Class 8: PCA Mini Project

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```r
colMeans(mtcars)
```

```
       mpg        cyl       disp         hp       drat         wt       qsec 
 20.090625   6.187500 230.721875 146.687500   3.596563   3.217250  17.848750 
        vs         am       gear       carb 
  0.437500   0.406250   3.687500   2.812500 
```

```r
apply(mtcars, 2, sd)
```

```
        mpg         cyl        disp          hp        drat          wt 
  6.0269481   1.7859216 123.9386938  68.5628685   0.5346787   0.9784574 
       qsec          vs          am        gear        carb 
  1.7869432   0.5040161   0.4989909   0.7378041   1.6152000 
```

```r
x <- scale(mtcars)
head(x)
```

```
                         mpg        cyl        disp         hp       drat
Mazda RX4          0.1508848 -0.1049878 -0.57061982 -0.5350928  0.5675137
Mazda RX4 Wag      0.1508848 -0.1049878 -0.57061982 -0.5350928  0.5675137
Datsun 710         0.4495434 -1.2248578 -0.99018209 -0.7830405  0.4739996
Hornet 4 Drive     0.2172534 -0.1049878  0.22009369 -0.5350928 -0.9661175
Hornet Sportabout -0.2307345  1.0148821  1.04308123  0.4129422 -0.8351978
Valiant           -0.3302874 -0.1049878 -0.04616698 -0.6080186 -1.5646078
                            wt       qsec         vs         am       gear
Mazda RX4         -0.610399567 -0.7771651 -0.8680278  1.1899014  0.4235542
Mazda RX4 Wag     -0.349785269 -0.4637808 -0.8680278  1.1899014  0.4235542
Datsun 710        -0.917004624  0.4260068  1.1160357  1.1899014  0.4235542
Hornet 4 Drive    -0.002299538  0.8904872  1.1160357 -0.8141431 -0.9318192
Hornet Sportabout  0.227654255 -0.4637808 -0.8680278 -0.8141431 -0.9318192
```

```
Valiant            0.248094592  1.3269868  1.1160357 -0.8141431 -0.9318192
                         carb
Mazda RX4          0.7352031
Mazda RX4 Wag      0.7352031
Datsun 710        -1.1221521
Hornet 4 Drive    -1.1221521
Hornet Sportabout -0.5030337
Valiant           -1.1221521
```

```r
round(colMeans(x),2)
```

```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb
   0    0    0    0    0    0    0    0    0    0    0
```

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

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

Remove “diagnosis” column - it is expert data to compare analysis results to.

```r
diagnosis <- wisc.df[, 1]
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

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

```
[1] 569
```

```r
dim(wisc.data)
```

```
[1] 569  30
```

```r
cols_means <- grep("_mean", colnames(wisc.data), value = T)
length(cols_means)
```

```
[1] 10
```

Q1. How many observations are in this dataset? 569 Q2. How many of the observations have a malignant diagnosis? 212 Q3. How many variables/features in the data are suffixed with _mean? 10

```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
"________"
```

```
[1] "________"
```

```r
apply(wisc.data, 2, sd)
```

```
            radius_mean            texture_mean          perimeter_mean 
           3.524049e+00            4.301036e+00            2.429898e+01 
              area_mean         smoothness_mean        compactness_mean 
           3.519141e+02            1.406413e-02            5.281276e-02 
         concavity_mean     concave.points_mean           symmetry_mean 
           7.971981e-02            3.880284e-02            2.741428e-02 
```

```
fractal_dimension_mean              radius_se             texture_se
          7.060363e-03           2.773127e-01           5.516484e-01
          perimeter_se                area_se          smoothness_se
          2.021855e+00           4.549101e+01           3.002518e-03
        compactness_se           concavity_se      concave.points_se
          1.790818e-02           3.018606e-02           6.170285e-03
           symmetry_se   fractal_dimension_se           radius_worst
          8.266372e-03           2.646071e-03           4.833242e+00
         texture_worst        perimeter_worst             area_worst
          6.146258e+00           3.360254e+01           5.693570e+02
      smoothness_worst      compactness_worst        concavity_worst
          2.283243e-02           1.573365e-01           2.086243e-01
  concave.points_worst         symmetry_worst fractal_dimension_worst
          6.573234e-02           6.186747e-02           1.806127e-02
```

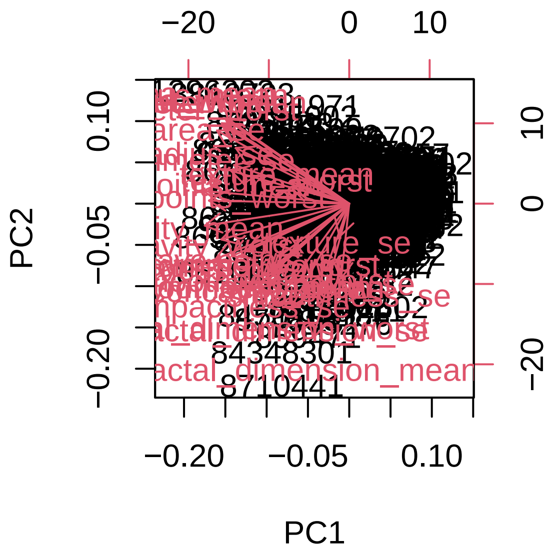
```r
wisc.pr <- prcomp(wisc.data, scale = TRUE)
summary(wisc.pr)
```

```
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. From your results, what proportion of the original variance is captured by the first principal components (PC1)? 44.27% Q5. How many principal components

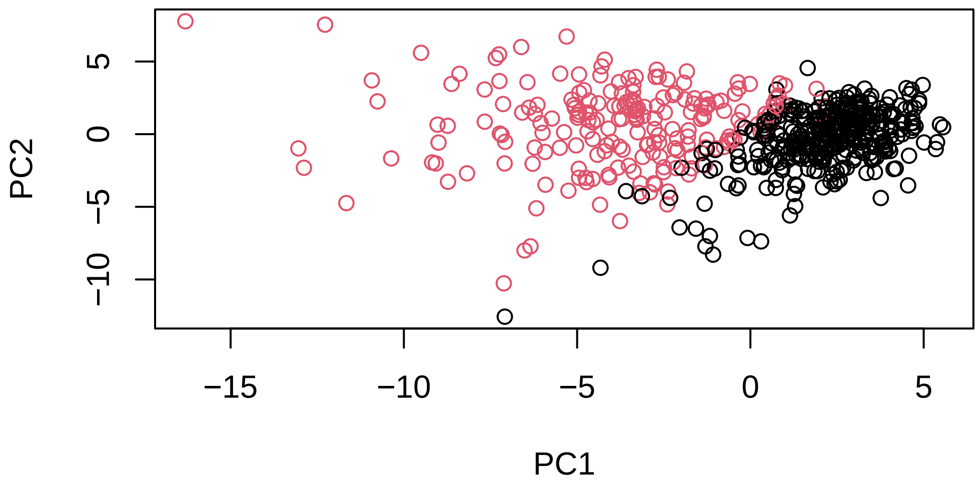
(PCs) are required to describe at least 70% of the original variance in the data? 3
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data? 7

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

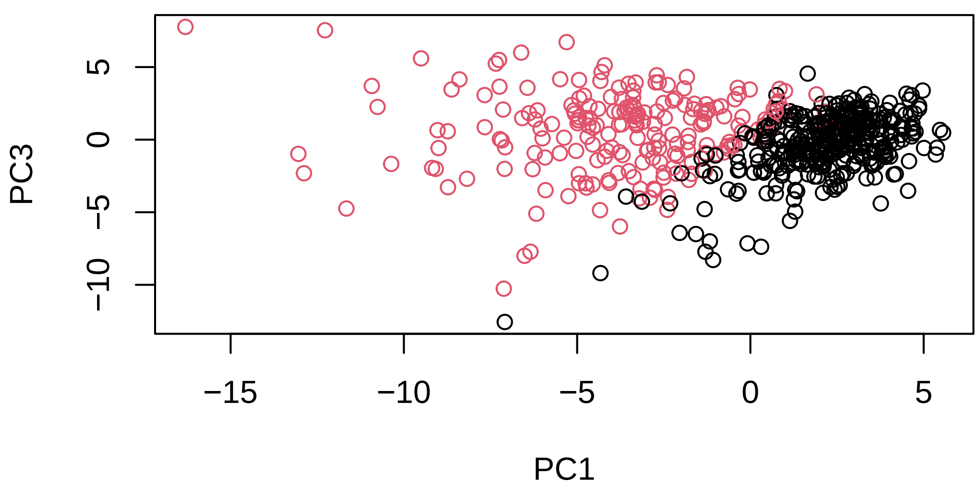


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why? This plot is very difficult to understand, as all of the data and words on it makes it so that nothing can really be discerned from it.

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




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

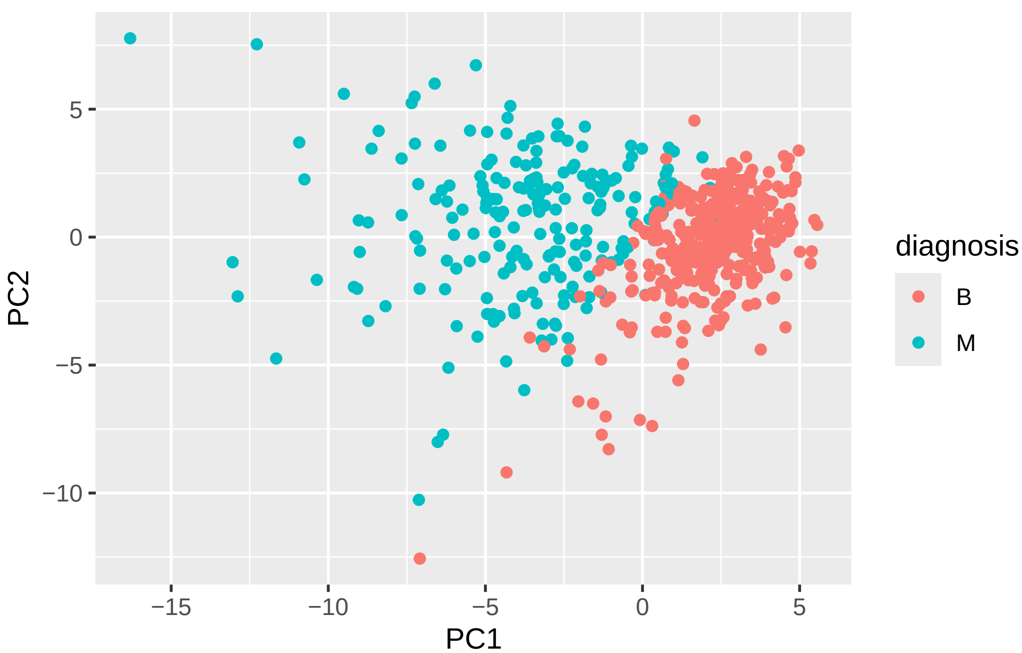


Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots? The plots are very similar but the distinction between the two categories is more blurry than the graph between principal components 1 and 2.

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

# Load the ggplot2 package
library(ggplot2)

# Make a scatter plot colored by diagnosis
ggplot(df) +
  aes(PC1, PC2, col= diagnosis) +
  geom_point()
```



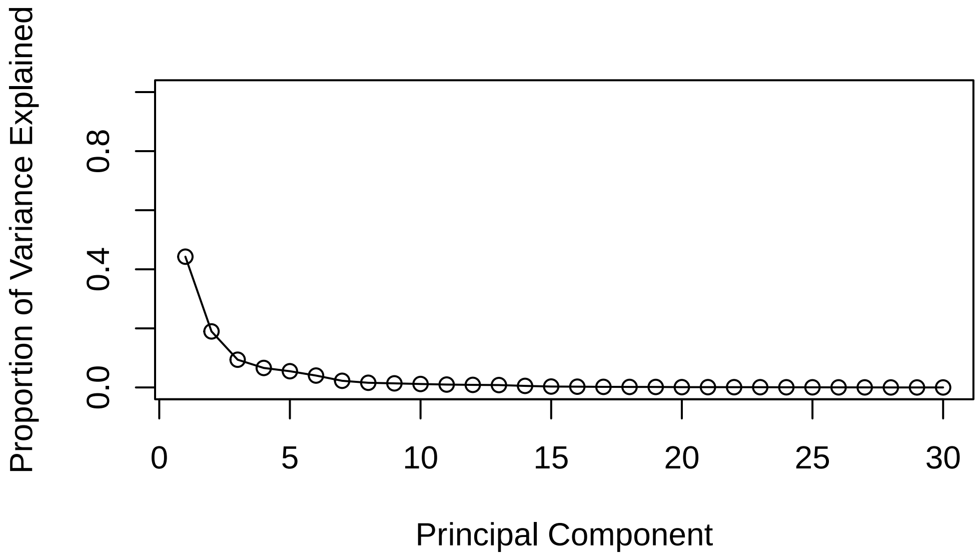

```
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

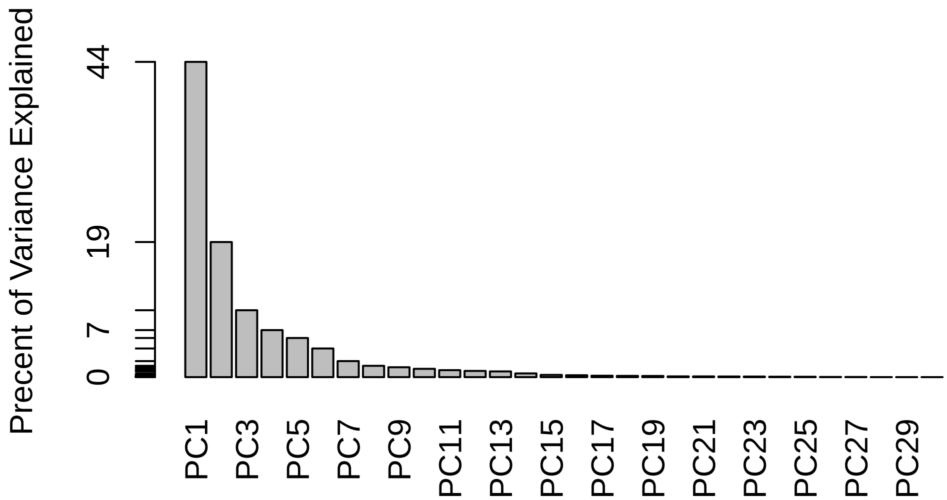
```r
var_tot <- sum(pr.var)
```

```r
# Variance explained by each principal component: pve
pve <- pr.var / var_tot

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



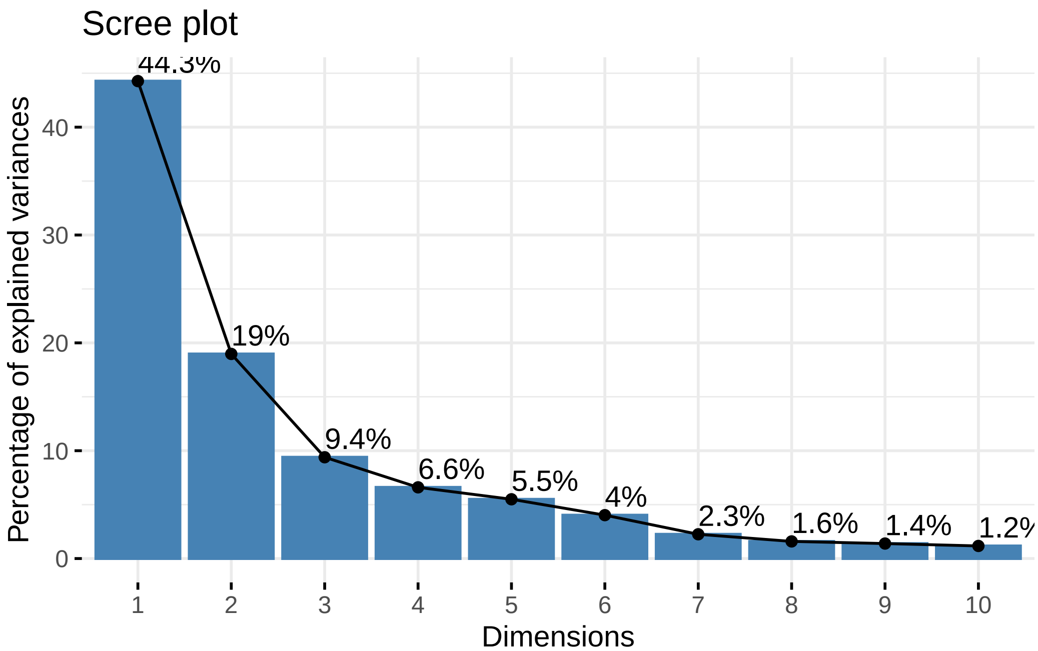

```r
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```




```r
## ggplot based graph
library(factoextra)
```

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

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




```r
y <- wisc.pr$rotation[,1]
y / sum(y)
```

```
            radius_mean            texture_mean          perimeter_mean
            0.043383214             0.020556671             0.045094513
              area_mean         smoothness_mean        compactness_mean
            0.043797925             0.028259160             0.047422804
         concavity_mean     concave.points_mean           symmetry_mean
            0.051211138             0.051697342             0.027382640
 fractal_dimension_mean               radius_se              texture_se
            0.012755860             0.040821935             0.003453976
           perimeter_se                 area_se           smoothness_se
            0.041881659             0.040205749             0.002879918
         compactness_se            concavity_se       concave.points_se
            0.033769452             0.030439216             0.036350605
            symmetry_se    fractal_dimension_se            radius_worst
            0.008422556             0.020327518             0.045185547
          texture_worst         perimeter_worst              area_worst
            0.020704269             0.046898471             0.044566001
       smoothness_worst       compactness_worst         concavity_worst
            0.025358298             0.041637884             0.045338328
   concave.points_worst          symmetry_worst fractal_dimension_worst
            0.049721874             0.024357858             0.026117621
```

```r
sum(y)
```

```
[1] -5.045787
```

```r
y
```

```
            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
```

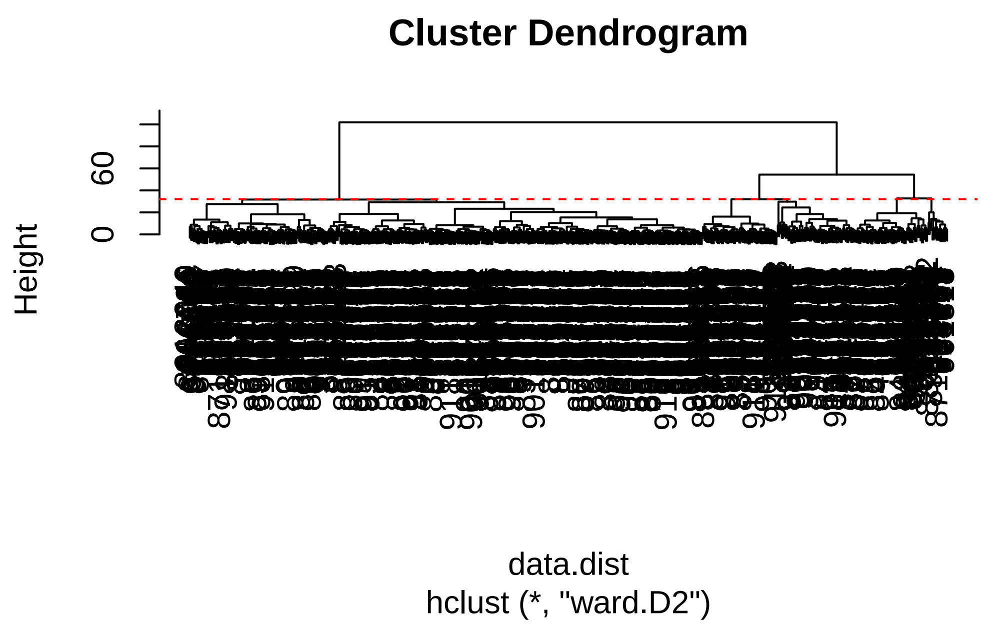
```r
summary(y)
```

```
    Min.  1st Qu.   Median     Mean  3rd Qu.     Max. 
-0.26085 -0.22687 -0.19314 -0.16819 -0.12417 -0.01453 
```

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? -0.26 out of the -5.04 variance is contributed by concave.points_mean, which is about 5.2%

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

```r
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(data.dist, method = "ward.D2")
plot(wisc.hclust)
abline(h = 32, col="red", lty=2)
```



Q11. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters? 32

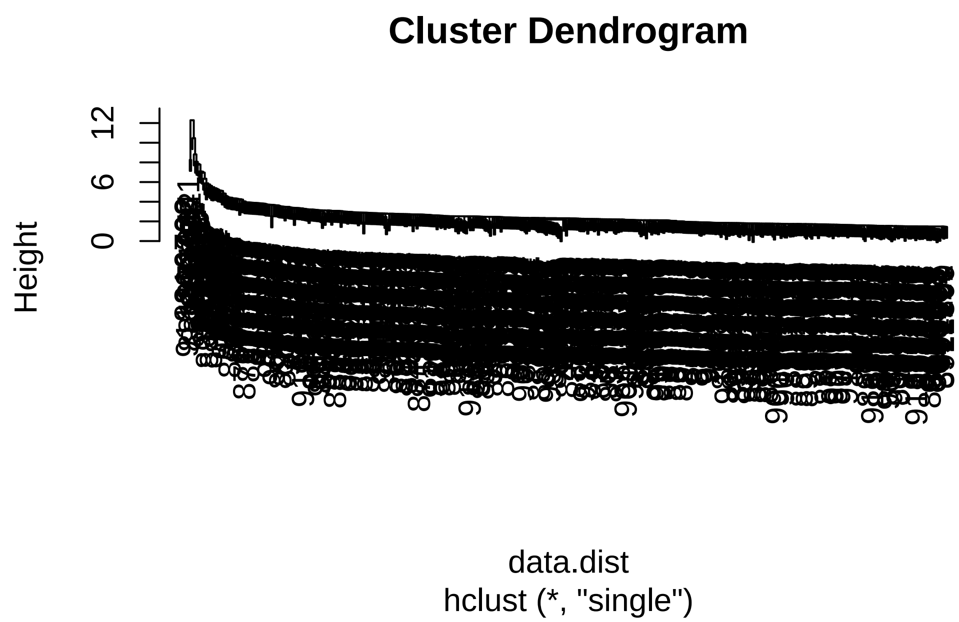
```r
wisc.hclust.clusters <- cutree(wisc.hclust, k = 4)
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1   0 115
                   2   6  48
                   3 337  48
                   4  14   1
```

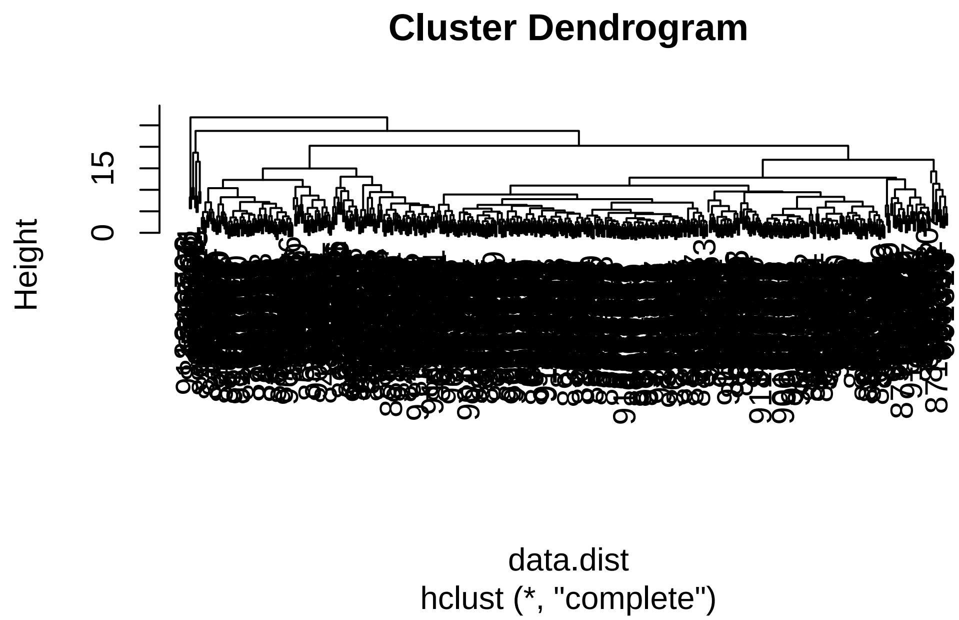
Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10? No, 4 groups yielded the best cluster vs diagnoses match.

Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning. My favorite results are given using the `complete` method, as it allows for the groups to be the most distinct, allowing for me to easily identify each group.

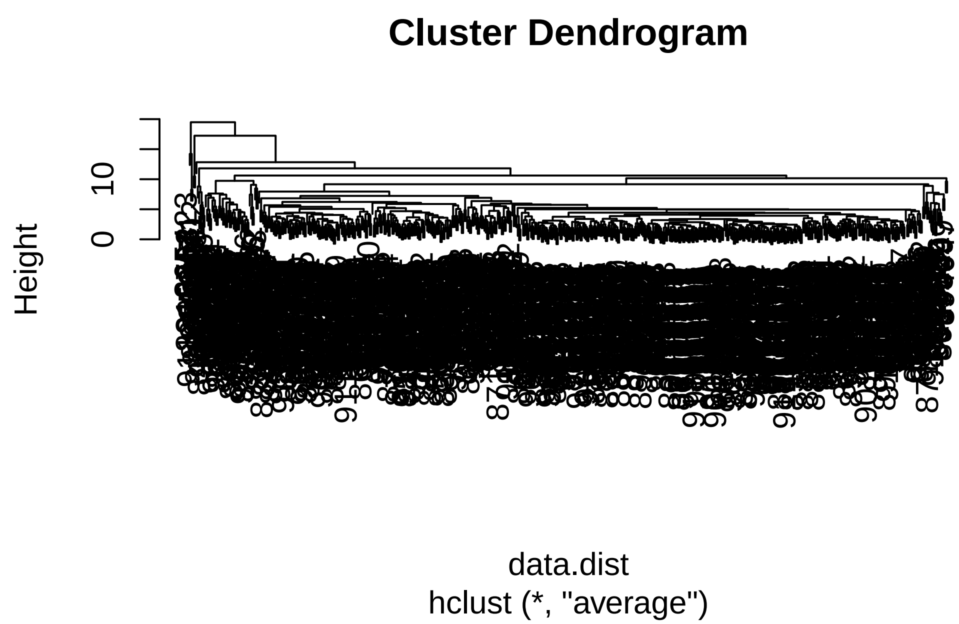
```
wisc.hclust <- hclust(data.dist, method = "single")
plot(wisc.hclust)
```



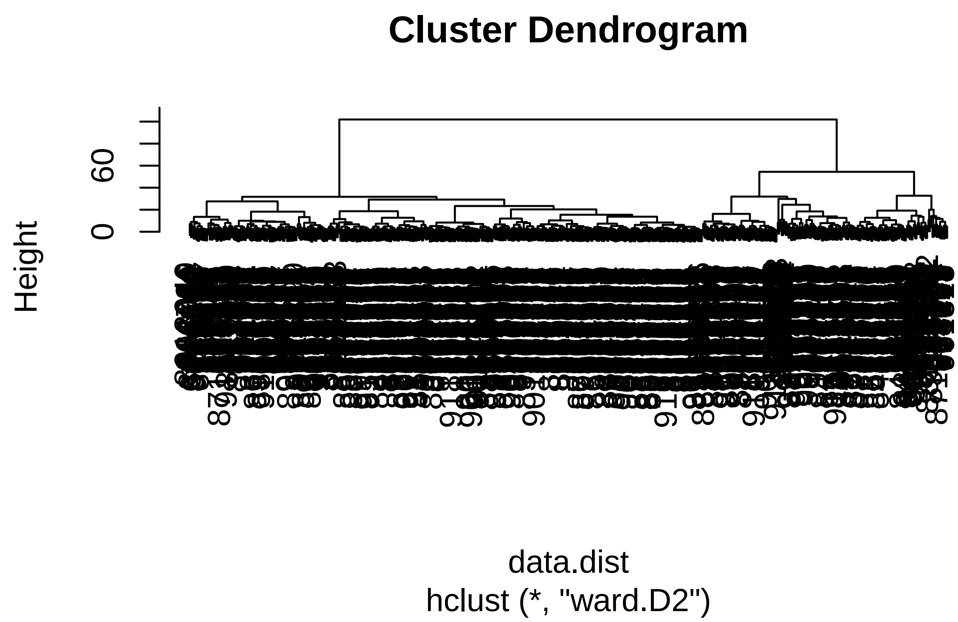

```
wisc.hclust <- hclust(data.dist, method = "complete")
plot(wisc.hclust)
```




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



```r
wisc.hclust <- hclust(data.dist, method = "ward.D2")
plot(wisc.hclust)
```



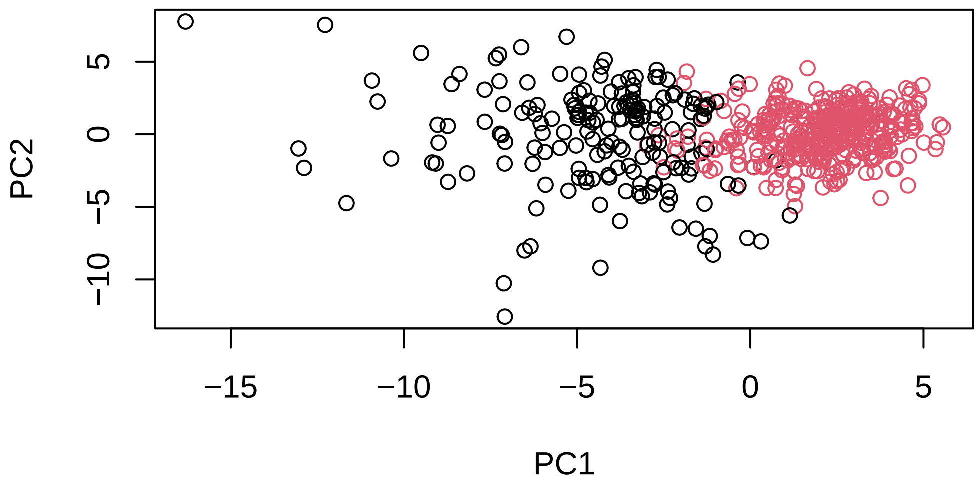

```r
wisc.pr.hclust <- hclust(data.dist, method = "ward.D2")
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
184 385
```

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

```
    diagnosis
grps   B   M
   1  20 164
   2 337  48
```

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



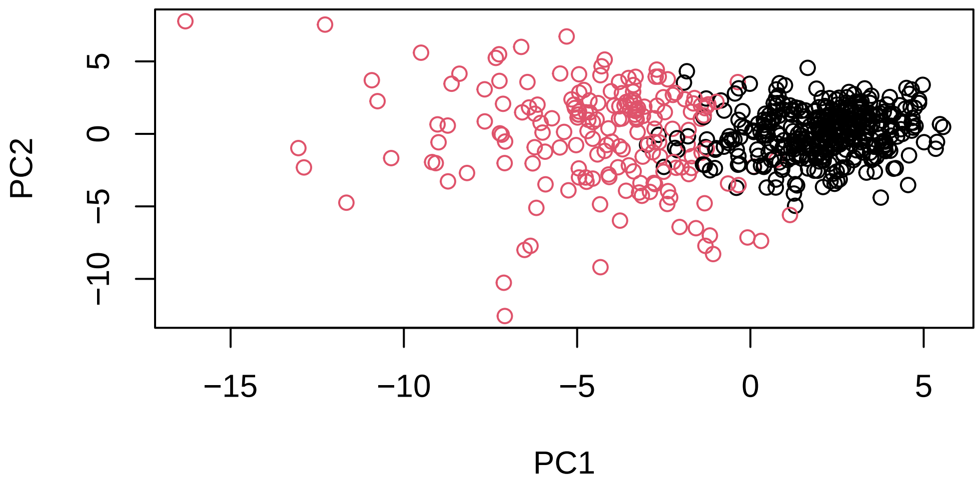

```
g <- as.factor(grps)
levels(g)
```

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

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

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

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




```
wisc.pr.hclust <- hclust(data.dist, 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  20 164
                      2 337  48
```

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

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

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

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

```
                     diagnosis
wisc.hclust.clusters   B   M
                   1   0 115
                   2   6  48
                   3 337  48
                   4  14   1
```

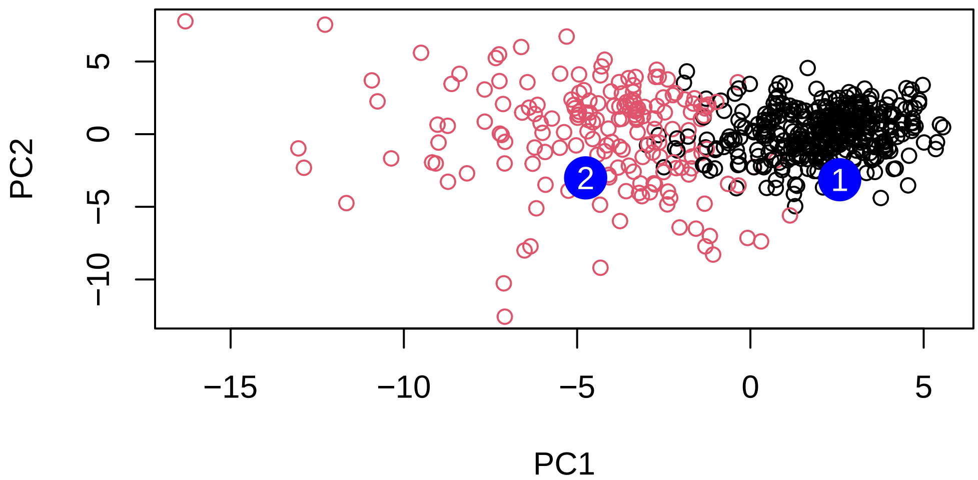
Q15. How well does the newly created model with four clusters separate out the two diagnoses? This model is good at not giving false positives, but there are still a decent amount of false negatives, which is something we would like to avoid.

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 I would say that the hierarchical clustering method did a little better than the k-means, as there were a similar amount of false positives detected in both, but the hclust method had far fewer false negatives, though still a lot.

```
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
```

```
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? We should prioritize patient 1, as they are in the region of the plot with the malignant results, so it is more likely that their tumor is malignant than patient 2.