class8

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Side_Note:

```r
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
```

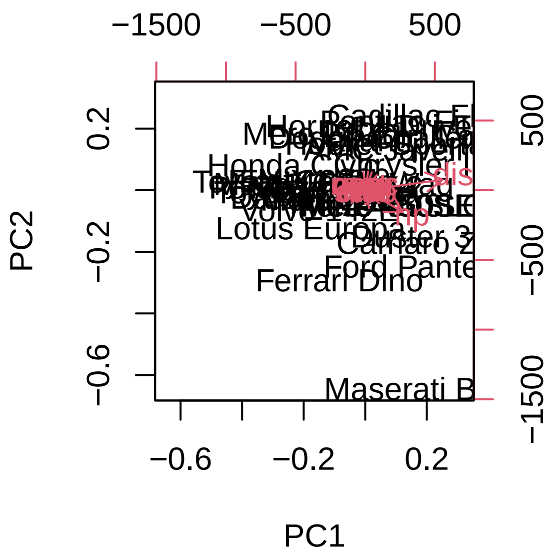
Let's look at "spread" via `sd()`

```r
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 
```

All the signal is goint to come from disp, because it has the largest standard deviation.

```r
pca<-prcomp(mtcars)
biplot(pca)
```



Let's try scaling the data:

```r
mtscale <- scale(mtcars)
head(mtscale)
```

```
                         mpg        cyl        disp         hp       drat
Mazda RX4          0.1508848 -0.1049878 -0.57061982 -0.5350928  0.5675137
Mazda RX4 Wag      0.1508848 -0.1049878 -0.57061982 -0.5350928  0.5675137
Datsun 710         0.4495434 -1.2248578 -0.99018209 -0.7830405  0.4739996
Hornet 4 Drive     0.2172534 -0.1049878  0.22009369 -0.5350928 -0.9661175
Hornet Sportabout -0.2307345  1.0148821  1.04308123  0.4129422 -0.8351978
Valiant           -0.3302874 -0.1049878 -0.04616698 -0.6080186 -1.5646078
                            wt       qsec         vs         am       gear
Mazda RX4         -0.610399567 -0.7771651 -0.8680278  1.1899014  0.4235542
Mazda RX4 Wag     -0.349785269 -0.4637808 -0.8680278  1.1899014  0.4235542
Datsun 710        -0.917004624  0.4260068  1.1160357  1.1899014  0.4235542
Hornet 4 Drive    -0.002299538  0.8904872  1.1160357 -0.8141431 -0.9318192
Hornet Sportabout  0.227654255 -0.4637808 -0.8680278 -0.8141431 -0.9318192
Valiant            0.248094592  1.3269868  1.1160357 -0.8141431 -0.9318192
                        carb
Mazda RX4          0.7352031
Mazda RX4 Wag      0.7352031
Datsun 710        -1.1221521
```

```
Hornet 4 Drive    -1.1221521
Hornet Sportabout -0.5030337
Valiant           -1.1221521
```

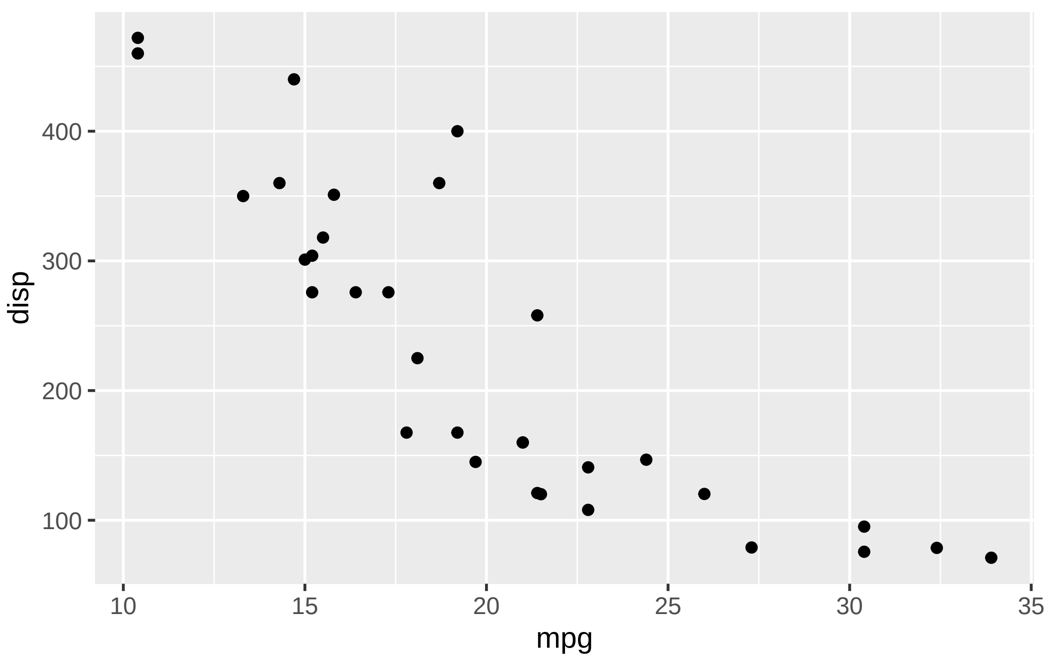
What is the mean of each dimension and column of mtscale?

```r
round(apply(mtscale, 2, sd), 3)
```

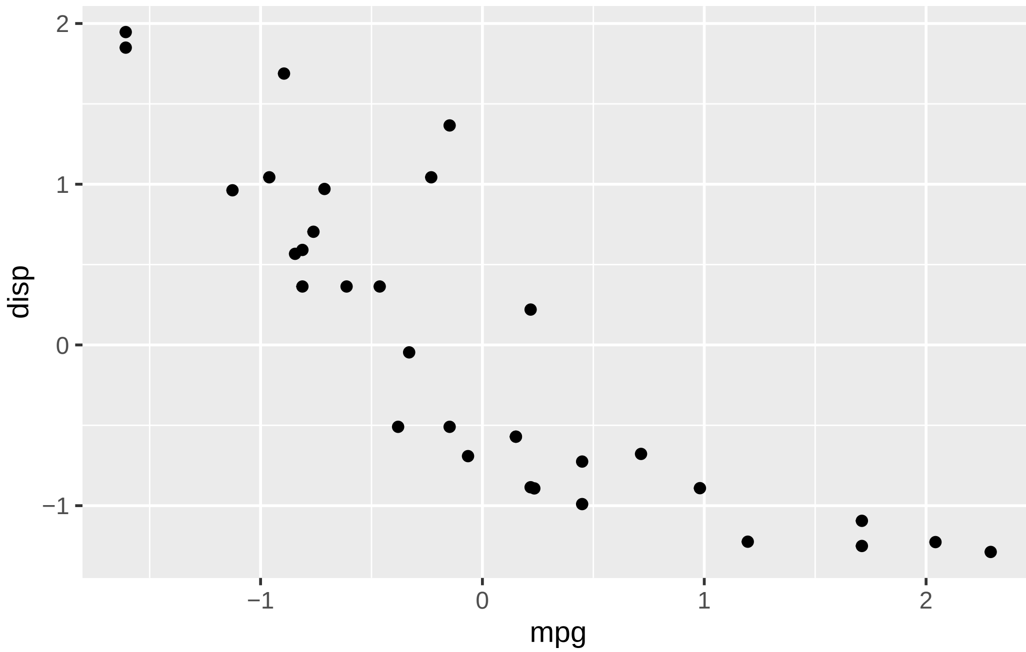
```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb
   1    1    1    1    1    1    1    1    1    1    1
```

Let's plot `mpg` vs. `disp` for both mtcars and the scaled data in `mtscale`.

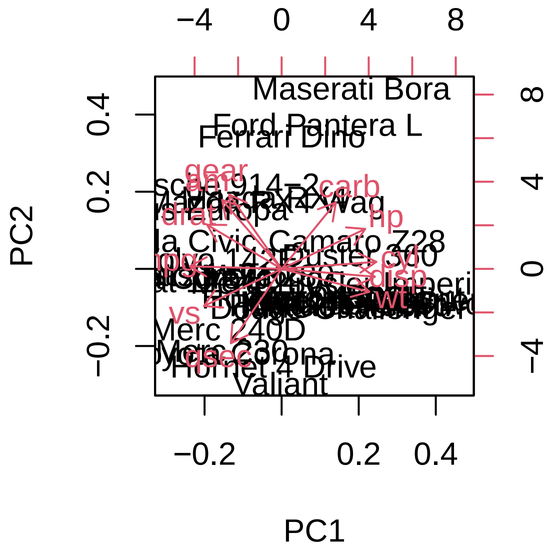
```r
library(ggplot2)

ggplot(mtcars) +
  aes(mpg,disp) +
  geom_point()
```



```r
ggplot(mtscale) +
  aes(mpg,disp) +
  geom_point()
```




```r
pca2 <- prcomp(mtscale)
  biplot(pca2)
```



Breast cancer

```
fna.data <- read.csv("C:/Users/eliso/Downloads/WisconsinCancer.csv", row.names = 1)
wisc.df <- data.frame(fna.data)
```

```
wisc.data <- wisc.df[,-1]
diagnosis <- factor(wisc.df[,1])
```

Q1. How many observations are in this dataset?

```
dim(wisc.data)
```

```
[1] 569  30
```

There are 569 observations in this data.

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

```r
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

There are 212 malignant diagnoses.

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

```r
length(grep("_mean", colnames(wisc.data)))
```

```
[1] 10
```

Ten variables in the data are suffixed with _mean.

PCA section

We want to scale our data before PCA by setting the `scale=TRUE` argument.

```r
# Check column means and standard deviations
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=TRUE)
```

How much variance captured in each principal component?

```r
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)?

44.27% of the original 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?

The first 3 PCs are required to describe at least 70% of the original variance in the data.

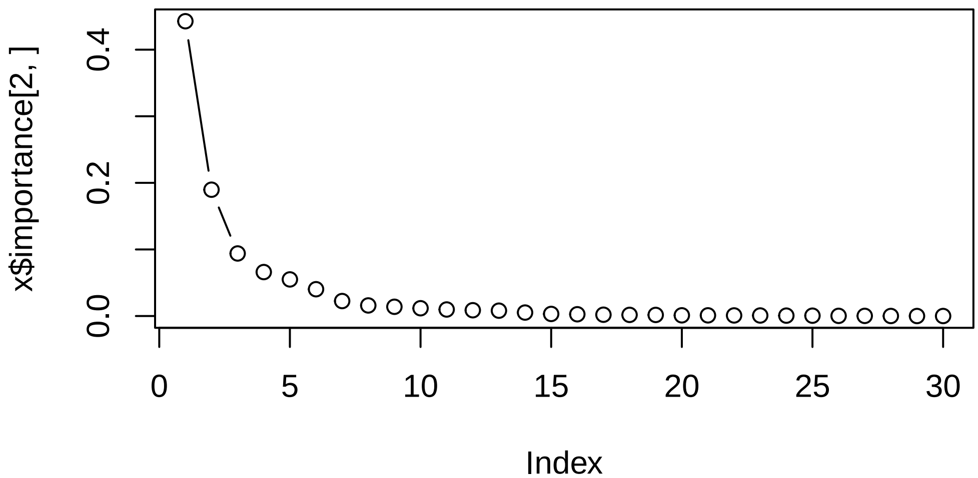
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

The first 7 PCs are required to describe at least 90% of the original variance in the data.

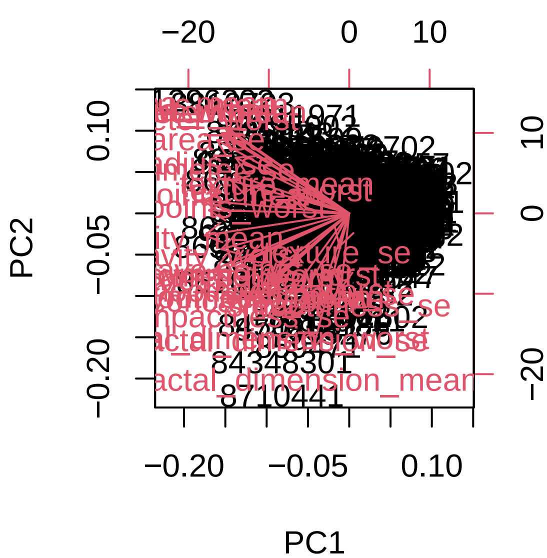
```r
x <- summary(wisc.pr)
x$importance
```

```
                            PC1      PC2      PC3      PC4      PC5      PC6
Standard deviation     3.644394 2.385656 1.678675 1.407352 1.284029 1.098798
Proportion of Variance 0.442720 0.189710 0.093930 0.066020 0.054960 0.040250
Cumulative Proportion  0.442720 0.632430 0.726360 0.792390 0.847340 0.887590
                             PC7       PC8       PC9      PC10      PC11
Standard deviation     0.8217178 0.6903746 0.6456739 0.5921938 0.5421399
Proportion of Variance 0.0225100 0.0158900 0.0139000 0.0116900 0.0098000
Cumulative Proportion  0.9101000 0.9259800 0.9398800 0.9515700 0.9613700
                            PC12      PC13      PC14      PC15      PC16
Standard deviation     0.5110395 0.4912815 0.3962445 0.3068142 0.2826001
Proportion of Variance 0.0087100 0.0080500 0.0052300 0.0031400 0.0026600
Cumulative Proportion  0.9700700 0.9781200 0.9833500 0.9864900 0.9891500
                            PC17      PC18      PC19      PC20      PC21
Standard deviation     0.2437192 0.2293878 0.2224356 0.1765203 0.1731268
Proportion of Variance 0.0019800 0.0017500 0.0016500 0.0010400 0.0010000
Cumulative Proportion  0.9911300 0.9928800 0.9945300 0.9955700 0.9965700
                            PC22      PC23      PC24      PC25      PC26
Standard deviation     0.1656484 0.1560155 0.1343689 0.1244238 0.0904303
Proportion of Variance 0.0009100 0.0008100 0.0006000 0.0005200 0.0002700
Cumulative Proportion  0.9974900 0.9983000 0.9989000 0.9994200 0.9996900
                             PC27      PC28       PC29       PC30
Standard deviation     0.08306903 0.0398665 0.02736427 0.01153451
Proportion of Variance 0.00023000 0.0000500 0.00002000 0.00000000
Cumulative Proportion  0.99992000 0.9999700 1.00000000 1.00000000
```

```
plot(x$importance[2,], typ="b")
```




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



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

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

$class
[1] "prcomp"
```

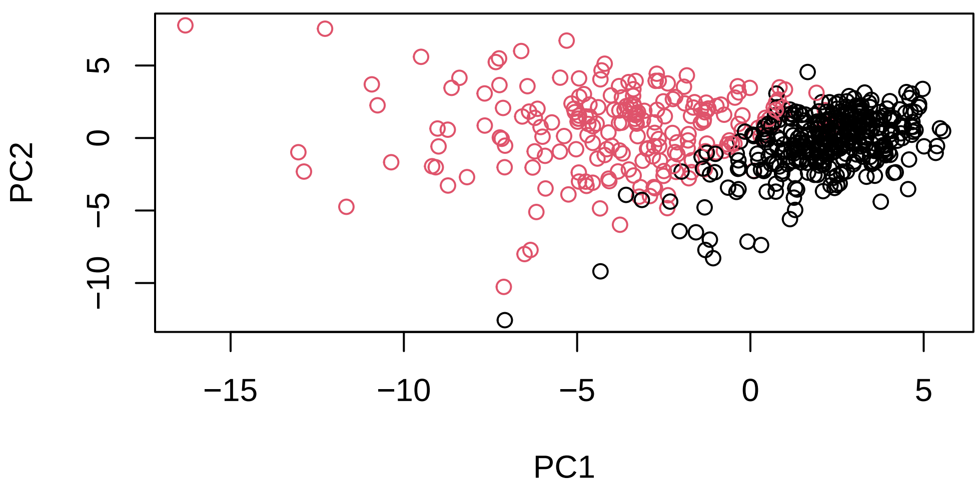
```r
head(wisc.pr$x)
```

```
               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
```

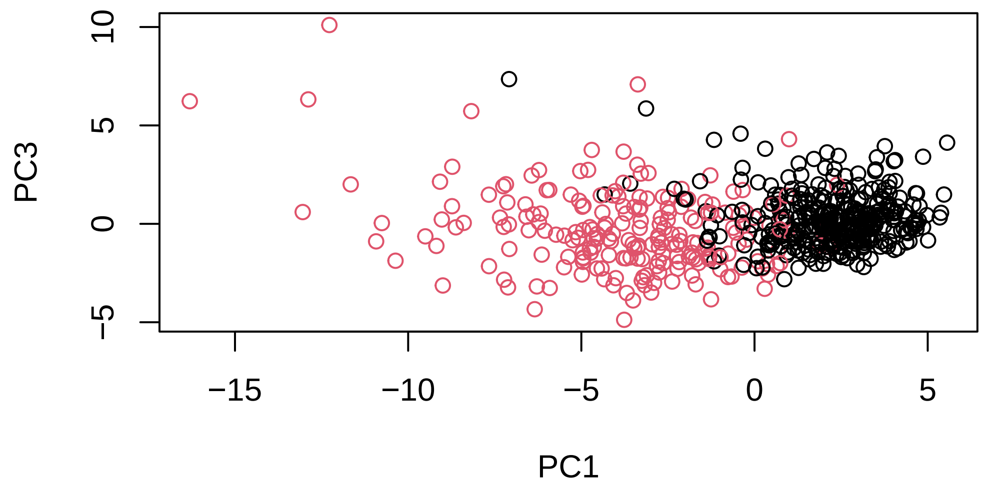
My main PC result figure

```
plot(wisc.pr$x, col=diagnosis)
```



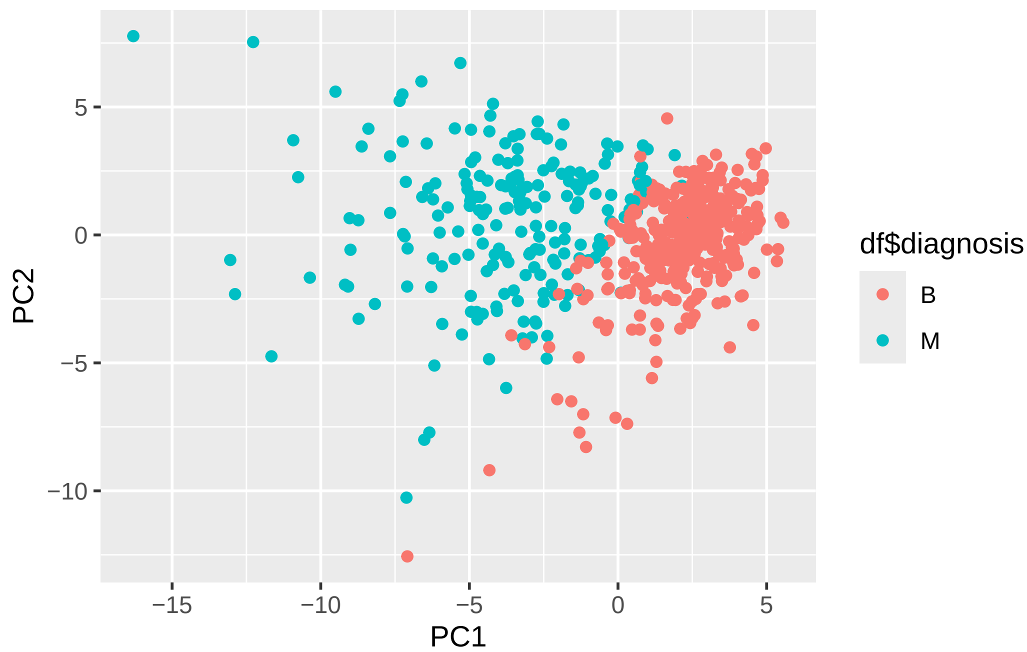
Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

```r
plot(wisc.pr$x[, c(1,3)], col = diagnosis)
```




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

# Load the ggplot2 package
library(ggplot2)

# Make a scatter plot colored by diagnosis
ggplot(df) +
  aes(PC1, PC2, col=df$diagnosis) +
  geom_point()
```

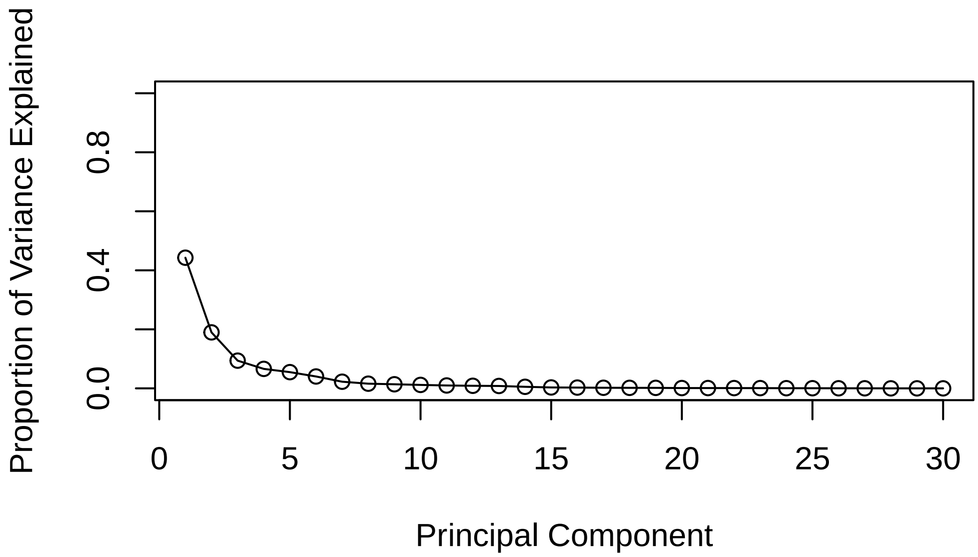
```
Warning: Use of `df$diagnosis` is discouraged.
i Use `diagnosis` instead.
```



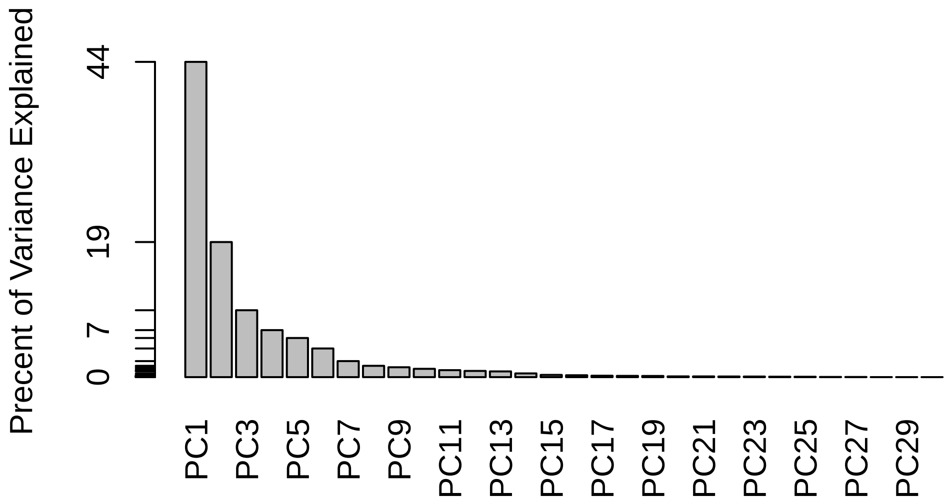

```
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

```
# Variance explained by each principal component: pve
pve <- pr.var / sum(pr.var)

# Plot variance explained for each principal component
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```




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



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? This tells us how much this original feature contributes to the first PC.

By printing the code below, we see that concave.points_mean = -0.26085376.

```
wisc.pr$rotation[,1]
```

```
            radius_mean            texture_mean          perimeter_mean
            -0.21890244             -0.10372458             -0.22753729
              area_mean         smoothness_mean        compactness_mean
            -0.22099499             -0.14258969             -0.23928535
         concavity_mean     concave.points_mean           symmetry_mean
            -0.25840048             -0.26085376             -0.13816696
 fractal_dimension_mean               radius_se              texture_se
            -0.06436335             -0.20597878             -0.01742803
           perimeter_se                 area_se           smoothness_se
            -0.21132592             -0.20286964             -0.01453145
         compactness_se            concavity_se       concave.points_se
            -0.17039345             -0.15358979             -0.18341740
            symmetry_se    fractal_dimension_se            radius_worst
```

```
          -0.04249842             -0.10256832             -0.22799663
        texture_worst         perimeter_worst              area_worst
          -0.10446933             -0.23663968             -0.22487053
     smoothness_worst       compactness_worst         concavity_worst
          -0.12795256             -0.21009588             -0.22876753
 concave.points_worst          symmetry_worst fractal_dimension_worst
          -0.25088597             -0.12290456             -0.13178394
```

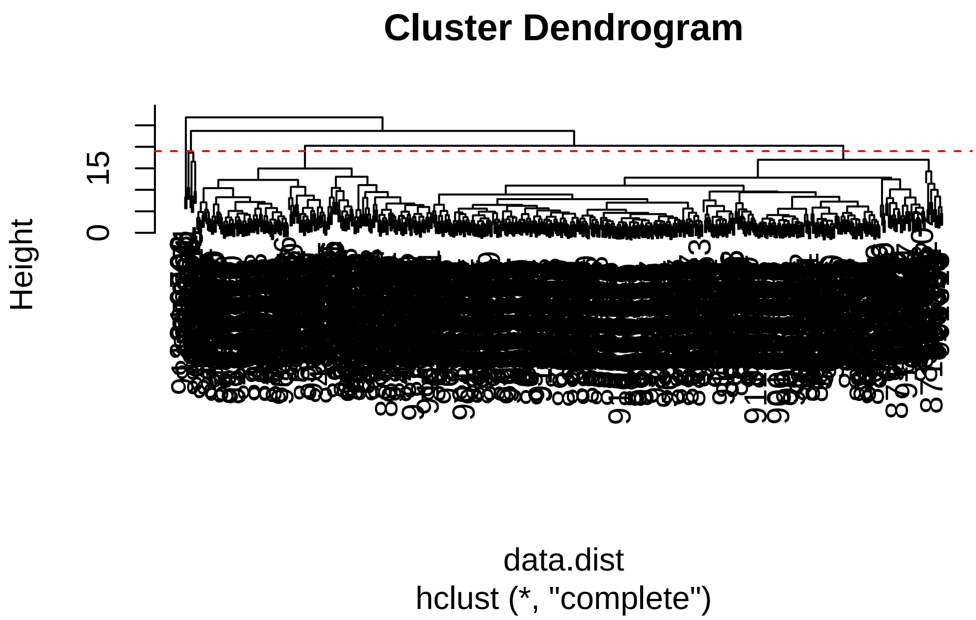
Hierarchical clustering

```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(data.dist, method="complete")
```

Q10. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

As determined below, the height at which the clustering model has 4 clusters is 19.

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




```
wisc.hclust.clusters <- cutree(wisc.hclust, h=19)
table(wisc.hclust.clusters, diagnosis)
```

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

Q11. OPTIONAL: Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10? How do you judge the quality of your result in each case?

Q12. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

After trying hclust() with each of the four methods, my favorite is ward.D2, because it put our data into two similarly sized groups, which fits what we know about our data by looking at the PCA plot where the points are neatly divided in two by diagnosis.

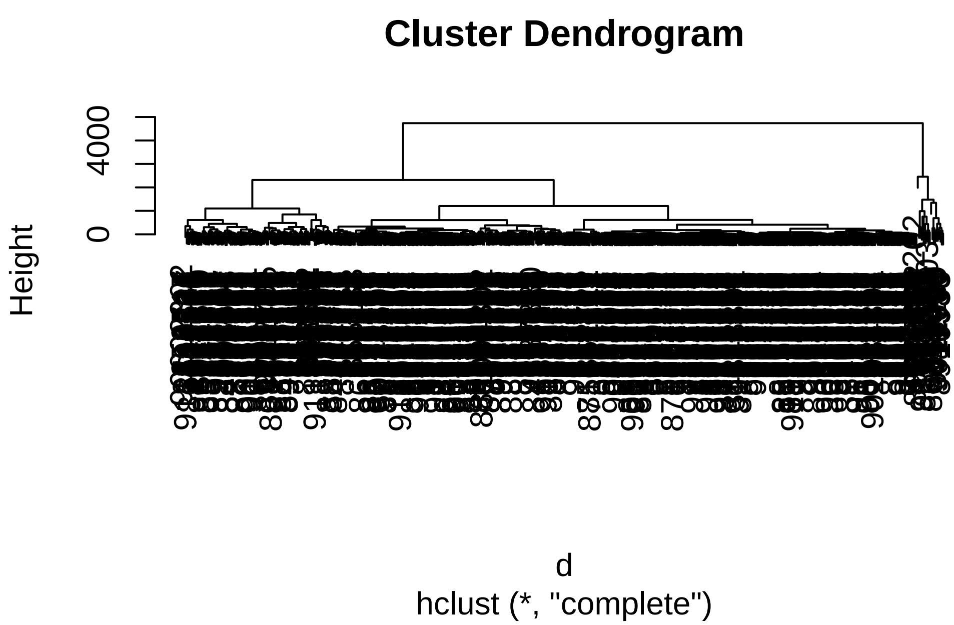
Clustering

Try to cluster the `wisc.data`.

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

```
  1   2
131 438
```

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



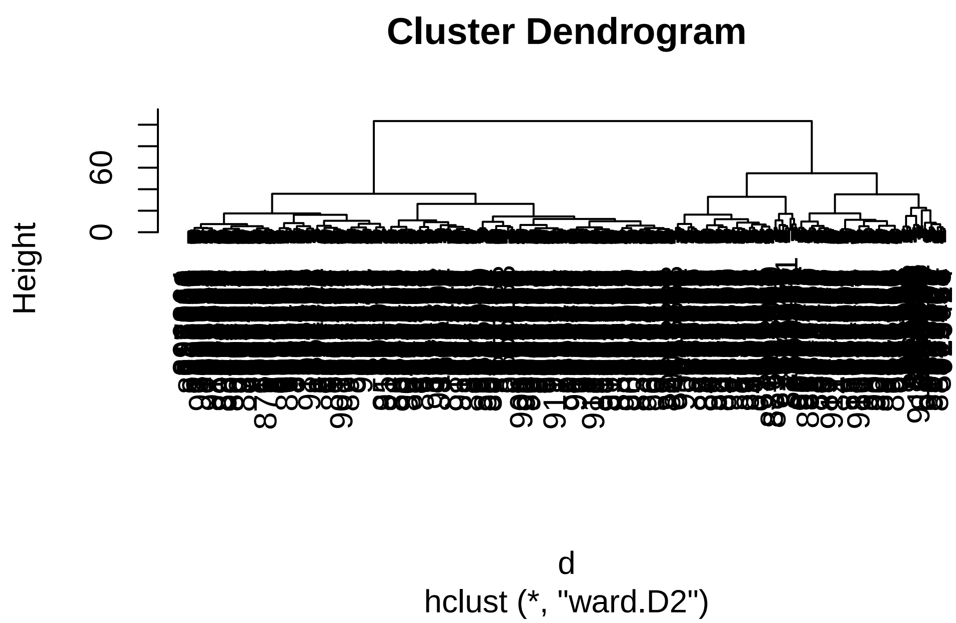

```r
grps <- cutree(hc, k=3)
table(grps)
```

```
grps
  1   2   3
549  19   1
```

Cluster in PC space

In other words, use my PCA results as a basis of clustering.

```
d <- dist(wisc.pr$x[,1:3])
hc <- hclust(d, method="ward.D2")
plot(hc)
```



Cut this tree to yield 2 groups/clusters

```
grps <- cutree(hc, k=2)
table(grps)
```

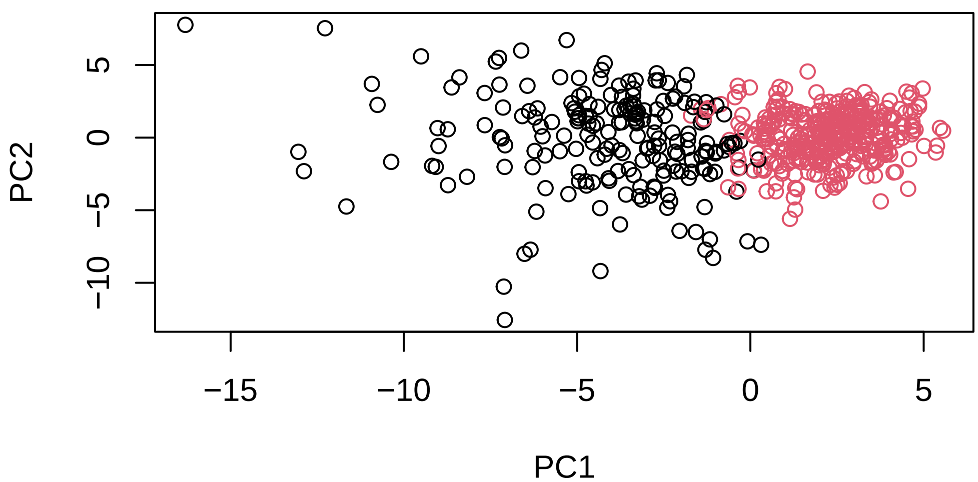
```
grps
  1   2 
203 366 
```

Compare to my expert M and B `diagnosis`

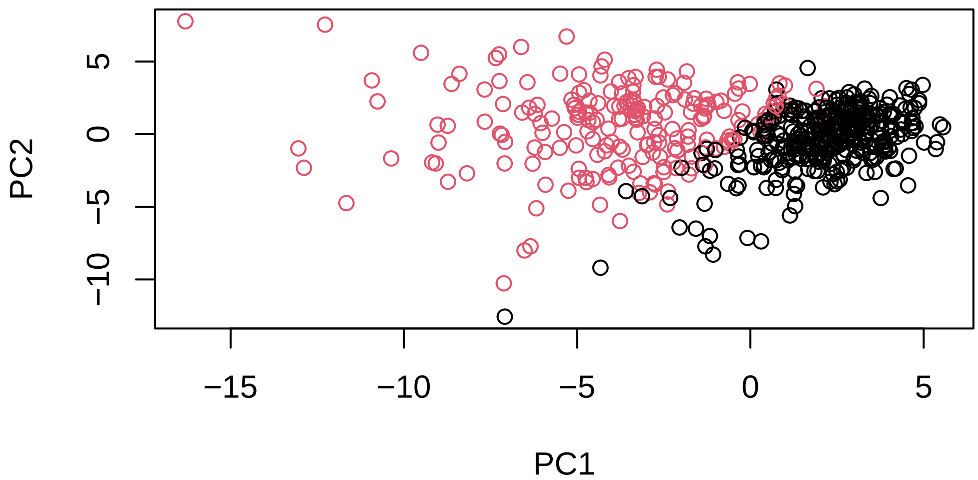
```
table(diagnosis, grps)
```

```
         grps
diagnosis   1   2
        B  24 333
        M 179  33
```

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




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



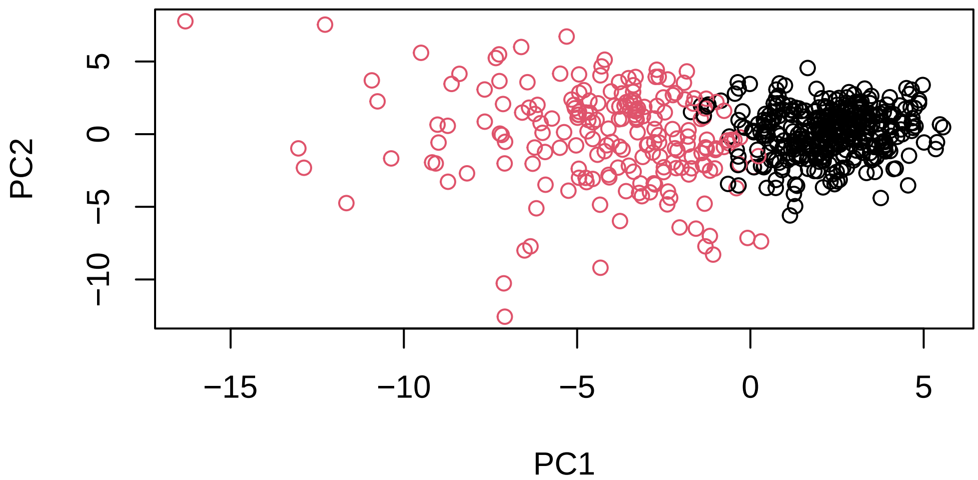

```
g <- as.factor(grps)
levels(g)
```

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

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

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

```
# Plot using our re-ordered factor
plot(wisc.pr$x[,1:2], col=g)
```




```
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
```

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

```
                       diagnosis
wisc.pr.hclust.clusters   B   M
                      1  28 188
                      2 329  24
```

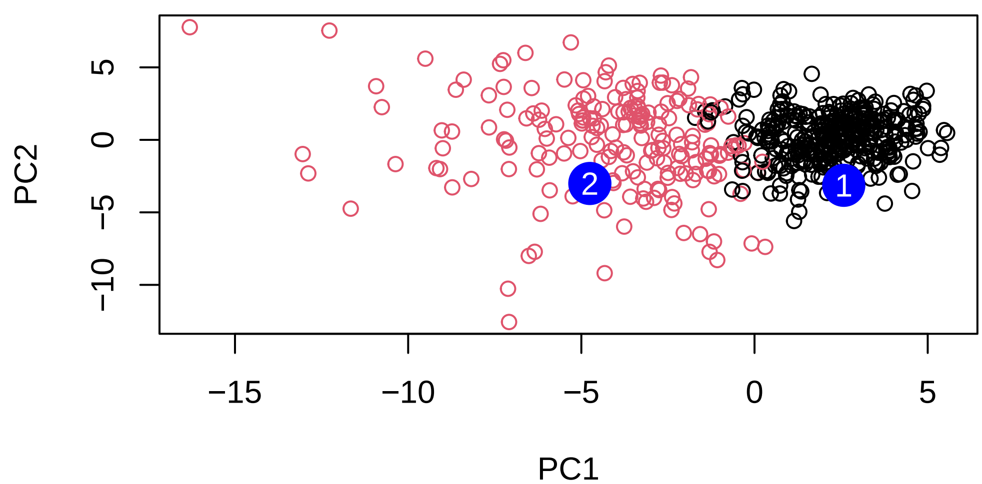
Prediction

```
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
```

```r
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")
```



Q16. Which of these new patients should we prioritize for follow up based on your results?

We should prioritize patient 2 for follow-up, since they are clustering with the samples that were diagnosed as malignant.