Class08Lab

Nancy Leon-Rivera

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Save your input data file into your Project directory

```
fna.data <- "WisconsinCancer.csv"
```

Complete the following code to input the data and store as wisc.df

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

```
          0.10960          0.15990         0.1974            0.12790
          0.14250          0.28390         0.2414            0.10520
          0.10030          0.13280         0.1980            0.10430
          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
```

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

There are 569 samples in this dataset

Q. How many cancer/non-cancer diagnosis samples are in this dataset?

```
Diagnosis <- wisc.df$diagnosis=="M"

sum(Diagnosis)
```

```
[1] 212
```

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

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

```
  B   M
357 212
```

Q. How amny columns/dimensions are there?

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

```
[1] 31
```

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

```
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 findpattern amtches here:

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

```
[1] 10
```

Tidy to remove diagnosis

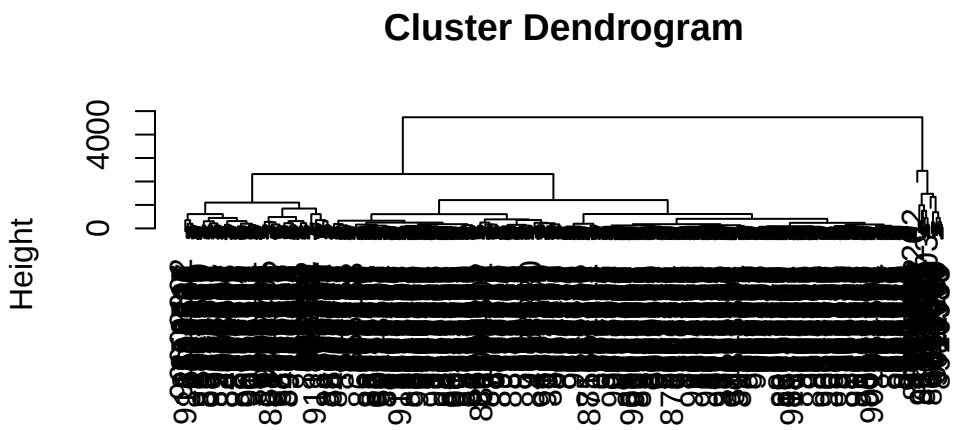
```
#Save the vector of this expert diagnosis for later and remove it from the sata to undergo cl

diagnosis <- wisc.df$diagnosis
```

```
#instead of remove the column you create a new data with the diagnosis data removed
wisc.data <- wisc.df[ ,-1]
```

##Cluster the dataset

Let's try `hclust`.

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



TO get some clusters out of this I can "cut" the tree at given height:

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

```
grps
  1   2
549  20
```

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

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

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

That is not that useful a clustering result...

##PCA should now be the first step for data analysis ##Principal Component Analysis (PCA)

Scaling data before analysis is often critical.

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

There's a data set in R called `mtcar` which has loads of numbers about old cars.

```
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 
```

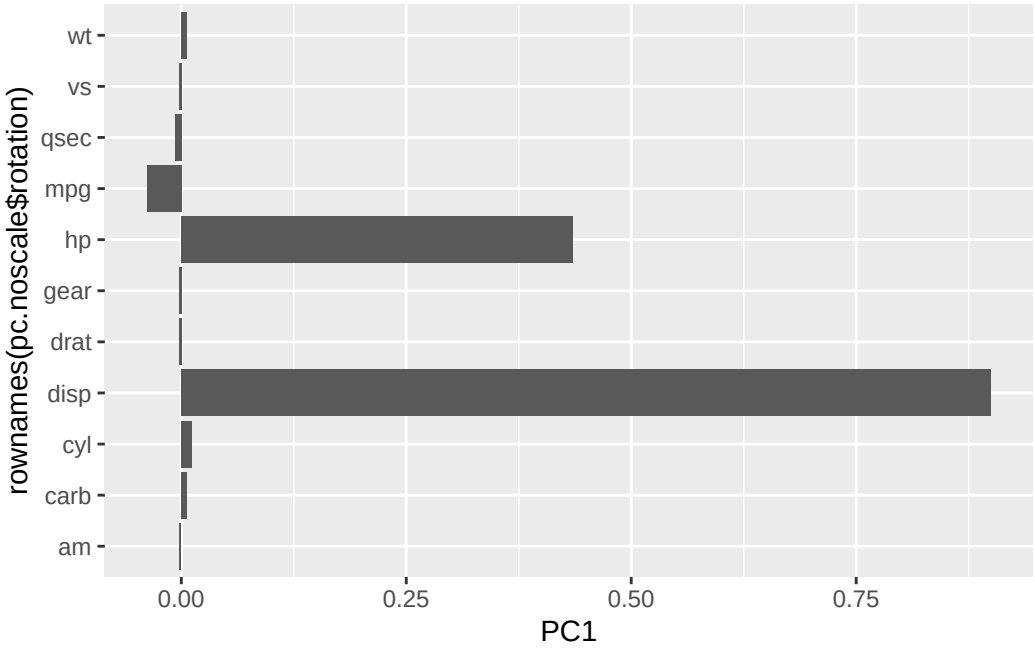
```
pc.noscale <- prcomp(mtcars, scale=F)
pc.scale <- prcomp(mtcars, scale=T)
```

Let's look at the loadings first:

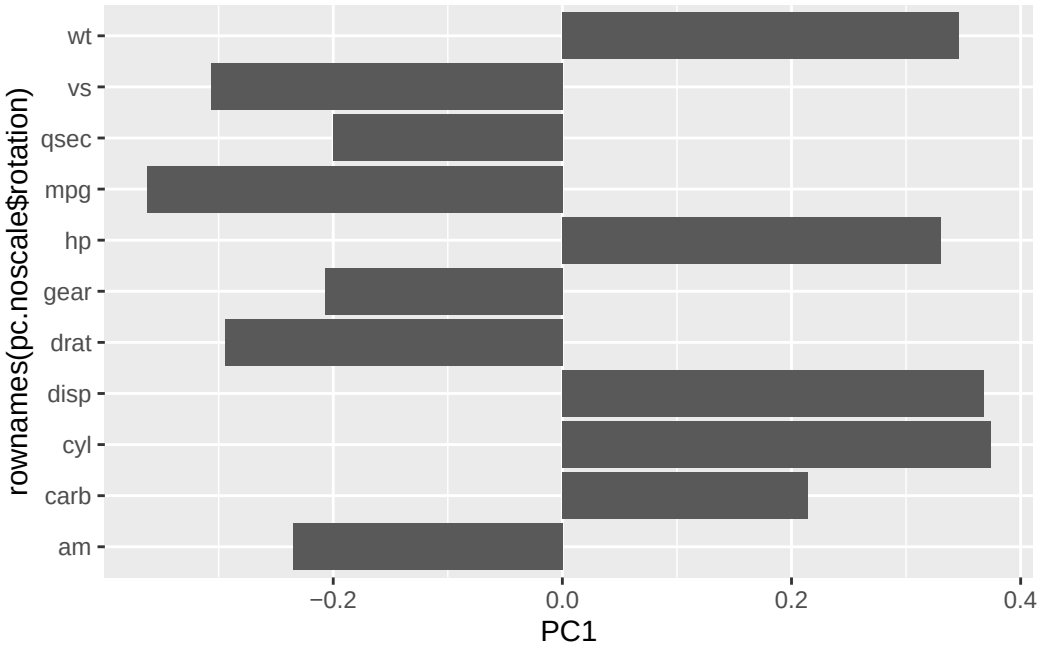
```
pc.noscale$rotation
```

```
              PC1           PC2           PC3           PC4          PC5
mpg  -0.038118199  0.009184847  0.982070847  0.047634784 -0.08832843
cyl   0.012035150 -0.003372487 -0.063483942 -0.227991962  0.23872590
disp  0.899568146  0.435372320  0.031442656 -0.005086826 -0.01073597
hp    0.434784387 -0.899307303  0.025093049  0.035715638  0.01655194
drat -0.002660077 -0.003900205  0.039724928 -0.057129357 -0.13332765
wt    0.006239405  0.004861023 -0.084910258  0.127962867 -0.24354296
qsec -0.006671270  0.025011743 -0.071670457  0.886472188 -0.21416101
vs   -0.002729474  0.002198425  0.004203328  0.177123945 -0.01688851
am   -0.001962644 -0.005793760  0.054806391 -0.135658793 -0.06270200
gear -0.002604768 -0.011272462  0.048524372 -0.129913811 -0.27616440
carb  0.005766010 -0.027779208 -0.102897231 -0.268931427 -0.85520810
              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
qsec -0.189564973  0.254844548  1.028515e-01 -0.095914479 -0.204240658
vs    0.102619063 -0.080788938  2.132903e-03  0.684043835  0.303060724
am    0.205217266  0.200858874  2.273255e-02 -0.572372433 -0.162808201
gear  0.334971103  0.801625551 -2.174878e-01  0.156118559  0.203540645
carb -0.283788381 -0.165474186 -3.972219e-03  0.127583043 -0.239954748
              PC11
mpg   0.0158569365
cyl  -0.1454453628
disp -0.0009420262
hp    0.0021526102
drat  0.0973818815
wt    0.0198581635
qsec -0.0110677880
vs   -0.6256900918
am   -0.7331658036
gear  0.1909325849
carb -0.0557957968
```

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

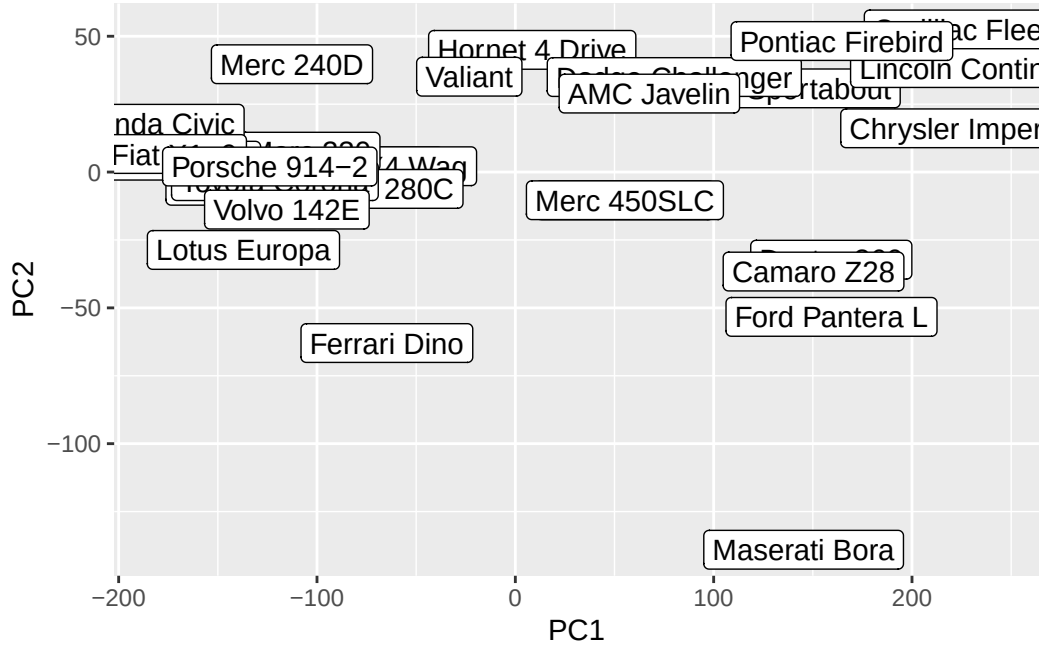



```
ggplot(pc.scale$rotation) +aes(PC1, rownames(pc.noscale$rotation)) +
  geom_col()
```



The main PC result figure is often called a “score plot” or “PC plot” etc…

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



##This is what scaleing does

```
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
```

```
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 mis-lead due to your data having different measurment units.

##Breast Cancer PC

We will scale our data.

```
pca <- prcomp(wisc.data, scale =T)
#if means and stdev are different scale data
```

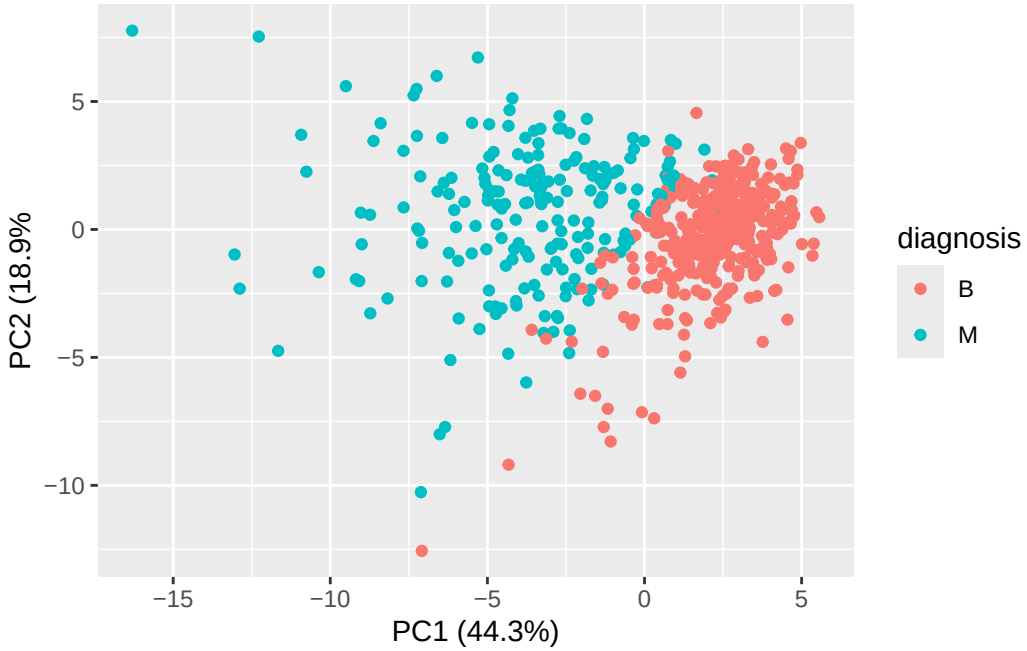
See how well we are doing:

```
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() + xlab("PC1 (44.3%)") +
  ylab("PC2 (18.9%")
```



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
```

```
##PC5
```

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

```
#can use stdev as vairance
attributes(pca)
```

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

$class
[1] "prcomp"
```

We can extract stdev and figure out the total variance

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

```
[1] 30
```

The proportion of variance captured in each PC

```
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
```

Cummulative variance captured

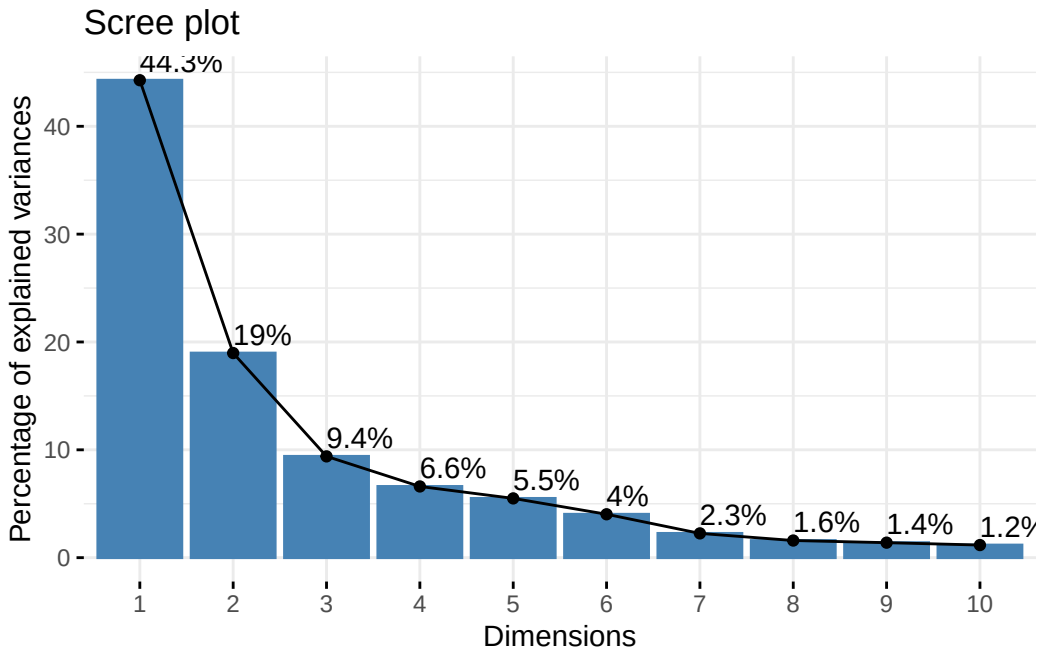
```
which(cumsum(v/sum(v)) >0.8)[1]
```

```
[1] 5
```

```
library(factoextra)
```

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

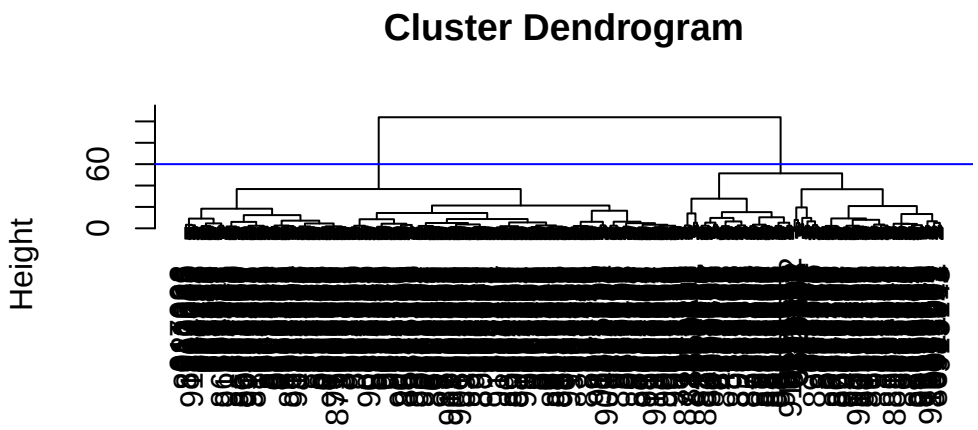
```
fviz_eig(pca, addlabels = TRUE)
```



##Combine PCA and clustering We caw 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. Use our `$x` PC scores and cluster in the PC1-2 subspace

```
hc.pca <- hclust(dist(pca$x[,1:2]), method="ward.D2")
plot(hc.pca)
abline(h=60, col="blue")
```



Q. Does your clustering help seperate cancer from on-cancer samples (i.e. diagnosis "M vsB"?

```
mb.grps <- cutree(hc.pca, h=60)
table(mb.grps)
```

```
mb.grps
  1   2
195 374
```

```
table(mb.grps, diagnosis)
```

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

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

Positive cancer samples “M” Negative non-cancer samples “B”

True our cluster/grp 1 False our cluster/grp 2

Q. How many true positive do we have?

Q. How many false positive do we have?

Sensitivity How many of the positives did we get right. TP/(TP+FN)

TN/(TN+FN)

##Prediction with our PCA Model

We can take new data(in this case from UofM) and project it onto our new variables (PCs).

Readd the UofM data first

```
url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
#Projection
npc <- predict(pca, 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
```

Base R plot

```r
plot(pca$x[,1:2], col=mb.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="red")
```