Class08 Mini Project

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Input the data into our document

```
wisc.df <- read.csv("WisconsinCancer.csv", 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
```

Wisc.df$diagnosis is a pathologist provided expert diagnosis, we will not use this for our unsupervised analysis as it is the "answer" to the question of which cells are malignant or benign.

To remove this, create a new data frame that omits the first column

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

Create a new separate vector called "diagnosis" that will contain the data from the diagnosis column of the original data set. We will store this as a factor (which is useful for plotting) and use this to check our results.

```
diagnosis <- as.factor(wisc.df[,1])
wisc.data <- wisc.df[,-1]
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
```

Exploratory data analysis

Q1. How many observations are in this dataset?

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

```
[1] 569
```

There are 569 observations in this set

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

```
table(wisc.df$diagnosis)
```

```
  B   M 
357 212 
```

There are 212 malignant diagnosis.

> Q3. How many variables/features in the data are suffized with "_mean"?

First find the column names

```
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"
```

Next I need to search within the column names for the suffix "_mean" pattern. The `grep()` function might help here.

```
#grep("search input", the data to search through)
grep("_mean", colnames(wisc.data))
```

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

```r
#only counts out how many, use `length()` to count it all at once
length(grep("_mean", colnames(wisc.data)))
```

```
[1] 10
```

There are 10 variables that are suffixed "_mean"

> How many dimensions are in this dataset?

```r
ncol(wisc.data)
```

```
[1] 30
```

Performing PCA

Check the 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 
```

Execute PCA with the prcomp() function on the wisc.data, scaling if appropriate, and assign the output model to wisc.pr.

```r
wisc.pr <- prcomp(wisc.data, scale=TRUE)
#take note that the measurements are not consistent throughout the data set, set the scale
```

Look at the summary of the results

```r
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% was captured

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

3 PCs capture over 70% of the original variance (look at the cumulative proportion)

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

7 PCs are required to describe at least 90% of the original variance

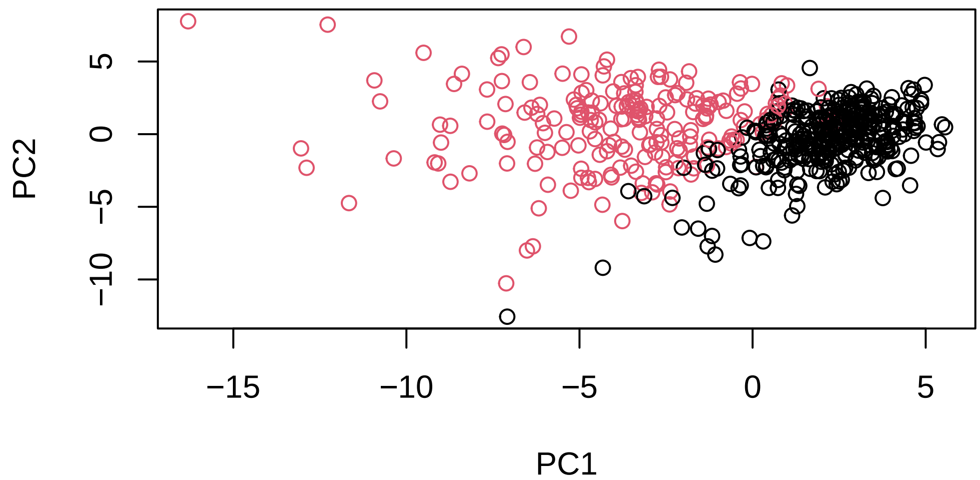
> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

It is difficult to understand as it overlaps too much and crowds the plot.

PC Plot

Time to create our own plot of PC1 vs PC2 (a.k.a score plot, PC-plot, etc.) The main result of PCA…

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

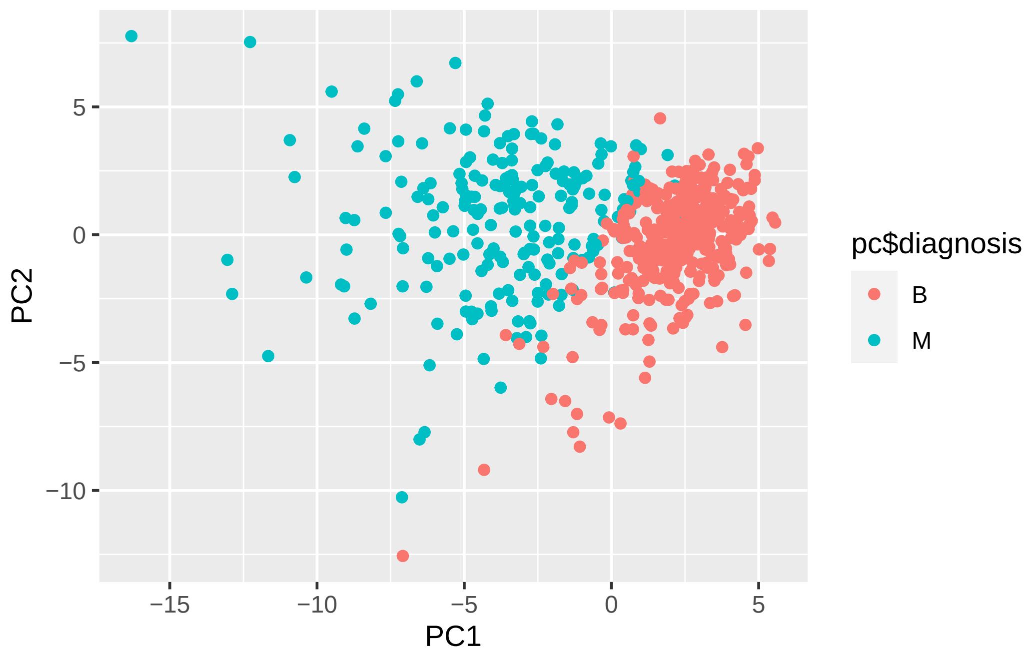


Can also run in ggplot2

```
library(ggplot2)

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

ggplot(pc, aes(PC1, PC2, col=pc$diagnosis)) +geom_point()
```



Variance explained

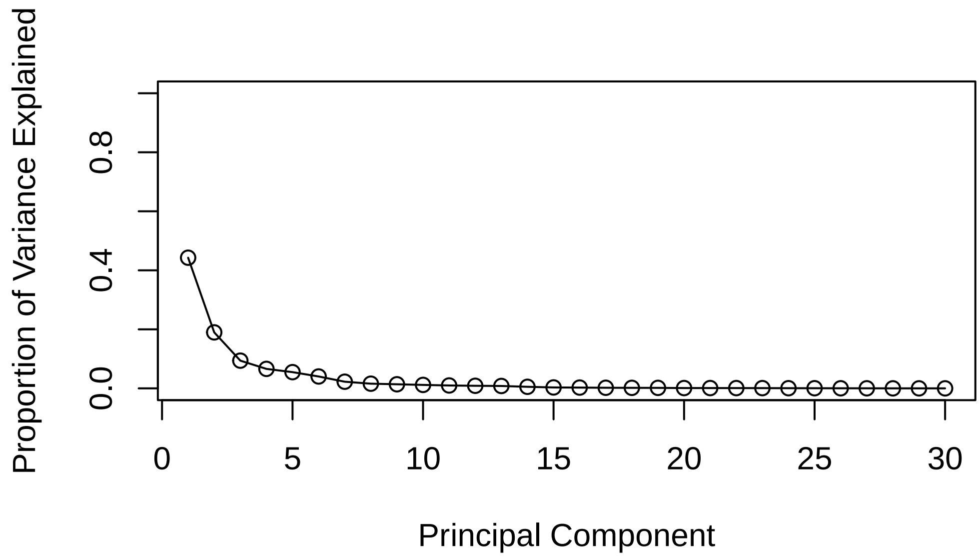
Calculate the variance of each component by squaring the sdev component of wisc.pr (ex. wisc.pr$sdev^2) and save it as pr.var

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

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

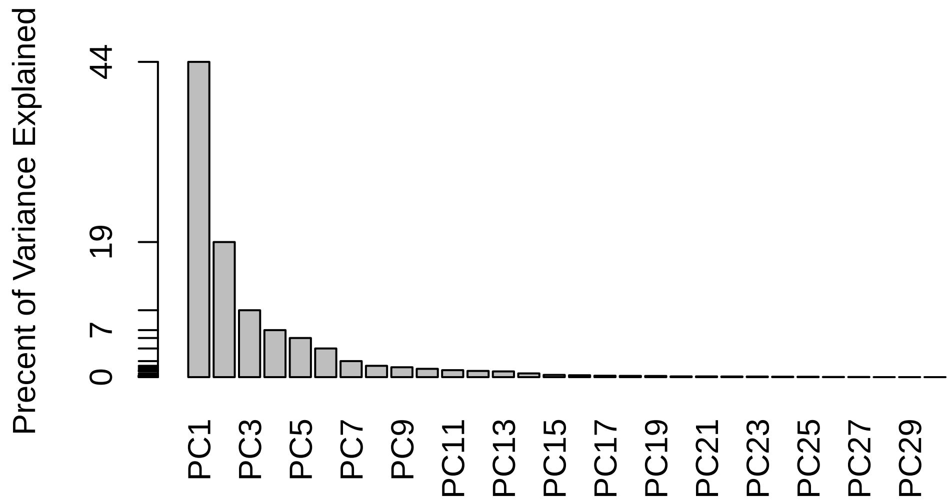
Calculate the variance explained by each principal component by dividing the total variance explained of all principal components. Assign this to a variable called pve and create a plot of the variance explained for each principal component

```
pve <- pr.var/sum(pr.var)
#plot variance
plot(pve, xlab = "Principal Component", ylab = "Proportion of Variance Explained", ylim=c(
```



Can also use in bar plot form

```
# 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)
```

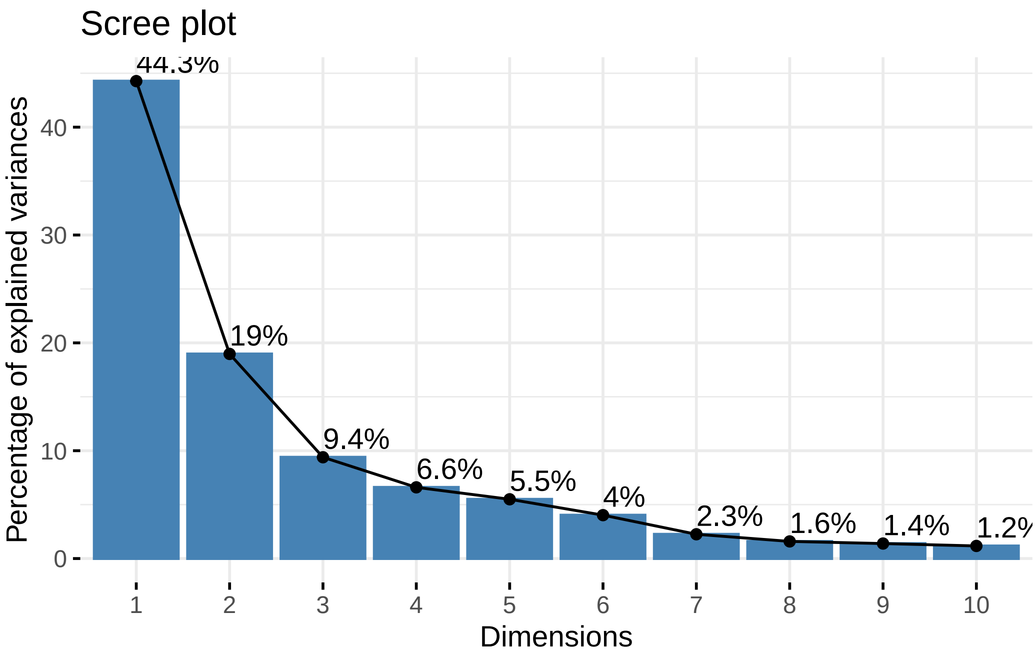


Optional Plot: can use a CRAN package for PCA known as `factoextra` Make sure to install it first and access with library

```
##ggplot based graph
#install.packages("factoextra")
library(factoextra)
```

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

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



Communicating PCA results

How much do the original variables contribute to the new PCs that were calculated? To get at this data, we can look at the `$rotation` component of he returned PCA object.

```
head(wisc.pr$rotation[,1:3])
```

```
                         PC1         PC2          PC3
radius_mean       -0.2189024  0.23385713 -0.008531243
texture_mean      -0.1037246  0.05970609  0.064549903
perimeter_mean    -0.2275373  0.21518136 -0.009314220
area_mean         -0.2209950  0.23107671  0.028699526
smoothness_mean   -0.1425897 -0.18611302 -0.104291904
compactness_mean  -0.2392854 -0.15189161 -0.074091571
```

Focus in on PC1

```
head(wisc.pr$rotation[,1])
```

```
    radius_mean      texture_mean    perimeter_mean         area_mean
     -0.2189024        -0.1037246        -0.2275373        -0.2209950
smoothness_mean compactness_mean
     -0.1425897        -0.2392854
```

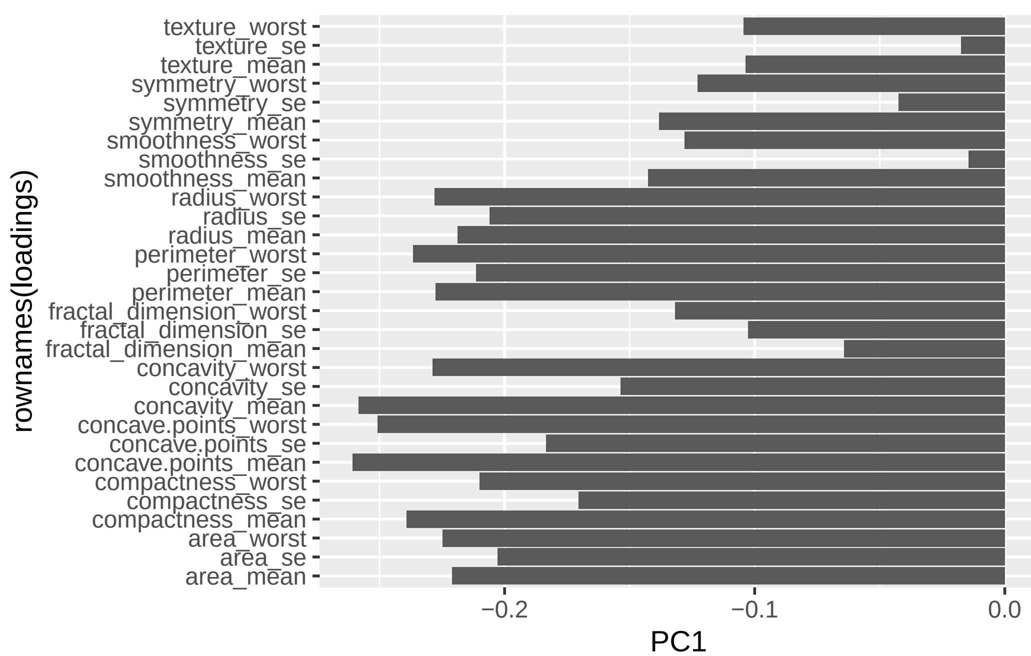
Q9. For the first principal component, what is the component of the loading vector (i.e. wisc.pr$rotation[,1]) for the feature concave.points_mean?

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

```
[1] -0.2608538
```

There is a complicated mix of variables that go together to make up PC1 - i.e. there are many of the original variables that react highly to PC1

```
loadings <- as.data.frame(wisc.pr$rotation)
ggplot(loadings) + aes(PC1, rownames(loadings)) + geom_col()
```



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

The minimum number required is 5 PC

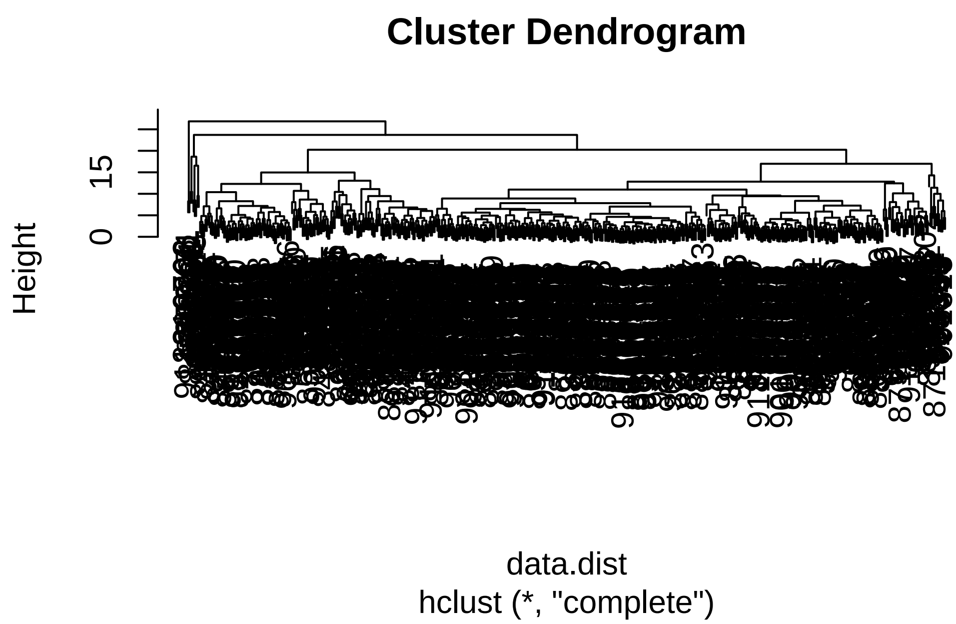
3. Heirarchal Clustering

Time to scale the data

```
data.scaled <- scale(wisc.data)
#calculate the (euclidean) distances between all pairs of observations in the new data set
data.dist <- dist(data.scaled)
#create a hierarchical clustering model using complete linkage
wisc.hclust <- hclust(data.dist, method="complete")
```

Plot the cluster

```
plot(wisc.hclust)
```



Cut the tree to yield cluster membership vector with `cutree()` function

```
grps <- cutree(wisc.hclust, k=4)
#can also do with h for height = 19
table(grps)
```

```
grps
```

```
  1   2   3   4 
177   7 383   2 
```

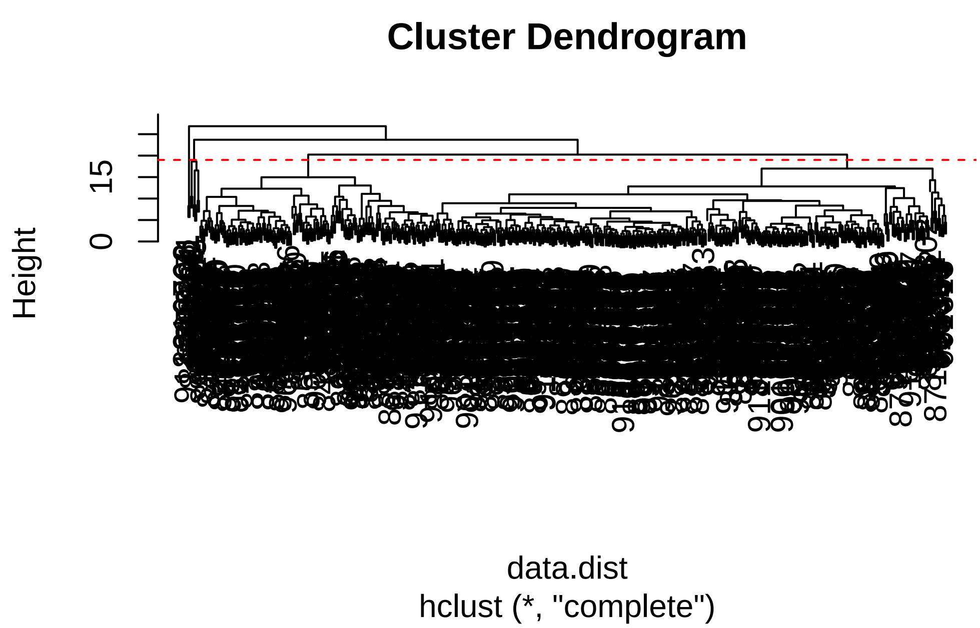
```r
table(grps, diagnosis)
```

```
    diagnosis
grps   B   M
   1  12 165
   2   2   5
   3 343  40
   4   0   2
```

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

h=19

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

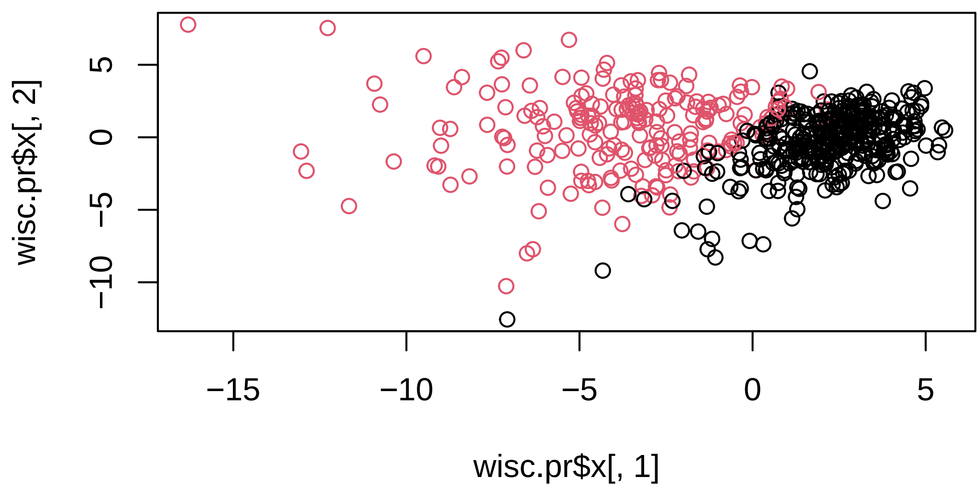


Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

Combine PCA and HCLUST

My PCA results were interesting as they showed a separation of M and B along PC1

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



I want to cluster my PCA results, that is use `wisc.pr$x` as input to `hclust()`

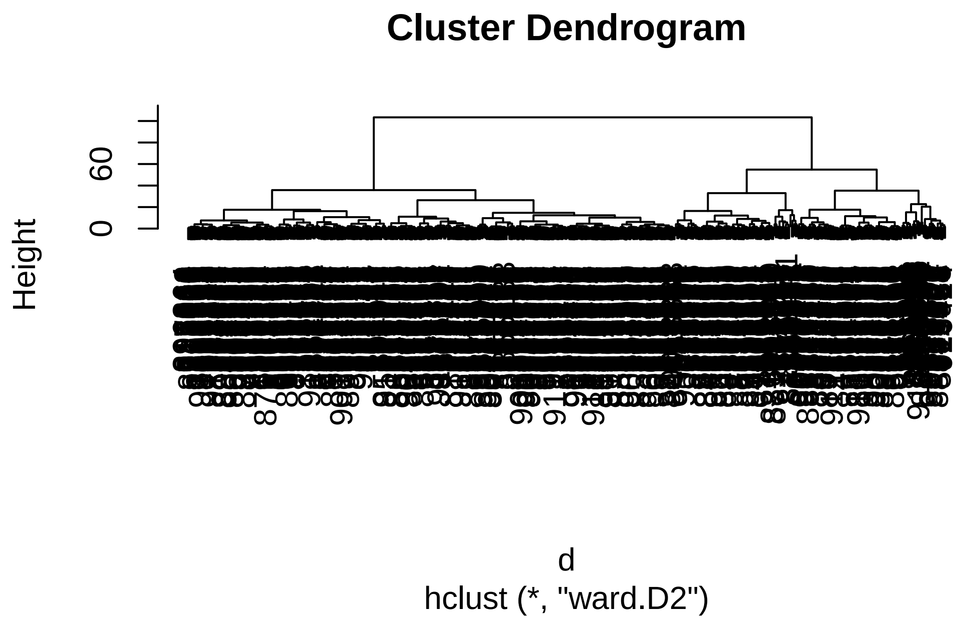
Try clustering 3 PCs first, PC1, PC2 and PC3 as input

```
d <- dist(wisc.pr$x[,1:3])

wisc.pr.hclust <- hclust(d,method="ward.D2")
```

And my tree figure

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

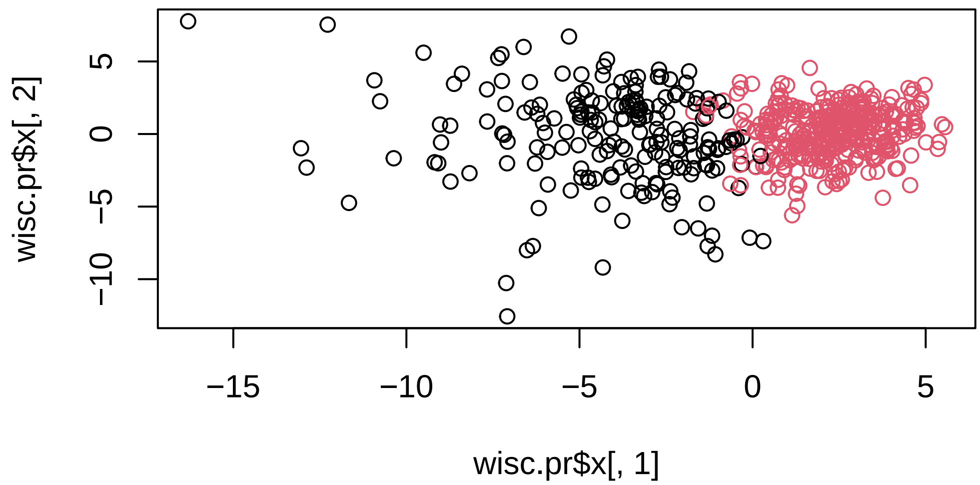


Let's cut this into 2 groups/clusters

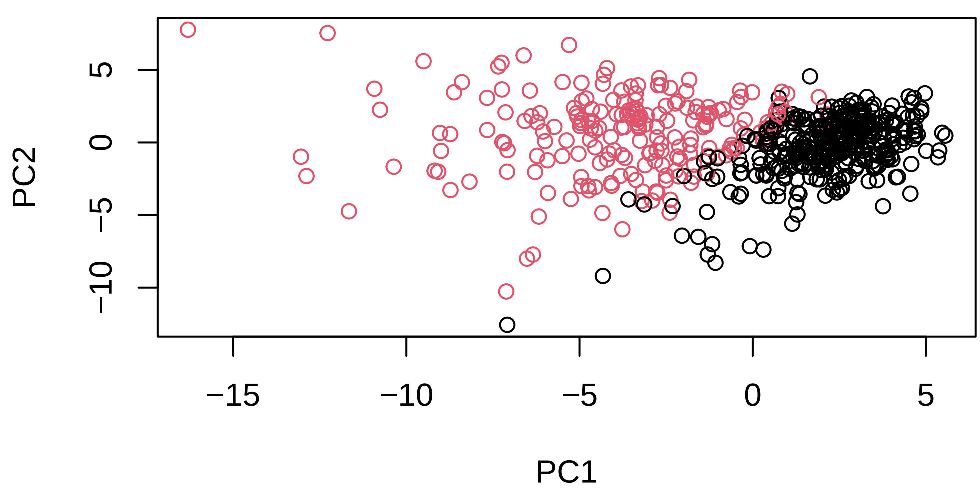
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
203 366
```

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




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



```
# just creates a color swap
```

How well do the two clusters separate the M and B diagnoses?

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

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

How accurate is this?

```
(179+333)/nrow(wisc.data)
```

```
[1] 0.8998243
```

2 clusters work better

> Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

The second method of setting an hclust of the wisc.pr$x as it scales and separates the data more in accordance to the percentage of the data that matches. When creating the cluster dendrogram it organizes and separates the groups into two nicer looking groups.

> Q14. Optional* How well does k-means separate the two diagnoses? How does it compare to your hclust results?

> Q15. How well does the newly created model with four clusters separate out the two diagnoses?

```
## 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")
```

Cut cluster into 2

```
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
# use table to compare results
table(wisc.pr.hclust.clusters, diagnosis)
```

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

How well does it work?

```r
(188+329)/nrow(wisc.data)
```

```
[1] 0.9086116
```

This is slightly more accurate at 90.86%