Class 8: PCR Mini Project

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Today we will do a complete analysis of some breast cancer biopsy data but first, let's revisit the main PCA function in R `prcomp()` and see what `scale=TRUE/FALSE` does.

```
head(mtcars)
```

```
                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

Find the mean value per column of this dataset.

```
apply(mtcars, 2, mean)
```

```
       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 
```

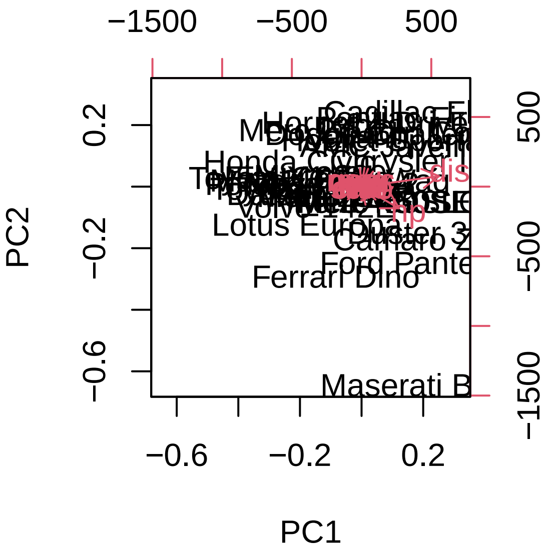
```
apply(mtcars, 2, sd)
```

```
        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 
```

It is clear that "disp" and "hp" have the highest mean values and the higest standard deviation. They will likely dominate any analysis I do on this dataset. Let's see.

```
pc.noscale <- prcomp(mtcars, scale = FALSE)
pc.scale <- prcomp(mtcars, scale=TRUE)
```

```
biplot(pc.noscale)
```



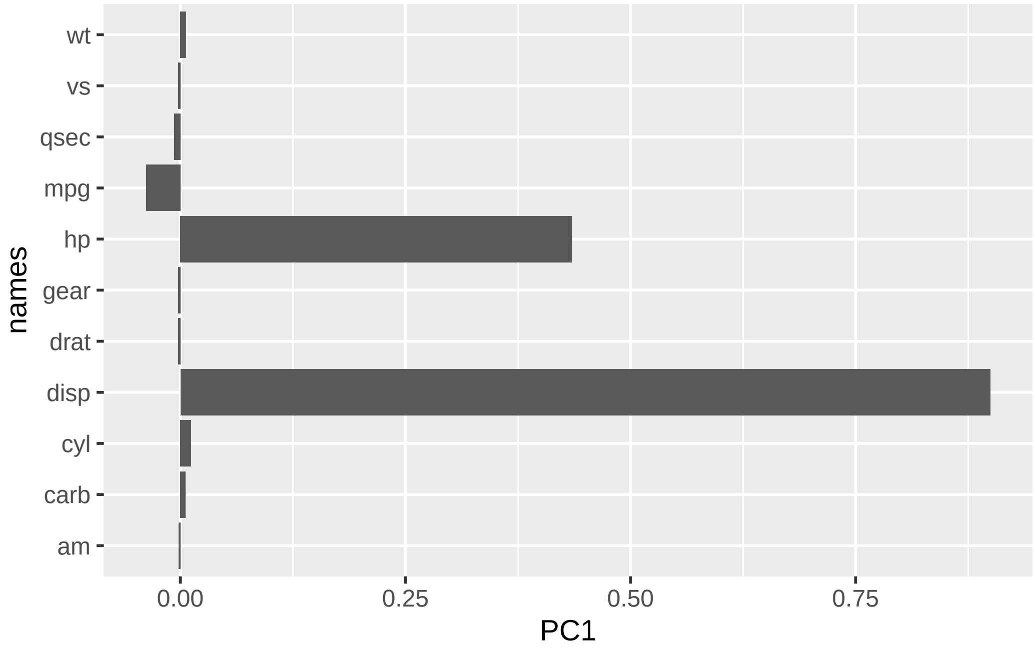
```
pc.noscale$rotation[,1]
```

```
        mpg         cyl        disp          hp        drat          wt 
-0.038118199  0.012035150  0.899568146  0.434784387 -0.002660077  0.006239405 
       qsec          vs          am        gear        carb 
-0.006671270 -0.002729474 -0.001962644 -0.002604768  0.005766010 
```

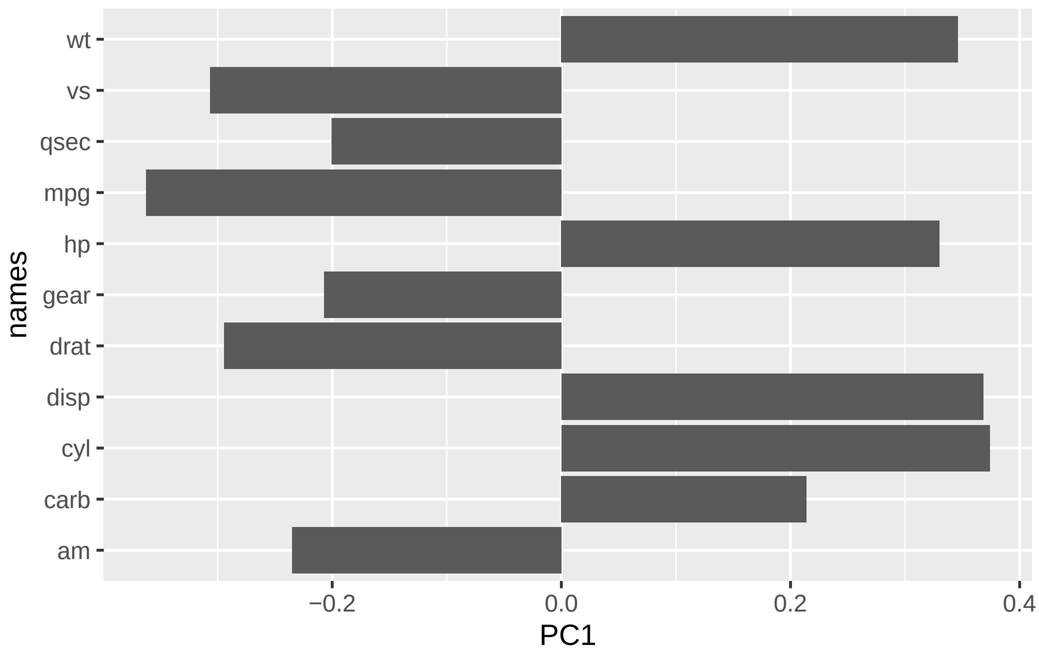
Plot the loadings

```
library(ggplot2)

r1 <- as.data.frame(pc.noscale$rotation)
r1$names <- rownames(pc.noscale$rotation)
```

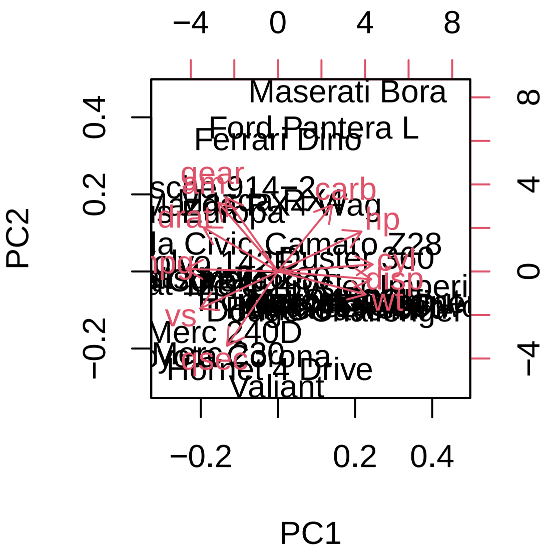
```r
ggplot(r1) +
aes(PC1, names) +
geom_col()
```



```r
r2 <- as.data.frame(pc.scale$rotation)
r2$names <- rownames(pc.scale$rotation)

ggplot(r2) +
aes(PC1, names) +
geom_col()
```



```r
biplot(pc.scale)
```



Take-home: Generally, we always want to set `scale=TRUE` when we do this type of analysis to avoid our analysis being dominated by individual variables with the larges variance just due to their unit of measurement.

FNA Breast Cancer Data

Load the data into R.

```
fna.data <- read.csv("WisconsinCancer.csv")

wisc.df <- data.frame(fna.data, 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
```

Q1. How many observations are in this dataset?

```r
nrow(wisc.df)
```

```
[1] 569
```

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

```r
sum(wisc.df$diagnosis == "M")
```

```
[1] 212
```

The `table()` function is super useful here:

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

```

  B   M 
357 212 
```

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

```
ncol(wisc.df)
```

```
[1] 31
```

```
colnames(wisc.df)
```

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

A useful function for this is `grep()`

```
length( #Tells us how _means were found
grep("_mean", colnames(wisc.df))) #Tells us which columns "_mean" were found
```

```
[1] 10
```

Before we go any further, we need to exclude the diagnosis column from any future analysis - this tells us whether a sample to cancer or non-cancer.

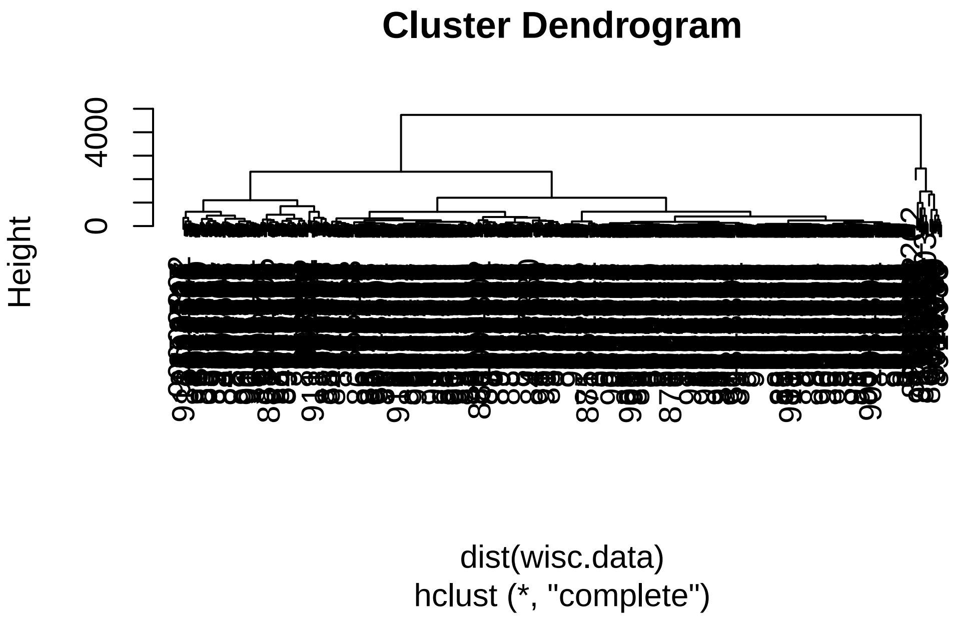
```
diagnosis <- as.factor(wisc.df$diagnosis)

head(diagnosis)
```

```
[1] M M M M M M
Levels: B M
```

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

Let's see if we cluster the `wisc.data` to find some structure in the dataset.

```
hc <- hclust(dist(wisc.data))

plot(hc)
```



Principal Component Analysis (PCA)

Performing PCA

```
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)?

0.4427

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

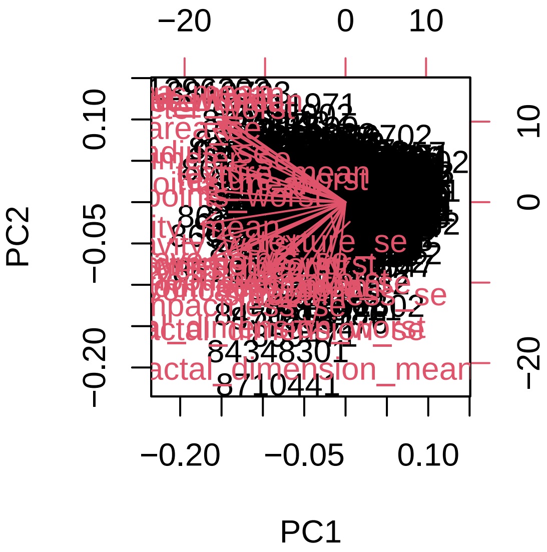
PC3

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

PC7

Interpreting PCA Results

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



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

This biplot sucks! It is difficult to understand because there's too many data points to actually understand.

We need to build our own PCA score plot of PC1 vs PC2.

```
attributes(wisc.pr)
```

```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"       

$class
[1] "prcomp"
```

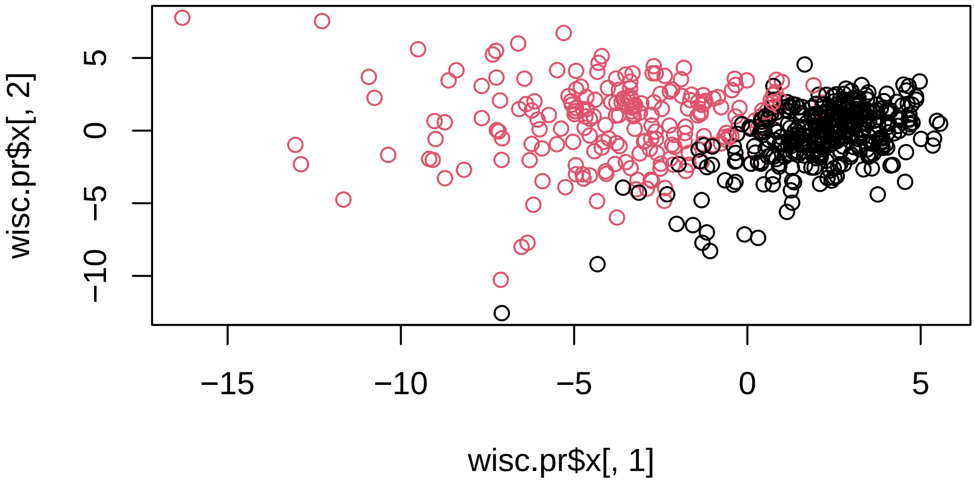
```r
head(wisc.pr$x)
```

```
               PC1        PC2        PC3       PC4        PC5         PC6
842302   -9.184755  -1.946870 -1.1221788 3.6305364  1.1940595  1.41018364
842517   -2.385703   3.764859 -0.5288274 1.1172808 -0.6212284  0.02863116
84300903 -5.728855   1.074229 -0.5512625 0.9112808  0.1769302  0.54097615
84348301 -7.116691 -10.266556 -3.2299475 0.1524129  2.9582754  3.05073750
84358402 -3.931842   1.946359  1.3885450 2.9380542 -0.5462667 -1.22541641
843786   -2.378155  -3.946456 -2.9322967 0.9402096  1.0551135 -0.45064213
                 PC7         PC8         PC9       PC10       PC11       PC12
842302    2.15747152  0.39805698 -0.15698023 -0.8766305 -0.2627243 -0.8582593
842517    0.01334635 -0.24077660 -0.71127897  1.1060218 -0.8124048  0.1577838
84300903 -0.66757908 -0.09728813  0.02404449  0.4538760  0.6050715  0.1242777
84348301  1.42865363 -1.05863376 -1.40420412 -1.1159933  1.1505012  1.0104267
84358402 -0.93538950 -0.63581661 -0.26357355  0.3773724 -0.6507870 -0.1104183
843786    0.49001396  0.16529843 -0.13335576 -0.5299649 -0.1096698  0.0813699
                PC13         PC14         PC15        PC16        PC17
842302    0.10329677 -0.690196797  0.601264078  0.74446075 -0.26523740
842517   -0.94269981 -0.652900844 -0.008966977 -0.64823831 -0.01719707
84300903 -0.41026561  0.016665095 -0.482994760  0.32482472  0.19075064
84348301 -0.93245070 -0.486988399  0.168699395  0.05132509  0.48220960
84358402  0.38760691 -0.538706543 -0.310046684 -0.15247165  0.13302526
843786   -0.02625135  0.003133944 -0.178447576 -0.01270566  0.19671335
                PC18       PC19        PC20         PC21        PC22
842302   -0.54907956  0.1336499  0.34526111  0.096430045 -0.06878939
842517    0.31801756 -0.2473470 -0.11403274 -0.077259494  0.09449530
84300903 -0.08789759 -0.3922812 -0.20435242  0.310793246  0.06025601
84348301 -0.03584323 -0.0267241 -0.46432511  0.433811661  0.20308706
84358402 -0.01869779  0.4610302  0.06543782 -0.116442469  0.01763433
843786   -0.29727706 -0.1297265 -0.07117453 -0.002400178  0.10108043
                PC23         PC24         PC25         PC26        PC27
842302    0.08444429  0.175102213  0.150887294 -0.201326305 -0.25236294
842517   -0.21752666 -0.011280193  0.170360355 -0.041092627  0.18111081
84300903 -0.07422581 -0.102671419 -0.171007656  0.004731249  0.04952586
84348301 -0.12399554 -0.153294780 -0.077427574 -0.274982822  0.18330078
84358402  0.13933105  0.005327110 -0.003059371  0.039219780  0.03213957
843786    0.03344819 -0.002837749 -0.122282765 -0.030272333 -0.08438081
                  PC28         PC29          PC30
842302   -0.0338846387  0.045607590  0.0471277407
842517    0.0325955021 -0.005682424  0.0018662342
84300903  0.0469844833  0.003143131 -0.0007498749
84348301  0.0424469831 -0.069233868  0.0199198881
```

```
84358402 -0.0347556386  0.005033481 -0.0211951203
843786    0.0007296587 -0.019703996 -0.0034564331
```

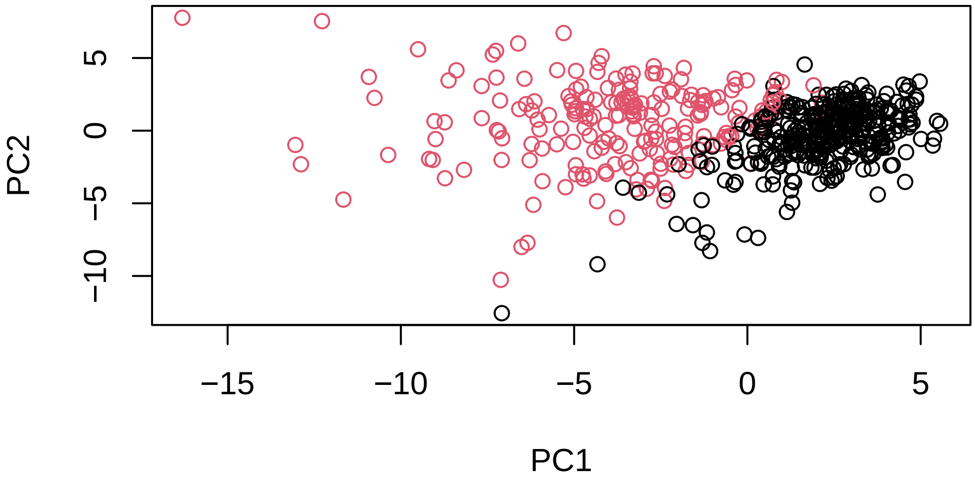
Plot of PC1 vs PC2 the first two columns

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



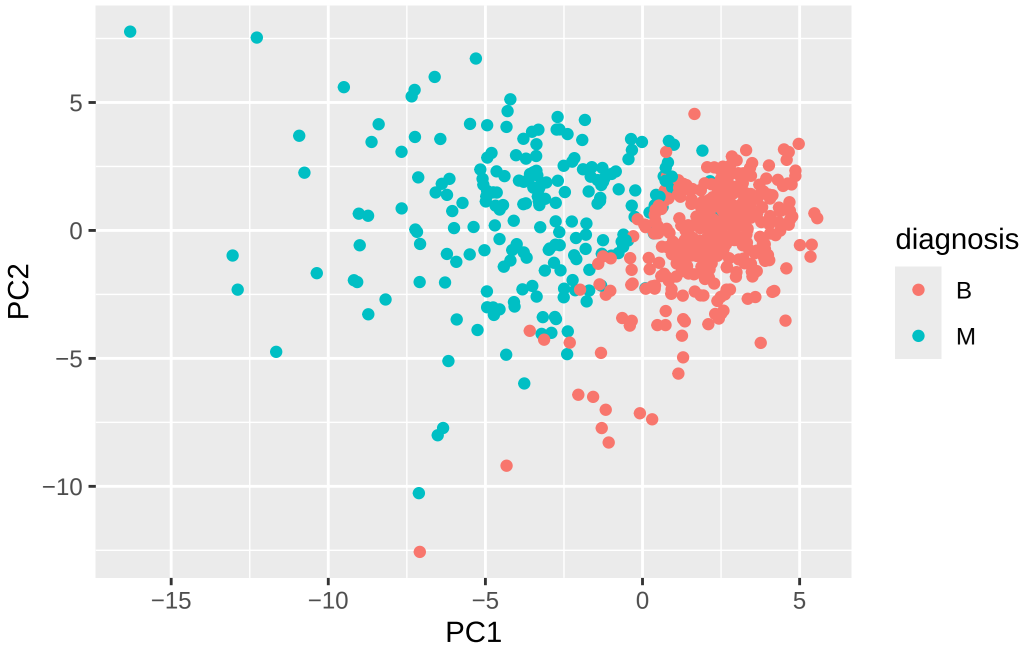
Let’s rename the axis.

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



Make a ggplot version of this score plot

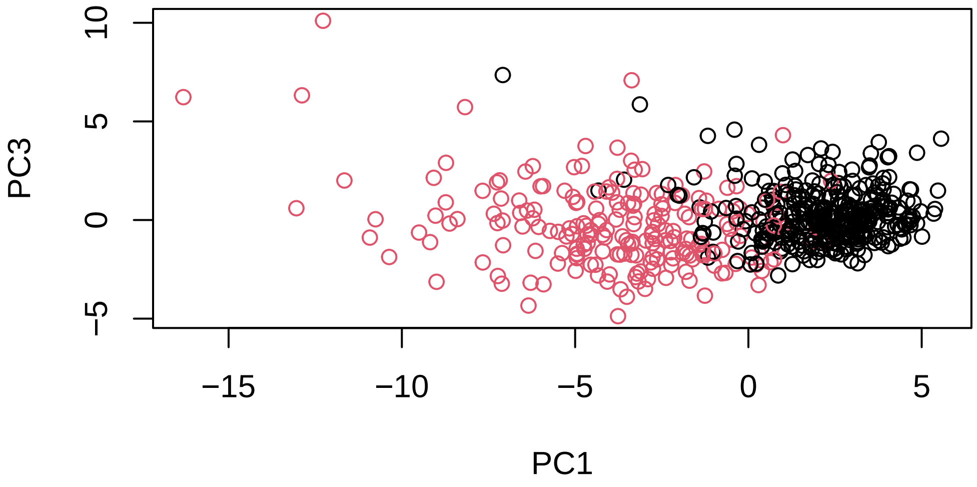
```r
pc <- as.data.frame(wisc.pr$x)

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



PCA compresses data into something that captures the essence of the original data -> takes a dataset with a lot of dimensions and flattens it into 2 or 3 dimensions so we can look at it.

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

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



Variance Explained

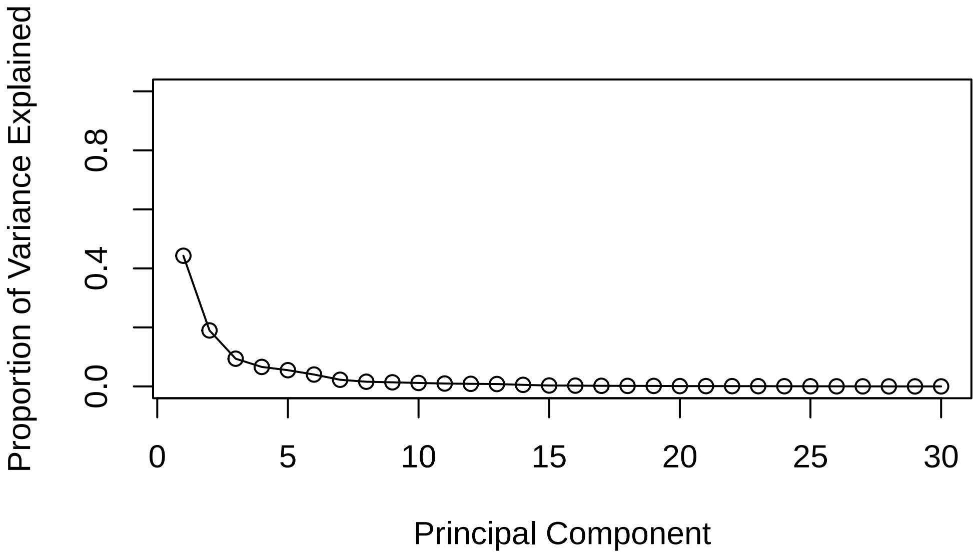
```
#Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

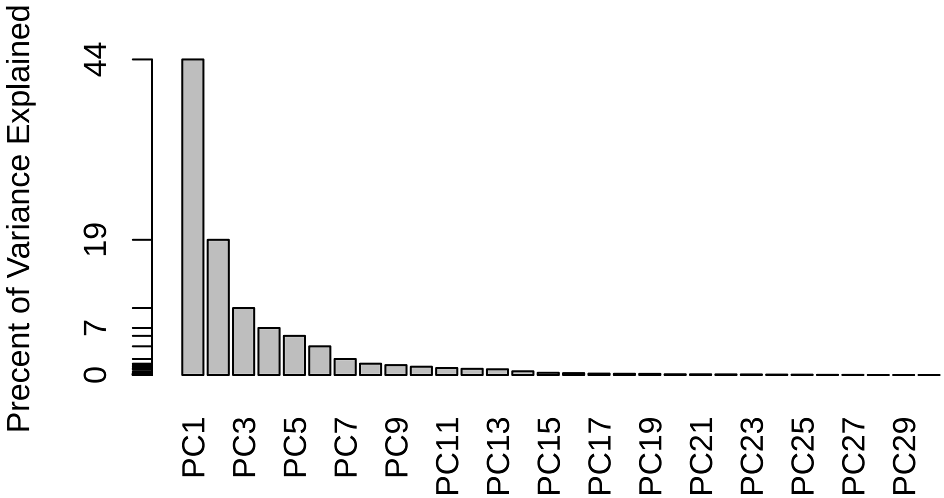
```
pr.var/sum(pr.var)
```

```
 [1] 4.427203e-01 1.897118e-01 9.393163e-02 6.602135e-02 5.495768e-02
 [6] 4.024522e-02 2.250734e-02 1.588724e-02 1.389649e-02 1.168978e-02
[11] 9.797190e-03 8.705379e-03 8.045250e-03 5.233657e-03 3.137832e-03
[16] 2.662093e-03 1.979968e-03 1.753959e-03 1.649253e-03 1.038647e-03
[21] 9.990965e-04 9.146468e-04 8.113613e-04 6.018336e-04 5.160424e-04
[26] 2.725880e-04 2.300155e-04 5.297793e-05 2.496010e-05 4.434827e-06
```

```
# 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")
```



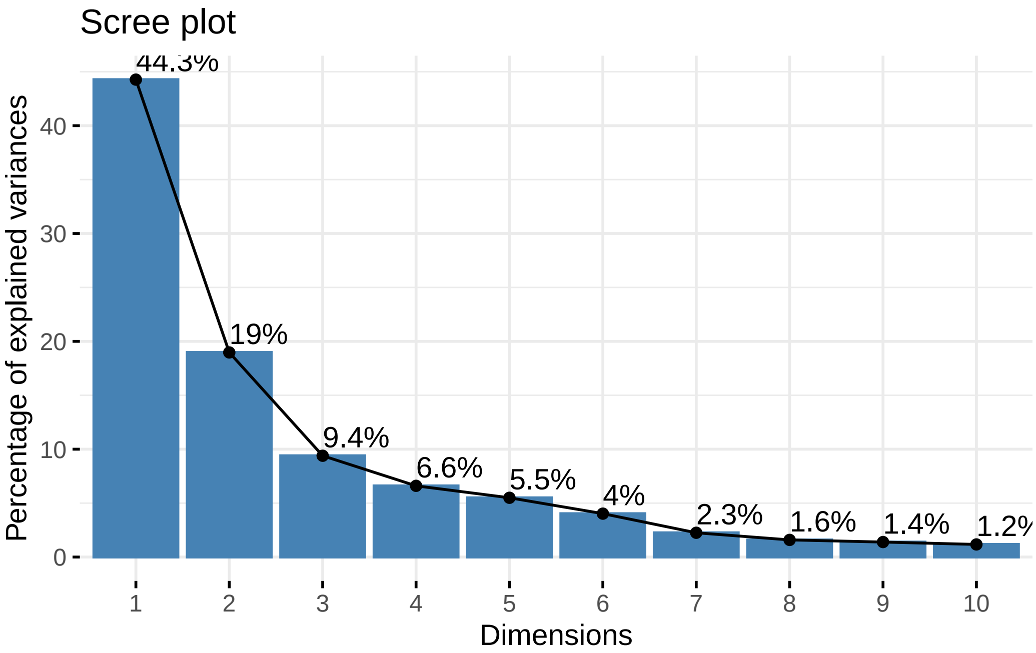
```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```



```
## ggplot based graph
#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

> 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
```

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

PC5

Hierarchal Clustering

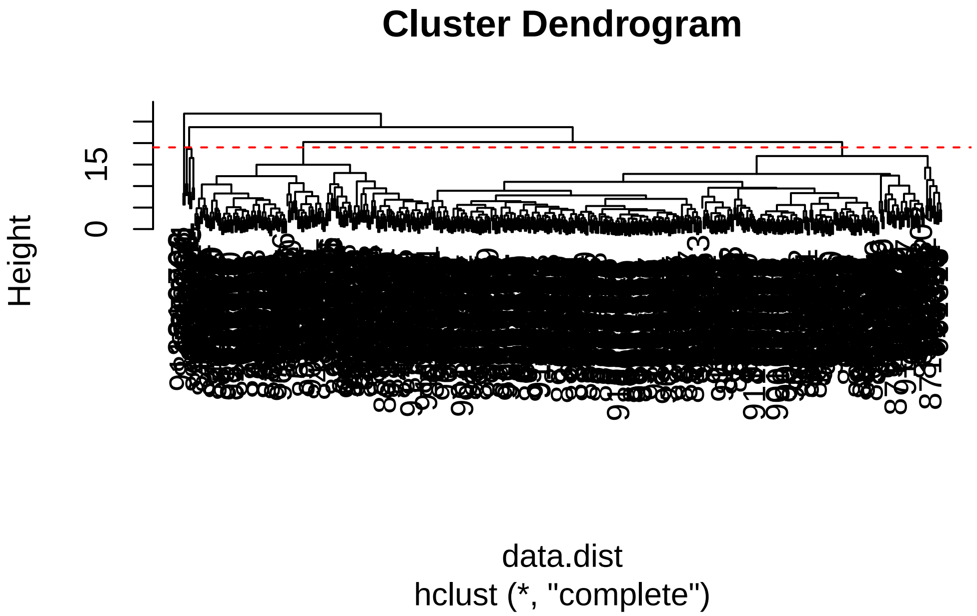
```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
```

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

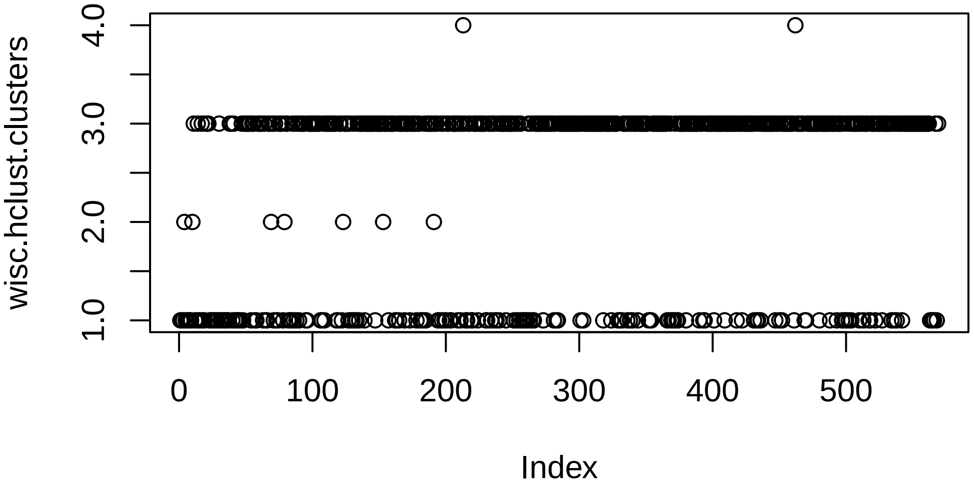
Results of Hierarchal Clustering

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

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



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

plot(wisc.hclust.clusters)
```



```r
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?

```r
wisc.hclust.clusters_2 <- cutree(wisc.hclust, k=2)
table(wisc.hclust.clusters_2, diagnosis)
```

```
                      diagnosis
wisc.hclust.clusters_2   B   M
                     1 357 210
                     2   0   2
```

```
wisc.hclust.clusters_3 <- cutree(wisc.hclust, k=3)
table(wisc.hclust.clusters_3, diagnosis)
```

```
                      diagnosis
wisc.hclust.clusters_3   B   M
                     1 355 205
                     2   2   5
                     3   0   2
```

```
wisc.hclust.clusters_6 <- cutree(wisc.hclust, k=6)
table(wisc.hclust.clusters_6, diagnosis)
```

```
                      diagnosis
wisc.hclust.clusters_6   B   M
                     1  12 165
                     2   0   5
                     3 331  39
                     4   2   0
                     5  12   1
                     6   0   2
```

```
wisc.hclust.clusters_10 <- cutree(wisc.hclust, k=10)
table(wisc.hclust.clusters_10, diagnosis)
```

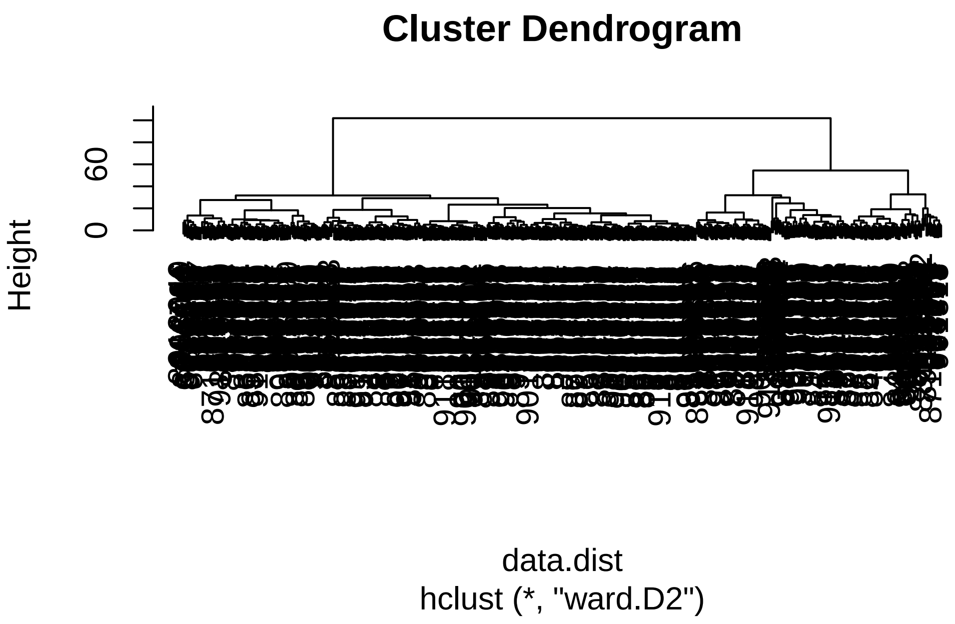
```
                       diagnosis
wisc.hclust.clusters_10   B   M
                     1   12  86
                     2    0  59
                     3    0   3
                     4  331  39
                     5    0  20
                     6    2   0
                     7   12   0
                     8    0   2
                     9    0   2
                     10   0   1
```

None of them were good, since every clustering method did not have distinct benign and malignant grouping.

Using Different Methods

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

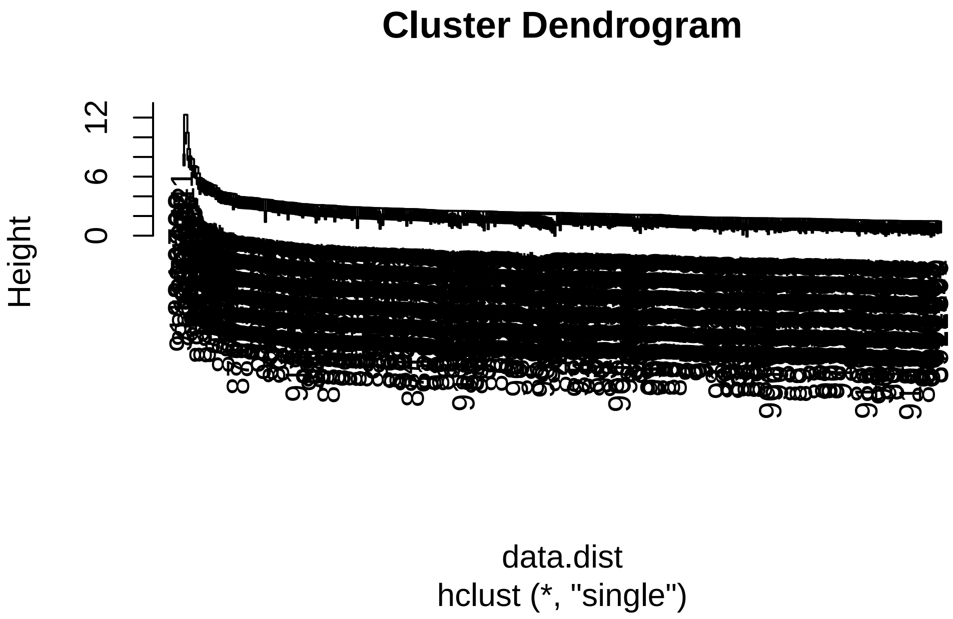
```
wisc.hclust_ward.d2 <- hclust(data.dist, "ward.D2")

plot(wisc.hclust_ward.d2)
```



```
wisc.hclust.clusters_d2 <- cutree(wisc.hclust_ward.d2, k=3)
table(wisc.hclust.clusters_d2, diagnosis)
```

```
                       diagnosis
wisc.hclust.clusters_d2   B   M
                      1   0 115
                      2  20  49
                      3 337  48
```

```
wisc.hclust_single <- hclust(data.dist, "single")

plot(wisc.hclust_single)
```



I like “ward.D2” because when using it to cluster, it can cluster them into groups that are more only malignant or benign compared to before.

Clustering in PC Space

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

```
               PC1        PC2        PC3
842302   -9.184755  -1.946870 -1.1221788
842517   -2.385703   3.764859 -0.5288274
84300903 -5.728855   1.074229 -0.5512625
84348301 -7.116691 -10.266556 -3.2299475
84358402 -3.931842   1.946359  1.3885450
843786   -2.378155  -3.946456 -2.9322967
```

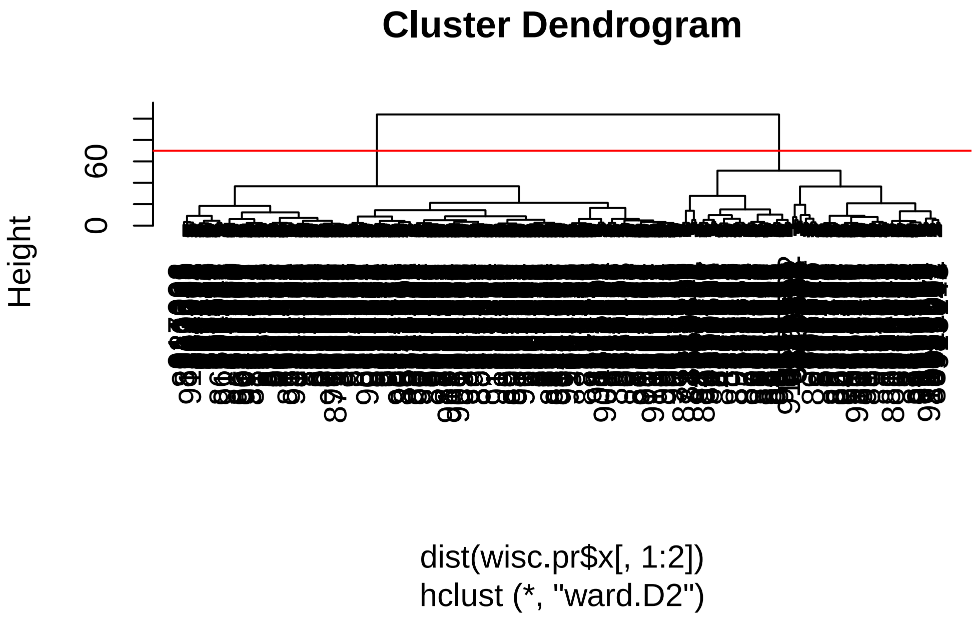
K-means Clustering (setting variables for future sections)

```
wisc.km <- kmeans(wisc.data, centers= 2, nstart= 20)
table(wisc.km$cluster, diagnosis)
```

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

Combining Methods

```
hc <- hclust(dist(wisc.pr$x[, 1:2]), method = "ward.D2")

plot(hc)
abline(h=70, col="red")
```



Cluster Membership Vector

```
grps <- cutree(hc, h=70)
table(grps)
```

```
grps
  1   2
195 374
```

```
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

Cross-table to see how my clustering groups correspond to the expert diagnosis vector of M and B values

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

```
    diagnosis
grps   B   M
   1  18 177
   2 339  35
```

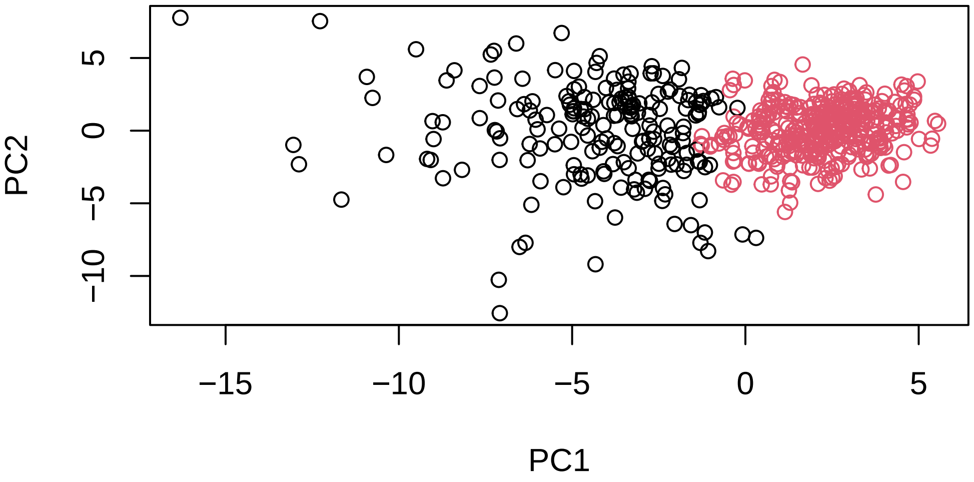
Group 1 has mostly malignant and group 2 has mostly benign.

Positive => cancer ("M") Negative => non-cancerous ("B")

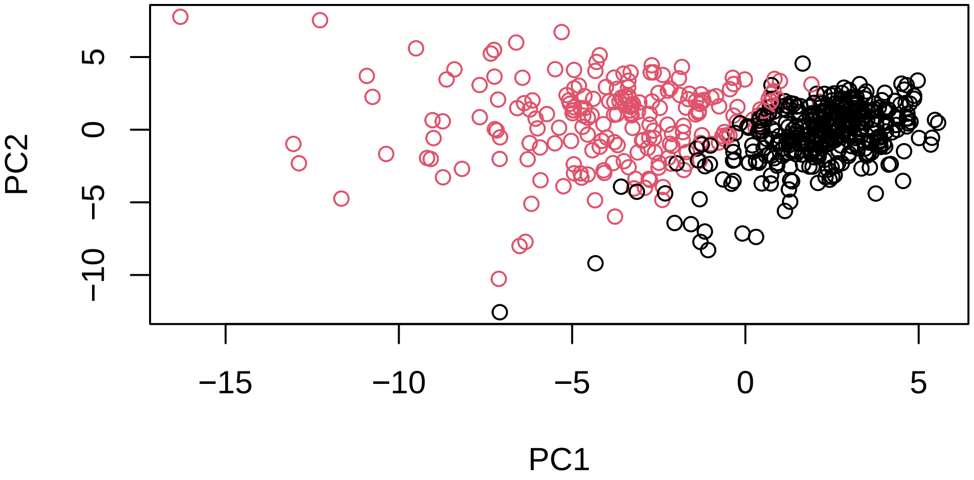
True = Cluster/Group 1 False = Cluster/Group 2

True Positive: 177 False Positive: 18 True Negative: 339 False Negative: 35

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



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



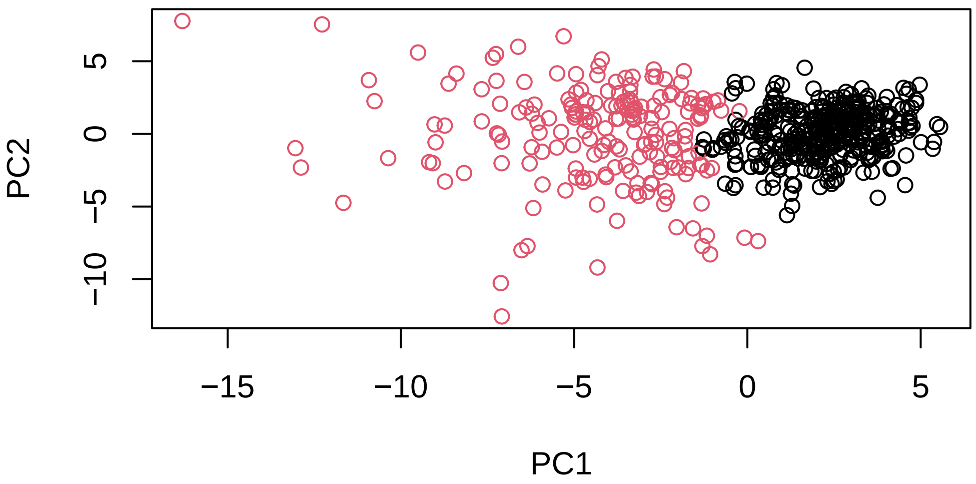
```
g <- as.factor(grps)
levels(g)
```

```
[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)
table(wisc.pr.hclust.clusters)
```

```
wisc.pr.hclust.clusters
  1   2 
216 353 
```

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

```
wisc.pr.hclust.clusters_4 <- cutree(wisc.pr.hclust, k=4)
table(wisc.pr.hclust.clusters_4)
```

```
wisc.pr.hclust.clusters_4
  1   2   3   4 
 45  79  92 353 
```

```
# Compare to actual diagnoses
table(wisc.pr.hclust.clusters_4, diagnosis)
```

```
                         diagnosis
wisc.pr.hclust.clusters_4   B   M
                        1   0  45
                        2   2  77
                        3  26  66
                        4 329  24
```

The newly created model with 4 clusters separates the two diagnoses out better, but the clusters still aren't distinctly only benign or malignant.

> Q 16. 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.

```
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  12 165
                   2   2   5
                   3 343  40
                   4   0   2
```

The k-means and hierarchical clustering models does a lot better in separating the diagnosis compared to previous sections. We can now have the data sorted into clusters of benign and malignant when before we only had the dendrogram clusters to base off of.

Sensitivity/Specificity

Sensitivity refers to a test's ability to correctly detect ill patients who do have the condition. In our example here the sensitivity is the total number of samples in the cluster identified as predominantly malignant (cancerous) divided by the total number of known malignant samples. In other words: TP/(TP+FN).

Specificity relates to a test's ability to correctly reject healthy patients without a condition. In our example specificity is the proportion of benign (not cancerous) samples in the cluster identified as predominantly benign that are known to be benign. In other words: TN/(TN+FN).

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

The ward.D2 clustering model has the best specificity.

```
#Specificity calculations for the k-means clustering model.
130/(130+82)
```

```
[1] 0.6132075
```

```
#Specificity calculations for the ward.D2 clustering model
165/(5+40+2+165)
```

```
[1] 0.7783019
```

The k-means clustering model has the best sensitivity.

```
#Sensitivity calculations model for the k-means clustering model
356/(356+1)
```

```
[1] 0.9971989
```

```
#Sensitivity calculations model for the ward.D2 clustering model
343/(343+2+12)
```

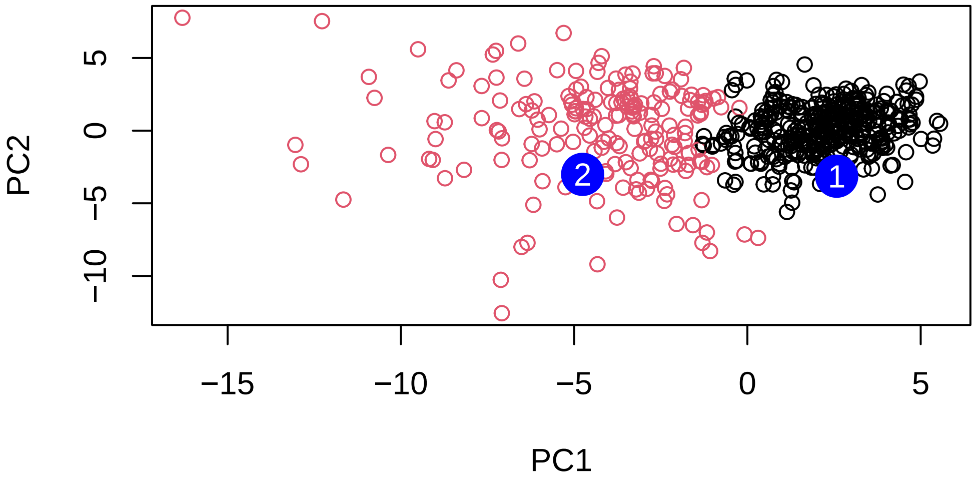
```
[1] 0.9607843
```

Prediction

We can use our PCA results (wisc.pr) to make predictions on new unseen data.

```
#url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
```

```
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 group 2 to follow up on based on our results. They are the group in the malignant diagnosis group.