class08

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```
# 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)

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

# Create diagnosis vector for later
diagnosis <- factor(wisc.df$diagnosis)
```

Q1. How many observations are in this dataset?

```
nrow(diagnosis)
```

```
NULL
```

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

```
sum(diagnosis=="M")
```

```
[1] 212
```

Q3. How many variables/features in the data are suffixed with _mean? 10

```
# 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
```

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

```r
# Look at summary of results
summary(wisc.pr)
```

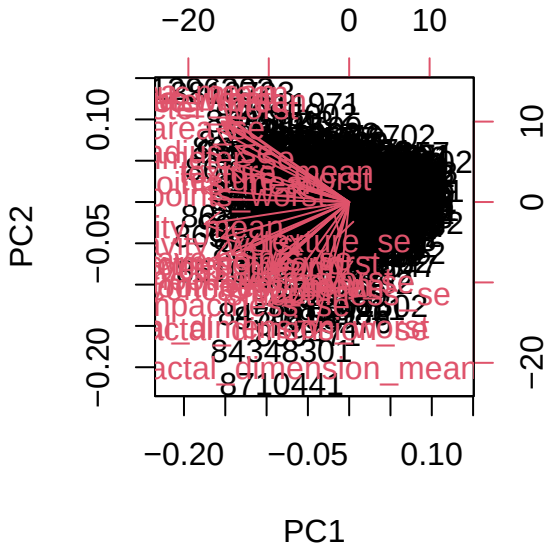
```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 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)? 0.4427

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

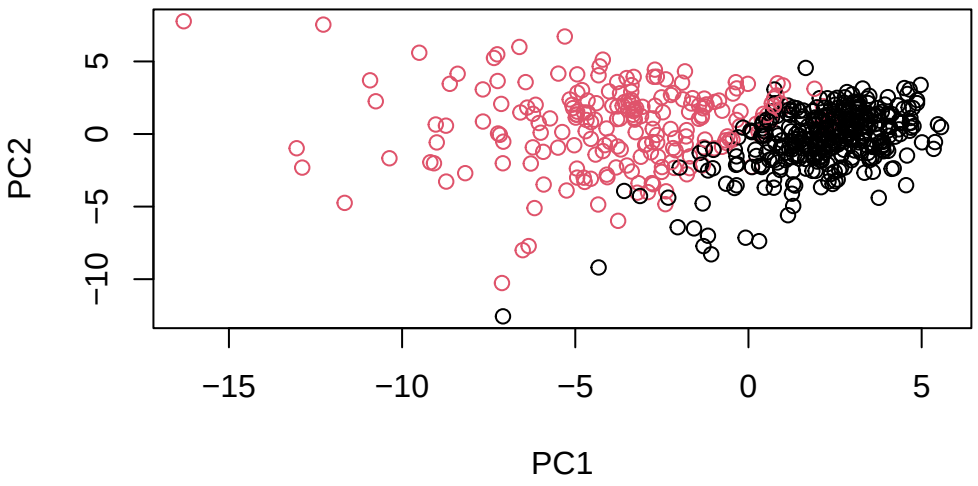
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data? 7

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



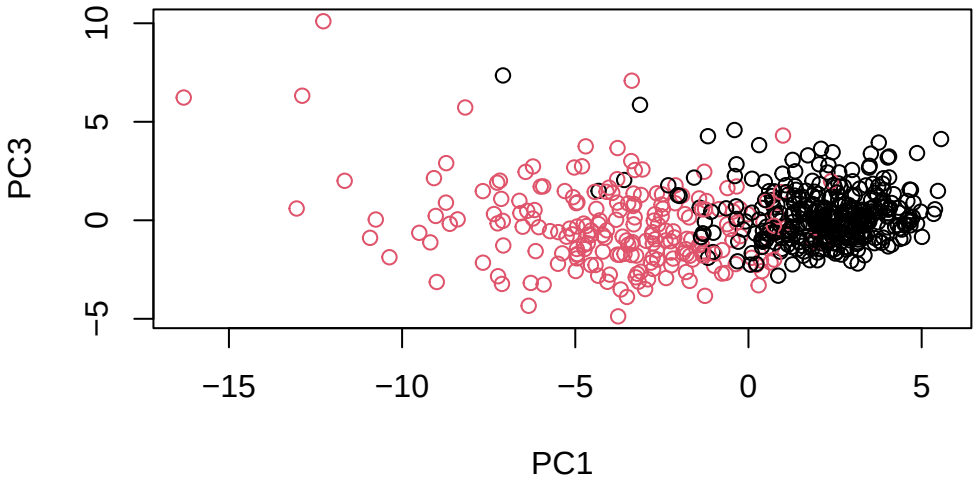
Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why? The data points are numbers instead of points and there are too many red descriptions. It would be better to have a colorcoded set of points and a legend to make the chart more readable.

```
# Scatter plot observations by components 1 and 2
plot( wisc.pr$x[,1:2] , col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots? The two PC's occupy different areas of the chart. They can be reasonable separated into two groupings.

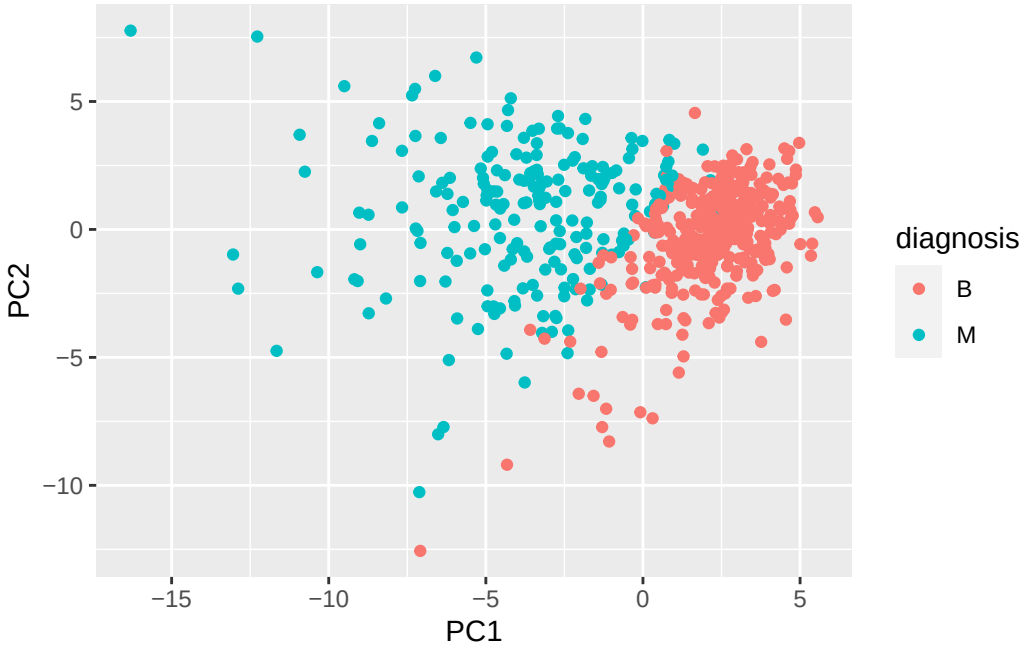
```
# Repeat for components 1 and 3
plot(wisc.pr$x[,1-3], col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```




```
# Create a data.frame for ggplot
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()
```

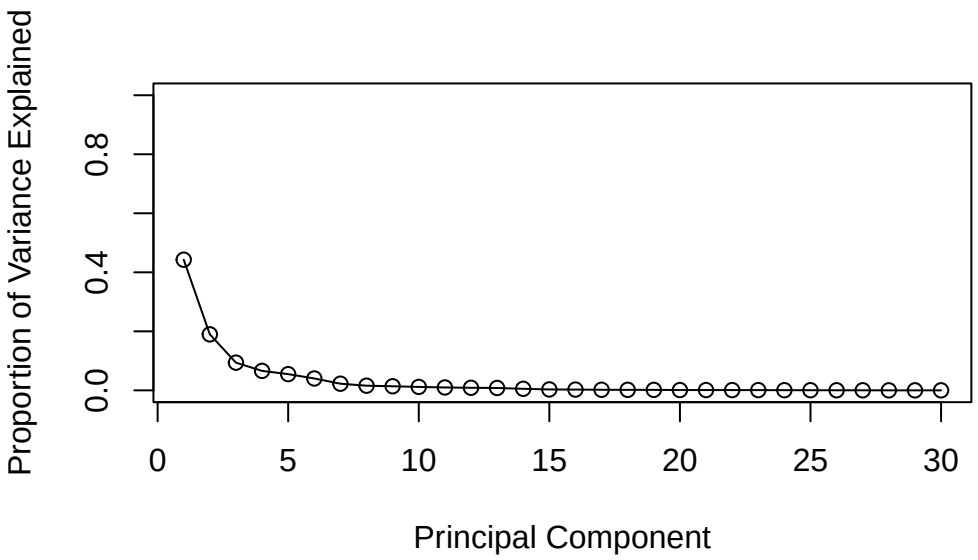



```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

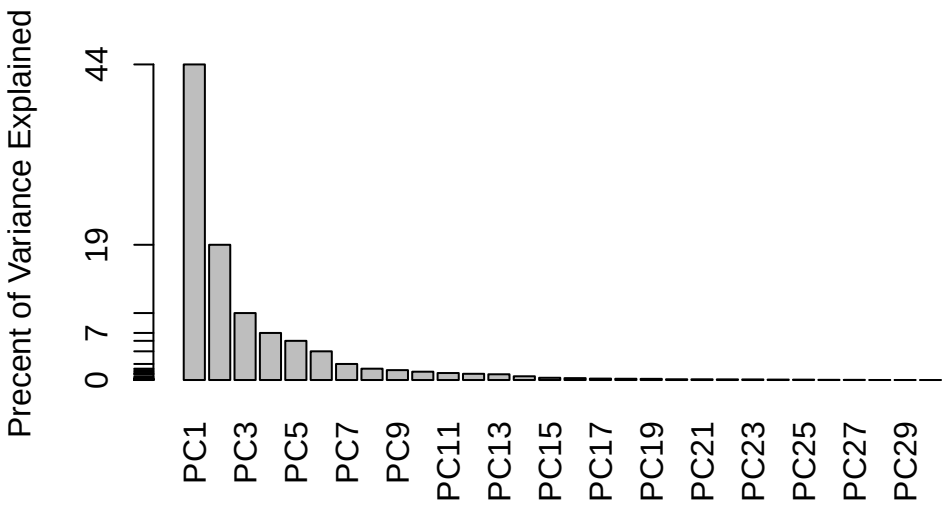
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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")
```



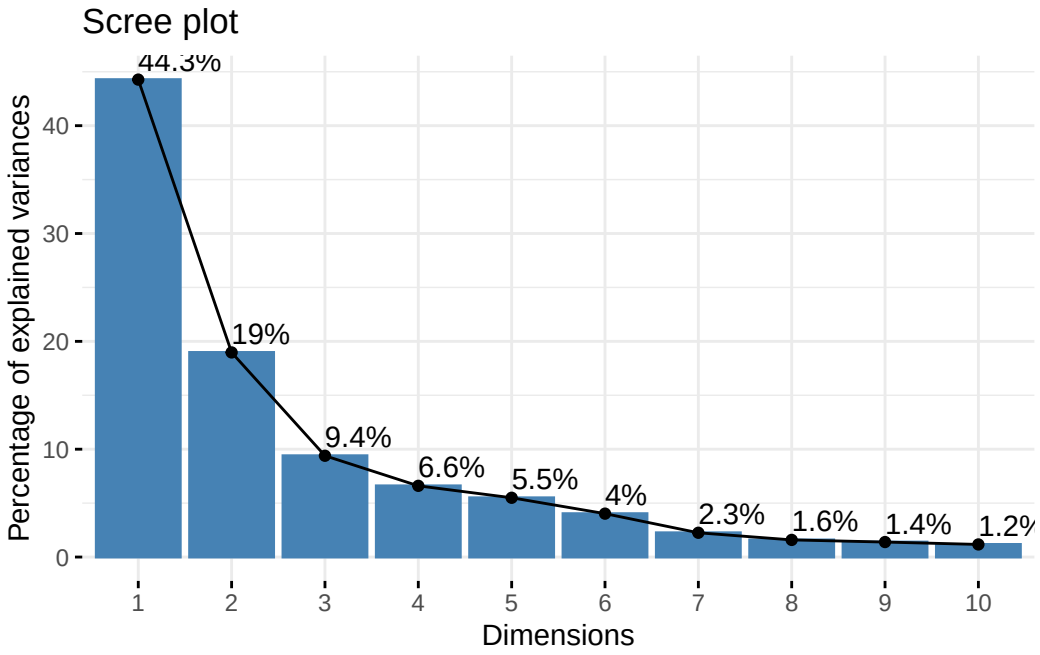

```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```




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

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

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




```
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
```

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? It is the weight that concave.points_mean has on the PC1 vector. It is -0.26085376

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

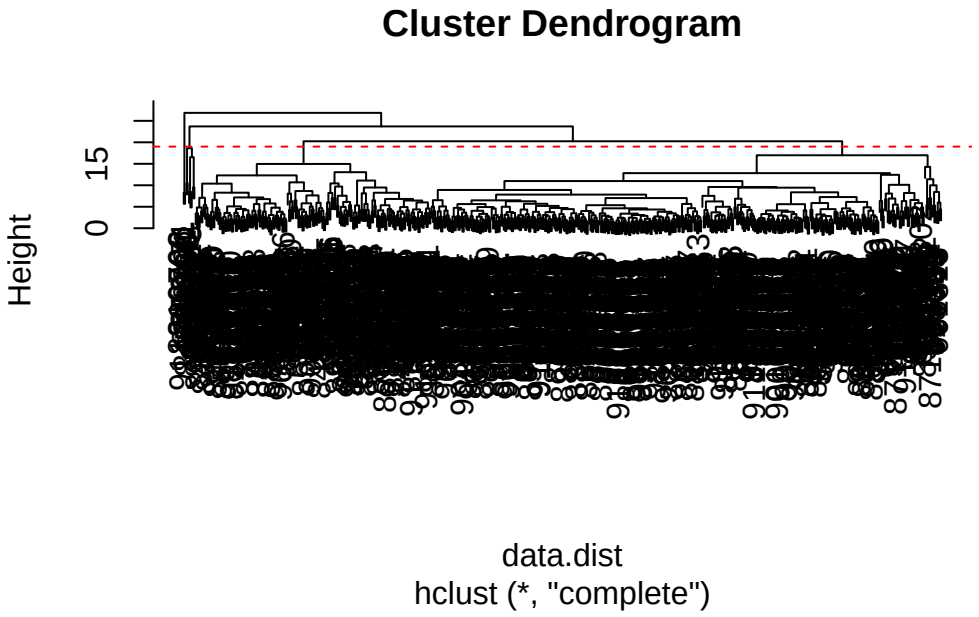
```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)

data.dist <- dist(data.scaled)

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

Q11. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters? At a height of 19

```
plot(wisc.hclust)
abline(a = 19, b = 0, col="red", lty=2)
```



```
wisc.hclust.clusters <- cutree(wisc.hclust, 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?

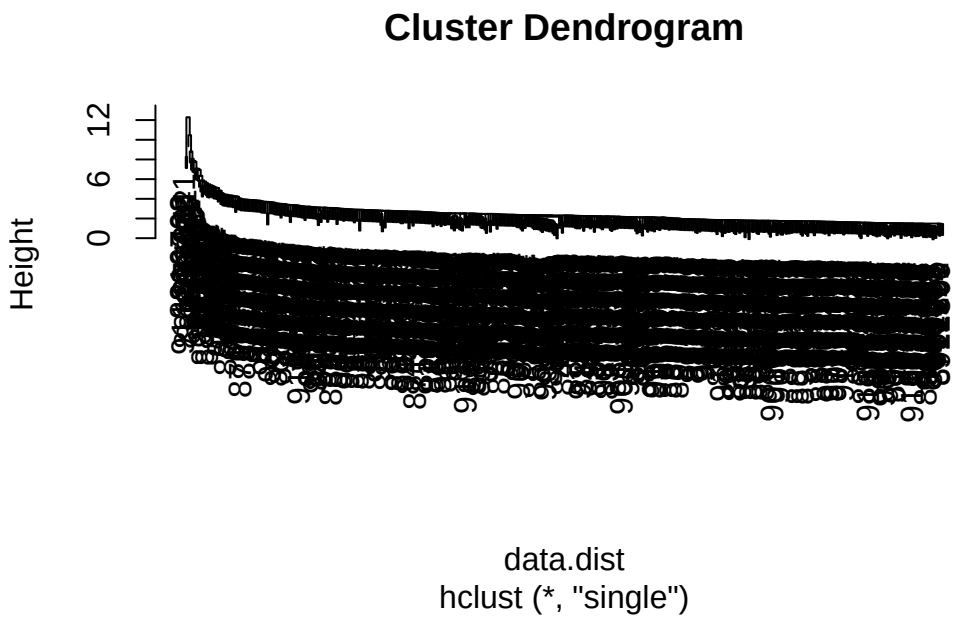
```
table(cutree(wisc.hclust, 2), diagnosis)
```

```
   diagnosis
      B   M
  1 357 210
  2   0   2
```

There are no better matchups. All other groupings between 2-10 do not increase the difference between the B and M groupings.

Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning. My favorite is complete linkage because it can be described as a "friends of friends" cluster strategy.

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




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

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

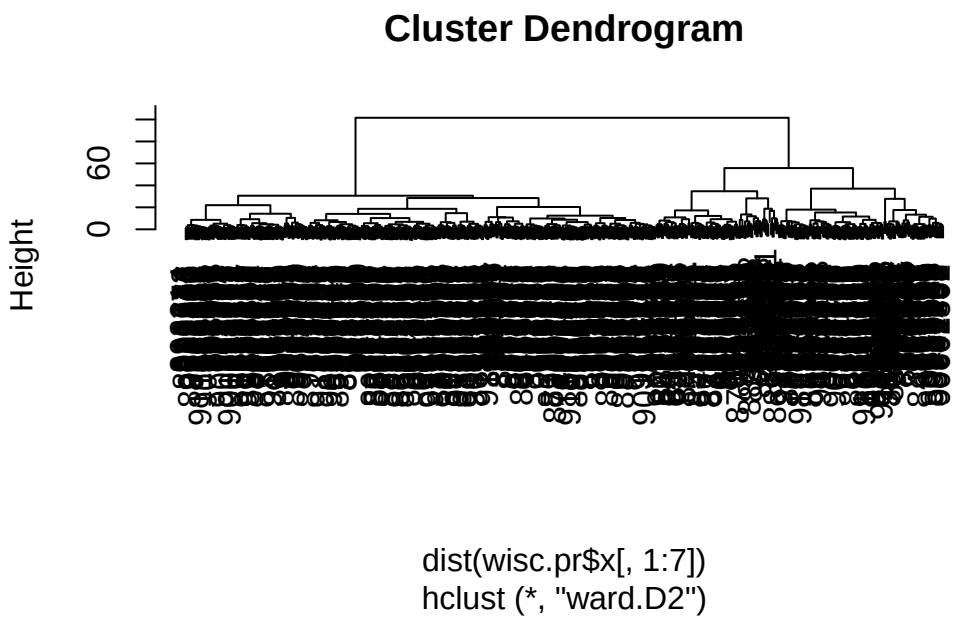
```
   diagnosis
      B   M
  1   14 175
  2 343  37
```

Q14. How well does k-means separate the two diagnoses? How does it compare to your hclust results? There are less "incorrect" groupings and there are only two categories instead of 4 which more accurately represents the diagnosis options.

```
table(wisc.hclust.clusters, wisc.km$cluster)
```

```
wisc.hclust.clusters   1   2
                   1 160  17
                   2   7   0
                   3  20 363
                   4   2   0
```

```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]), "ward.D2")
plot(wisc.pr.hclust)
```



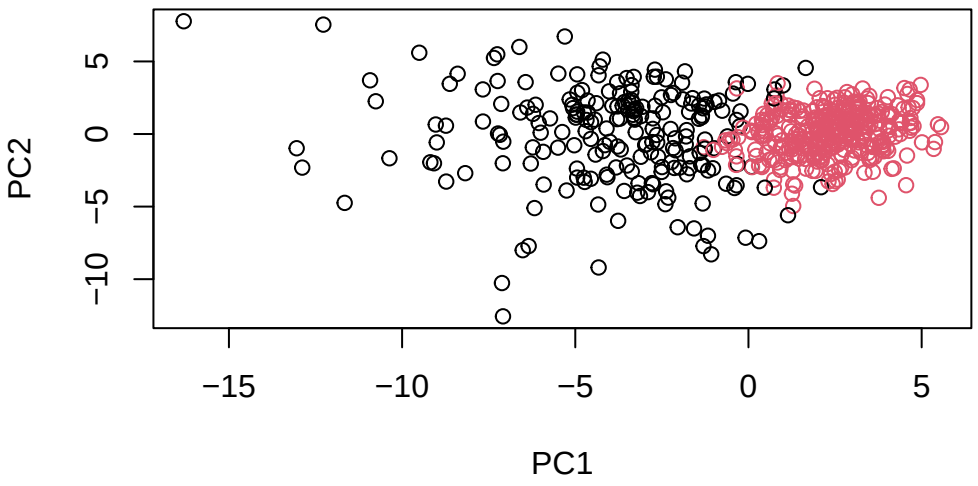

```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
216 353
```

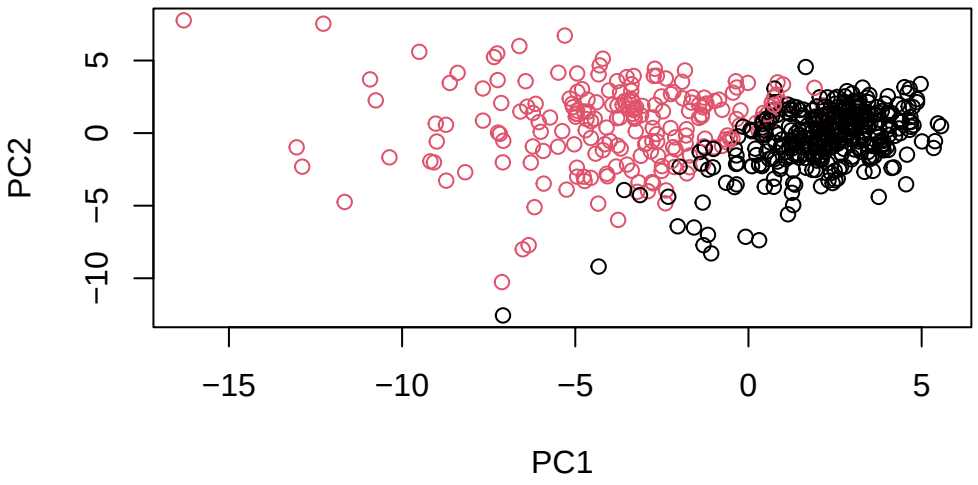
```
table(grps, diagnosis)
```

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

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




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



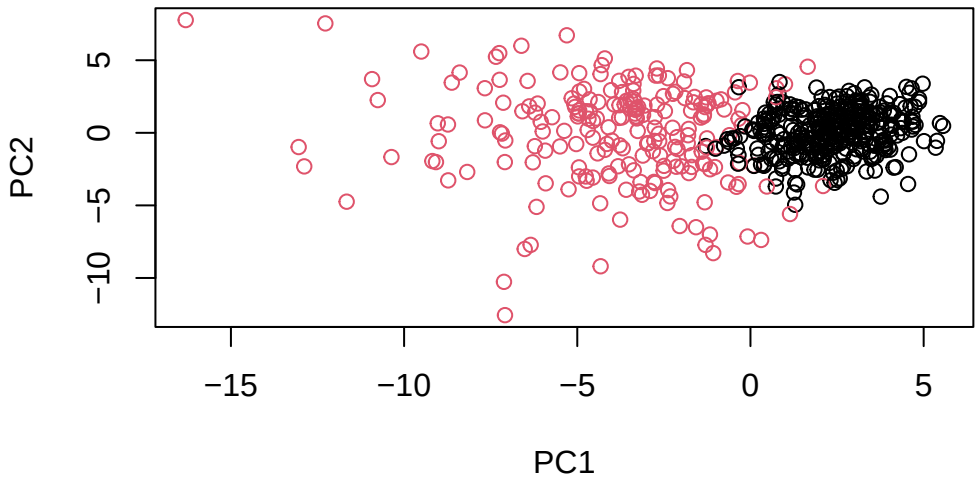
```
g <- as.factor(grps)
levels(g)
```

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

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

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

```
# Plot using our re-ordered factor
plot(wisc.pr$x[,1:2], col=g)
```




```
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method="ward.D2")
```

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

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

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

Q15. How well does the newly created model with four clusters separate out the two diagnoses? this model does a decent job of separating out the two diagnoses, with around a 25% error rate. It is comparable to the other methods.

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

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

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

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

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. The hierarchical method is better because it does not contain unecessary clusters. However, the actual separation of diagnoses types is not significantly better.

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

```
km.tp <- 175
km.fn = 212
km.sens <- km.tp / (km.tp + km.fn)
km.sens
```

```
[1] 0.4521964
```

```
km.tn <- 343
km.spec <- km.tn / (km.tn + km.fn)
km.spec
```

```
[1] 0.618018
```

```
hc.tp <- 165
hc.fn <- 212
hc.sens <- hc.tp / (hc.tp + hc.fn)
hc.sens
```

```
[1] 0.4376658
```

```
hc.tn <- 343
hc.spec <- hc.tn / (hc.tn + hc.fn)
hc.spec
```

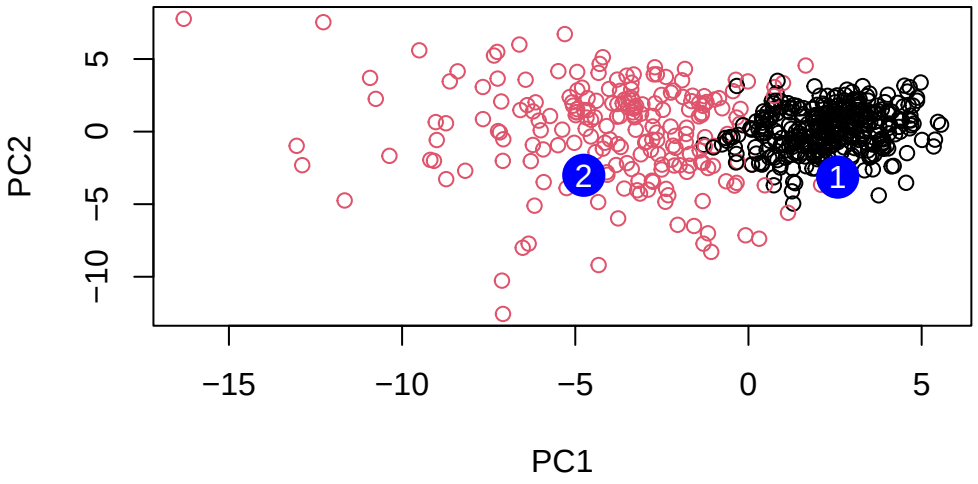
```
[1] 0.618018
```

kmeans has a higher sensitivity and they both have the same selectivity

```
#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
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? patient two should have a follow up because they were grouped with the malignant diagnoses