Class 8: Mini Project

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Analyzing the data

```
# Save your input data file into your Project directory
wisc.df <- read.csv("WisconsinCancer.csv")
```

Q1. How many observations are in the data?

```
• nrow(wisc.df)
```

```
[1] 569
```

There are 569 observations

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

```
# extracting out the diagnosis column
diagnosis <- wisc.df$diagnosis

# new variable without the first column
wisc.data <- wisc.df[,-1]

# information from the diagnosis column
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

There are 212 observations with a malignant diagnosis

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

```r
grep("_mean", colnames(wisc.df))
```

```
[1]  3  4  5  6  7  8  9 10 11 12
```

- There are 10 variables

Principle Component Analysis (PCA)

Scaling the data to order it better, making sure all the observations are numeric

```r
# checking column means and standard deviation
x <- wisc.data[,-1]

colMeans(wisc.data[,-1])
```

```
            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(x,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
# applying PCA
wisc.pr <- prcomp(x, 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
```

```
y <- summary(wisc.pr)
```

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?

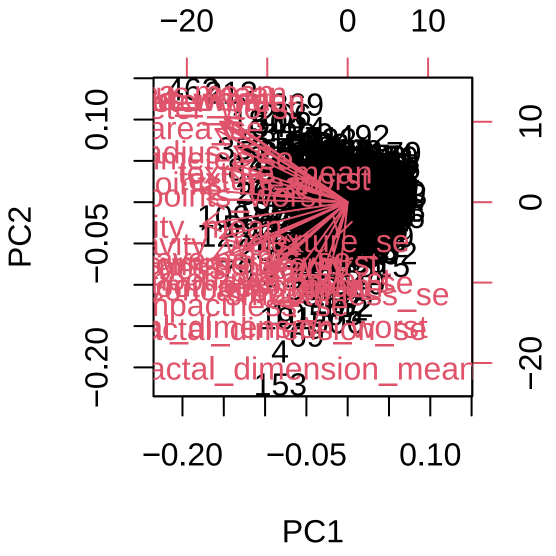
up to PC3

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

up to PC7

Interpreting PCA results

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

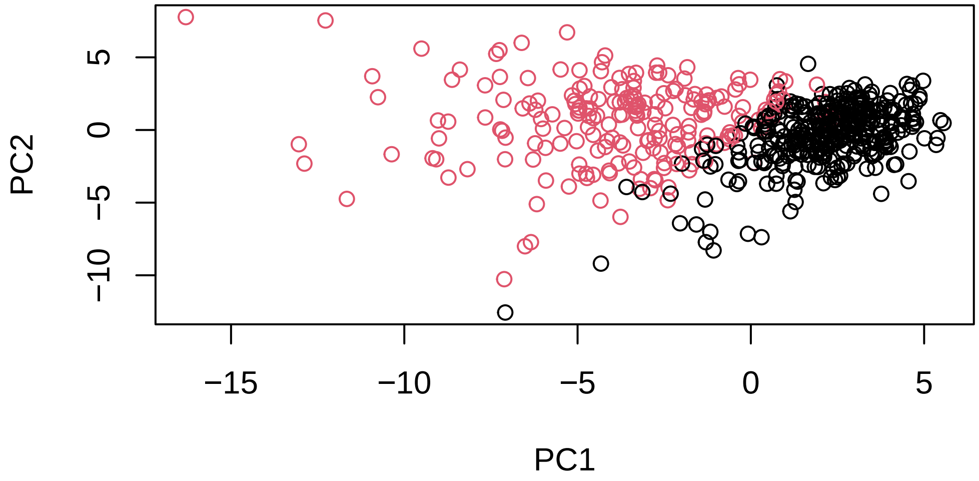


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

There is a huge cluster of numbers and words clustered in the center of the graph. It is very difficult to understand as it's not readable and doesn't provide any information.

Building a better plot

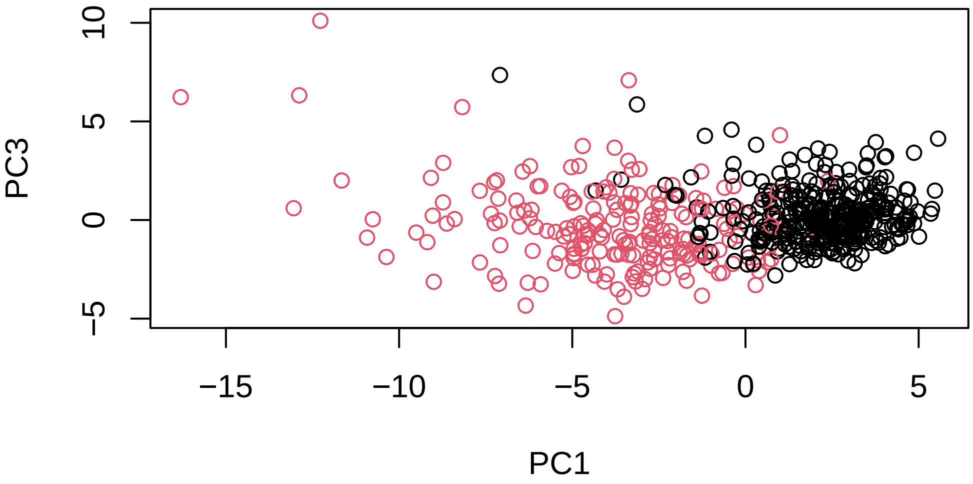
```
# Scatter plot observations by components 1 and 2
plot(wisc.pr$x[,1], wisc.pr$x[,2], col=as.factor(diagnosis), xlab="PC1", ylab="PC2")
```



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

PC3 and PC1 had more overlapping data while PC2 and PC1 had a cleaner plot with more separation.

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



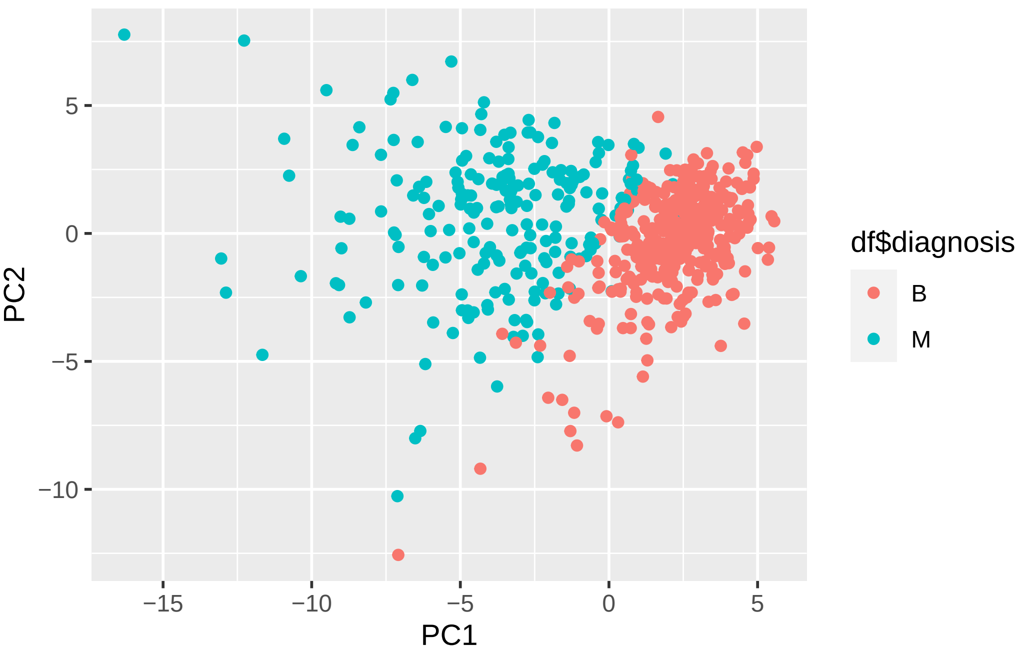
Using GGplot2

```
# 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=df$diagnosis) + geom_point()
```

```
Warning: Use of `df$diagnosis` is discouraged.
i Use `diagnosis` instead.
```



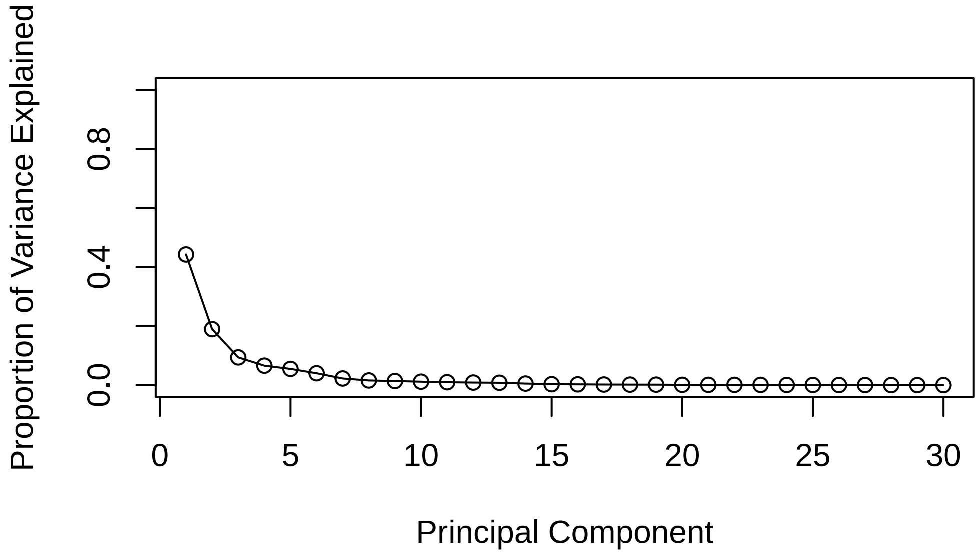
Showing variance

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

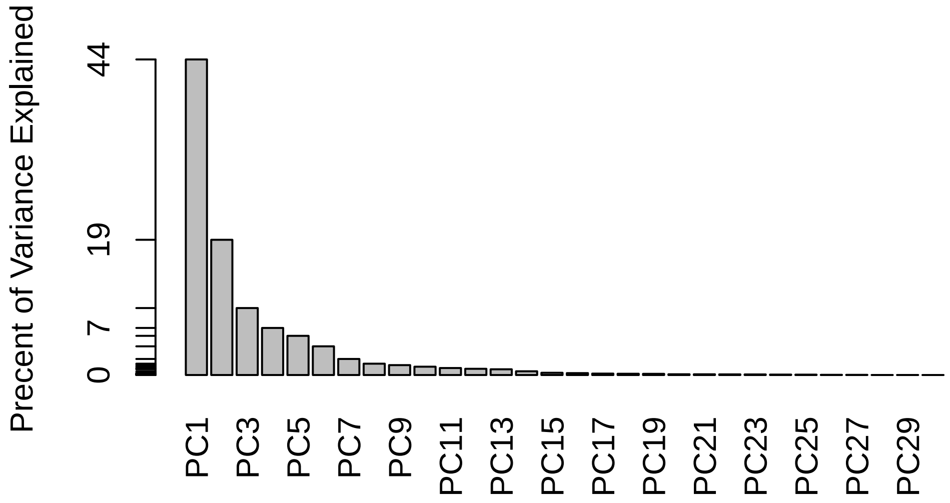
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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 )
```



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.

component of loading vector PC1 for feature concave.points_mean: -0.26085376

Comparing that with the other data from various principal components, we can see that this particular data from PC1 is not the only negative value as PC28 and PC29 have much more negative values (-8.88 and -4.21) that would contribute more to the overall mapping of the data.

```
# loading vector
wisc.pr$rotation["concave.points_mean",1]
```

```
[1] -0.2608538
```

Hierarchical clustering

```
# First scaling the data
data.scaled <- scale(x)
```

```
# Calculating the distance between all pairs of observations
data.dist <- dist(data.scaled)
```

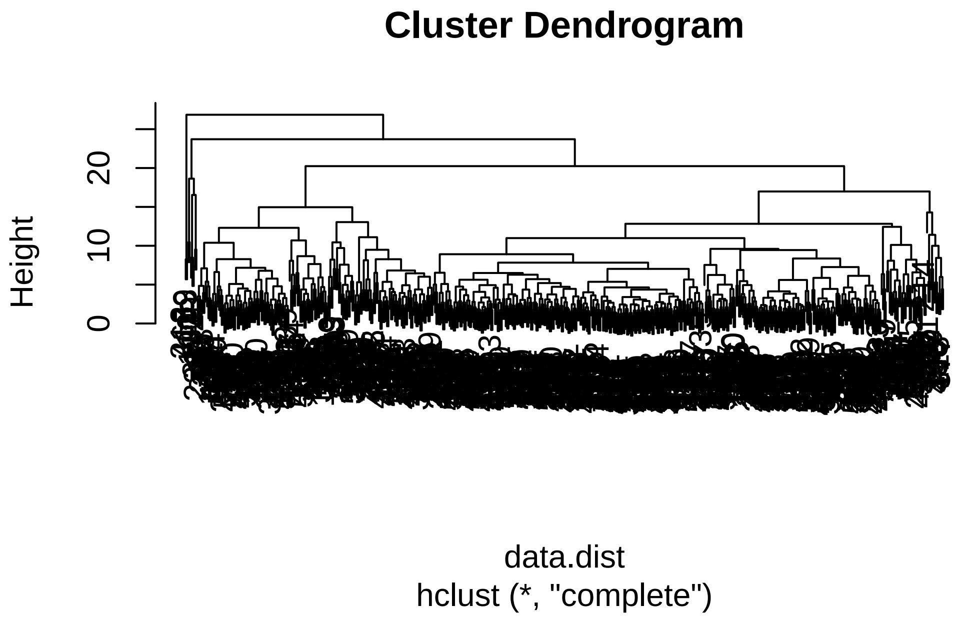
```
# Hierarchical clustering model using complete linkage
wisc.hclust <- hclust(data.dist, method="complete")
wisc.hclust
```

```

Call:
hclust(d = data.dist, method = "complete")

Cluster method   : complete 
Distance         : euclidean 
Number of objects: 569 
```

```
# Plotting the model
plot(wisc.hclust)
```

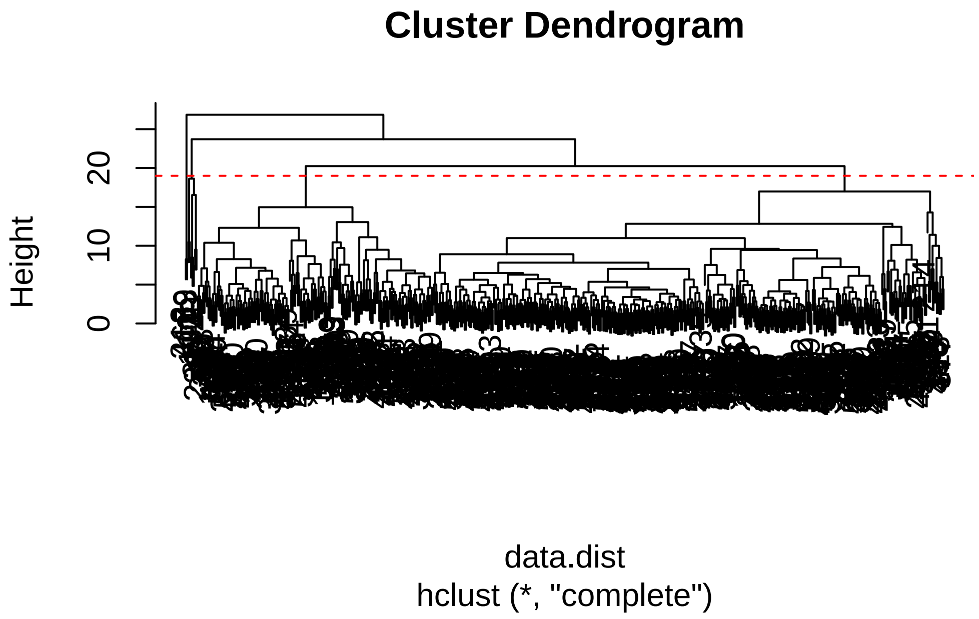


Results of hierarchical clustering

Q10. Using the `plot()` and `abline()` functions, what is the height at which the clustering model has 4 clusters?

Around height 19, the clustering model would have 4 clusters

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



Selecting number of clusters

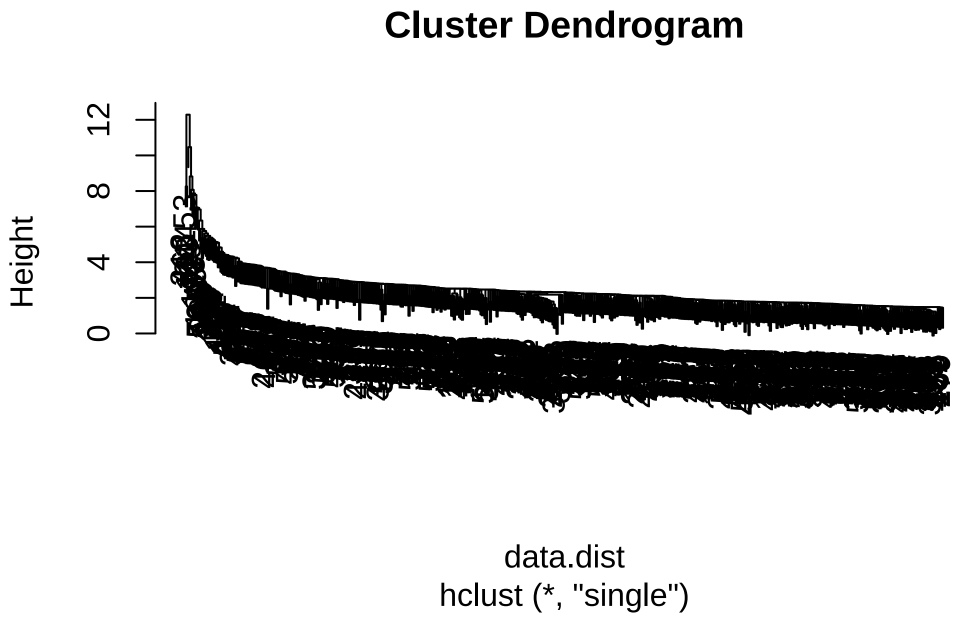
```
# Cutting the tree to only have 4 clusters
wisc.hclust.clusters <- cutree(wisc.hclust, h=19)
```

```
# Comparing the cluster membership to actual diagnoses
table(wisc.hclust.clusters, diagnosis)
```

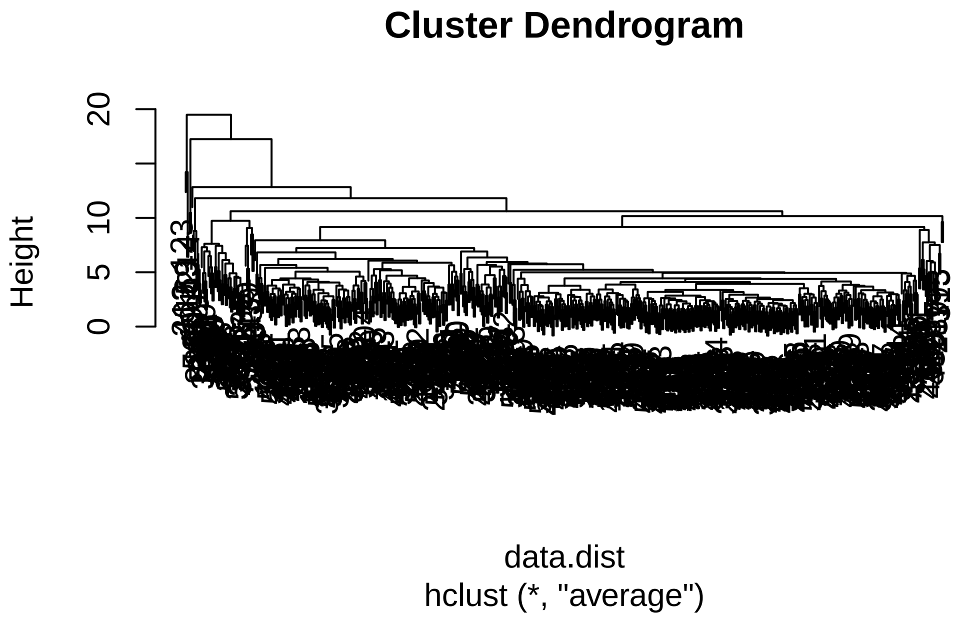
```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   2   5
                   3 343  40
                   4   0   2
```

Using different methods

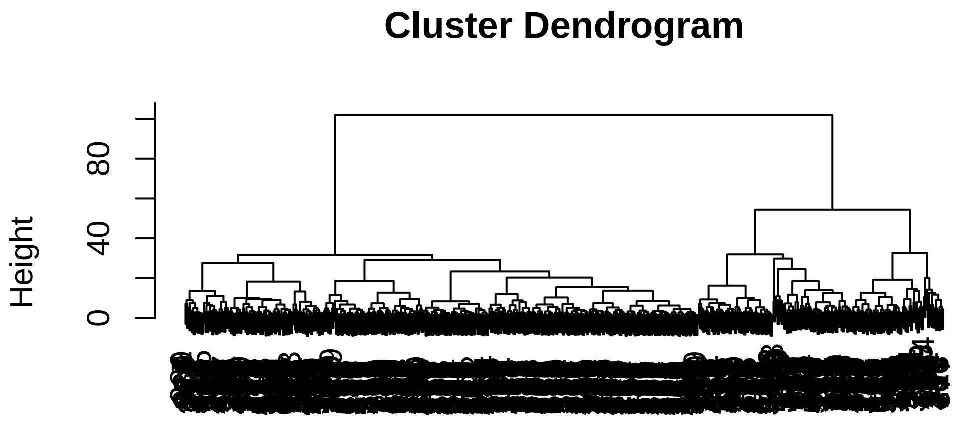
```
# Hierarchical clustering model using single linkage
wisc.hclust.single <- hclust(data.dist, method="single")
plot(wisc.hclust.single)
```



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



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



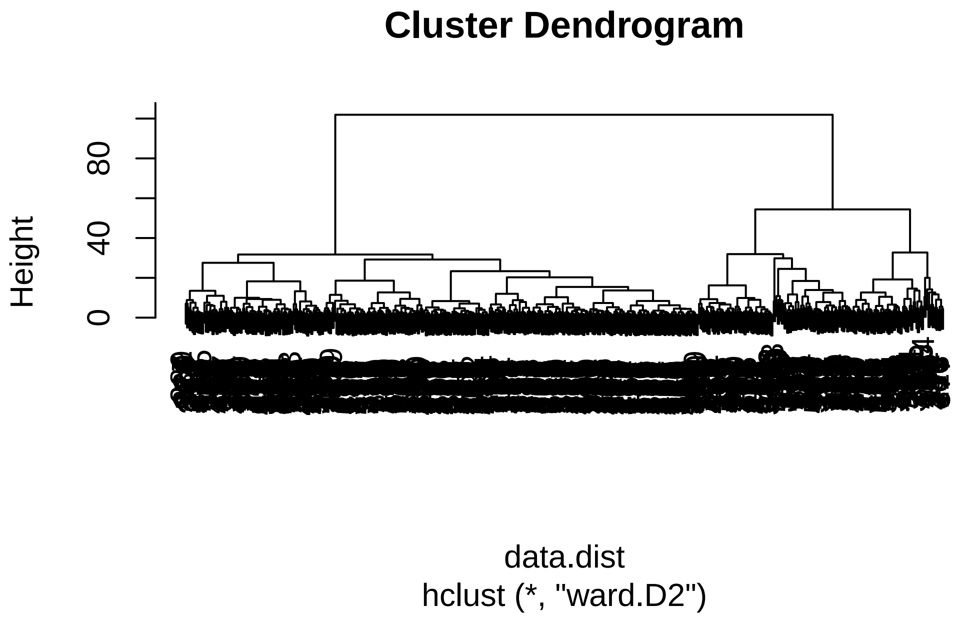
data.dist
hclust (*, "ward.D2")

Q12. Which method gives your favorite results for the same `data.dist` dataset? Explain your reasoning.

The complete method gives my favorite results for the dataset as it is much clearer than the other methods. The branching is more separated and clearer to see and interpret. Though the ward.D2 method gives very distinct branches towards the top which may be significant when analyzing the data.

Combining methods

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



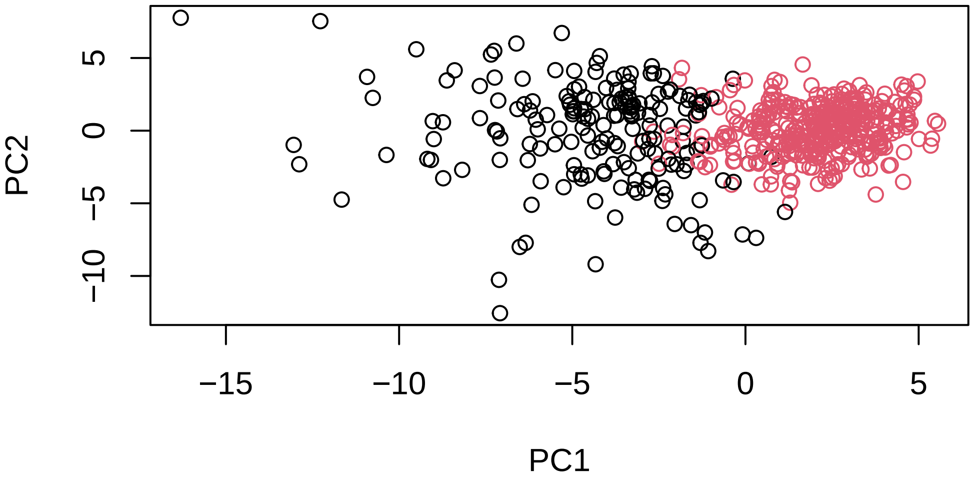
```
# analyzing the two main branches
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2 
184 385 
```

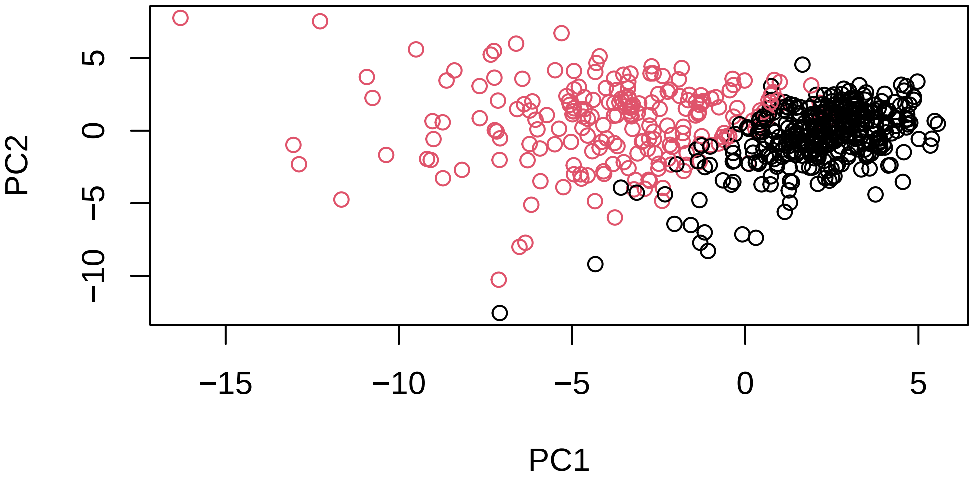
```
table(grps, diagnosis)
```

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

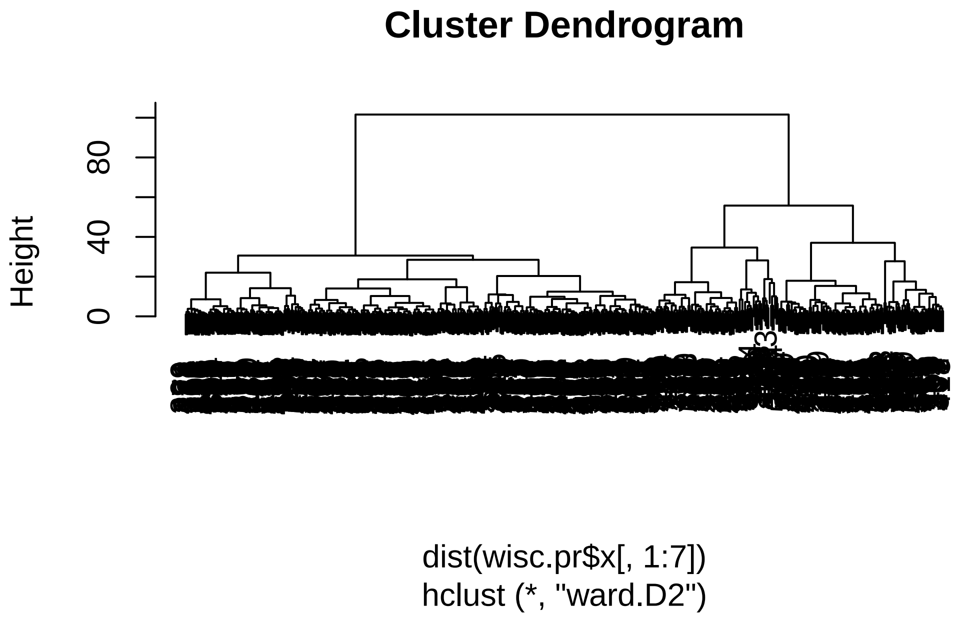
```
plot(wisc.pr$x[,1:2], col=grps)
```



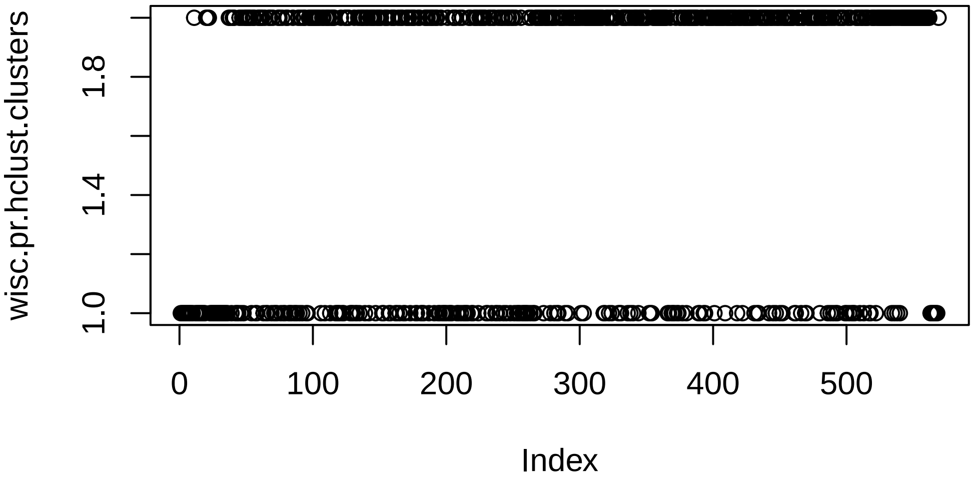
```
#swapping the colors
plot(wisc.pr$x[,1:2], col=as.factor(diagnosis))
```



```
# 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")
plot(wisc.pr.hclust)
```



```
# Cutting into 2 clusters
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
plot(wisc.pr.hclust.clusters)
```



Q13. **How well does the newly created model with four clusters separate out the two diagnoses?**

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

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

In cluster 1, there are more instances of malignant cells whereas in cluster 2, there are more benign cells. To compare this to the actual diagnoses, we can add up the clusters most number of cells and divide them by the total (569): (188+329)/569 = 0.909

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.

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

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

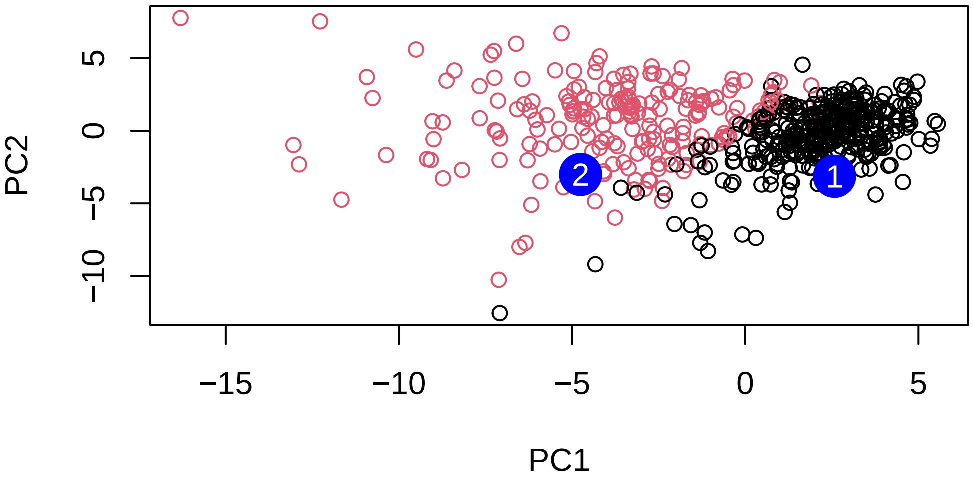
Cluster 1 has a high number of cells total, with the majority of them being malignant cells. Cluster 2 also has more malignant cells. Cluster 3 has the most number total cells with most of them being benign. In cluster 4, there are only 2 total cells with those being malignant.

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
```

```
plot(wisc.pr$x[,1:2], col=as.factor(diagnosis))
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



Q16. Which of these new patients should we prioritize for follow up based on your results?

Patient 2 should be prioritized as their principle component showcased more malignant cells that may pose a threat to their health.