Lab 8: PCA Mini Project

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Today we will do a complete analysis of some breast cancer biopsy data but first let's revist the main PCA function in R `pccomp()` 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
```

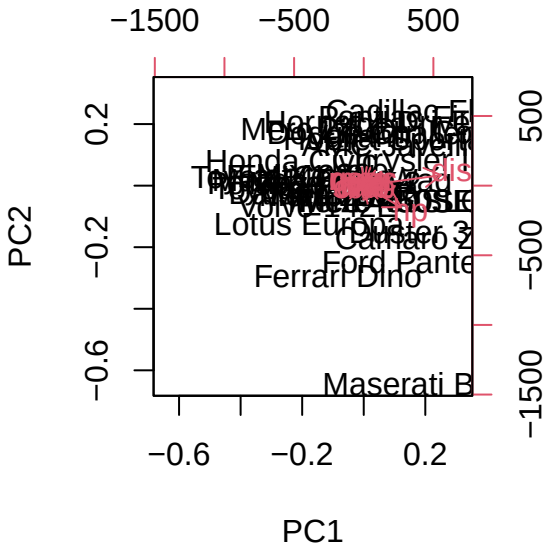
```
apply(mtcars,2,sd)
```

```
       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 highest sd here. THey will likely dominate any anylysis I do on this dataset. Let's see

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

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



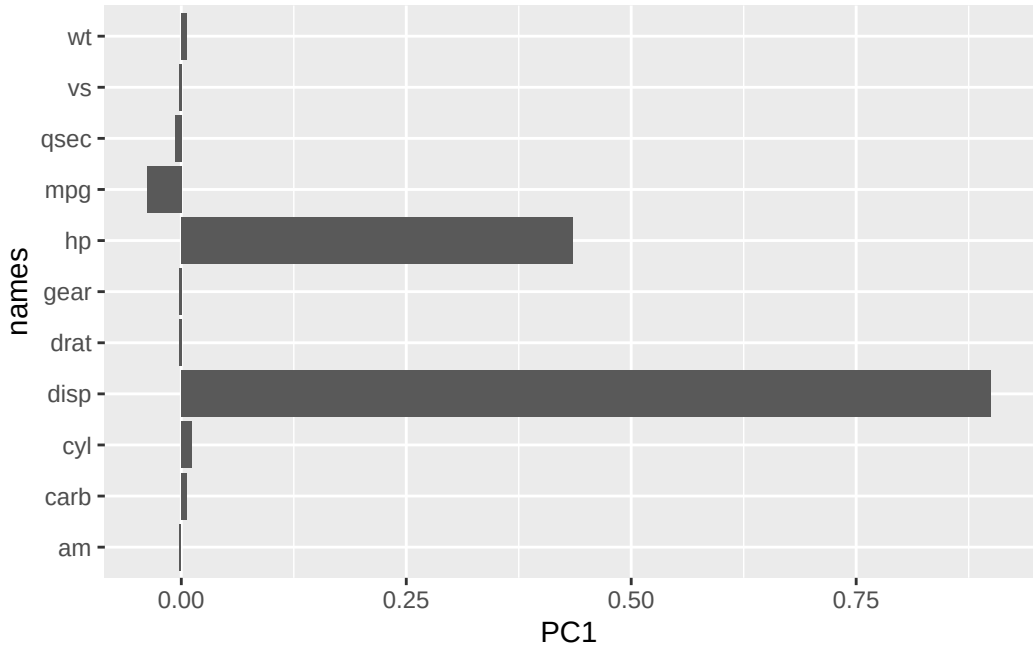

```
pc.noscale$rotation[,1]
```

```
         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
```

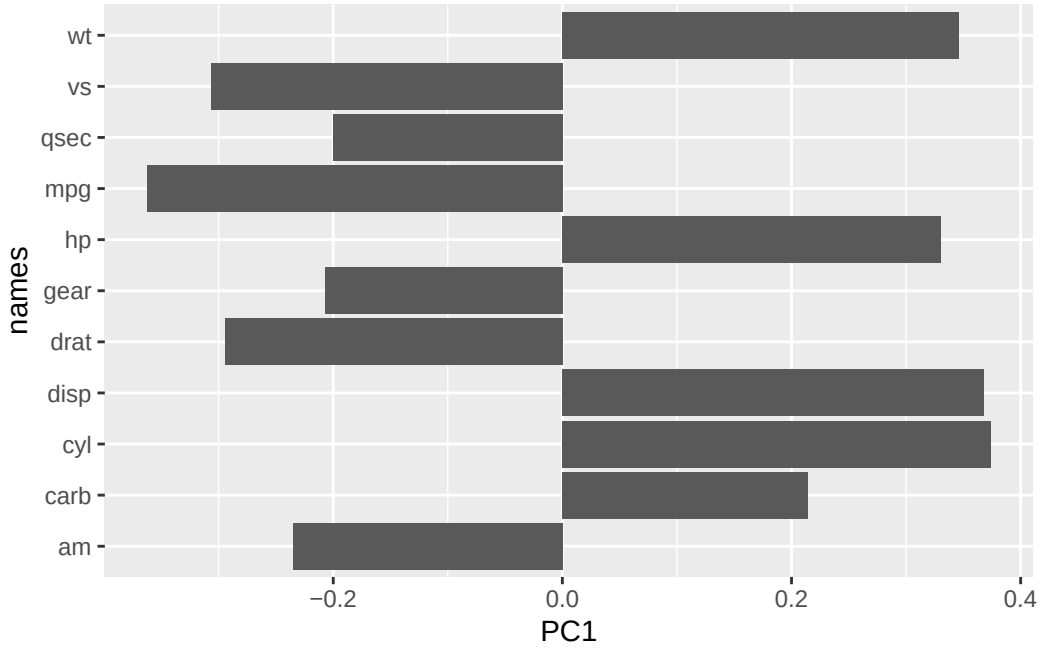
Plot the loadings

```
library(ggplot2)

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

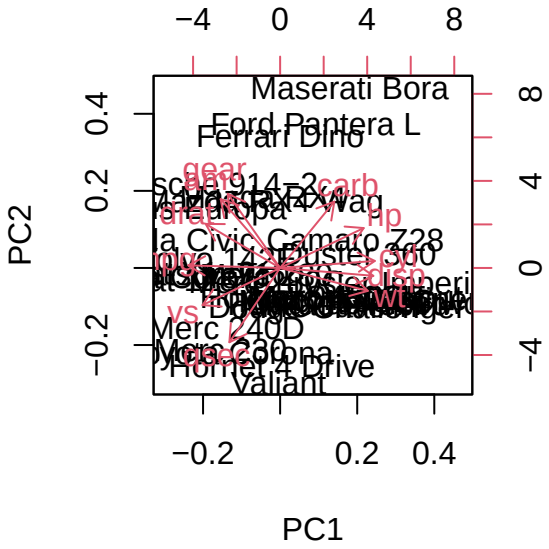
```
ggplot(r1)+
  aes(PC1, names) +
  geom_col()
```




```
library(ggplot2)

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: 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 largest variance just due to their unit of measurement.

#FNA Breast Cancer data

Load the data into 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
```

Q1. How many observations are in this dataset?

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

```
[1] 569
```

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

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

```
[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.

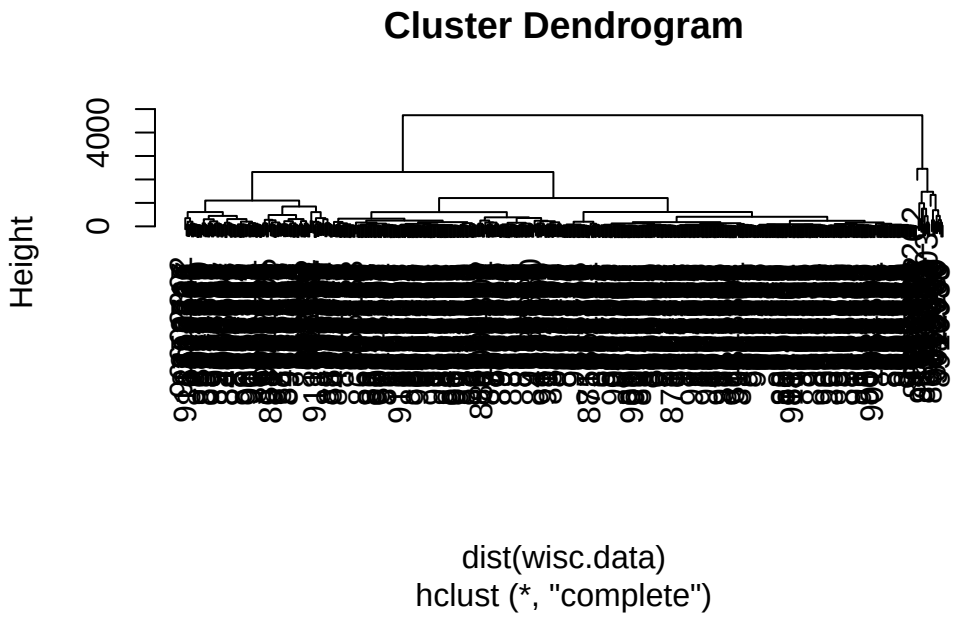
```
diagnosis = as.factor(wisc.df$diagnosis)
head(diagnosis)
```

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

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

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

```
hc = hclust(dist(wisc.data))
plot(hc)
```



Principal Component Anaylsis (PCA)

```
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
```

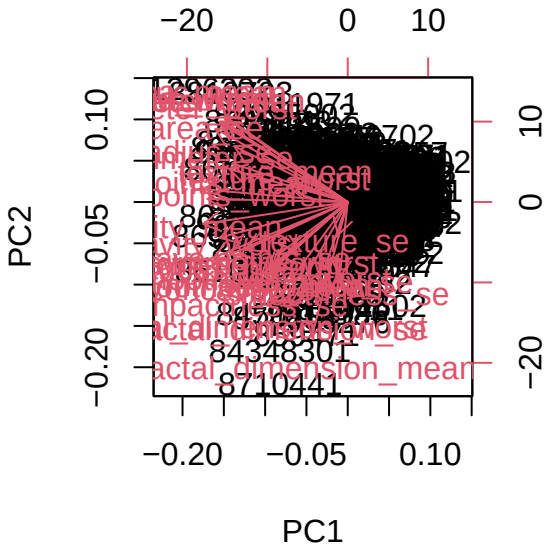
```
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
                           PC8    PC9    PC10   PC11    PC12    PC13    PC14
Standard deviation     0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 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)? PC1 has 44.27% of the original variance

Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data? You need 3 PCs to describe at least 70% of the original variance.

Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data? You need 7 PCs to descibe at least 90% of the original variance.

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



Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why? It is really difficult to understand because all of the subject numbers are stacked on top of one another.

This biplot sucks! We need to build our own PCA score plot of PCI vs PC2

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

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

$class
[1] "prcomp"
```

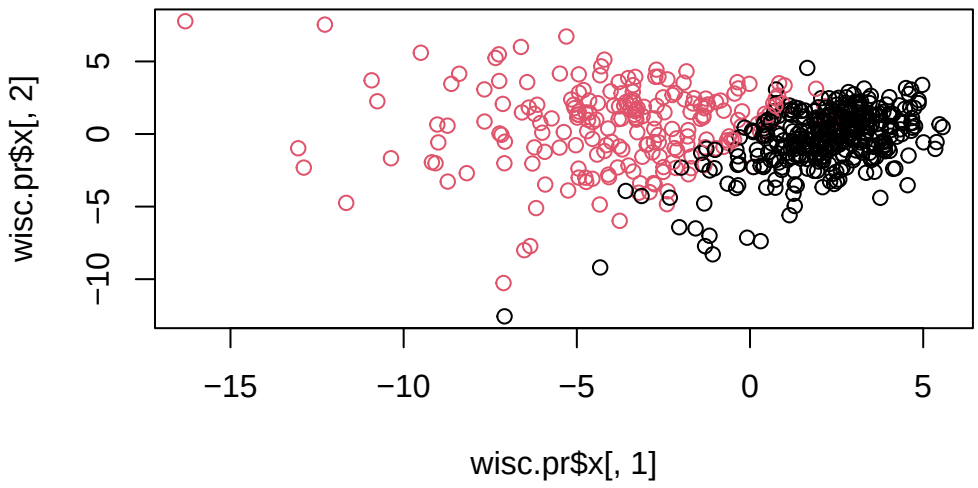
```
head(wisc.pr$x)
```

```
               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
```

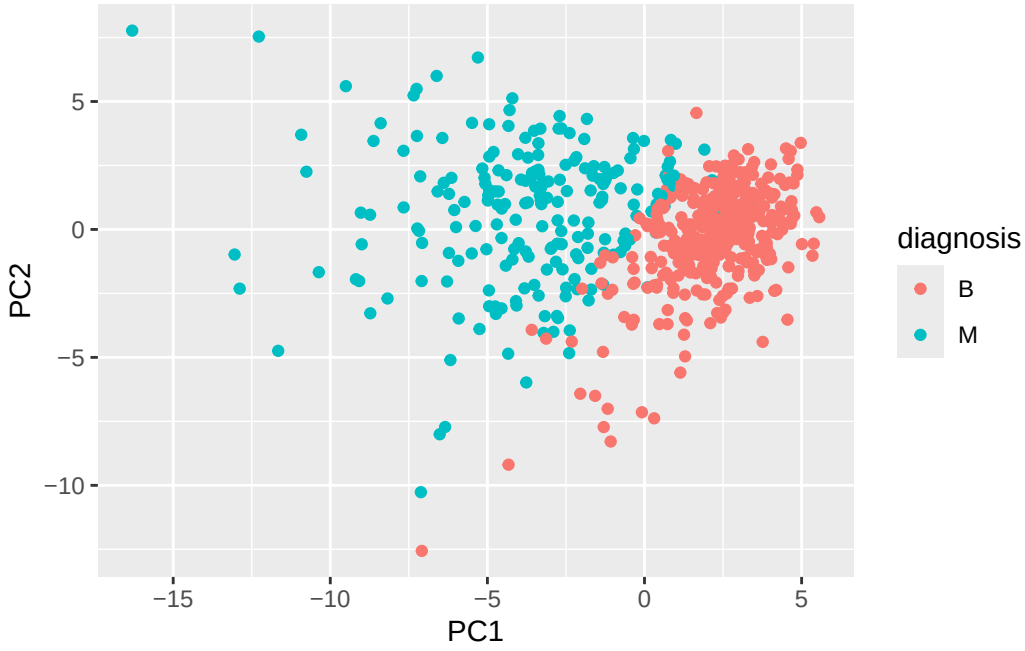
Plot of PC1 vs PC2 the first 2 columns

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



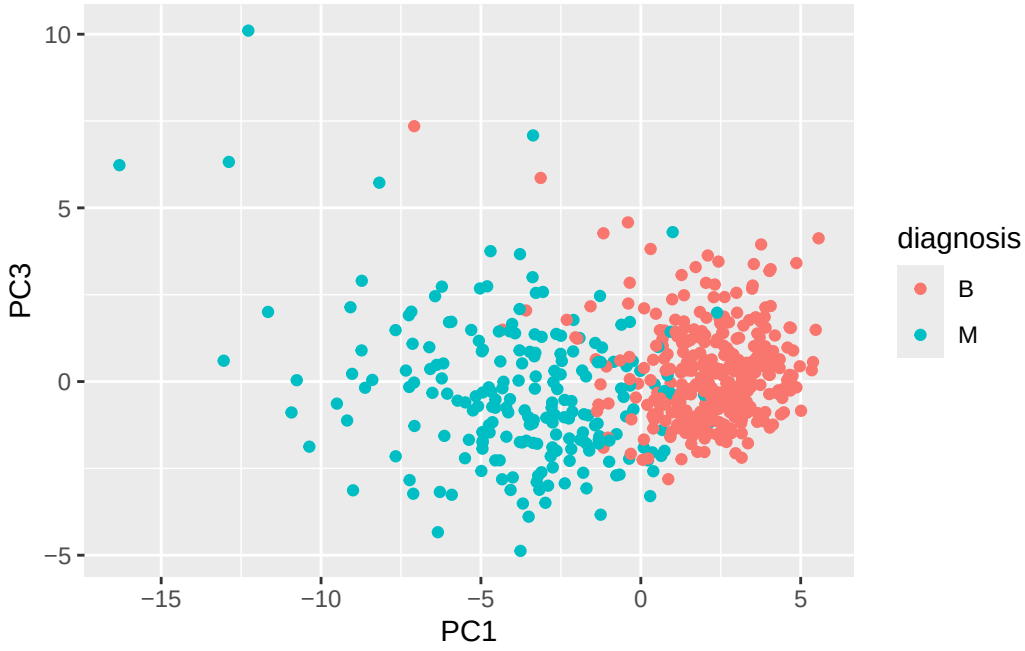
Make a ggplot version of this score plot

```
pc2 = as.data.frame(wisc.pr$x)

ggplot(pc2) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point()
```



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

```
pc = as.data.frame(wisc.pr$x)

ggplot(pc) +
  aes(PC1, PC3, col=diagnosis) +
  geom_point()
```



These plots have very similar clustering meaning that the benign and malignant tumors most likely have very similar data However PC3 seems to have less variance.

Variance

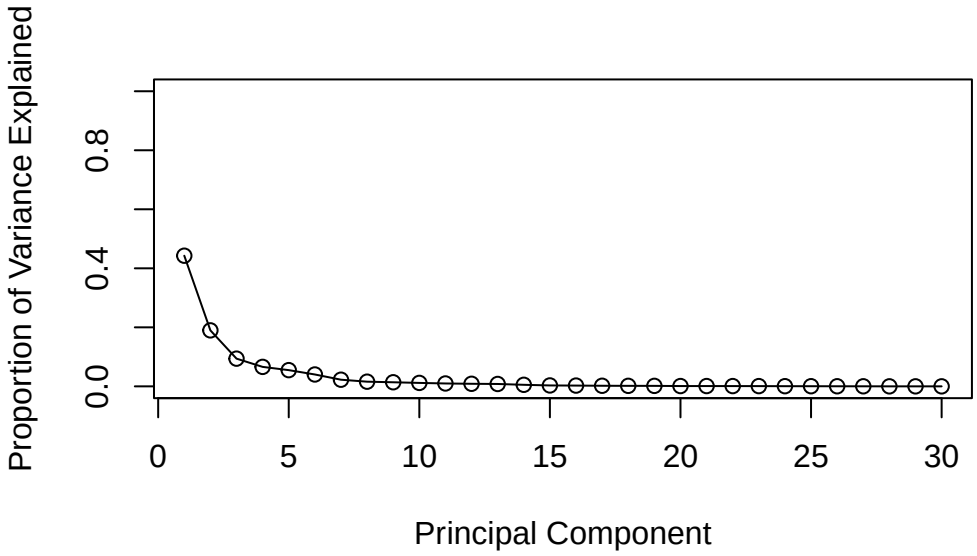
Trying to find a hint as to which natural number it may be.

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

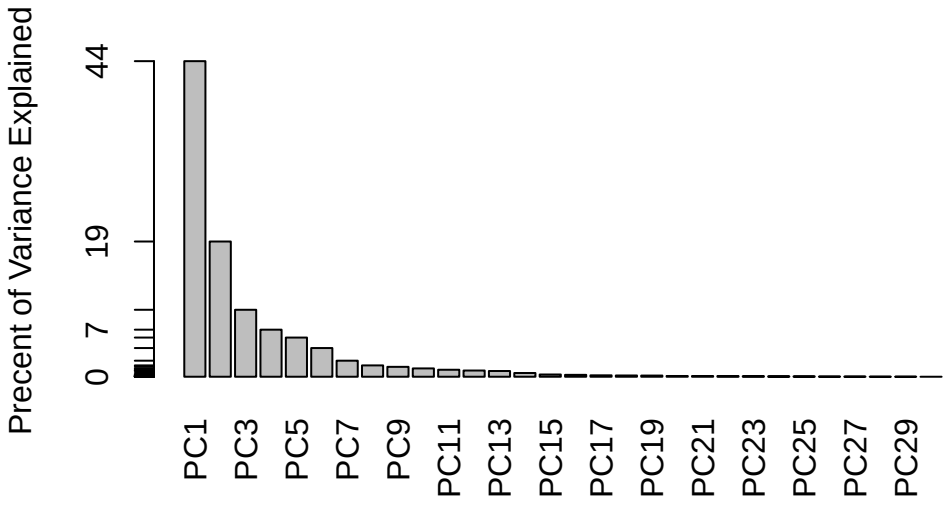
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

Finding the variance explained by each principal component

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

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




```
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 )
```



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
```

The component of the loading vector for `concave.points_mean` is -0.26085376

Q10. What is the minimum number of principal components required to explain 80% of the variance of the data? You need 5 PCs to explain 80% of the variance of the data.

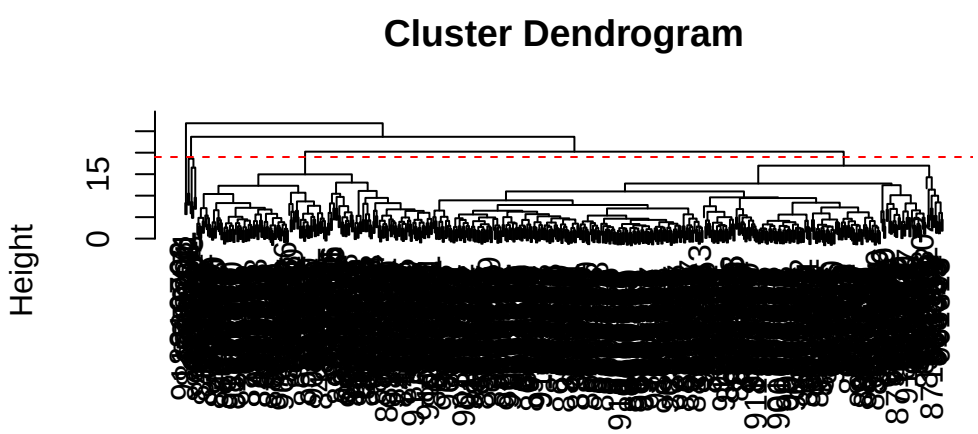
##Hierarchical Clustering

Scaling the data

```
data.scaled = scale(wisc.data)

data.dist = dist(data.scaled)

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

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)
```



There are 4 clusters at 19.

Cutting the tree

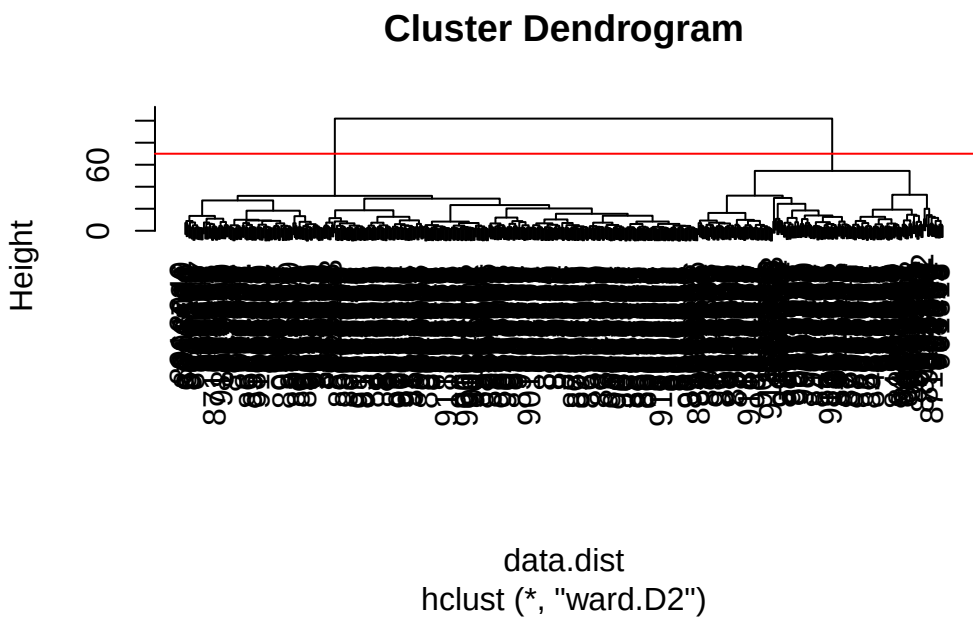
```
wisc.hclust.cluster = cutree(wisc.hclust, h=19)

table(wisc.hclust.cluster, diagnosis)
```

```
                    diagnosis
wisc.hclust.cluster   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? No, if we cut into 2 or 10 clusters, we will end up with false negatives and false positives.

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

```
wisc.pr.hclust = hclust(data.dist, method="ward.D2")
plot(wisc.pr.hclust)
abline(h=70, col="red")
```



"ward.D2" is my favorite due to the fact that it is the least condensed an the easiest to look at.

##Cluster membership vector

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

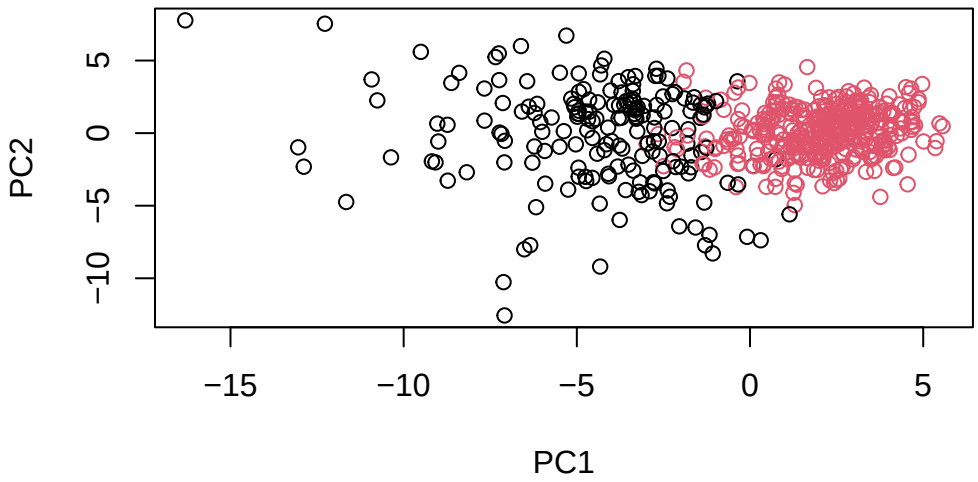
```
grps
  1   2
184 385
```

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  20 164
   2 337  48
```

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



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

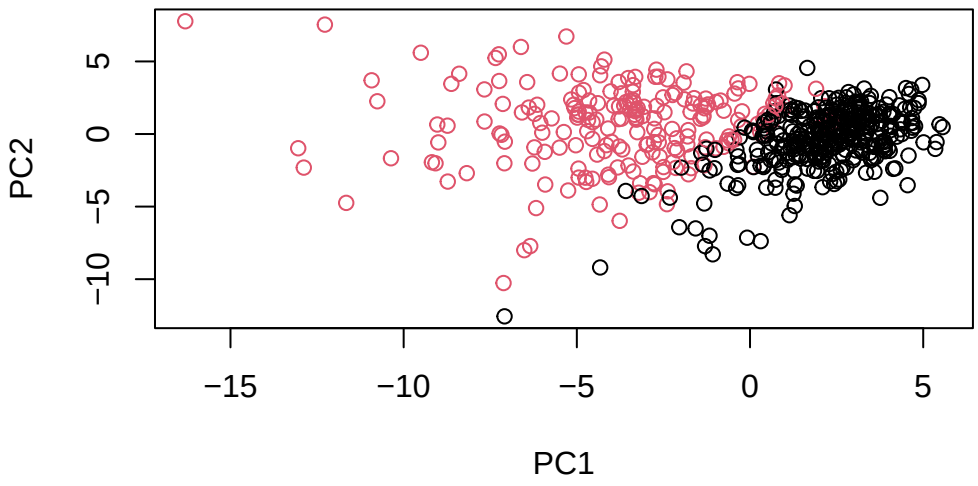
Positive = cancer M Negative = non-cancer B

True = cluster/grp 1 False grp 2

True Positive = 164 False Positive = 20 True Negative = 337 False Negative = 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. The models used seperate the diagnoses pretty well, but they are still a little bit inaccurate.

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



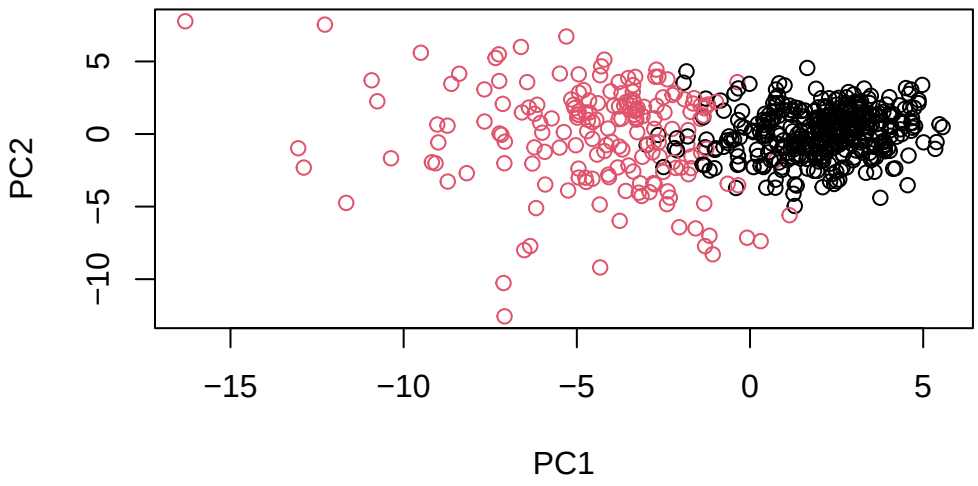

```
g = as.factor(grps)
levels(g)
```

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

```
g = relevel (g,2)
levels(g)
```

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

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

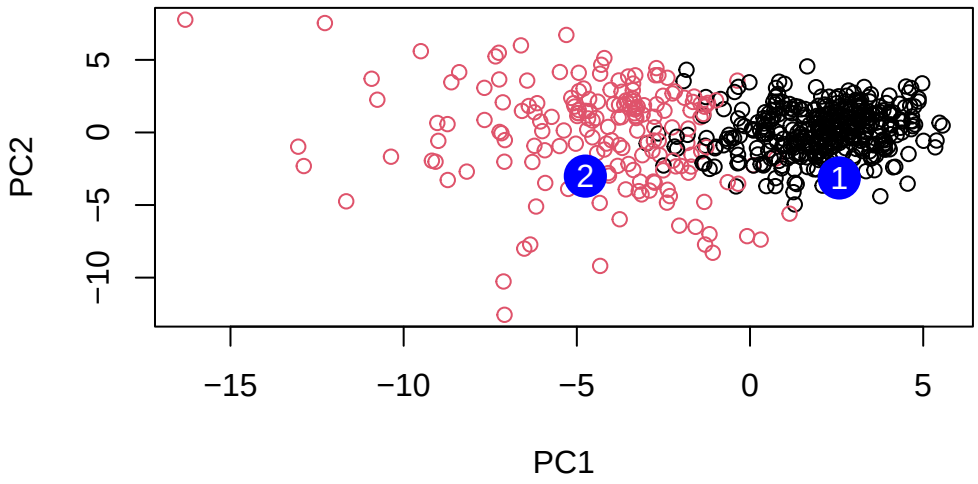


We can use our PCA results (wisc.pr) to make predictions on new unseen data.

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



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

Sensitivity:

```
164/(164+20)
```

```
[1] 0.8913043
```

Specificity

```
337/(337+48)
```

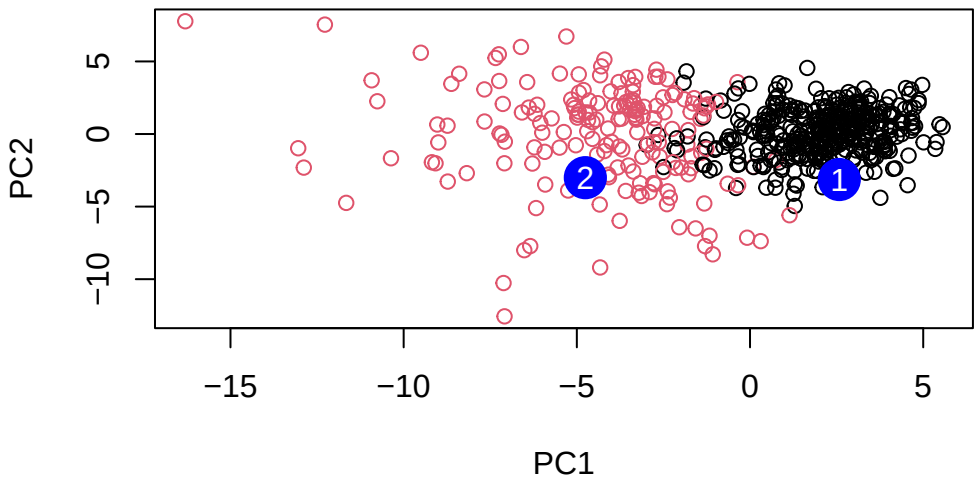
```
[1] 0.8753247
```

##Prediction Using predict funciton to project data into new PCA space

```
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 patients that are in group 2