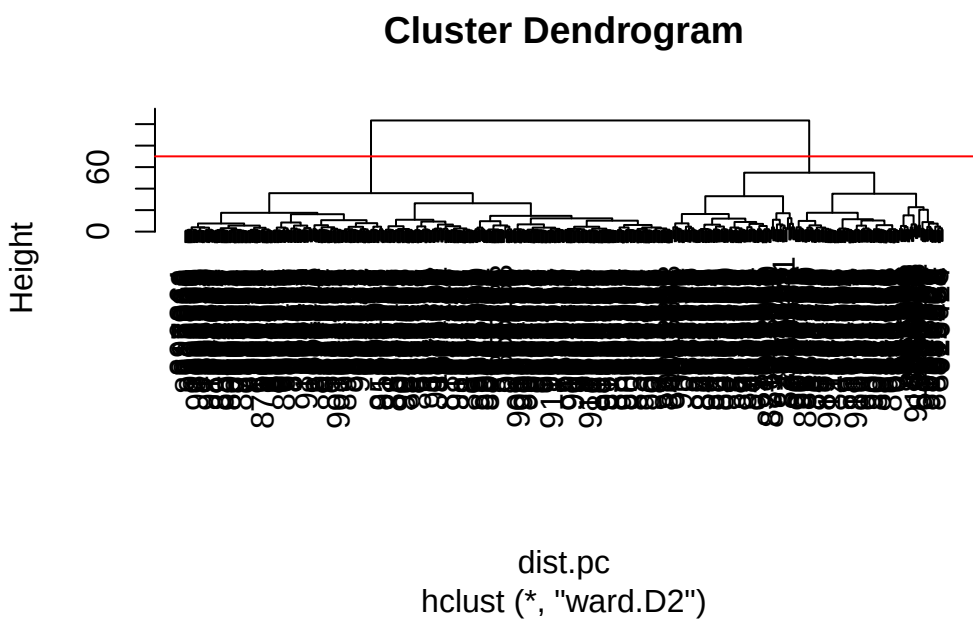
Combinding Methods (PCA and Clustering)

Clustering the original data was not very productive. The PCA results looked promising. Here we combine these methods by clustering from our PCA results. In other words, "clustering in PC space"... not using the original data but our PCA data (PC1, PC2, PCn...).

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

View the tree...

```
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.

> Q15. How well does the newly created model with four clusters separate out the two diagnoses? - Note for 15/16: we did not perform k-means clustering in class and this section was optional.

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

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

Separates well. Separates into true positives = 179, false negatives = 33, false positives = 24, true negatives = 333.

> 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. How does this clustering grps compare to the expert diagnosis?

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

```
   diagnosis
      B   M
  1 337  78
  2  20 134
```

We did not perform k-means cluster in class. However, on my own, k-means clustering separated into true positives = 134, false negatives = 78, false positives = 20, true negatives = 337. Separate similarly, although h-clustering + PCA does a better job with sensitivity, specificity is slightly larger for k-means clustering.

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

We can calculate the sensitivity (how well h-clustering + PCA can detect positives/malignant).

Sensitivity (h-clustering + PCA): TP/(TP+FN)

```
179/(179+33)
```

```
[1] 0.8443396
```

We can calculate the specificity (how well h-clustering + PCA can detect negatives/benign).

Specificity (h-clustering + PCA): TN/(TN+FP)

```
333/(333 + 24)
```

```
[1] 0.9327731
```

Sensitivity (k-means clustering): TP/(TP+FN)

```
134/(134+78)
```

```
[1] 0.6320755
```

Specificity (k-means clustering): TN/(TN+FP)

```
337/(337 + 20)
```

```
[1] 0.9439776
```

H-clustering + PCA has a higher sensitivity (0.8443396 > 0.6320755), while specificity is slightly larger for k-means clustering (0.9439776 > 0.9327731).

Prediction

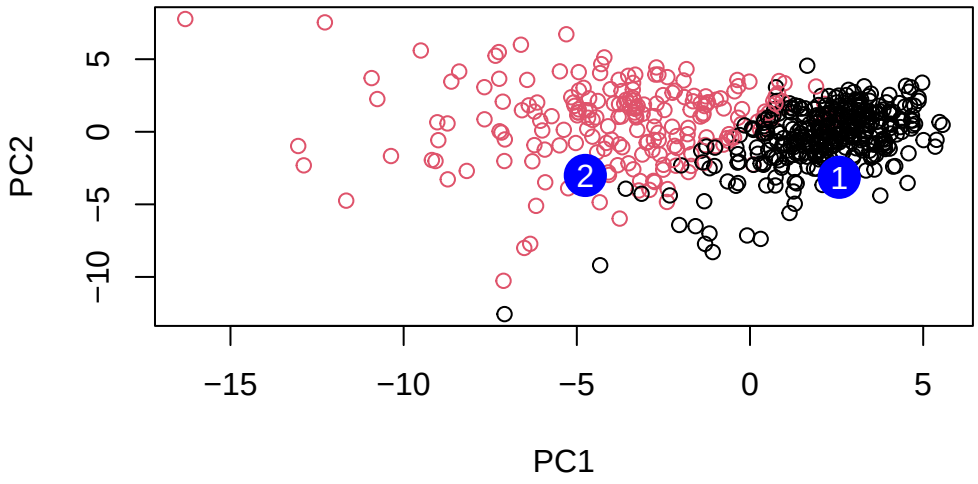
We can use our PCA model for prediction with new input patient samples.

```
#url <- "new_samples.csv"
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 <- factor(diagnosis)
```

```
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?

- Should follow up with patient 2.