Class08MiniProject

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Today we wiill practice applying our PCA and clustering methods from the last class on some breast cancer FNA data.

Get the dataset into R

To get the csv file into R, right click on the web link to the file, select "save link as" and save the file into the folder where this R project is. Use `row.names = 1` to make the patient identifier the name of the row

```r
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
```

Dataset basic exploration

> Q. How many samples/patients are in this dataset?

There are 569 samples in the dataset (example of in line code)

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

```
[1] 569
```

> Q. How many cancer/non-cancer diagnosis samples are there?

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

```
[1] 212
```

The `table()` function is a super useful utility for counting up the number of observations of each type

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

```

  B   M 
357 212 
```

> Q. How many columns/dimensions are there?

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

```
[1] 31
```

> Q. How many columns are suffixed with "_mean"?

```r
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"
```

The `grep()` function can help us find pattern matches

```r
x <- grep("_mean", colnames(wisc.df))
length(x)
```

```
[1] 10
```

Tidy to remove diagnosis

Save a vector of this expert diagnosis for later and remove it from the data to undergo clustering, PCA etc….

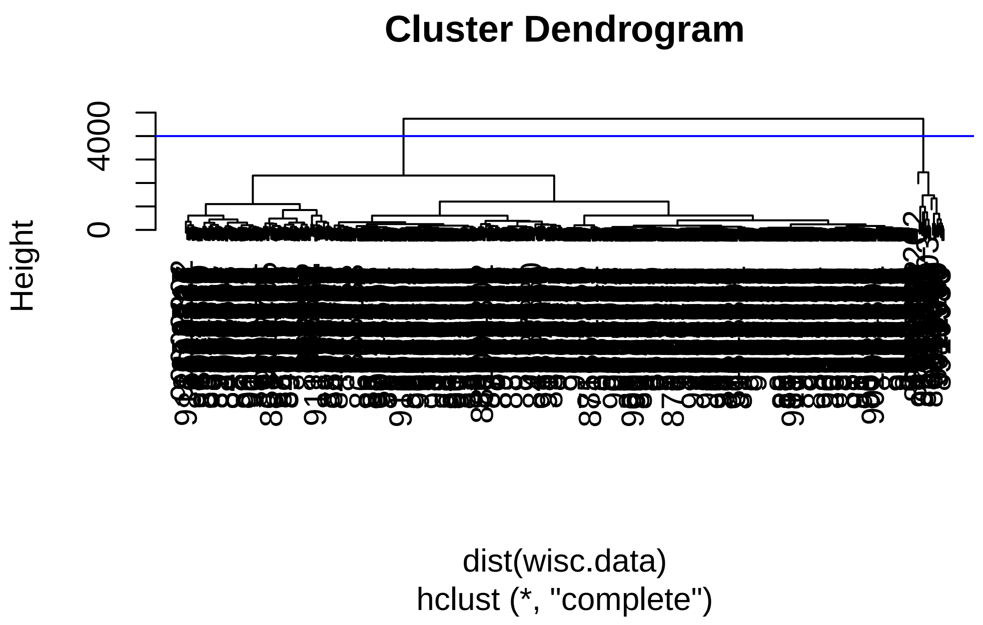
```r
diagnosis <- wisc.df$diagnosis
```

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

Cluster the dataset

Let's try a `hclust()`.

```r
hc.raw <- hclust(dist(wisc.data))
plot(hc.raw)
abline(h=4000, col="blue")
```



To get some clusters out of this I can “cut” the tree at a given height

```r
grps <- cutree(hc.raw, h=4000)
table(grps)
```

```
grps
  1   2 
549  20 
```

To see the correspondance of our cluster `grps` with the expert `diagnosis` I can use `table()`

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

```
    diagnosis
grps   B   M
   1 357 192
   2   0  20
```

That is not that useful of a clustering result.....

Principal Component Analysis (PCA)

Scaling data before analysis is often critical.

Side-note: The default for `prcomp()` is `scale=FALSE`

```
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
```

```
colMeans(mtcars)
```

```
       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
```

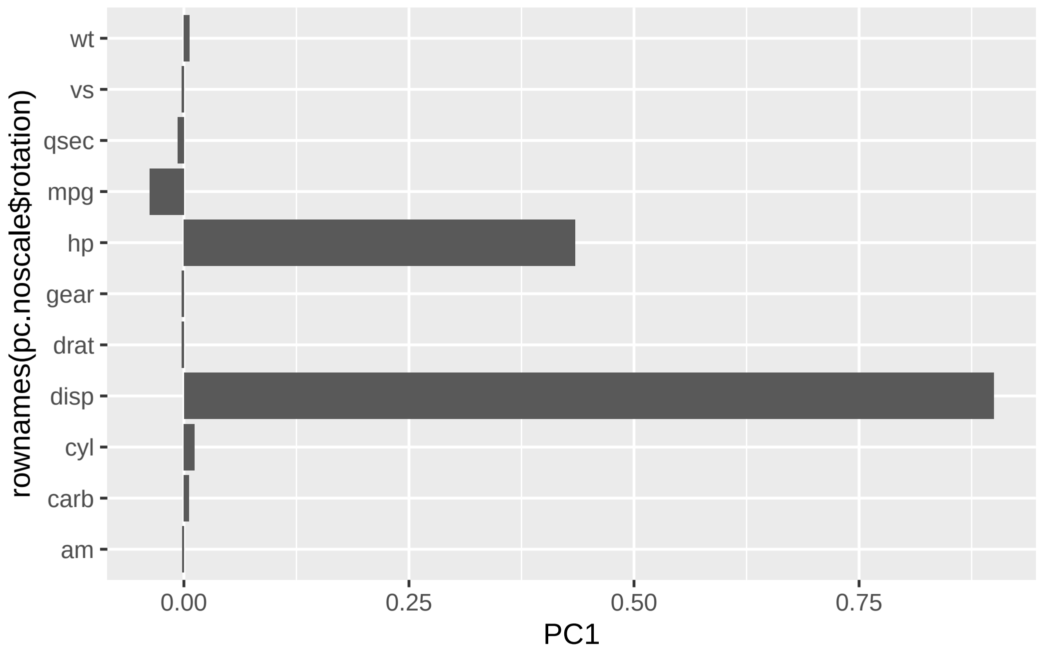
```
pc.noscale <-  prcomp(mtcars, scale=FALSE)
pc.scale <- prcomp(mtcars, scale=TRUE)
```

Let's look at the laodings first:

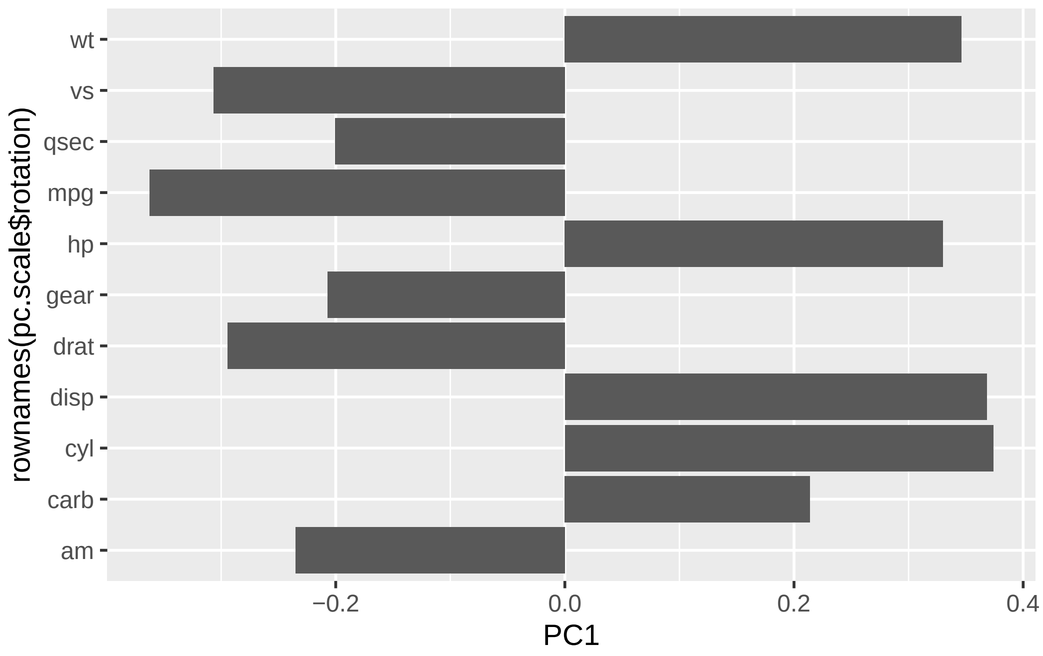
```
head(pc.noscale$rotation)
```

```
              PC1          PC2         PC3          PC4         PC5
mpg  -0.038118199  0.009184847  0.98207085  0.047634784 -0.08832843
cyl   0.012035150 -0.003372487 -0.06348394 -0.227991962  0.23872590
disp  0.899568146  0.435372320  0.03144266 -0.005086826 -0.01073597
hp    0.434784387 -0.899307303  0.02509305  0.035715638  0.01655194
drat -0.002660077 -0.003900205  0.03972493 -0.057129357 -0.13332765
wt    0.006239405  0.004861023 -0.08491026  0.127962867 -0.24354296
              PC6          PC7           PC8          PC9         PC10
mpg  -0.143790084 -0.039239174 -2.271040e-02 -0.002790139  0.030630361
cyl  -0.793818050  0.425011021  1.890403e-01  0.042677206  0.131718534
disp  0.007424138  0.000582398  5.841464e-04  0.003532713 -0.005399132
hp    0.001653685 -0.002212538 -4.748087e-06 -0.003734085  0.001862554
drat  0.227229260  0.034847411  9.385817e-01 -0.014131110  0.184102094
wt   -0.127142296 -0.186558915 -1.561907e-01 -0.390600261  0.829886844
              PC11
mpg   0.0158569365
cyl  -0.1454453628
disp -0.0009420262
hp    0.0021526102
drat  0.0973818815
wt    0.0198581635
```

```r
library(ggplot2)
ggplot(pc.noscale$rotation) + aes(PC1, rownames(pc.noscale$rotation)) + geom_col()
```

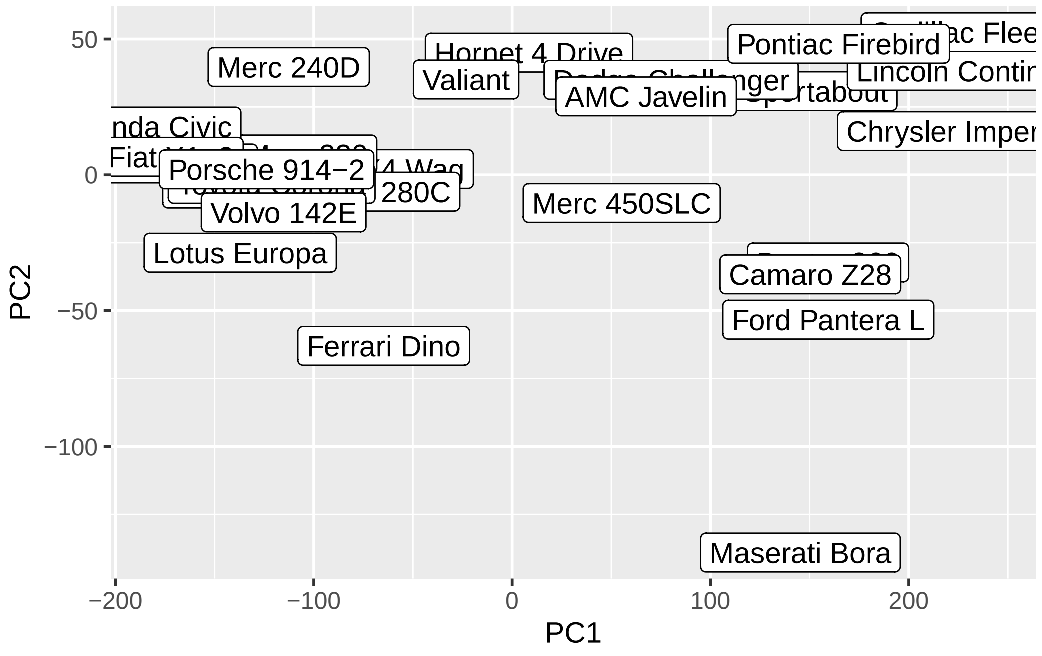


```r
ggplot(pc.scale$rotation) + aes(PC1, rownames(pc.scale$rotation)) + geom_col()
```

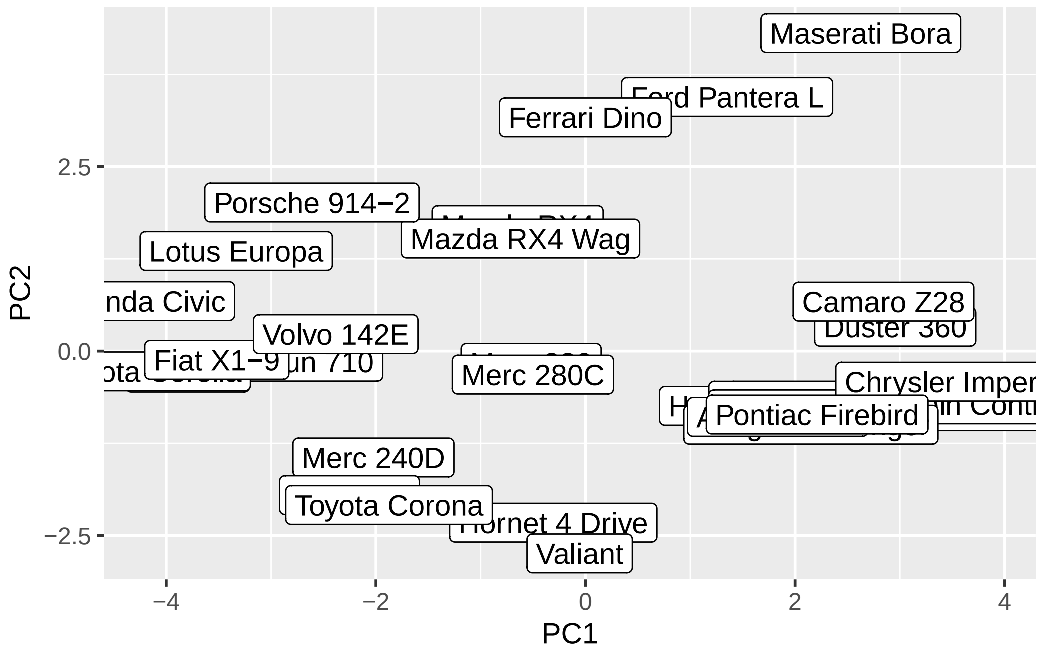


The main PC result figure is often called a “score plot” or “PC plot” or “PC1 vs PC2 plot”

```
ggplot(pc.noscale$x) + aes(PC1, PC2, label=rownames(pc.noscale$x)) + geom_point() + geom_labe
```



```
ggplot(pc.scale$x) + aes(PC1, PC2, label=rownames(pc.scale$x)) + geom_point() + geom_label()
```



What does scaling actually do??

```r
x <- scale(mtcars)
round(colMeans(x))
```

```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb 
   0    0    0    0    0    0    0    0    0    0    0 
```

```r
round(apply(x, 2, sd))
```

```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb 
   1    1    1    1    1    1    1    1    1    1    1 
```

> **Key-point** Generally we want to scale our data before analysis to avoid being misled due to our data having different measurment units.

Breast Cancer PCA

```r
pca <- prcomp(wisc.data, scale=T)
```

see how well we are doing

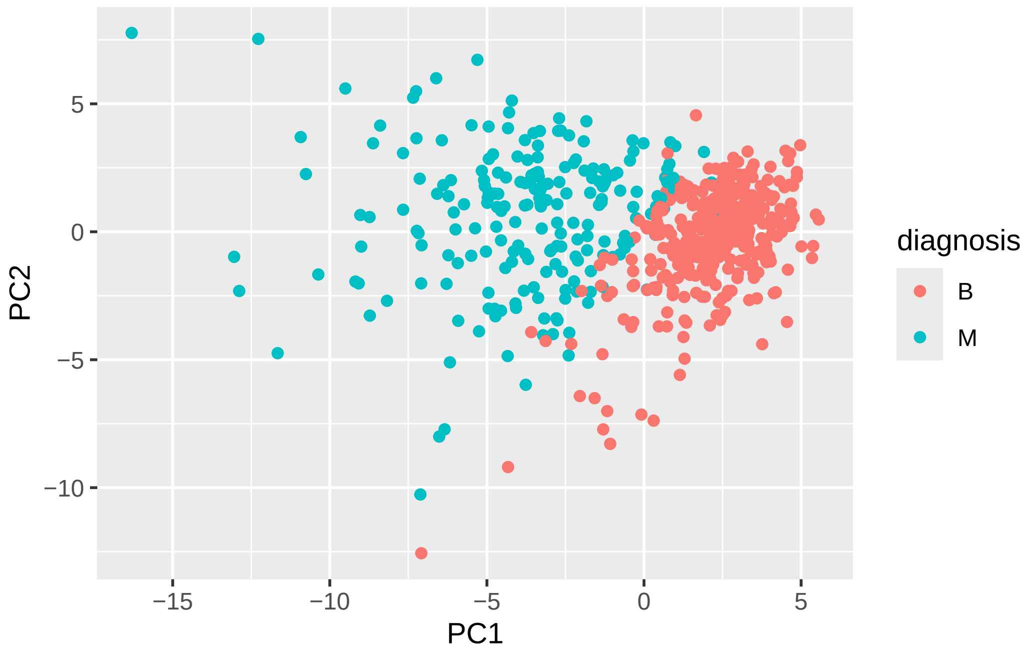
```r
summary(pca)
```

```
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
```

Our PC plot

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



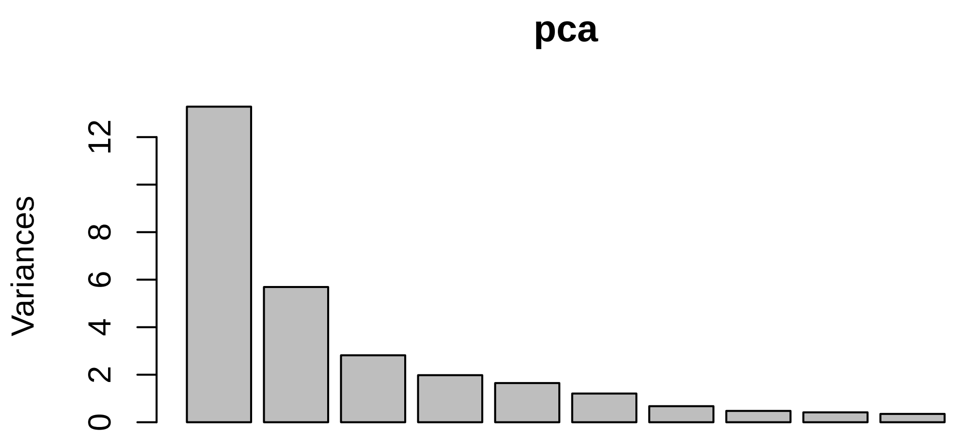
Q. How many PCs capture 80% of the original variance in the dataset?

```
summary(pca)
```

```
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
```

```
plot(pca)
```



Q. Use ggplot to plot a "scree-plot" of the variance per PC

```
attributes(pca)
```

```
$names
```

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

$class
[1] "prcomp"
```

W can extract the sdev and figure out the variance

```r
v <- pca$sdev^2
sum(v)
```

```
[1] 30
```

the proportion of variance captured in each PC

```r
round(v/sum(v), 2)
```

```
 [1] 0.44 0.19 0.09 0.07 0.05 0.04 0.02 0.02 0.01 0.01 0.01 0.01 0.01 0.01 0.00
[16] 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
```

cumulative variance captured

```r
cumsum(v/sum(v))
```

```
 [1] 0.4427203 0.6324321 0.7263637 0.7923851 0.8473427 0.8875880 0.9100953
 [8] 0.9259825 0.9398790 0.9515688 0.9613660 0.9700714 0.9781166 0.9833503
[15] 0.9864881 0.9891502 0.9911302 0.9928841 0.9945334 0.9955720 0.9965711
[22] 0.9974858 0.9982971 0.9988990 0.9994150 0.9996876 0.9999176 0.9999706
[29] 0.9999956 1.0000000
```

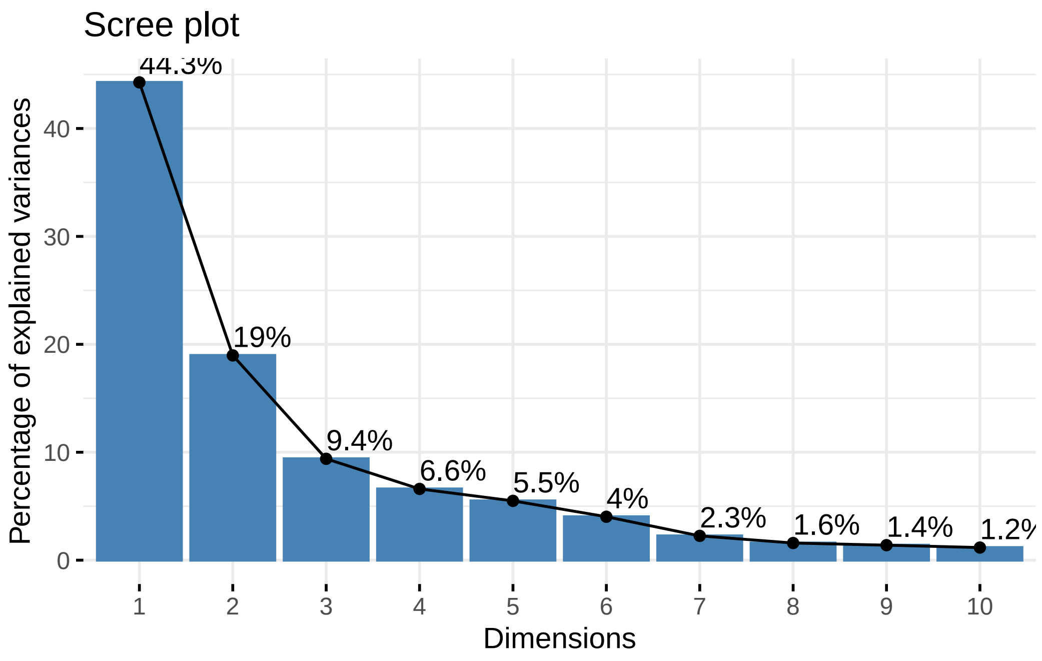
```r
which(cumsum(v/sum(v)) > 0.8)
```

```
 [1]  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29
[26] 30
```

```r
library(factoextra)
```

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

```r
fviz_eig(pca, addlabels = TRUE)
```

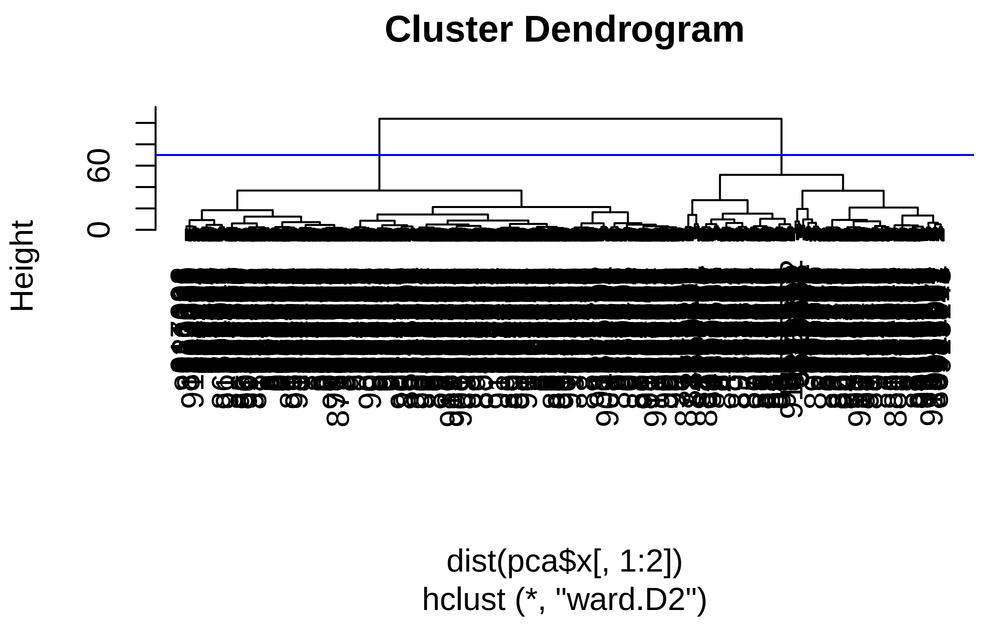


Combine PCA and clustering

We saw earlier that clustering the raw data alone did not provide useful results.

We can use our new PC variables (our PCs) as a basis for clustering. We can use our $x PC scores

```r
hc.pca <- hclust(dist(pca$x[,1:2]), method="ward.D2")
plot(hc.pca)
abline(h=70, col = "blue")
```



> Q. Does your clustering help separate cancer from non-cancer samples (i.e. diagnosis "M" vs "B")?

```r
grps <- cutree(hc.pca, h=70)
table(grps, diagnosis)
```

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

```r
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

Positive cancer samples "M" Negativenon-cancer "B"

True is our cluster grp 1 False is our cluster grp2

> Q. How many true positives do we have?

```r
sens <- table(grps, diagnosis)
sens[1,2]
```

```
[1] 177
```

> Q. How many false positives fo we have?

```r
sens[2,2]
```

```
[1] 35
```

Sensitivity: TP/(TP+FN) Specificity: TN/(TN+FN)

Prediction with our PCA model

We can take new data and project it onto our new variables (PCs)

read the UofM data

```r
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
```

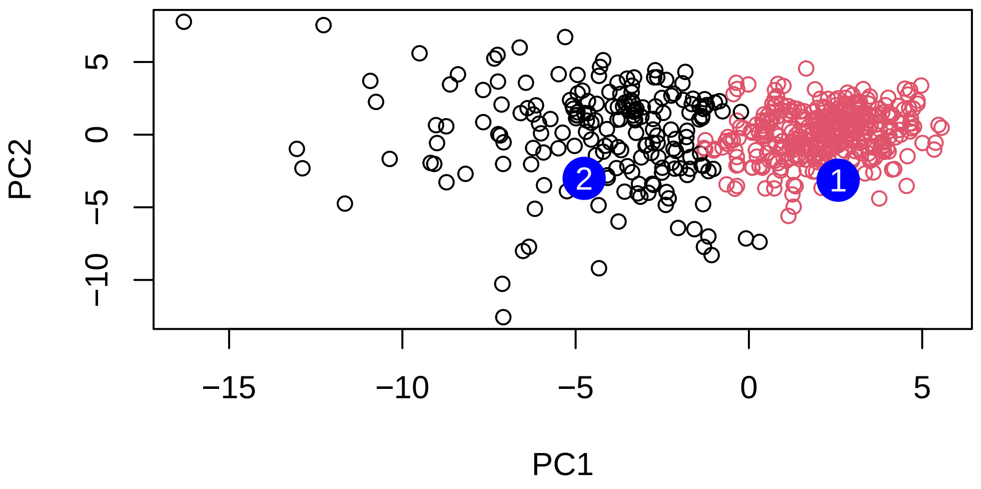
Peojection

```r
npc <- predict(pca, newdata=new)
```

Base R plot

```r
plot(pca$x[,1:2], col=grps)

# add the new points
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



Patient 2 is inside the malignant cluster