Class 8: Mini Project

Courtney Anderson (PID:A69038035)

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".

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 Import

Read in data and name it; edit the roles:

```r
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
```

Remove the first column; we dont want to add patient IDs:

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

Create a diagnosis vector:

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

Exploring my data

```r
head(wisc.data)
```

```
         radius_mean texture_mean perimeter_mean area_mean smoothness_mean
842302         17.99        10.38         122.80    1001.0         0.11840
842517         20.57        17.77         132.90    1326.0         0.08474
84300903       19.69        21.25         130.00    1203.0         0.10960
```

```
84348301       11.42        20.38          77.58     386.1         0.14250
84358402       20.29        14.34         135.10    1297.0         0.10030
843786         12.45        15.70          82.57     477.1         0.12780
        compactness_mean concavity_mean concave.points_mean symmetry_mean
842302           0.27760         0.3001             0.14710        0.2419
842517           0.07864         0.0869             0.07017        0.1812
84300903         0.15990         0.1974             0.12790        0.2069
84348301         0.28390         0.2414             0.10520        0.2597
84358402         0.13280         0.1980             0.10430        0.1809
843786           0.17000         0.1578             0.08089        0.2087
        fractal_dimension_mean radius_se texture_se perimeter_se area_se
842302                 0.07871    1.0950     0.9053        8.589  153.40
842517                 0.05667    0.5435     0.7339        3.398   74.08
84300903               0.05999    0.7456     0.7869        4.585   94.03
84348301               0.09744    0.4956     1.1560        3.445   27.23
84358402               0.05883    0.7572     0.7813        5.438   94.44
843786                 0.07613    0.3345     0.8902        2.217   27.19
        smoothness_se compactness_se concavity_se concave.points_se
842302       0.006399        0.04904      0.05373           0.01587
842517       0.005225        0.01308      0.01860           0.01340
84300903     0.006150        0.04006      0.03832           0.02058
84348301     0.009110        0.07458      0.05661           0.01867
84358402     0.011490        0.02461      0.05688           0.01885
843786       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
```

```r
head(diagnosis)
```

```
[1] M M M M M M
Levels: B M
```

Q1. How many observations are in this dataset?

```r
nrow(wisc.data)
```

```
[1] 569
```

There are 569 observations in this data set.

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

```r
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

212 observations have been a malignant diagnosis.

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

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

```
[1] 10
```

10 variables are suffixed with _mean.

Principal Component Analysis

The main function in base R for PCA is called `prcomp()`. An optional argument `scal` should nearly always be switched to`scale=TRUE` for this function.

Performing PCA

Check column means and standard deviations:

```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 
```

Perform PCA and inspect summary:

```
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)? 44% of the original variance is captured by PC1.

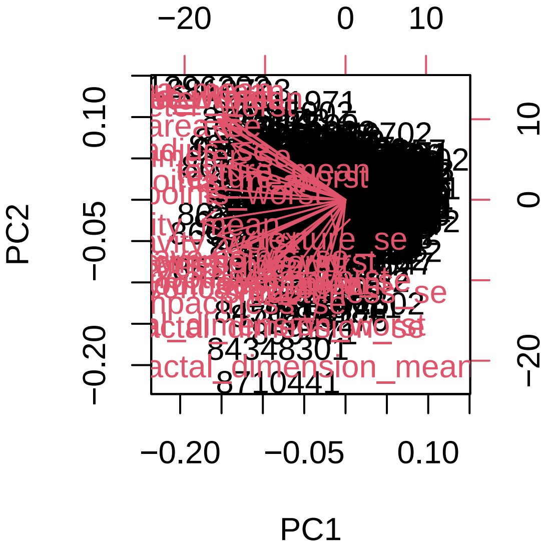
Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data? Three principle components would be required to describe at least 70% of the original variance of the data.

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

Interpreting PCA Results

Create a biplot:

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

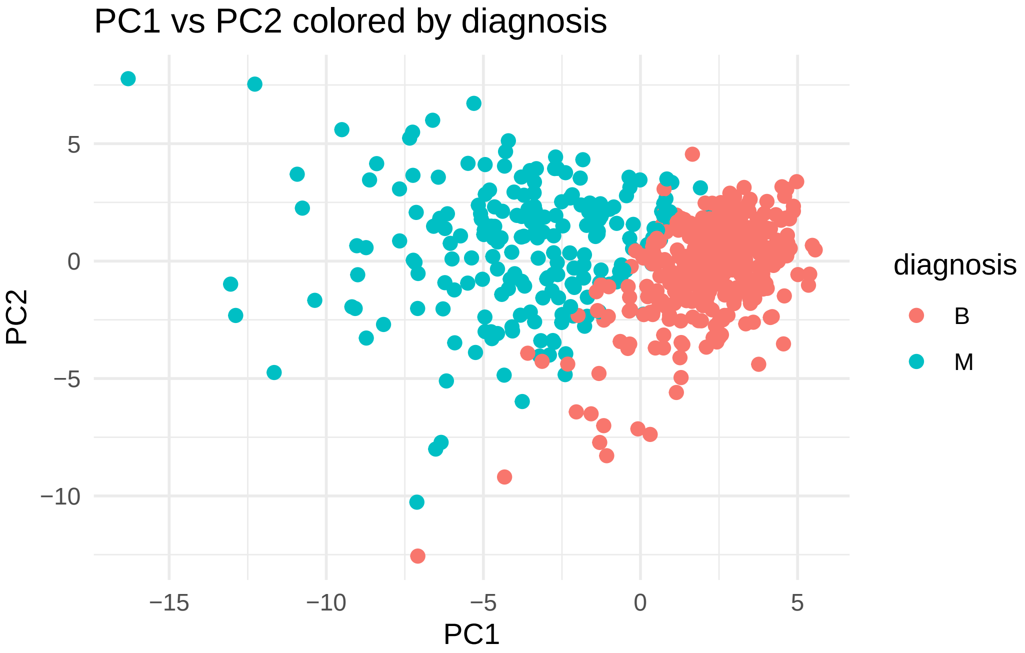


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why? This plot is very difficult to understand because everything is overlapping.

Create a scatterplot:

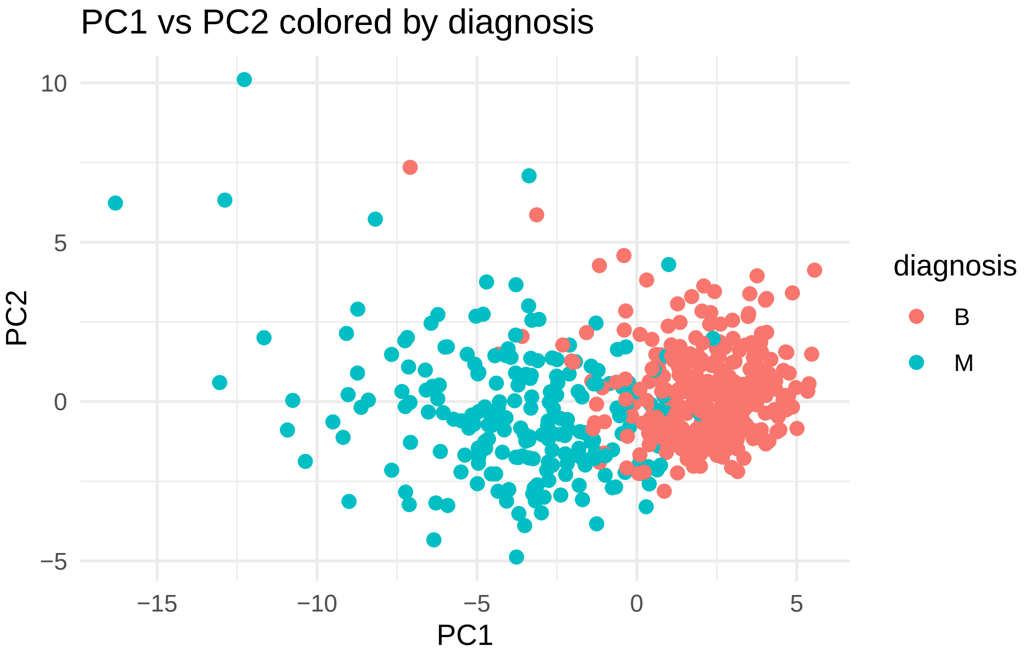
```r
library(ggplot2)

ggplot(wisc.pr$x, aes(x = PC1, y = PC2, color = diagnosis)) +
  geom_point(size = 2) +
  labs(x = "PC1", y = "PC2", title = "PC1 vs PC2 colored by diagnosis") +
  theme_minimal()
```



Create a similar plot for components 1 and 3:

```r
ggplot(wisc.pr$x, aes(x = PC1, y = PC3, color = diagnosis)) +
  geom_point(size = 2) +
  labs(x = "PC1", y = "PC2", title = "PC1 vs PC2 colored by diagnosis") +
  theme_minimal()
```

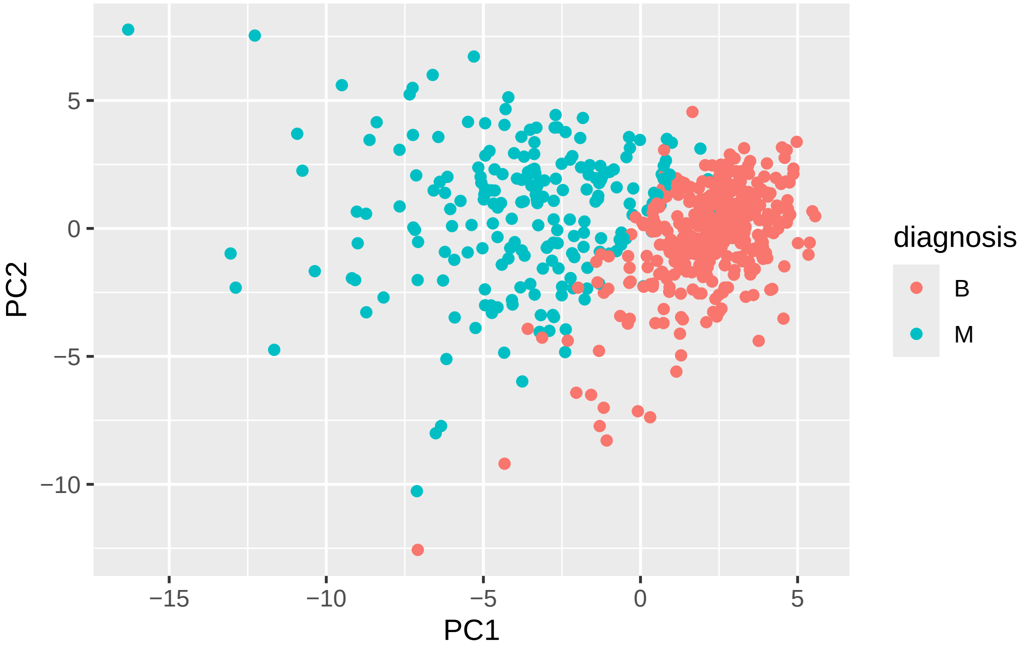


Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots? In the second plot, the points appear to be shifted downward.

Create plots using ggplot:

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

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



Variance Explained: Making Scree Plots

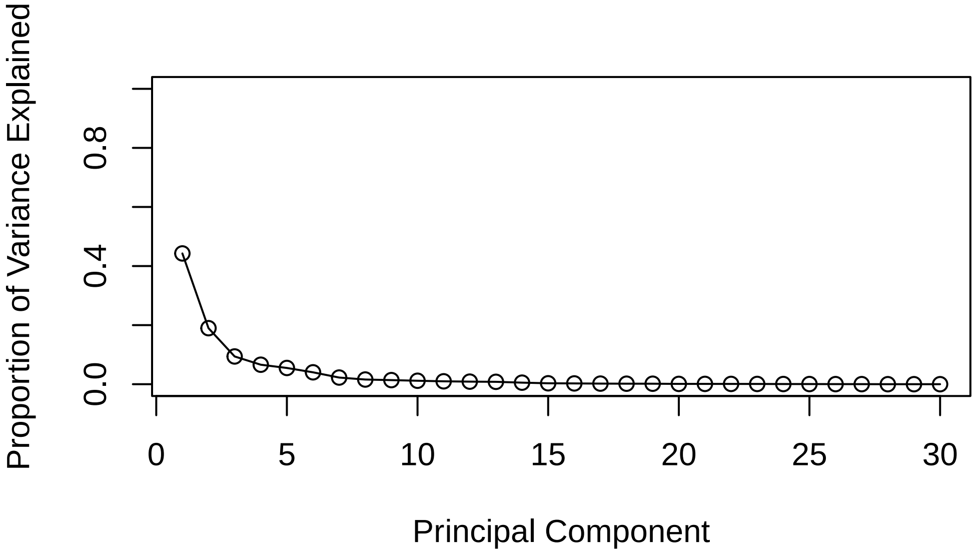
Calculate the variance of each component:

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

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

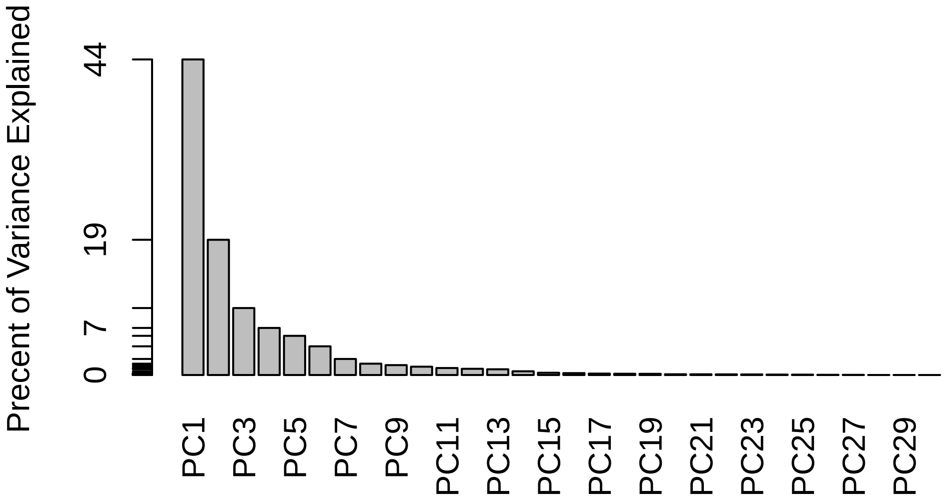
Explain and plot variance:

```
pve <- wisc.pr$sdev^2 / sum(wisc.pr$sdev^2)
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



Create an alternate scree plot:

```
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? This tells us how much this original feature contributes to the first PC.

```
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
```

> The feature for concave points mean is -0.26085376.

Hierarchical Clustering

Scale the original data:

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

Calculate the distances between all pairs of observations in the new scaled dataset:

```
data.dist <- dist(data.scaled, method= "euclidean")
```

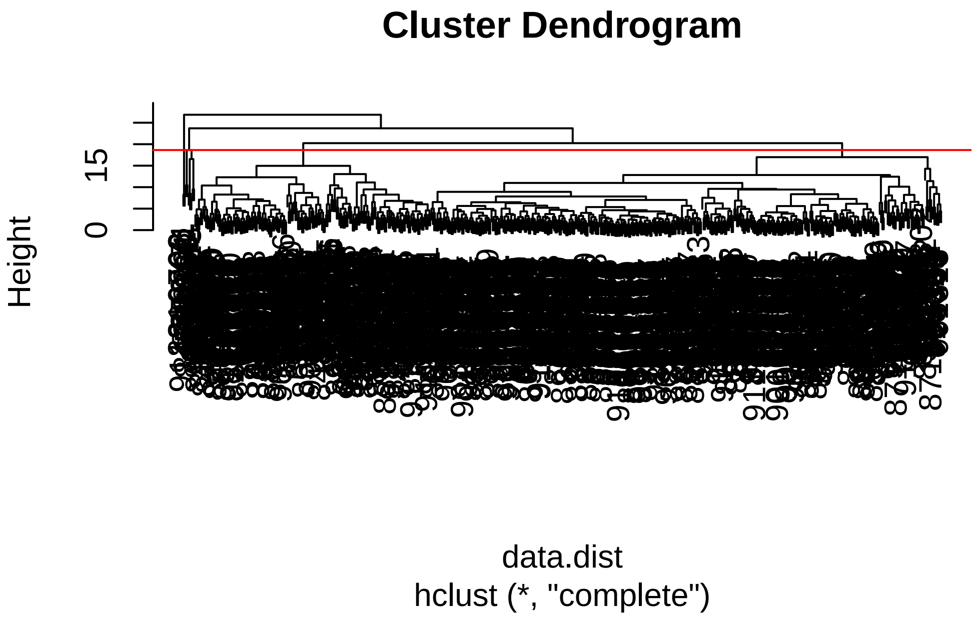
Create a hierarchical clustering using complete linkage:

```
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?

```
plot(wisc.hclust)
abline(h = wisc.hclust$height[length(wisc.hclust$height) - 3], col = "red")
```



Selecting number of clusters

Use cutree to cut the tree so that it has 4 clusters; show a table:

```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
```

> Q11. OPTIONAL: Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10? How do you judge the quality of your result in each case? Skipped.

Using Different Methods

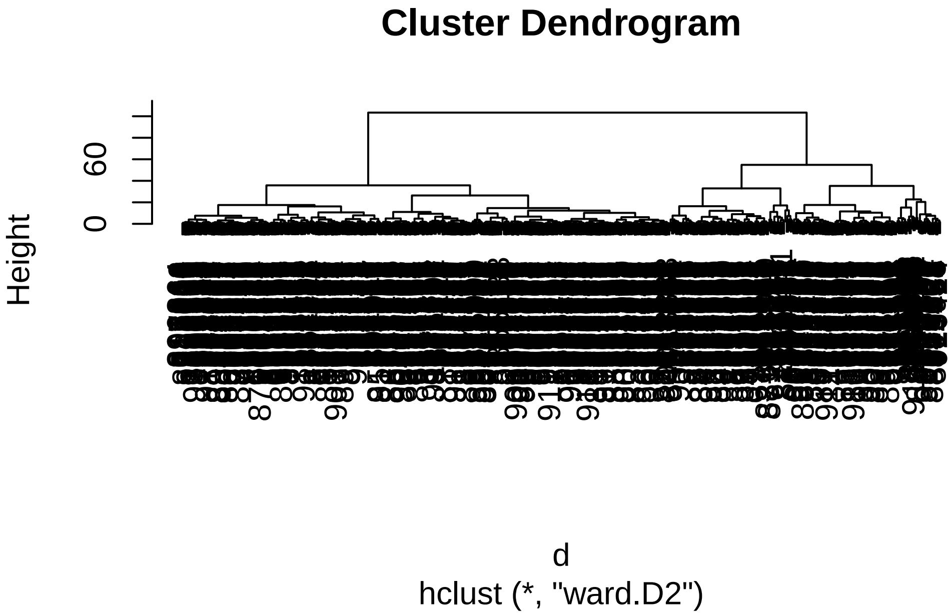
> Q12. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning. My favorite is the ward.d2 method. I like the ward.d2

message because its easier to interpret.

Combining methods

Create a Ward clustering

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



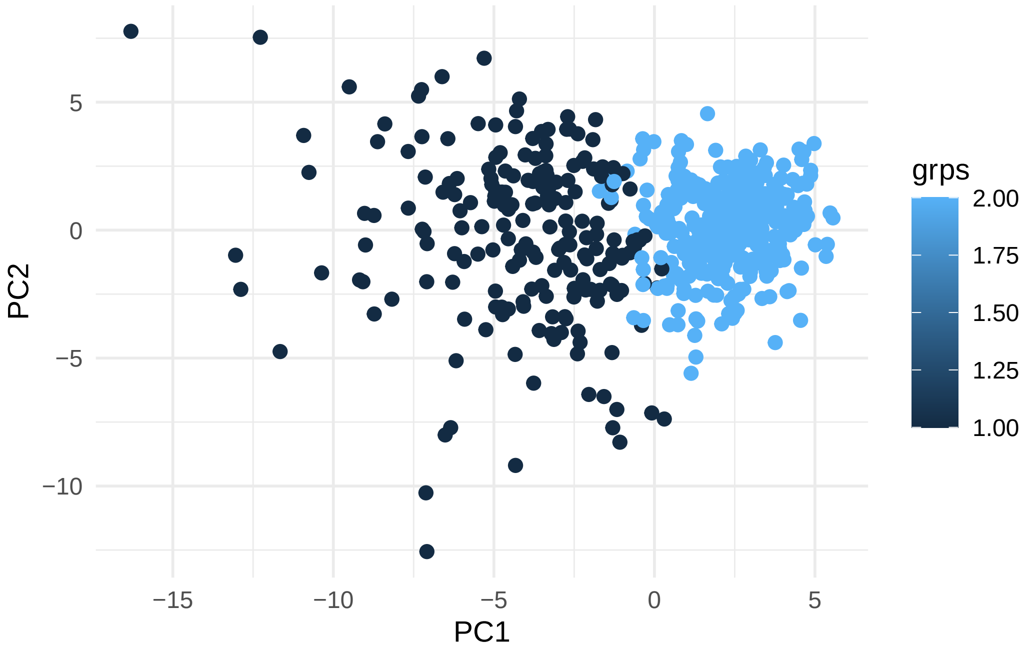
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
203 366
```

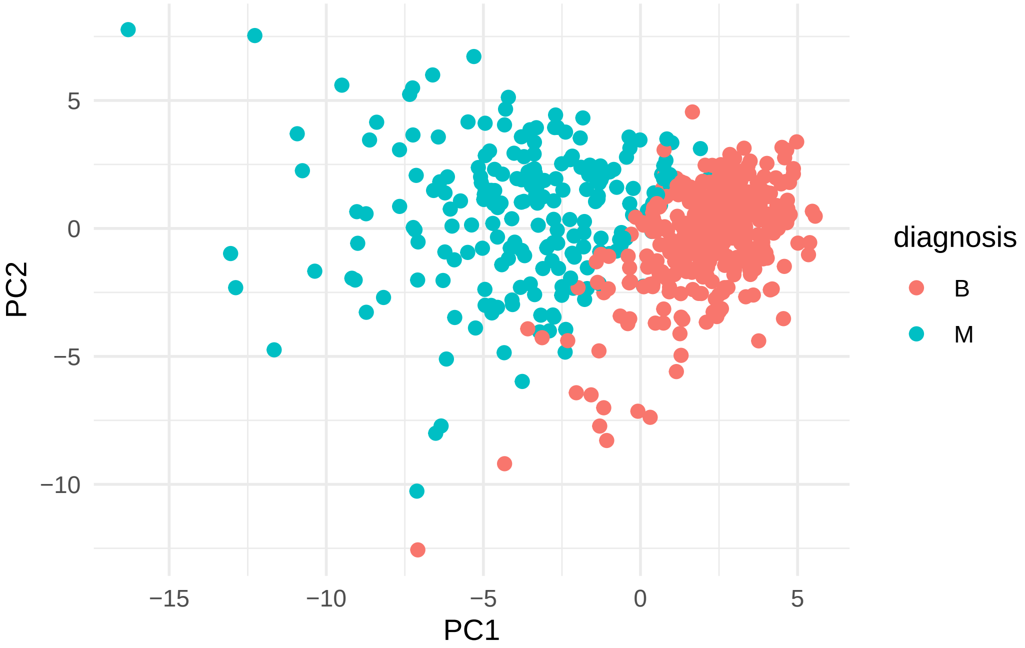
```
table(grps, diagnosis)
```

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

```
ggplot(wisc.pr$x, aes(x = PC1, y = PC2, color = grps)) +
  geom_point(size = 2) +
  labs(x = "PC1", y = "PC2") +
  theme_minimal()
```



```
ggplot(wisc.pr$x, aes(x = PC1, y = PC2, color = diagnosis)) +
  geom_point(size = 2) +
  labs(x = "PC1", y = "PC2") +
  theme_minimal()
```



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

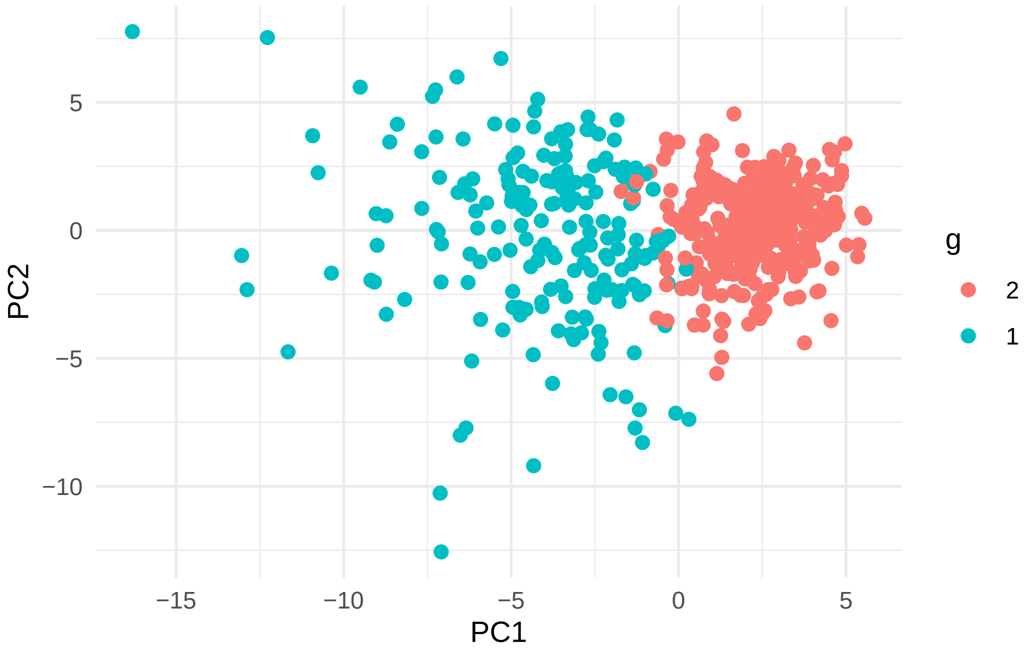
```
[1] "1" "2"
```

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

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

Plot your reordered factor:

```r
ggplot(wisc.pr$x, aes(x = PC1, y = PC2, color = g)) +
  geom_point(size = 2) +
  labs(x = "PC1", y = "PC2") +
  theme_minimal()
```



I skipped the rgl and plotly packages.

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

> Q13. How well does the newly created model with four clusters separate out the two diagnoses? It does a really good job at separating the two diagnoses. I can easily tell that group 1 associates with mostly malignant whereas group 2 mostly associates with benign tumors.

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

```
wisc.hclust.clusters   B   M
                   1  12 165
                   2   2   5
```

```
  3 343  40
  4   0   2
```

Q14. How well do the 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. In the previous sections, the hierarchical models we're hard to interpret.The method that uses PCA is easier to interpret to make accurate predictions.

Sensitivity/Specificity

Q15. OPTIONAL: Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity? Skipped.

Prediction

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

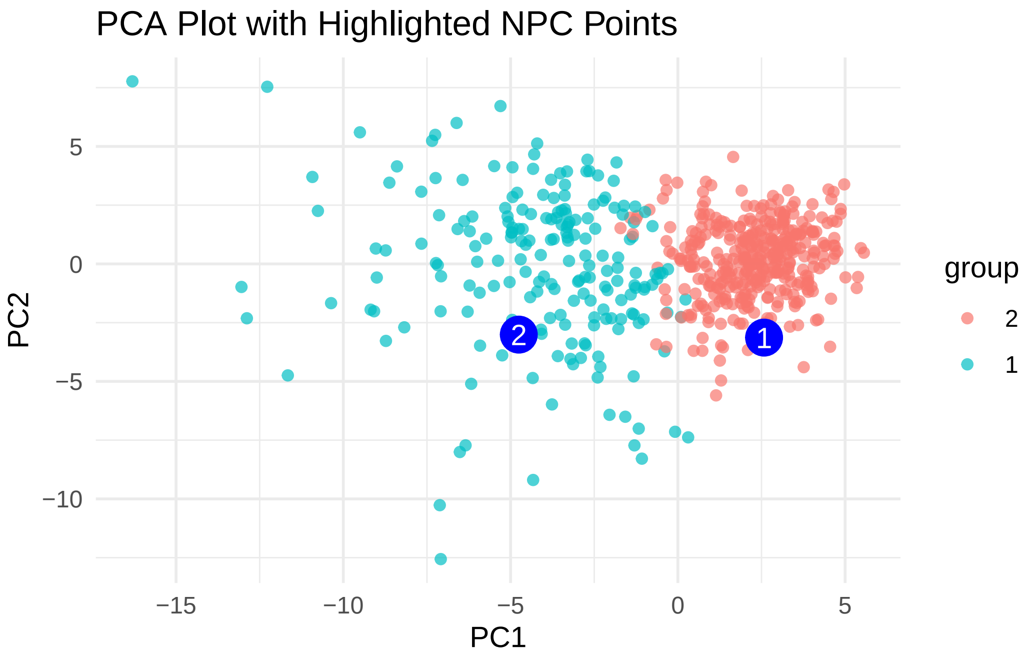
```
           PC1       PC2        PC3        PC4       PC5        PC6        PC7
[1,]  2.576616 -3.135913  1.3990492 -0.7631950  2.781648 -0.8150185 -0.3959098
[2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698 -1.2189945  0.8193031
            PC8       PC9       PC10      PC11      PC12      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
```

```r
library(ggplot2)

# Create a data frame for the PCA points
pca_df <- data.frame(PC1 = wisc.pr$x[, 1],
                     PC2 = wisc.pr$x[, 2],
                     group = as.factor(g))

# Create a data frame for npc points
npc_df <- data.frame(PC1 = npc[, 1],
                     PC2 = npc[, 2],
                     label = as.factor(c(1, 2)))

# Plot with ggplot2
ggplot(pca_df, aes(x = PC1, y = PC2, color = group)) +
  geom_point(alpha = 0.7) +
  geom_point(data = npc_df, aes(x = PC1, y = PC2),
             color = "blue", size = 6) +
  geom_text(data = npc_df, aes(label = label),
            color = "white", size = 4) +
  labs(x = "PC1", y = "PC2",
       title = "PCA Plot with Highlighted NPC Points") +
  theme_minimal()
```



Q16. Which of these new patients should we prioritize for follow up based on your results? Patient 2 needs to be prioritized for a check up since their tumor most likely will be malignant (since they fall into group 1). For group 1: TP=188 and FP=28