mini-project

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#1 Looking at the data

```
# 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)
```

Then remove the diagnosis column

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

#i also gotta get rid of the last column because i got an extra 'x' one
wisc.data <- wisc.data[, -c(ncol(wisc.data))]
```

The diagnosis columns here

```
# Create diagnosis vector for later
diagnosis <- wisc.df[,1]
```

Q1. How many observations are in this dataset?

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

```
[1] 569  30
```

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

```
[1] 569
```

There are 569 patients with 31 observations (columns)

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

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

```
[1] 212
```

```
# can also do it another way
table(wisc.df$diagnosis)
```

```
  B   M
357 212
```

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

```
colnames(wisc.data)
```

```
 [1] "radius_mean"             "texture_mean"
 [3] "perimeter_mean"          "area_mean"
 [5] "smoothness_mean"         "compactness_mean"
 [7] "concavity_mean"          "concave.points_mean"
 [9] "symmetry_mean"           "fractal_dimension_mean"
[11] "radius_se"               "texture_se"
[13] "perimeter_se"            "area_se"
[15] "smoothness_se"           "compactness_se"
[17] "concavity_se"            "concave.points_se"
[19] "symmetry_se"             "fractal_dimension_se"
[21] "radius_worst"            "texture_worst"
[23] "perimeter_worst"         "area_worst"
[25] "smoothness_worst"        "compactness_worst"
[27] "concavity_worst"         "concave.points_worst"
[29] "symmetry_worst"          "fractal_dimension_worst"
```

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

```
 [1]  1  2  3  4  5  6  7  8  9 10
```

So there are 10 features suffixed with _mean

#2 PCA section

First see if the data needs to be scaled

```
# 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
```

The values are very distinct from each other so scaling is needed, then call prcomp()

```
# Perform PCA on wisc.data by completing the following code
#df <- wisc.data[, -c(ncol(wisc.data))]

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)?

PC1 accounts for 44.27% of the variance

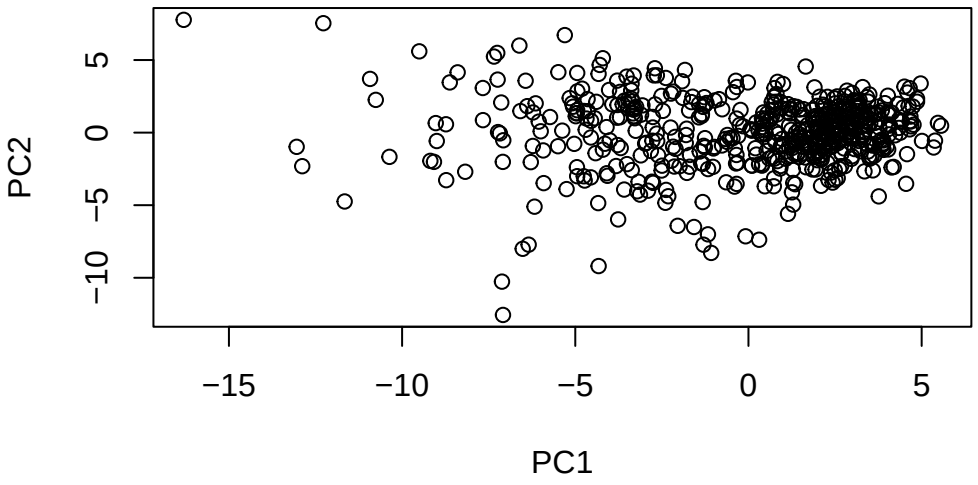
> Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

We need PC1, 2, and 3 to account for at least 70% of the total variance

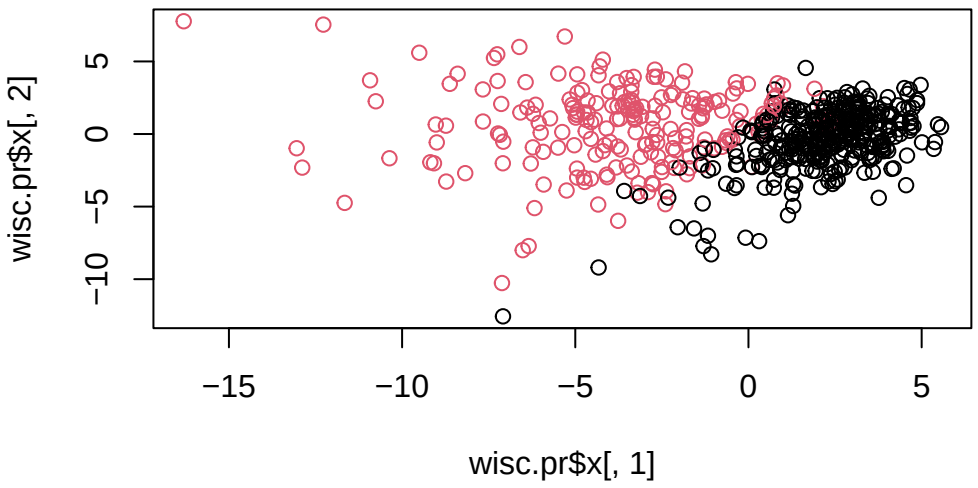
> Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

For at least 90% we need 7 PCs

```
plot(wisc.pr$x)
```




```
plot(wisc.pr$x[,1], wisc.pr$x[,2], col=(as.logical(diagnosis=="M")+9))
```

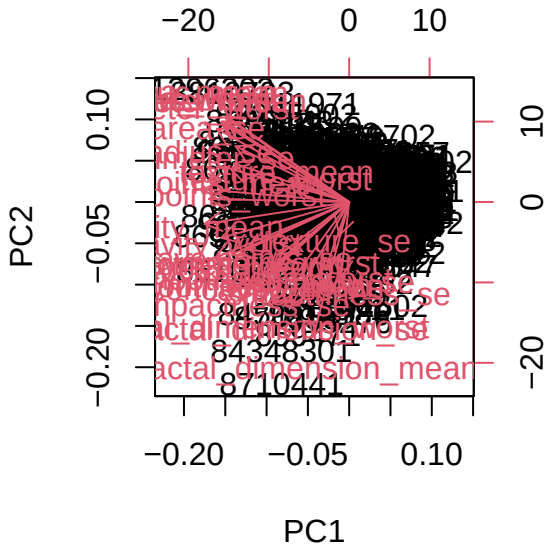



```
v <- summary(wisc.pr)
pcvar <- v$importance[3,]
pcvar["PC1"]
```

```
    PC1
0.44272
```

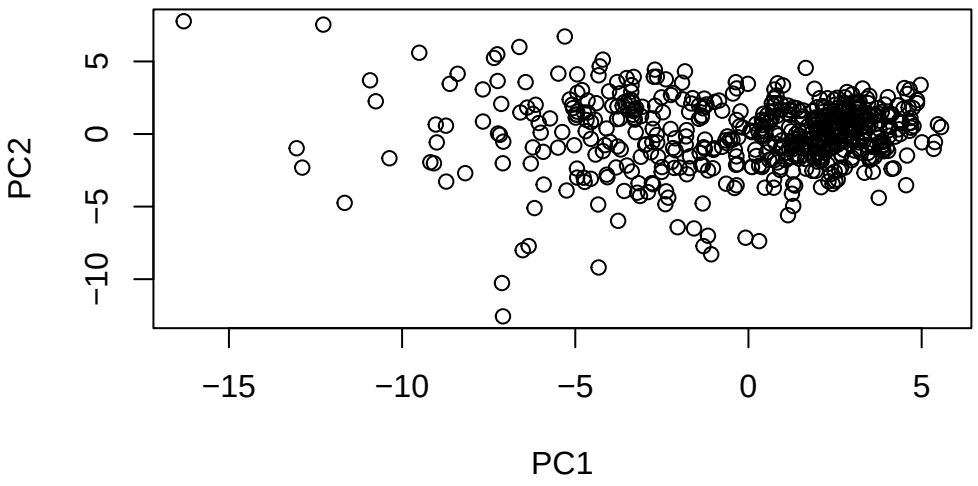
make a biplot of the PCA

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



The biplot is very messy so we will make a ggplot one instead

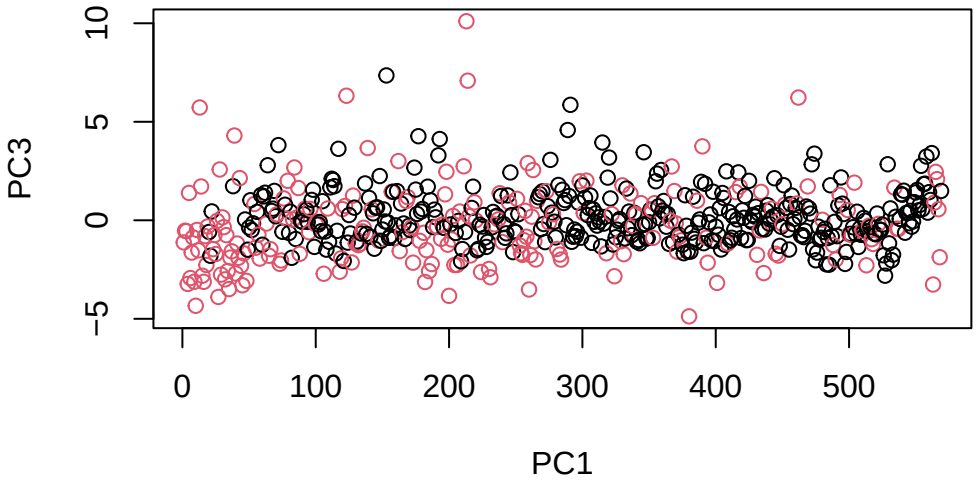
```
# Scatter plot observations by components 1 and 2
plot(wisc.pr$x[,1], wisc.pr$x[,2] , col = as.logical((diagnosis=="M")+1) ,
     xlab = "PC1", ylab = "PC2")
```



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

PC1 and PC3 are not very informative

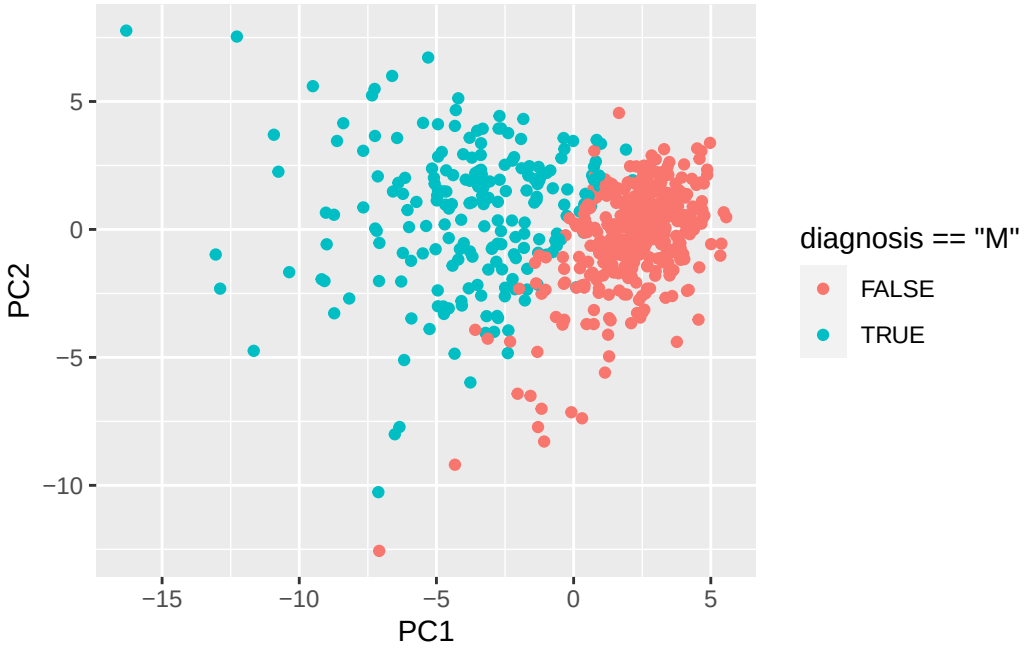
```
plot(wisc.pr$x[,3], col = (diagnosis=="M")+1,
     xlab = "PC1", ylab = "PC3")
```




```
# 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=="M") +
  geom_point()
```



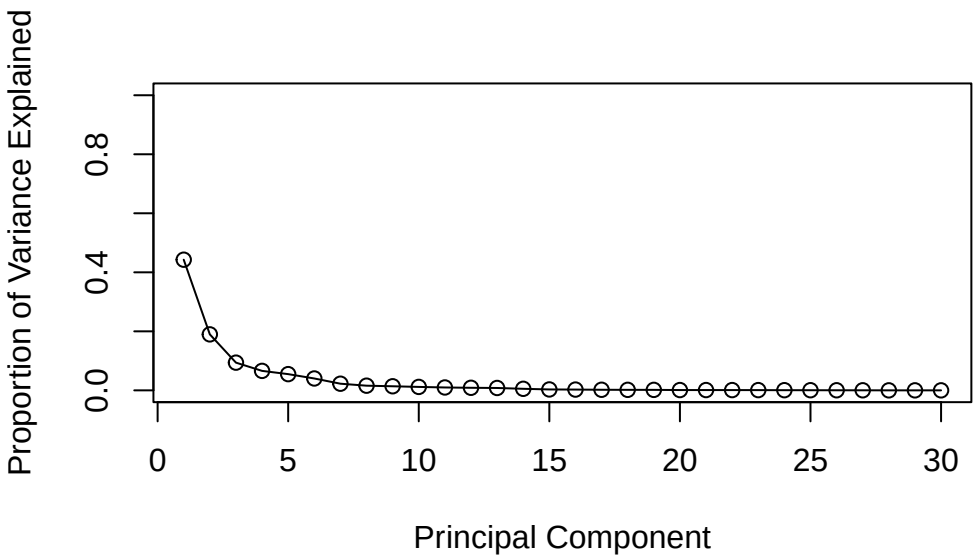
Variance

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

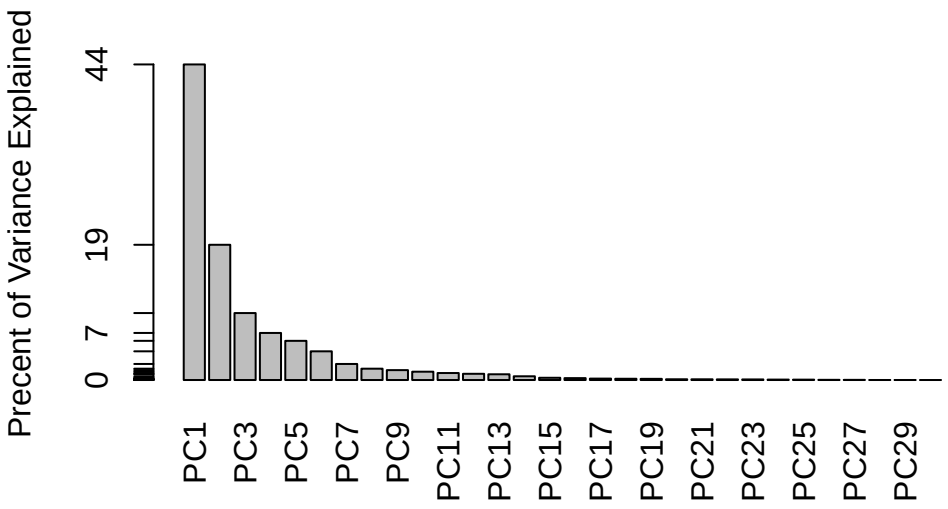
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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.

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

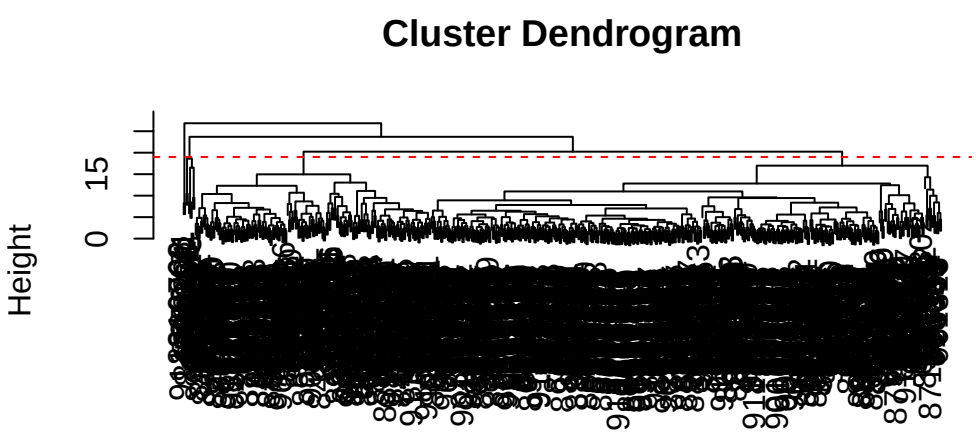
```
[1] -0.2608538
```

#Heirarchical clustering

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

at height 19 it splits it into 4 clusters

```
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(data.dist, method = "complete")
plot(wisc.hclust)
abline(h=19, col="red", lty=2)
```



#number of 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
```

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?

I used 3 PCs and compared the Table from my PC to the diagnosis table to see if they matched. If i only use 2 clusters I get something very similar to the diagnosis but if i increase to 3 PCs I start to see difference between them.

```
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
```

#Clustering in PC space

```
d.pc <- dist(wisc.pr$x[,1:3])
wisc.pr.hc <- hclust(d.pc, method="ward.D2")
#plot(wisc.pr.hc)
grps <- cutree(wisc.pr.hc, k=2)
table(grps)
```

```
grps
  1   2
203 366
```

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

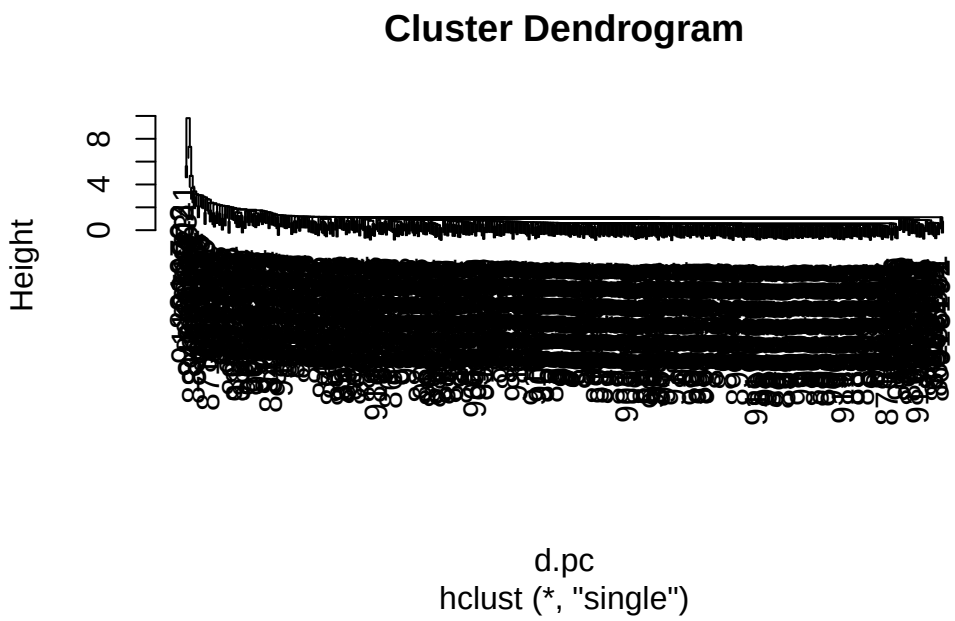
```
table(diagnosis, grps)
```

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

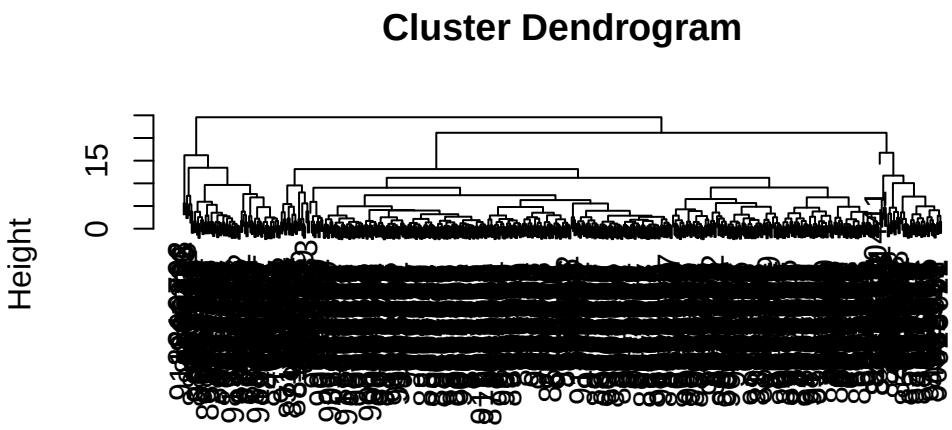
Q12. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

The ward method gave me the best looking histogram so i prefer that one. It also minimizes the variance between the samples, but in this case I think it also has the biggest height which makes it in my opinion better to distinguish M vs B.

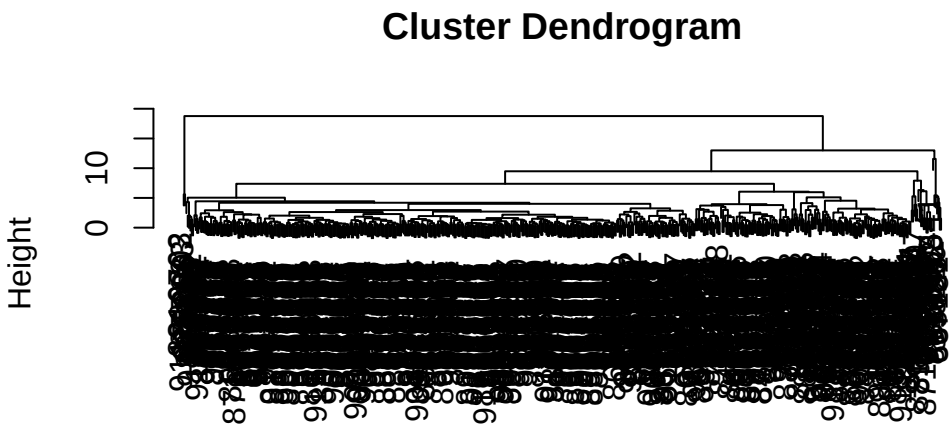
```
single_hc <- hclust(d.pc, method="single")
plot(single_hc)
```



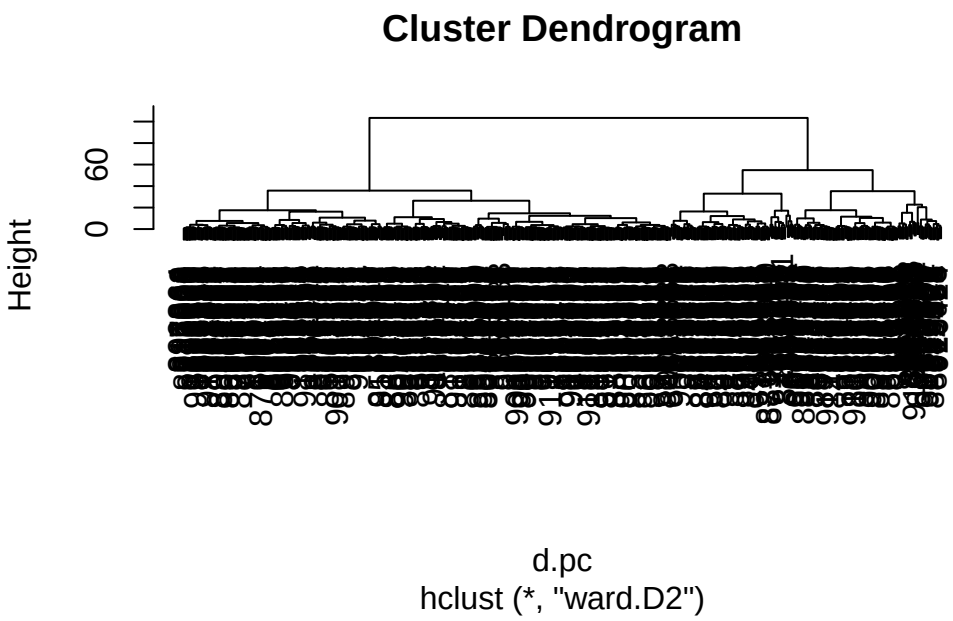

```
complete_hc <- hclust(d.pc, method="complete")
plot(complete_hc)
```




```
average_hc <- hclust(d.pc, method="average")
plot(average_hc)
```

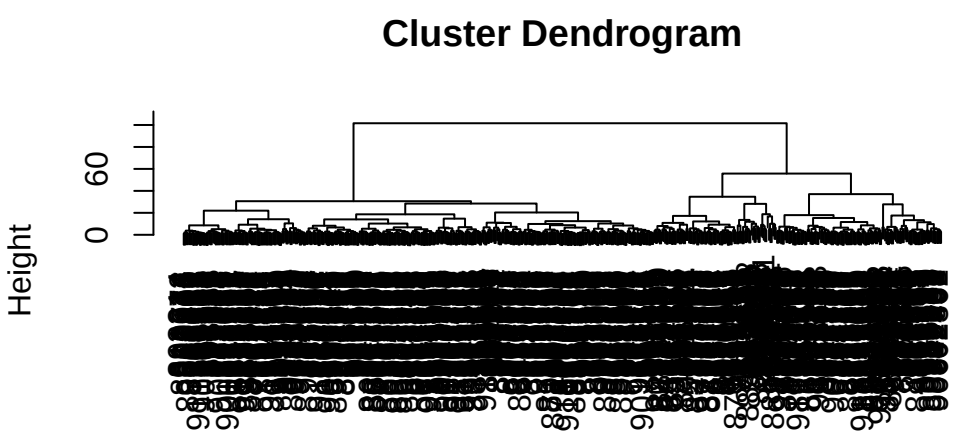


```
wardD2_hc <- hclust(d.pc, method="ward.D2")
plot(wardD2_hc)
```



Clustering on PCA results

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



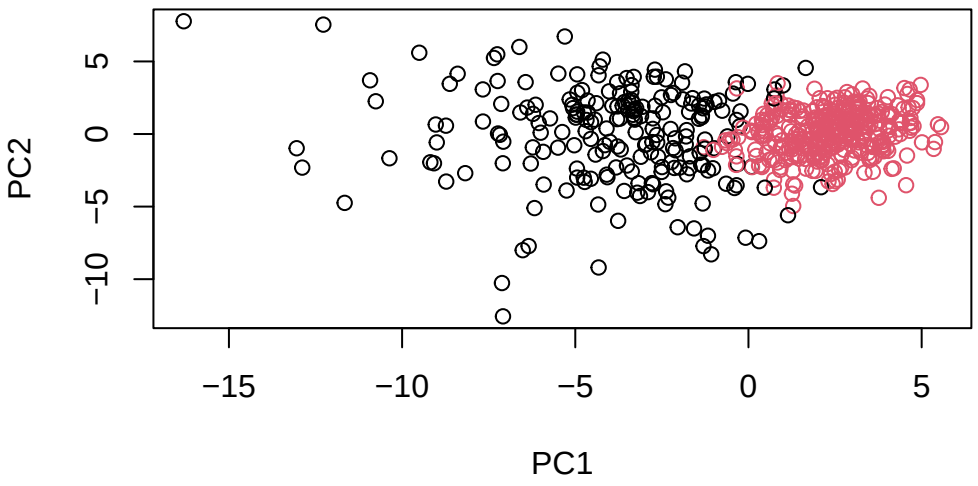

```
grps <- cutree(wisc.pr.hc, k=2)
table(grps)
```

```
grps
  1   2
216 353
```

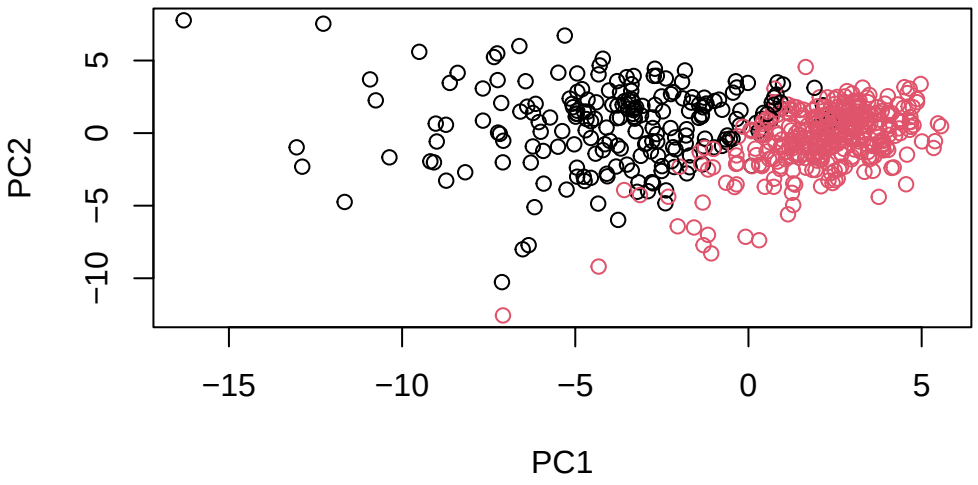
```
table(grps, diagnosis)
```

```
    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=="M")+2)
```



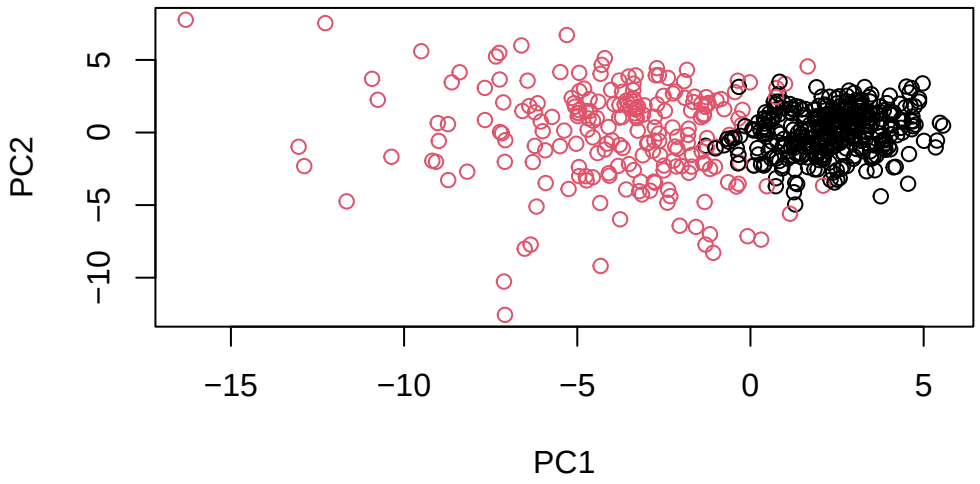
```
g <- as.factor(grps)
levels(g)
```

```
[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)
```




```
#library(rgl)
#plot3d(wisc.pr$x[,1:3], xlab="PC 1", ylab="PC 2", zlab="PC 3", cex=1.5, size=1, type="s",
```

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

When using 2 clusters it does not make much difference if i use 70% variance or 90% variance (7PCs). But when I use more clusters it becomes tricky to say which one is really malignant because clusters 2 and 3 have 77 and 66 tumors in it but they are most malign. Cluster 1 since it has 0 B is more likely to include M.

```
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
```

```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:3]), 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  24 179
                      2 333  33
```

```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]), method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=4)
table(wisc.pr.hclust.clusters, diagnosis)
```

```
                     diagnosis
wisc.pr.hclust.clusters   B   M
                      1   0  45
                      2   2  77
                      3  26  66
                      4 329  24
```

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.

```
  print("kmeans")
```

```
[1] "kmeans"
```

```
  km <- kmeans(wisc.data, centers=4, nstart=20)
  table(km$cluster,diagnosis)
```

```
   diagnosis
      B   M
  1 262   6
  2  94  87
  3   1 100
  4   0  19
```

```
  print("hclust")
```

```
[1] "hclust"
```

```
  wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]), method="ward.D2")
  wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=4)
  table(wisc.pr.hclust.clusters, diagnosis)
```

```
                      diagnosis
wisc.pr.hclust.clusters   B   M
                      1   0  45
                      2   2  77
                      3  26  66
                      4 329  24
```

Comparing hclust vs kmean it looks like the groups for hclust are a lot different. For kmeans there was a group with 94 and 87 B and M in the same group which is a bad cluster because it does not differentiate them. The h clust had bigger differences in the clusters. hcluster 4 has 24 false negatives and 329 true negatives while kmeans has 24 false negatives and 262 true negatives. So in distinguishing bening i would do hclust. For malign it is trickier because they are present in all 4 clusters regardless of the method so that one is trickier but kmeans seems to distinguigh better.

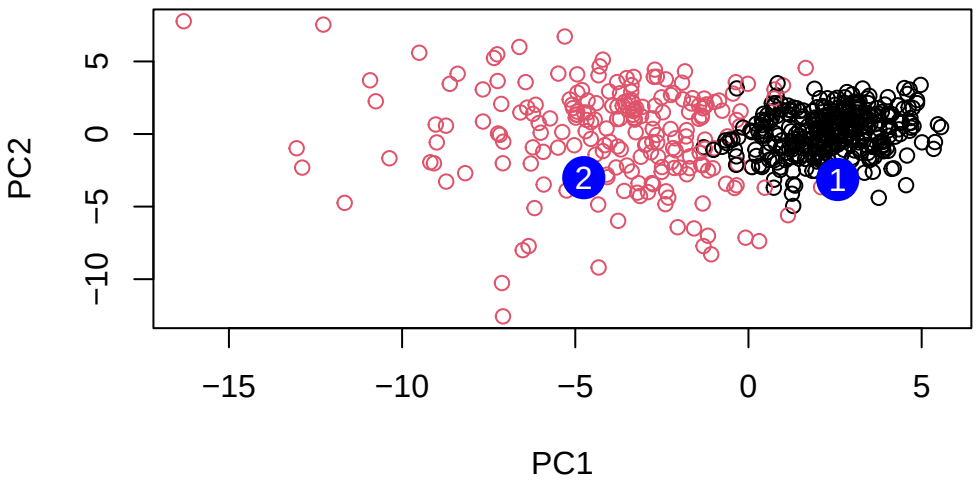
Q15. OPTIONAL: Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

I think the best model was when we took the first 2 components and assigned it 4 different clusters, that was the closest to the expert's opinion.

```
#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=g)
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?

based on this patient #2 is more urgent because their tumor is not as clustered to the benign as #1.