Class08 MiniProject

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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/FLASE` 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 
```

Standard deviation per column:

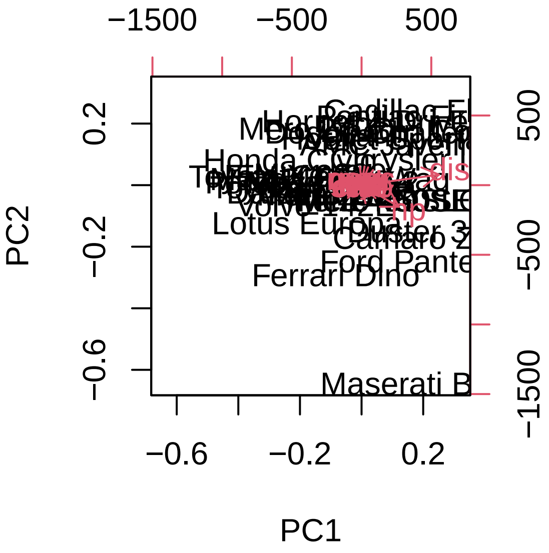
```
apply(mtcars, 2, sd)
```

```
        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 “disp” and “hp” have the highest mean values and the highest standard deviation here. They will likely dominate any analysis I do on this dataset. Let’s see…

```r
pca.noscale <- prcomp(mtcars, scale=FALSE)

pca.scale <- prcomp(mtcars, scale=TRUE)
```

```r
biplot(pca.noscale)
```



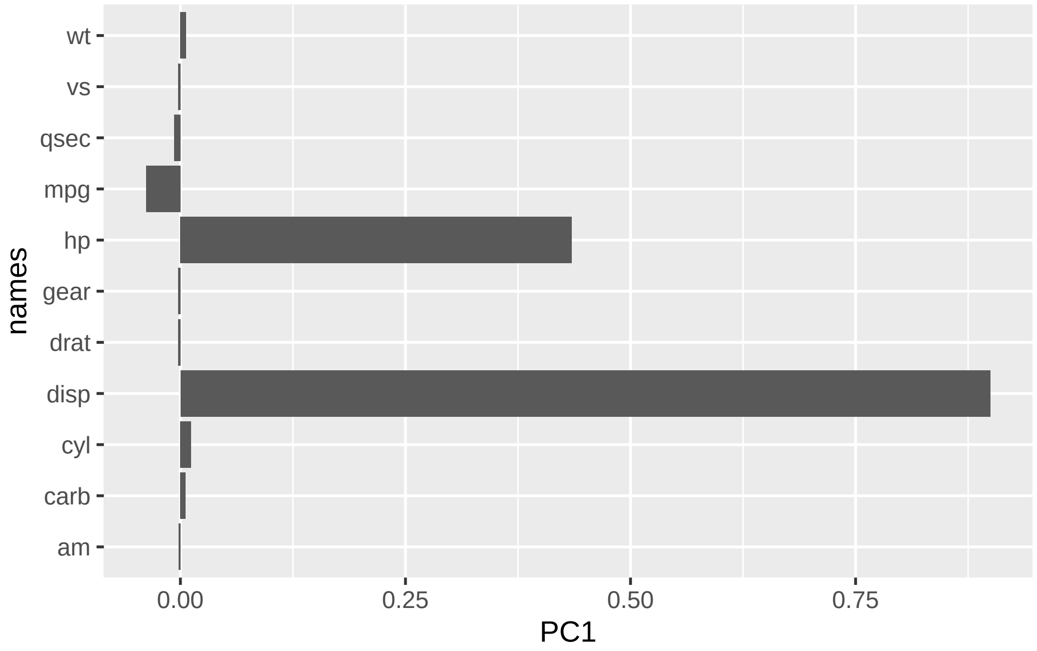
```r
pca.noscale$rotation[,1]
```

```
          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
```

We can see how displacement and hp are the main two componenets that contribute to this dataset.

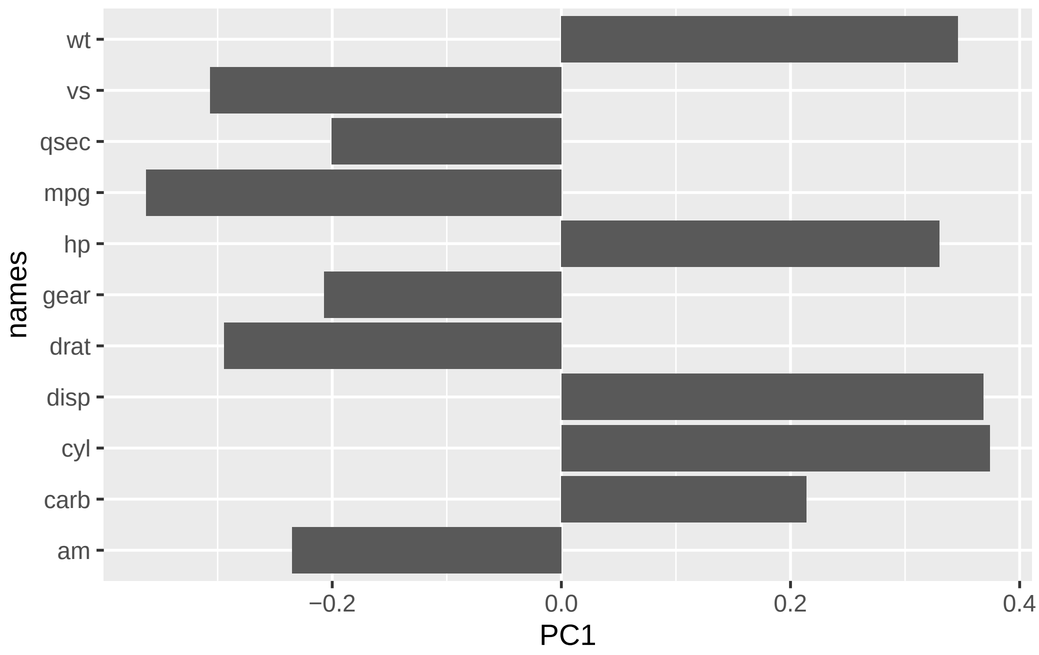
plot the loadings

```
library(ggplot2)
r1 <- as.data.frame(pca.noscale$rotation)
r1$names <- rownames(pca.noscale$rotation)

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

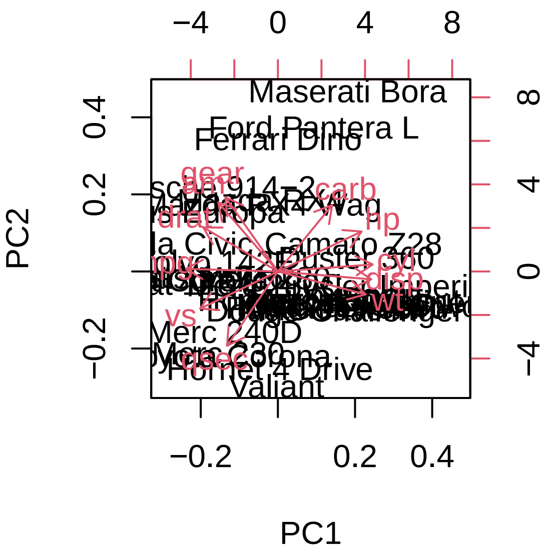


We can see the values that dominate this dataset with the largest varition and standard deviation in this plot above.

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

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



```
biplot(pca.scale)
```



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

FNA Breast Cancer Data

Load the data into R.

```r
wisc.df <- read.csv("WisconsinCancer (1).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
```

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 also 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
```

There are 31 total columns in the dataset with the names:

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

```
[1] 10
```

Before we continue, we need to exclude the diagnoses column from any further analysis. The column `diagnosis` is an expert provided diagnosis whether the cell is malignant or not. This tells use whether a sample is cancerous or non-cancerous.

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

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

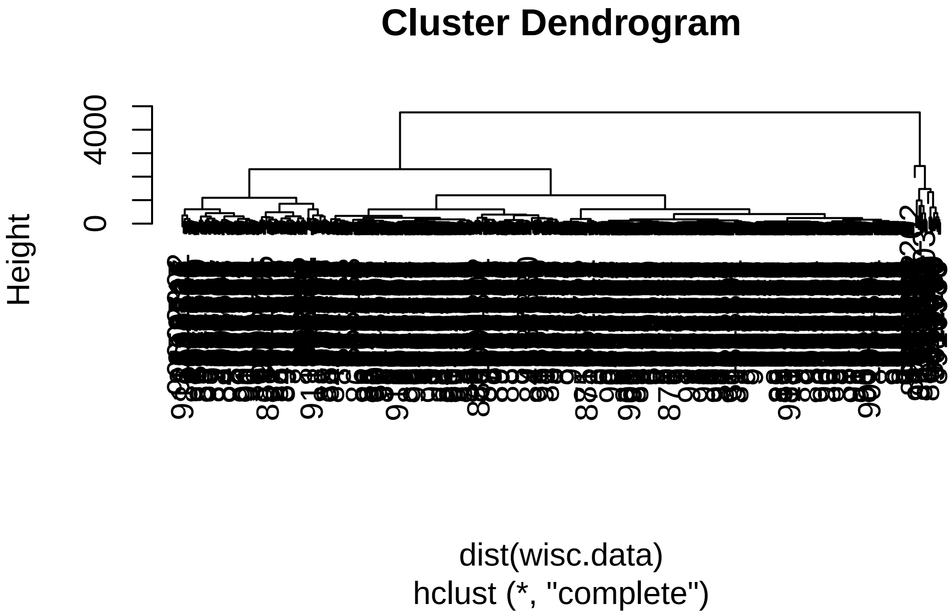
To remove this column:

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

Performing PCA

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

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



Principal Component Analysis(PCA)

First, check the mean and standard deviation of the columns to check if the data needs to be scaled.

```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
```

```r
wisc.pr <- prcomp(wisc.data, 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
```

> Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)?

~44% of variance is captured by PC1.

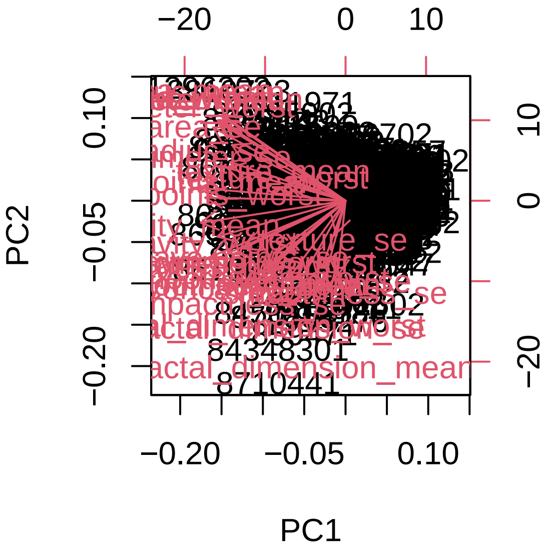
> Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

To describe at least 70% of the original variance, three PCs are required.

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

To describe at leas 90% of the original variance, 7 PCs are required.

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



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

This plot has a lot of data points that are impacted by the variables. However, this dataset is very large, and this biplot only works for smaller datasets. This plot is not helpful for a large dataset, so we need to build our own PCA score plot of PC1 vs. PC2.

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

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

$class
[1] "prcomp"
```

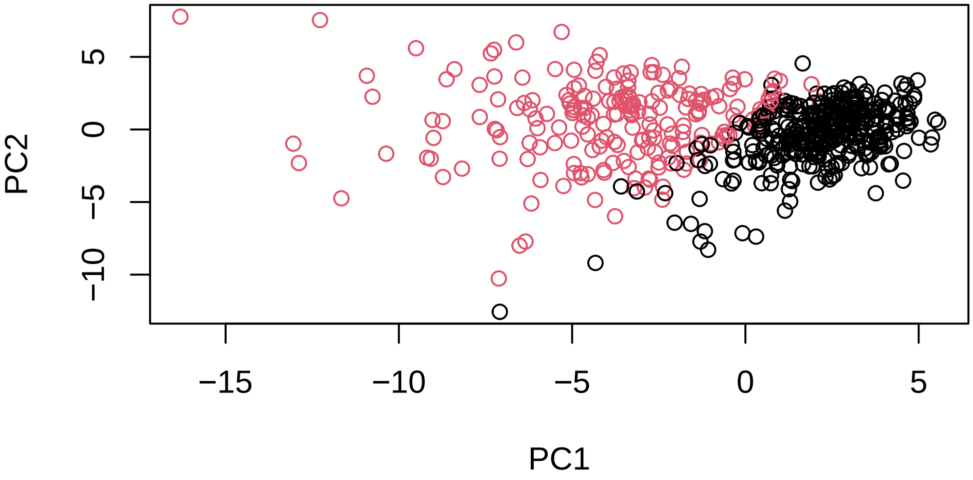
```r
head(wisc.pr$x)
```

```
               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
```

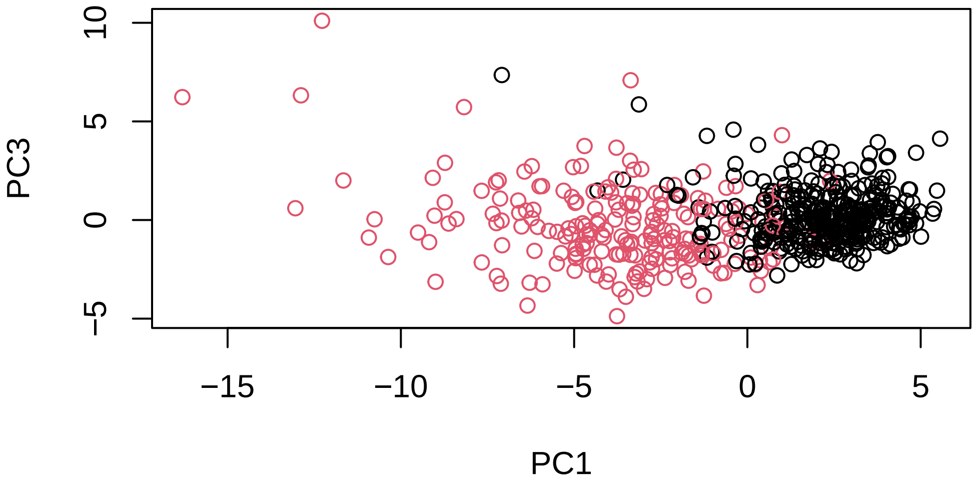
Plot of PC1 vs PC2(the first two columns).

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



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

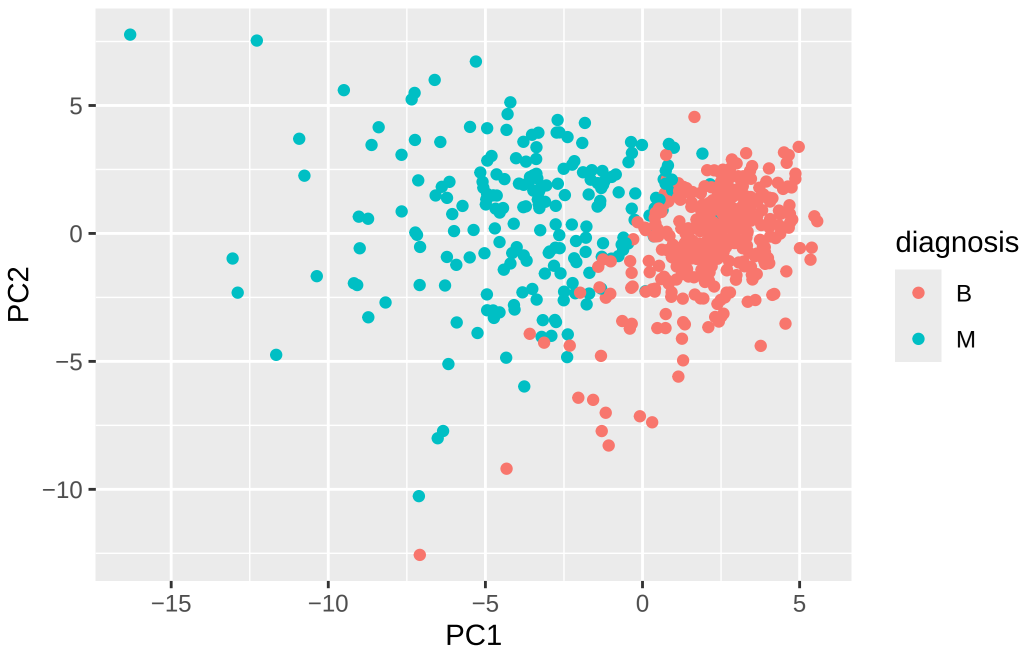
```
plot(wisc.pr$x[,1], wisc.pr$x[,3], col=diagnosis, xlab="PC1", ylab="PC3")
```



This plot has less separation between the two subgroups because PC3 explains less variance in the original dataset than PC2.

Make a ggplot version of PC1 vs PC2 score plot:

```
pc <- as.data.frame(wisc.pr$x)
library(ggplot2)
ggplot(pc) + aes(PC1, PC2, col=diagnosis) + geom_point()
```



This PCA plot shows a separation of Malignant(turquoise) from benign(red) samples. Each point represents a sample and its measured cell characteristics in the dataset. The general idea is that cells with similar characteristics should cluster.

Variance Explained

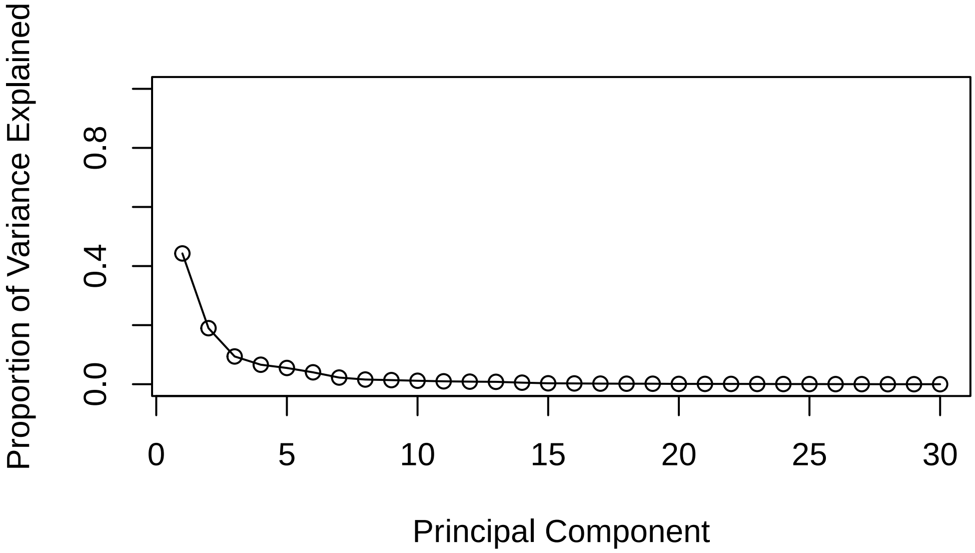
calculate the variance of each principal component by squaring the sdev component of `wisc.pr`.

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

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

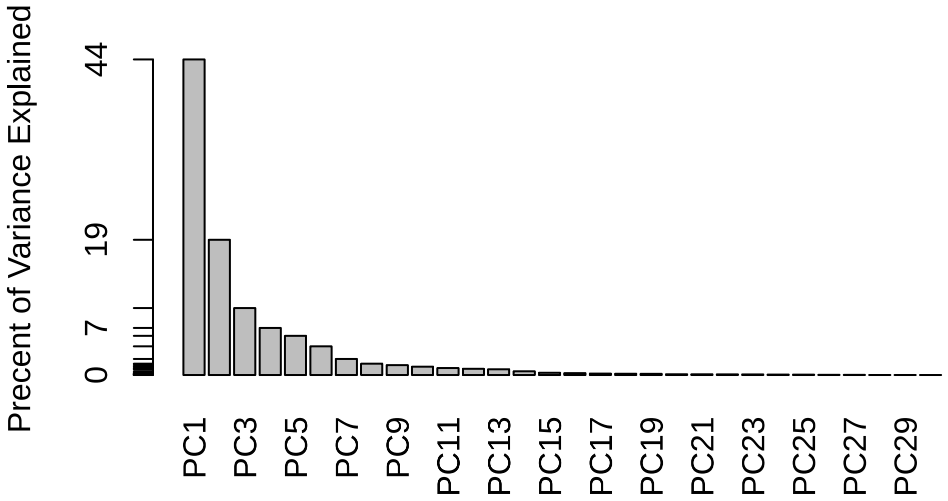
Now calculate the variance explained by each PC by dividing by the total variance explained of all PCs.

```
pve <- pr.var/sum(pr.var)

plot(pve, xlab="Principal Component", ylab="Proportion of Variance Explained", ylim=c(0,1), 
```



Now plot as a bar plot:

```
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 )
```

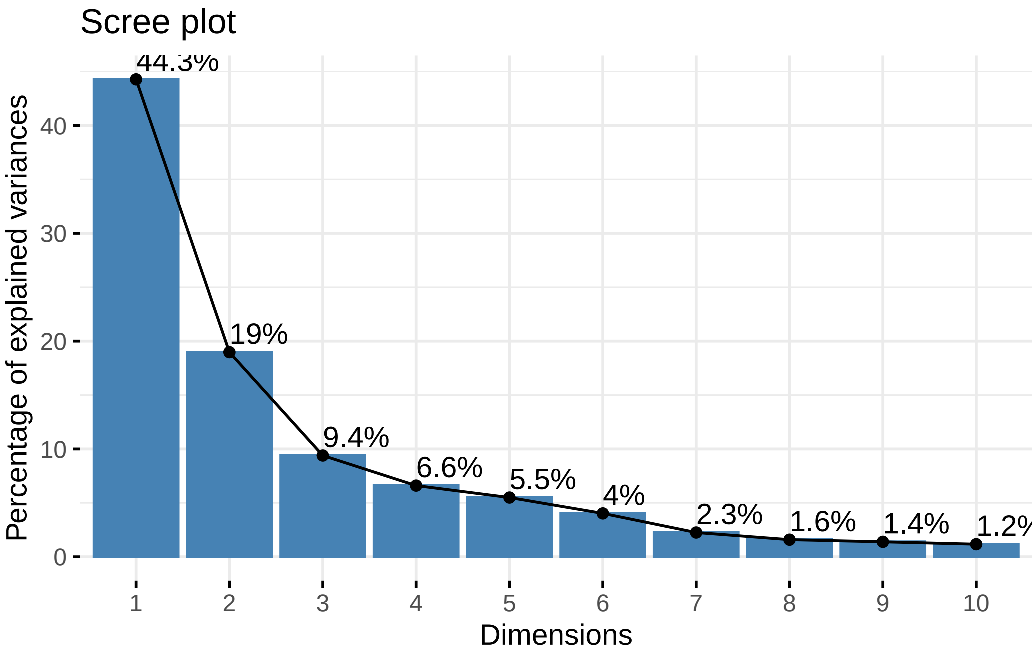


ggplot based graph:

```
#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

Loadings, represented as vectors, explain the mapping from the original features to the principal components.

> 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?

```r
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?

The minimum number of PCs required to explain 80% of the variance of the data is four according to the ggplot-based graph of variance.

Hierarchical Clustering

To perform hierarchical clustering on the original data, we first must scale the data using the `scale()` function.

```
data.scaled <- scale(wisc.data)
```

Calculate the distances between all pairs of observation in the new scaled data.

```
data.dist <- dist(data.scaled)
```

Create a hierarchical clustering model using complete linkage:

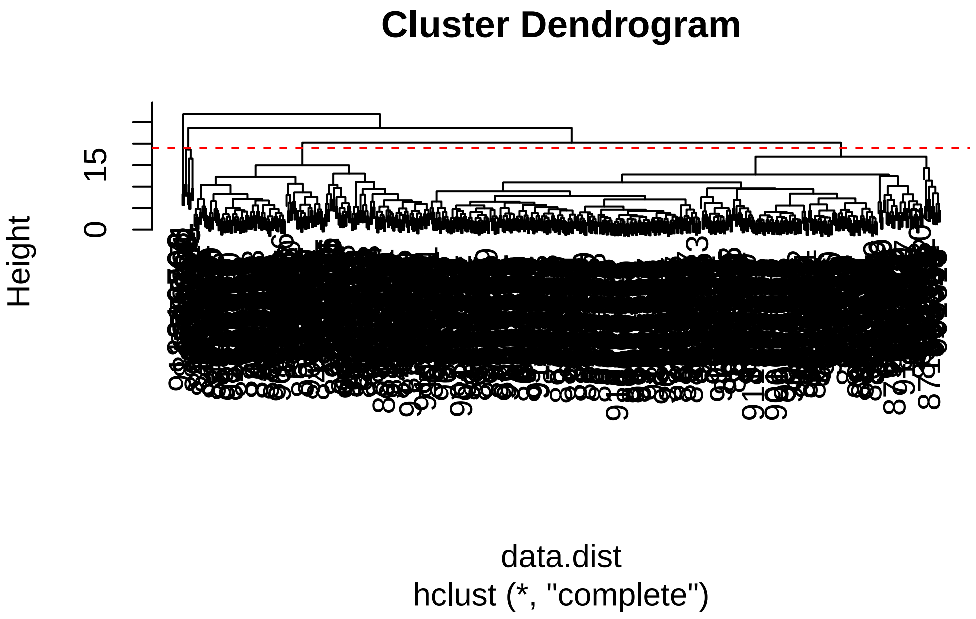
```
wisc.hclust <- hclust(data.dist, method="complete")
```

Now plot using `plot()` and `abline()`functions:

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

At height h=19, we can cut the cluster model into four clusters.

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



Selecting Number of Clusters

When performing supervised learning, use clustering to create new features may or may not improve the performance of the final model.

Use `cutree()` to cut the tree into 4 clusters.

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

Compare the cluster membership to 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
```

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

```
wisc.hclust.clusters <- cutree(wisc.hclust, k=5)
table(wisc.hclust.clusters, diagnosis)
```

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

We can see that as the number of clusters increases, it becomes a “messier” system. These clusters are not indicative for being malignant or benign. Depending on the data, the number of clusters varies on what is considered “better” for analysis.

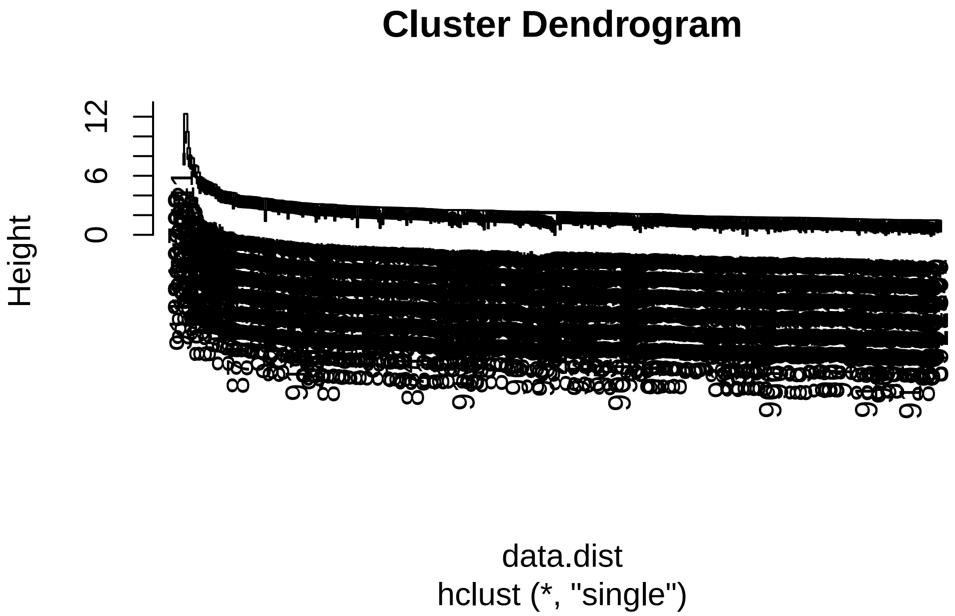
Using Different Methods.

There are a number of different methods to combine points during hierarchical clustering procedure, including "single", "complete", "average", and "ward.D2".

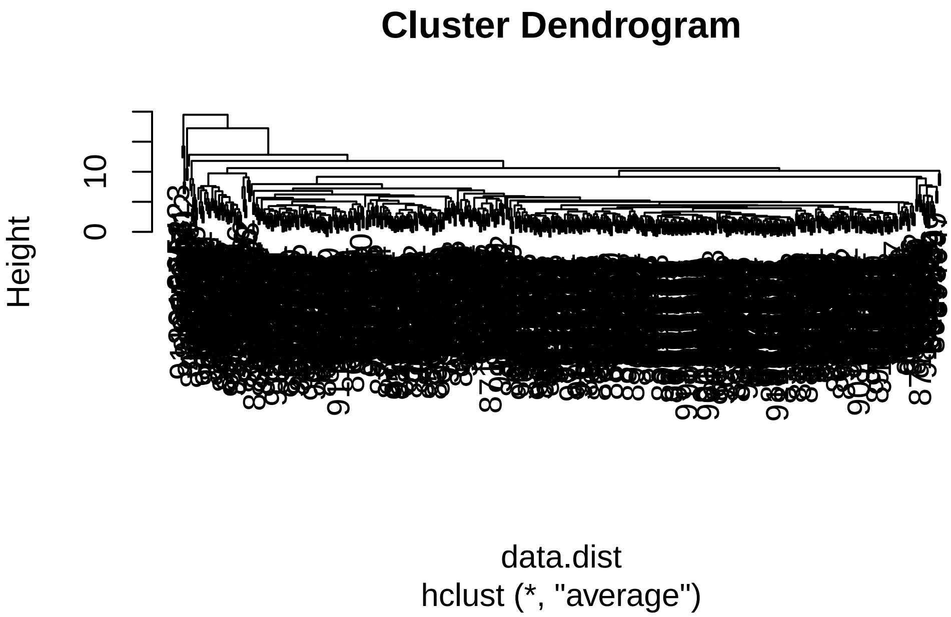
> Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

Each method has its own benefits depending on the dataset and analysis being conducted. for the data.dist dataset, my favorite is the "ward.D2" method because this gives the most well-separated clusters compared to the other methods. This method minimizes the amount of variance within clusters, while the other methods cluster based on the distances of variance between points. In these methods, we see skewed dendrograms compared to the dendrogram using the ward.D2 method.

```r
wisc.hclust.single <- hclust(data.dist, method="single")
plot(wisc.hclust.single)
```



```r
wisc.hclust.average <- hclust(data.dist, method="average")
plot(wisc.hclust.average)
```

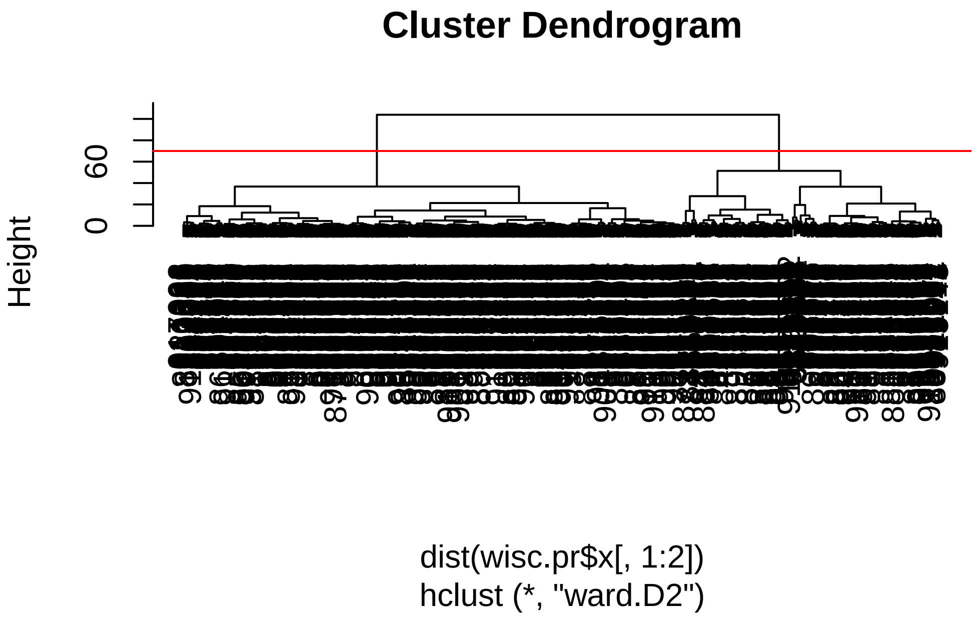


Clustering on PCA Results

In earlier sections, we see that PCA models requires significantly fewer features to describe 70, 80, and 95% of the variability in the data. Let's see if PCA improves or degreades the perfromance of hierarchial clustering.

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

```
plot(wisc.pr.hclust)
abline(h=70, col="red")
```



Cluster membership vector

```
grps <- cutree(wisc.pr.hclust, 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
```

positive => cancer M negative => non-cancer B

True positive = cluster/grps 1 False positive => grp 2

True positive 177 False positive 18 True negative 339 False negative 35

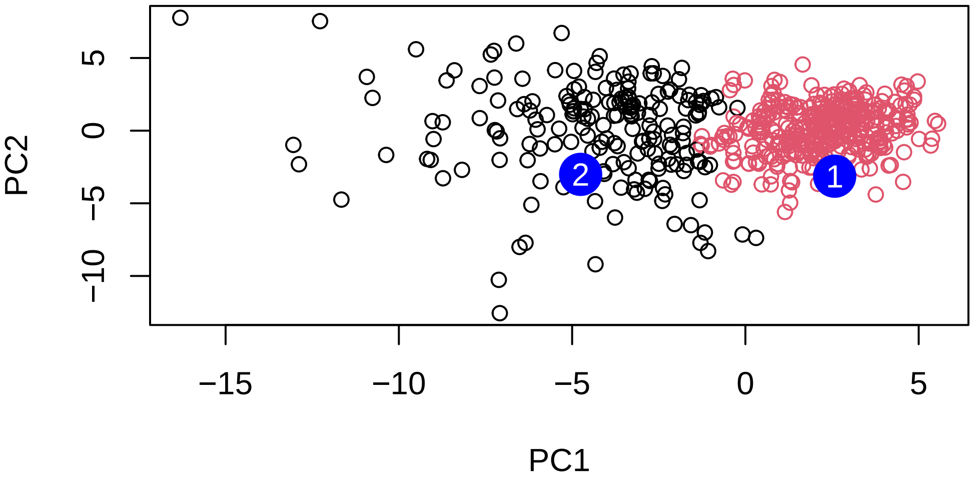
we want to optimize true positive and true negatives, and minimize false positives/negatives.

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

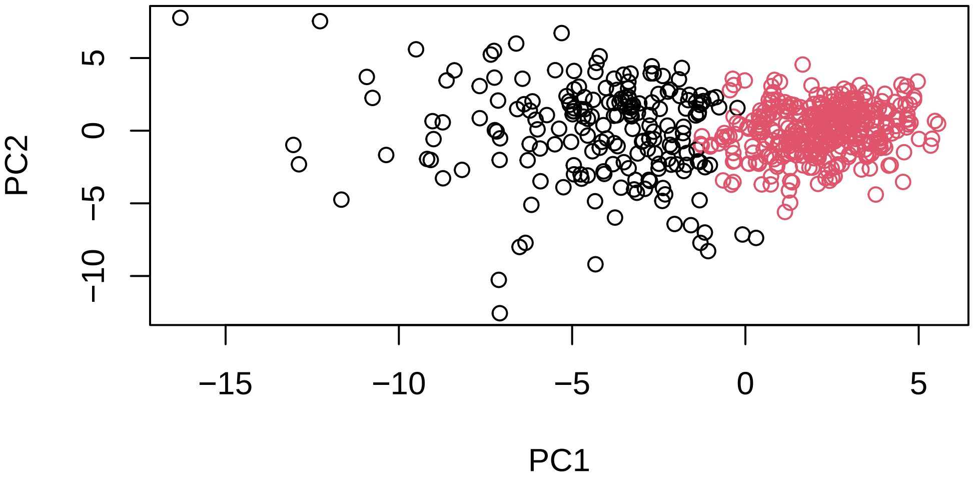
```
#url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
npc
```

```
           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
```

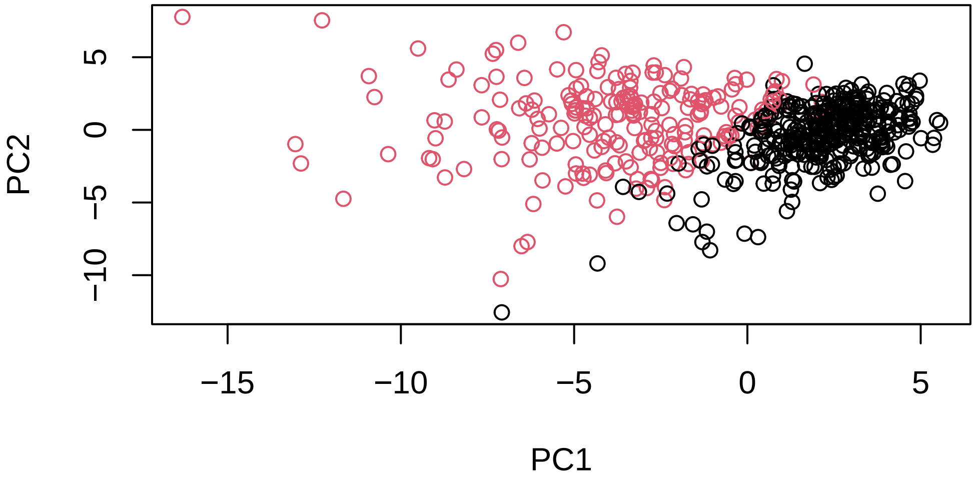
```
plot(wisc.pr$x[,1:2], col=grps)
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



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



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



We perform a color swap to reorder the levels so that cluster 2, which is mostly "B" comes out first with the first color(black) and cluster 1 gets the second color (red), which aligns mostly with "M".

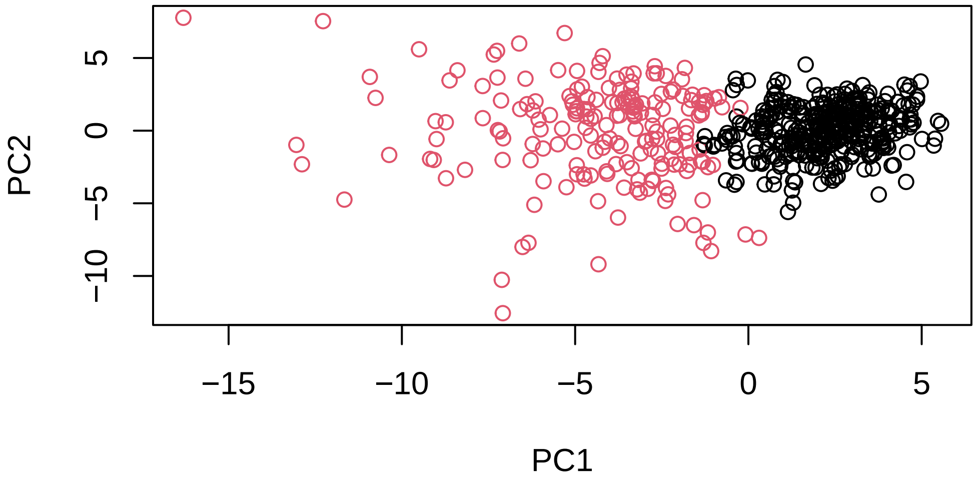
```
g <- as.factor(grps)
levels(g)
```

```
[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)
```



We can also look in 3D with the `rgl` or `plotly` packages. This step will be skipped to avoid difficulties in the PDF report.

```
g2 <- relevel(g, 2)
levels(g2)
```

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

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

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

Use `table()` to compare the results from you new hierarchical clustering model with the actual diagnoses.

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

We can see that there is greater and cleaner separation between B and M, but we still see false positives and negatives in the clusters.

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

```
                       diagnosis
wisc.pr.hclust.clusters   B   M
                      1  20 164
                      2 337  48
```

> Q16. How well do the k-means and hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.km$cluster and wisc.hclust.clusters) with the vector containing the actual diagnoses.

Note that wisc.km was not created since this was a part of the optional K-means clustering section. We can see that hierarchical clustering has more clusters than k-means clustering, but this is a more messy outcome. K-means clustering only has two clusters, which has less messy clustering, but we still see the presence of false negatives and false positives. Both methods are not perfect to cluster the diagnoses, resulting in some false results.

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

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

Sensitivity/Specificity

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

Specificity related 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?

K-means clustering:

-sensitivity: (175)/(175+14)=0.92 –> better at identifying malignant cases

-specificity: (343)/(343+37)=0.90

Hierarchical clustering using `wisc.pr.hclust.clusters`:

-sensitivity: (188)/(28+188)=0.87

-Specificity: (329)/(329+24)= 0.93–> better at identifying benign cases

The k-means clustering procedure resulted in the clustering model with the best specificity because this is better at identifying malignant cases. The hierarchical clustering methods is the best at identifying true negatives() and has the best specificity with less false negatives.

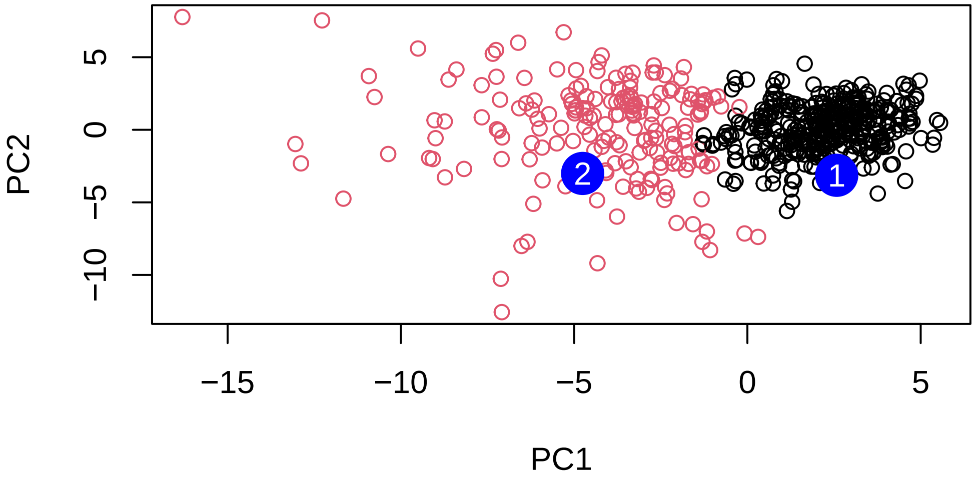
Prediction

we will use the `predict()` function that will take our PC model from before and **new cancer cell data** and project that data onto out PCA space.

```
#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")
```



Q18. Which of these new patients should we prioritize for follow up based on your results?

We should prioritize a follow-up with patient 1 because that cluster is closer together compared to the red cluster where patient 2 is. Since the black cluster is closer together, this limits the number of false positives and false negatives that could result from the tests, and therefore we can trust whether or not patient 1 has cancer that is malignant.