Class 09

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1. Exploratory data analysis

Preparing the data

Read Wisconsin Breast Cancer Diagnostic Data Set:

```
fna.data <- 'WisconsinCancer.csv'
wisc.df <- read.csv(fna.data, 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
```

Drop diagnosis in data and save diagnosis for plot:

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

head(wisc.data)
```

```
##          radius_mean texture_mean perimeter_mean area_mean smoothness_mean
## 842302         17.99        10.38         122.80    1001.0         0.11840
## 842517         20.57        17.77         132.90    1326.0         0.08474
## 84300903       19.69        21.25         130.00    1203.0         0.10960
## 84348301       11.42        20.38          77.58     386.1         0.14250
## 84358402       20.29        14.34         135.10    1297.0         0.10030
## 843786         12.45        15.70          82.57     477.1         0.12780
##          compactness_mean concavity_mean concave.points_mean symmetry_mean
## 842302            0.27760         0.3001             0.14710        0.2419
## 842517            0.07864         0.0869             0.07017        0.1812
## 84300903          0.15990         0.1974             0.12790        0.2069
## 84348301          0.28390         0.2414             0.10520        0.2597
## 84358402          0.13280         0.1980             0.10430        0.1809
## 843786            0.17000         0.1578             0.08089        0.2087
##          fractal_dimension_mean radius_se texture_se perimeter_se area_se
## 842302                  0.07871    1.0950     0.9053        8.589  153.40
## 842517                  0.05667    0.5435     0.7339        3.398   74.08
## 84300903                0.05999    0.7456     0.7869        4.585   94.03
## 84348301                0.09744    0.4956     1.1560        3.445   27.23
## 84358402                0.05883    0.7572     0.7813        5.438   94.44
## 843786                  0.07613    0.3345     0.8902        2.217   27.19
##          smoothness_se compactness_se concavity_se concave.points_se
## 842302        0.006399        0.04904      0.05373           0.01587
## 842517        0.005225        0.01308      0.01860           0.01340
## 84300903      0.006150        0.04006      0.03832           0.02058
## 84348301      0.009110        0.07458      0.05661           0.01867
## 84358402      0.011490        0.02461      0.05688           0.01885
## 843786        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
```

```
head(diagnosis)
```

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

Exploratory data analysis

Answer the following quesiton:

Q1. How many observations are in this dataset?

```
q1ans <- nrow(wisc.data)
q1ans
```

```
## [1] 569
```

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

```
q2ans <- sum(diagnosis == 'M')
q2ans
```

```
## [1] 212
```

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

```
varsName <- colnames(wisc.data)
varsName[grep('_mean', x = varsName)]
```

```
##  [1] "radius_mean"            "texture_mean"           "perimeter_mean"
##  [4] "area_mean"              "smoothness_mean"        "compactness_mean"
##  [7] "concavity_mean"         "concave.points_mean"    "symmetry_mean"
## [10] "fractal_dimension_mean"
```

```
q3ans <- sum(grepl('_mean', x = varsName))
q3ans
```

```
## [1] 10
```

2. Principal Component Analysis

Performing PCA

Check column mean and standard deviation for dataset:

```
colmean <- colMeans(wisc.data)
colsd <- apply(wisc.data,2,sd)
colmean
```

```
##             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
```

```
colsd
```

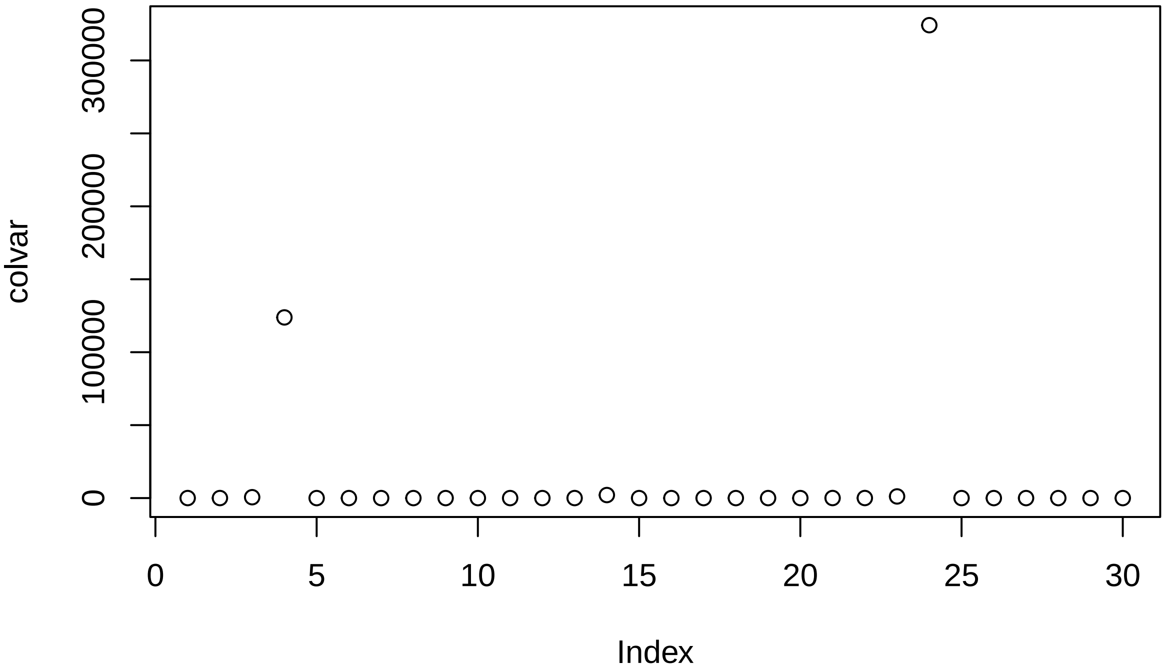
```
##             radius_mean            texture_mean          perimeter_mean
##            3.524049e+00            4.301036e+00            2.429898e+01
##               area_mean         smoothness_mean        compactness_mean
##            3.519141e+02            1.406413e-02            5.281276e-02
##          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
```

Inspect variance:

```
colvar <- colsd * colsd
colvar
```

```
##              radius_mean            texture_mean          perimeter_mean
##             1.241892e+01            1.849891e+01            5.904405e+02
##                area_mean         smoothness_mean        compactness_mean
##             1.238436e+05            1.977997e-04            2.789187e-03
##           concavity_mean     concave.points_mean           symmetry_mean
##             6.355248e-03            1.505661e-03            7.515428e-04
##   fractal_dimension_mean               radius_se              texture_se
##             4.984872e-05            7.690235e-02            3.043159e-01
##             perimeter_se                 area_se           smoothness_se
##             4.087896e+00            2.069432e+03            9.015114e-06
##           compactness_se            concavity_se       concave.points_se
##             3.207029e-04            9.111982e-04            3.807242e-05
##              symmetry_se    fractal_dimension_se            radius_worst
##             6.833290e-05            7.001692e-06            2.336022e+01
##            texture_worst         perimeter_worst              area_worst
##             3.777648e+01            1.129131e+03            3.241674e+05
##         smoothness_worst       compactness_worst         concavity_worst
##             5.213198e-04            2.475477e-02            4.352409e-02
##     concave.points_worst          symmetry_worst fractal_dimension_worst
##             4.320741e-03            3.827584e-03            3.262094e-04
```

```
plot(colvar)
```



Now perform the PCA on data set:

```
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp(x = wisc.data, scale. = TRUE)
```

Look at the summary of PCA:

```
# Look at summary of results
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
```

Answer the following questions:

Q4. From your results, what proportion of the original variance is captured by the first principal

> components (PC1)?

0.4427

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

3 (PC1-3)

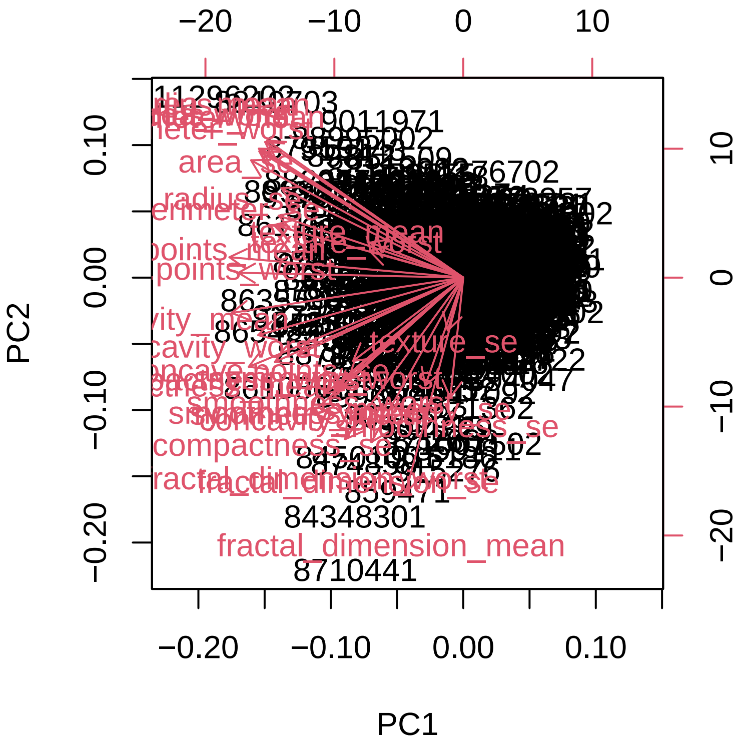
> Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

7 (PC1-7)

Interpreting PCA results

Look at result using `biplot()`:

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

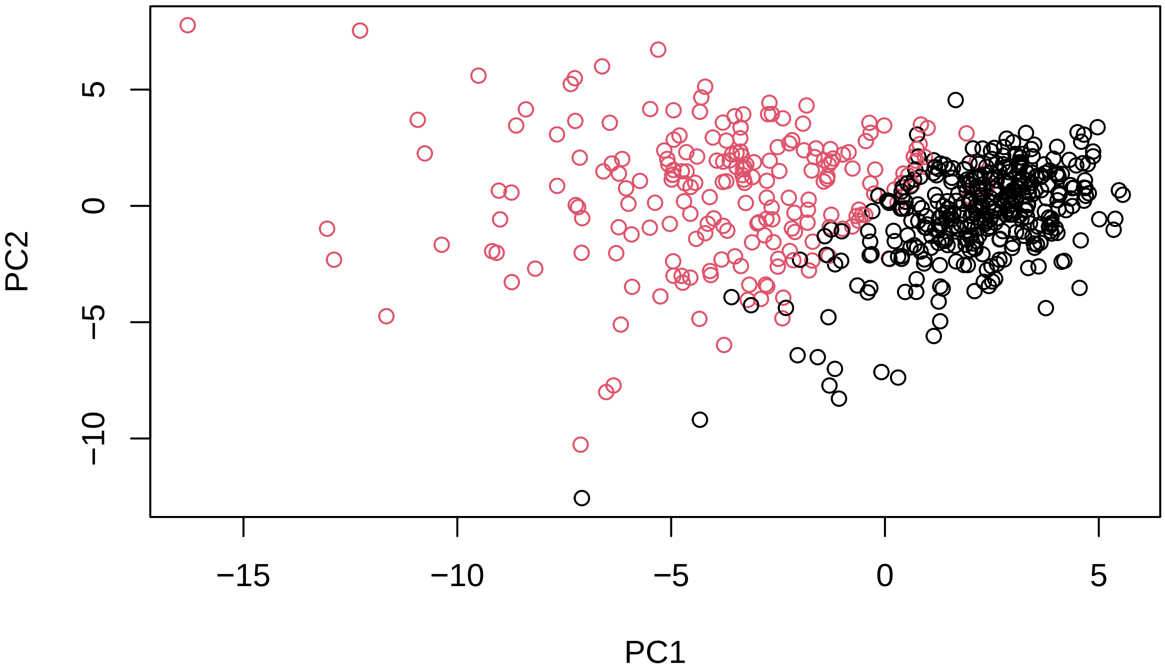


> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

It is difficult to understand because all dimensions and patients are squeezed in two PC.

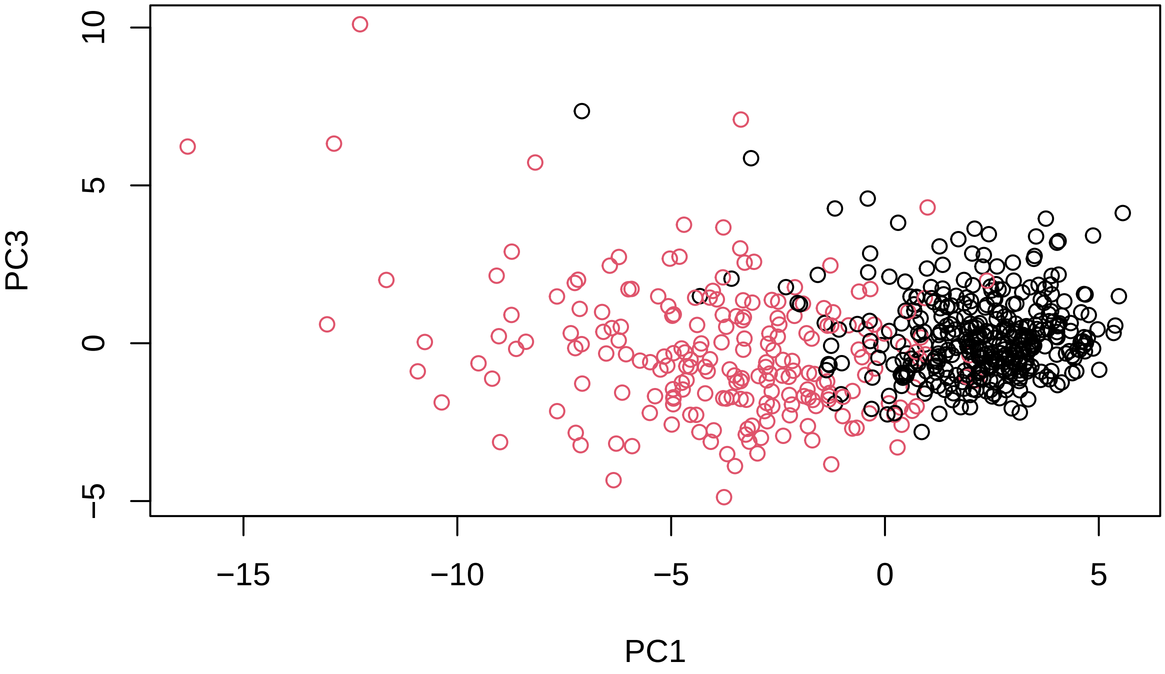
Look at first two PC using `plot()`:

```
# Scatter plot observations by components 1 and 2
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?

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



Two groups overlap more than PC1 and PC2.

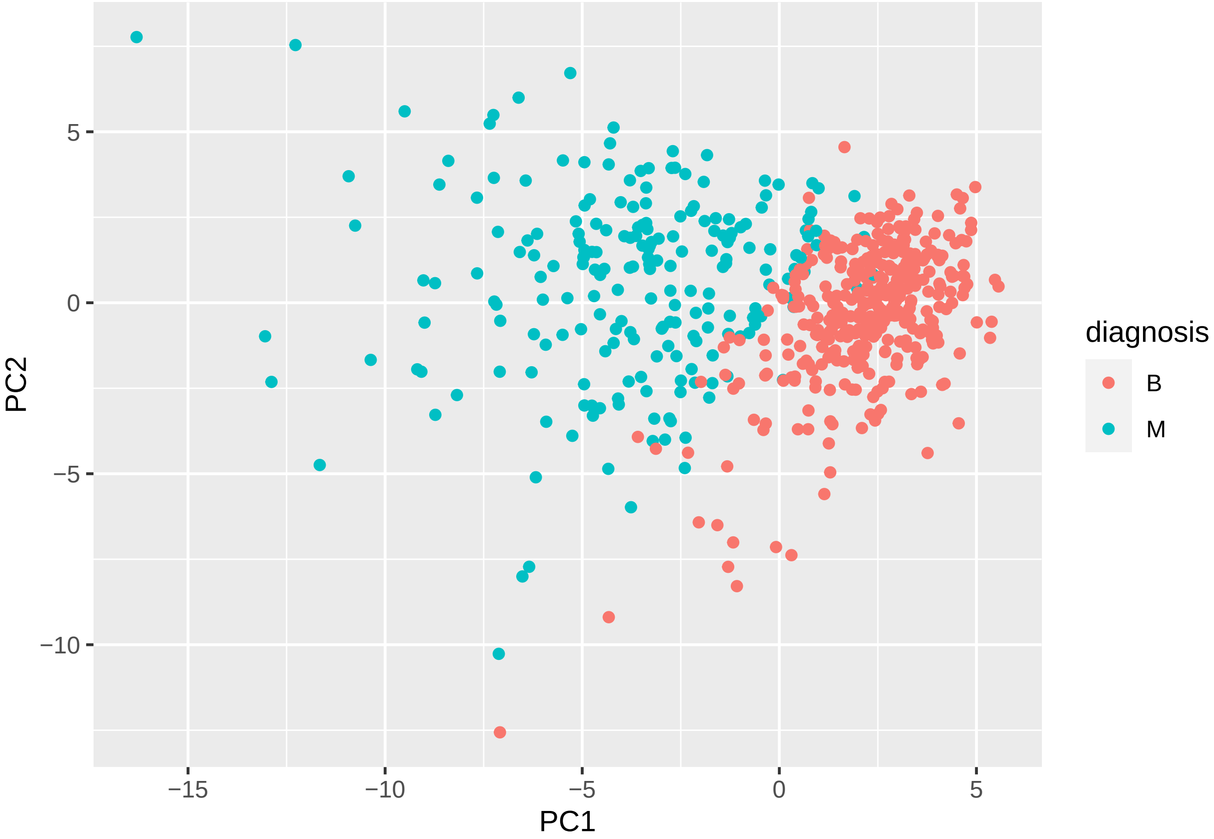
Using ggplot() to plot the result:

```
# Create a data.frame for ggplot
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=diagnosis) +
  geom_point()
```



Variance explained

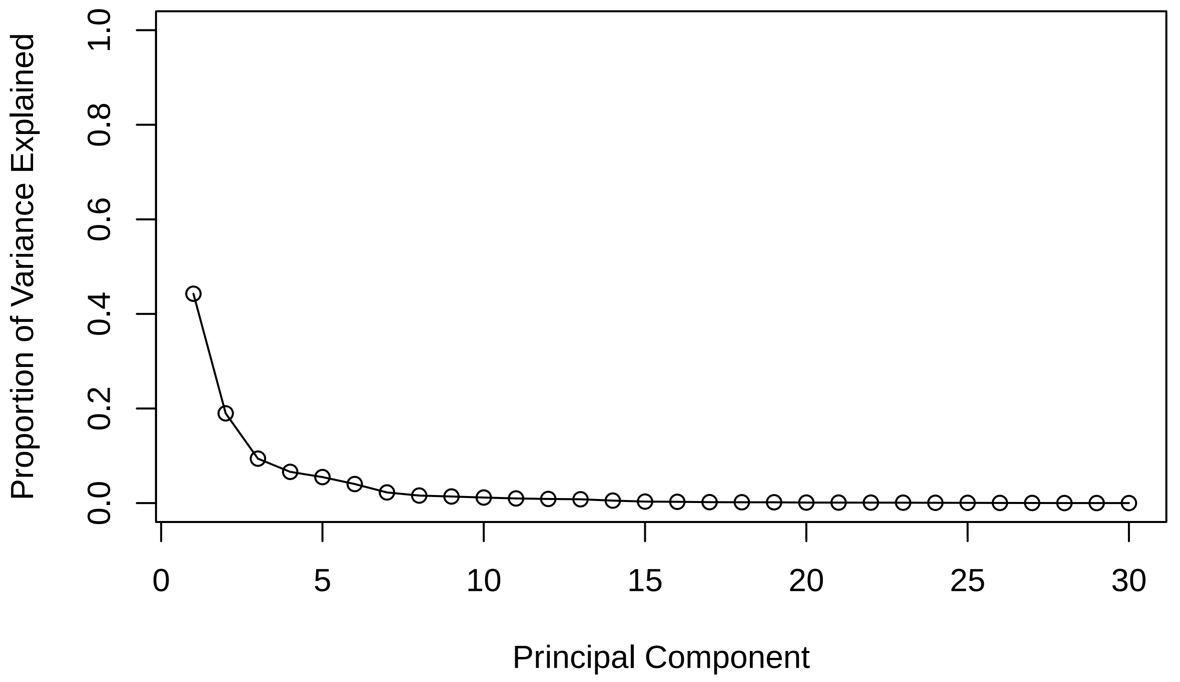
Examine the variance explained by each PC:

```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

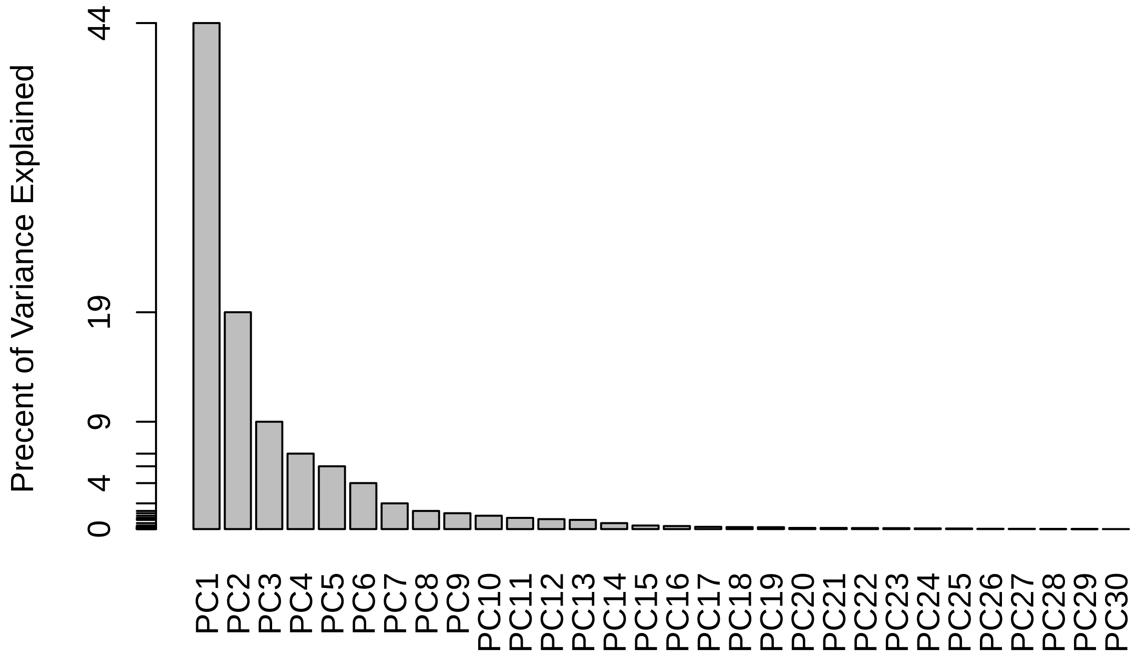
```
## [1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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 )
```



Communicating PCA results

Answering following questions:

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?

```r
cumsum(pve)
```

```
##  [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
q10ans <- length(pve) - sum(cumsum(pve) >= 0.8) + 1
```

Scale the data using `scale()`:

```r
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
head(data.scaled)
```

```
##          radius_mean texture_mean perimeter_mean  area_mean smoothness_mean
## 842302     1.0960995   -2.0715123      1.2688173  0.9835095       1.5670875
## 842517     1.8282120   -0.3533215      1.6844726  1.9070303      -0.8262354
## 84300903   1.5784992    0.4557859      1.5651260  1.5575132       0.9413821
## 84348301  -0.7682333    0.2535091     -0.5921661 -0.7637917       3.2806668
## 84358402   1.7487579   -1.1508038      1.7750113  1.8246238       0.2801253
## 843786    -0.4759559   -0.8346009     -0.3868077 -0.5052059       2.2354545
##          compactness_mean concavity_mean concave.points_mean symmetry_mean
## 842302          3.2806281     2.65054179           2.5302489   2.215565542
## 842517         -0.4866435    -0.02382489           0.5476623   0.001391139
## 84300903        1.0519999     1.36227979           2.0354398   0.938858720
## 84348301        3.3999174     1.91421287           1.4504311   2.864862154
## 84358402        0.5388663     1.36980615           1.4272370  -0.009552062
## 843786          1.2432416     0.86554001           0.8239307   1.004517928
##          fractal_dimension_mean  radius_se texture_se perimeter_se    area_se
## 842302                2.2537638  2.4875451 -0.5647681    2.8305403  2.4853907
## 842517               -0.8678888  0.4988157 -0.8754733    0.2630955  0.7417493
## 84300903             -0.3976580  1.2275958 -0.7793976    0.8501802  1.1802975
## 84348301              4.9066020  0.3260865 -0.1103120    0.2863415 -0.2881246
## 84358402             -0.5619555  1.2694258 -0.7895490    1.2720701  1.1893103
## 843786                1.8883435 -0.2548461 -0.5921406   -0.3210217 -0.2890039
##          smoothness_se compactness_se concavity_se concave.points_se
## 842302      -0.2138135     1.31570389    0.7233897        0.66023900
## 842517      -0.6048187    -0.69231710   -0.4403926        0.25993335
## 84300903    -0.2967439     0.81425704    0.2128891        1.42357487
## 84348301     0.6890953     2.74186785    0.8187979        1.11402678
## 84358402     1.4817634    -0.04847723    0.8277425        1.14319885
## 843786       0.1562093     0.44515196    0.1598845       -0.06906279
##          symmetry_se fractal_dimension_se radius_worst texture_worst
## 842302     1.1477468           0.90628565    1.8850310   -1.35809849
## 842517    -0.8047423          -0.09935632    1.8043398   -0.36887865
## 84300903   0.2368272           0.29330133    1.5105411   -0.02395331
## 84348301   4.7285198           2.04571087   -0.2812170    0.13386631
## 84358402  -0.3607748           0.49888916    1.2974336   -1.46548091
## 843786     0.1340009           0.48641784   -0.1653528   -0.31356043
##          perimeter_worst area_worst smoothness_worst compactness_worst
## 842302         2.3015755  1.9994782        1.3065367         2.6143647
## 842517         1.5337764  1.8888270       -0.3752817        -0.4300658
## 84300903       1.3462906  1.4550043        0.5269438         1.0819801
## 84348301      -0.2497196 -0.5495377        3.3912907         3.8899747
## 84358402       1.3373627  1.2196511        0.2203623        -0.3131190
## 843786        -0.1149083 -0.2441054        2.0467119         1.7201029
##          concavity_worst concave.points_worst symmetry_worst
## 842302         2.1076718            2.2940576      2.7482041
## 842517        -0.1466200            1.0861286     -0.2436753
## 84300903       0.8542223            1.9532817      1.1512420
## 84348301       1.9878392            2.1738732      6.0407261
## 84358402       0.6126397            0.7286181     -0.8675896
## 843786         1.2621327            0.9050914      1.7525273
##          fractal_dimension_worst
## 842302                 1.9353117
## 842517                 0.2809428
## 84300903               0.2012142
## 84348301               4.9306719
## 84358402              -0.3967505
## 843786                 2.2398308
```

3. Hierarchical clustering

Calculate the (Euclidean) distances between all pairs of observations in the new scaled dataset and assign the result to data.dist.

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

```
## [1] 10.309426  6.771675 10.463467  8.663413  8.402233  9.843286
```

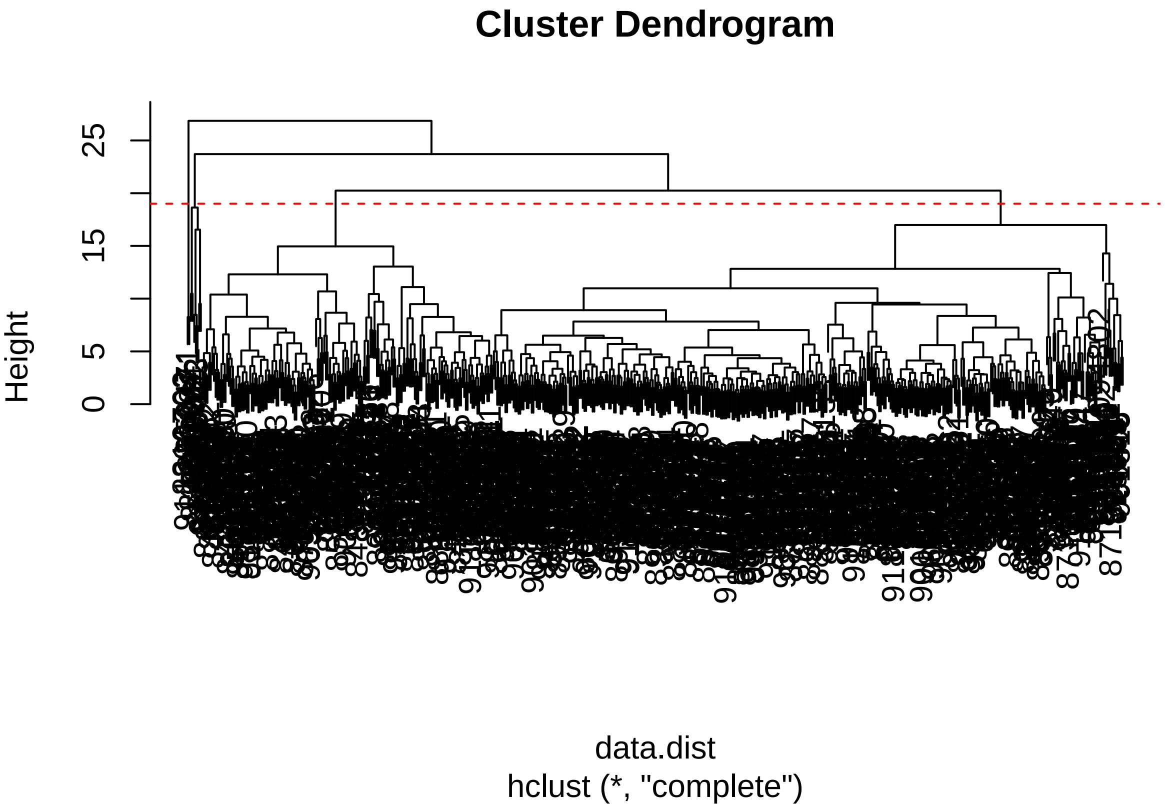
Create a hierarchical clustering model using complete linkage. Manually specify the method argument to `hclust()` and assign the results to wisc.hclust.

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

Results of hierarchical clustering

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

```
plot(wisc.hclust)
abline(a = 19, b = 0, col="red", lty=2)
```



The height is 19.

Selecting number of clusters

Cut the tree sp that it has 4 clusters:

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

```
desireNumClst <-  (2:10)
for (i in desireNumClst) {
  wisc.hclust.clusters <- cutree(wisc.hclust, k = i)
  tbl <- table(wisc.hclust.clusters, diagnosis)
  print(tbl)
}
```

```
##                     diagnosis
## wisc.hclust.clusters   B   M
##                    1 357 210
##                    2   0   2
##                     diagnosis
## wisc.hclust.clusters   B   M
##                    1 355 205
##                    2   2   5
##                    3   0   2
##                     diagnosis
## wisc.hclust.clusters   B   M
##                    1  12 165
##                    2   2   5
##                    3 343  40
##                    4   0   2
##                     diagnosis
## wisc.hclust.clusters   B   M
##                    1  12 165
##                    2   0   5
##                    3 343  40
##                    4   2   0
##                    5   0   2
##                     diagnosis
## wisc.hclust.clusters   B   M
##                    1  12 165
##                    2   0   5
##                    3 331  39
##                    4   2   0
##                    5  12   1
##                    6   0   2
##                     diagnosis
## wisc.hclust.clusters   B   M
##                    1  12 165
##                    2   0   3
##                    3 331  39
##                    4   2   0
##                    5  12   1
##                    6   0   2
##                    7   0   2
##                     diagnosis
## wisc.hclust.clusters   B   M
##                    1  12  86
##                    2   0  79
##                    3   0   3
##                    4 331  39
##                    5   2   0
##                    6  12   1
##                    7   0   2
##                    8   0   2
##                     diagnosis
## wisc.hclust.clusters   B   M
##                    1  12  86
##                    2   0  79
##                    3   0   3
##                    4 331  39
##                    5   2   0
##                    6  12   0
##                    7   0   2
##                    8   0   2
##                    9   0   1
##                     diagnosis
## wisc.hclust.clusters   B   M
##                   1  12  86
##                   2   0  59
##                   3   0   3
##                   4 331  39
##                   5   0  20
##                   6   2   0
##                   7  12   0
##                   8   0   2
##                   9   0   2
##                   10  0   1
```

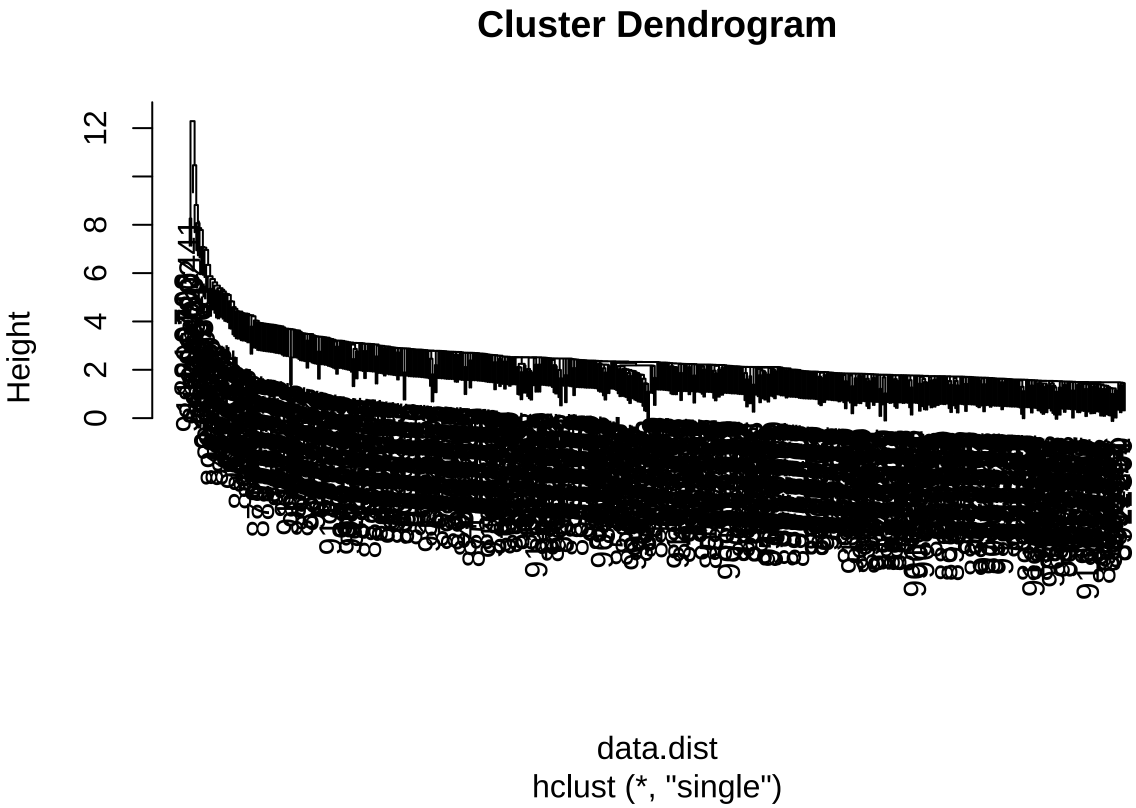
4 and 5 clusters give a better results than the others since 1-3 does not separate data well and cluster above 5 gives too many extra clusters with few datapoint.

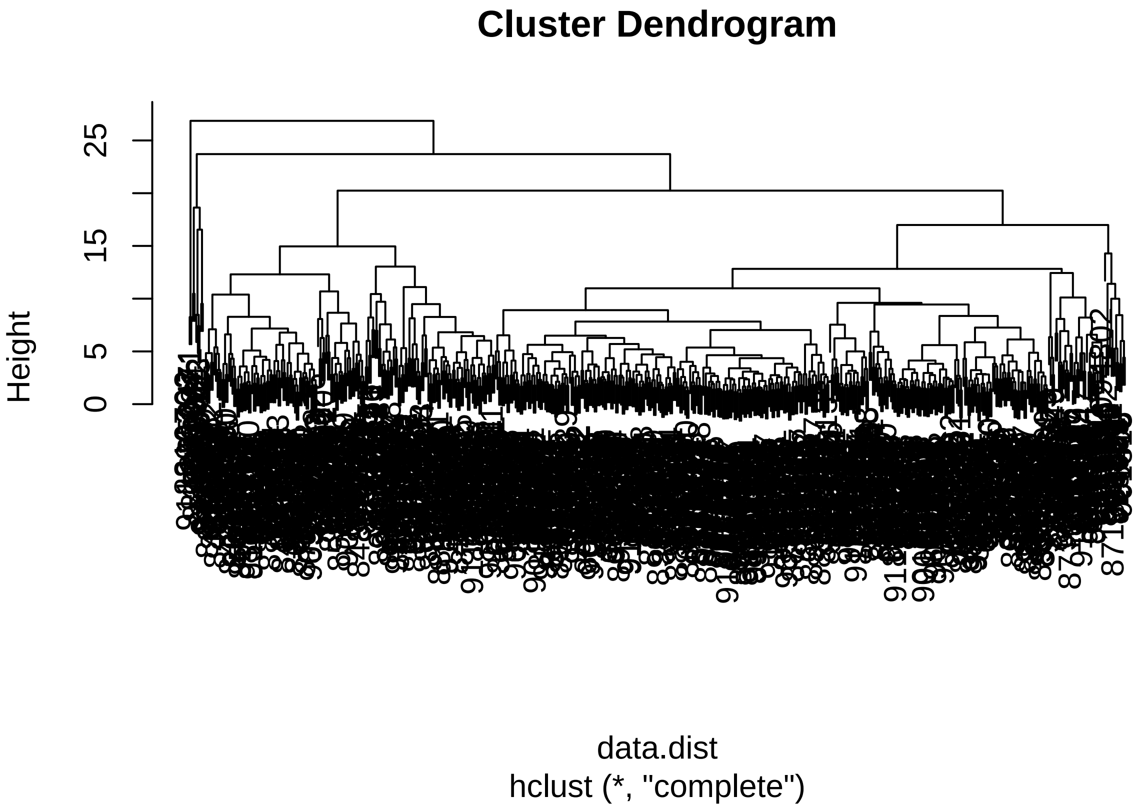
Using different methods

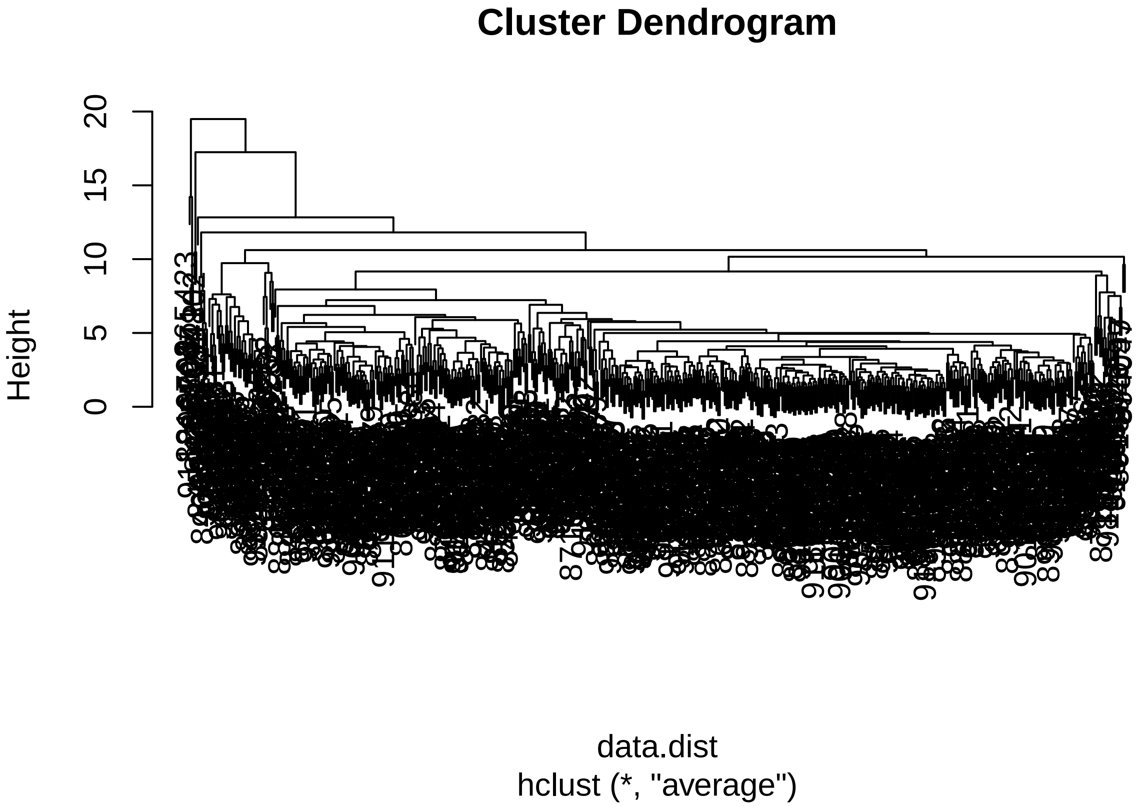
We can use different method to cluster data.

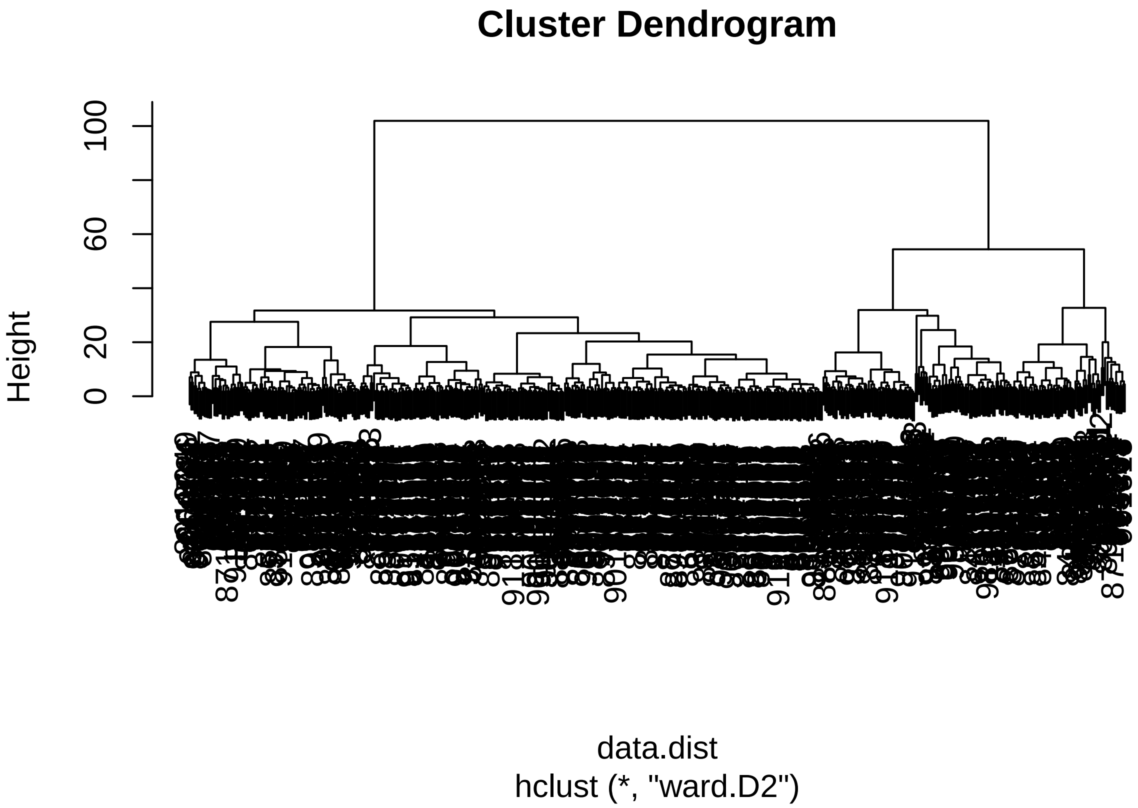
> Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

```
methodV = c("single", "complete", "average", "ward.D2")
for (i in methodV) {
  wisc.hclust <- hclust(data.dist, method = i)
  plot(wisc.hclust)
}
```




Cluster Dendrogram
Height
0
5
15
25
data.dist
hclust (*, "complete")


Cluster Dendrogram
Height
0
5
10
15
20
data.dist
hclust (*, "average")



“ward.D2” is better because it creates the balanced clusters compare to the other methods.

4. OPTIONAL: K-means clustering

K-means clustering and comparing results

Create a k-means model on wisc.data:

```r
wisc.km <- kmeans(scale(wisc.data), centers = 2, nstart = 20)
summary(wisc.km)
```

```
##              Length Class  Mode   
## cluster      569    -none- numeric
## centers       60    -none- numeric
## totss          1    -none- numeric
## withinss       2    -none- numeric
## tot.withinss   1    -none- numeric
## betweenss      1    -none- numeric
## size           2    -none- numeric
## iter           1    -none- numeric
## ifault         1    -none- numeric
```

Use the `table()` function to compare the cluster membership of the k-means model (wisc.km$cluster) to the actual diagnoses contained in the diagnosis vector.

```r
table(wisc.km$cluster, diagnosis)
```

```
##    diagnosis
##       B   M
##   1 343  37
##   2  14 175
```

> Q14. How well does k-means separate the two diagnoses? How does it compare to your hclust results?

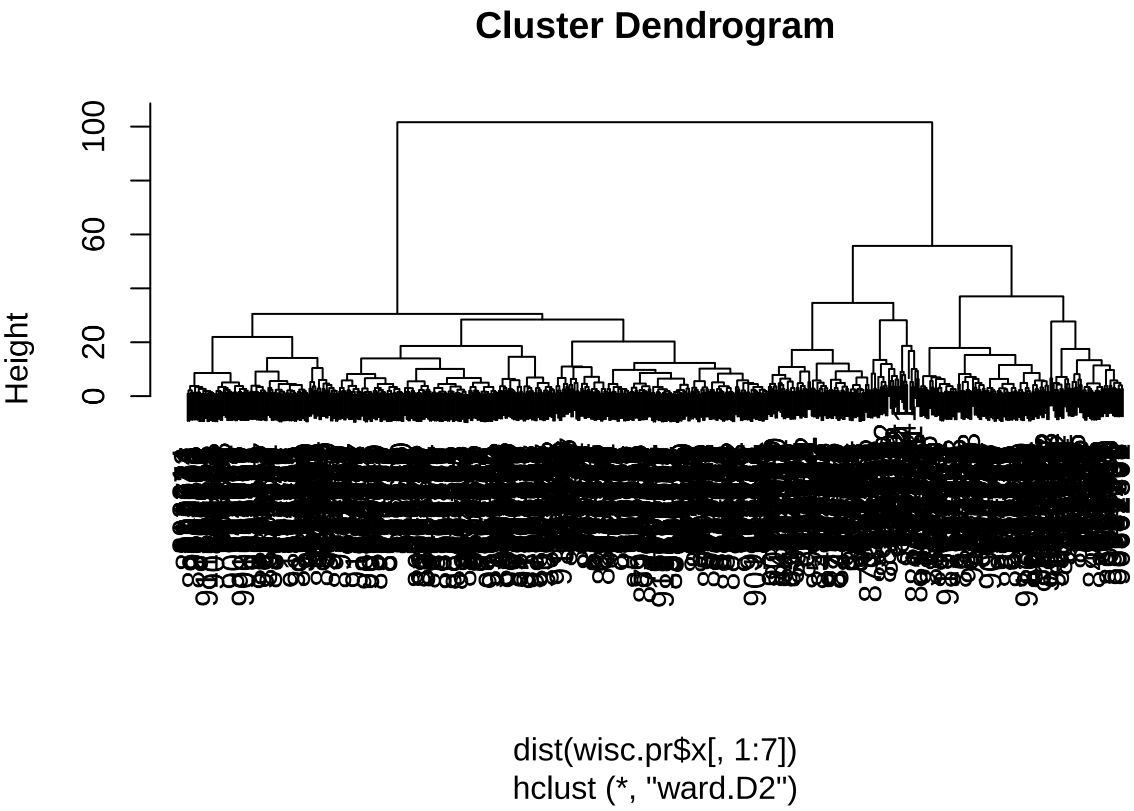
The k-means separate the diagnosis effectively with less number of clusters than hclust.

5. Combining methods

Clustering on PCA results

Using the minimum number of principal components required to describe at least 90% of the variability in the data, create a hierarchical clustering model with the linkage method="ward.D2".

```
  wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method = 'ward.D2')
  plot(wisc.pr.hclust)
```



Cut into two clusters:

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

```
## grps
##   1   2
## 216 353
```

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

```
##     diagnosis
## grps   B   M
##    1  28 188
##    2 329  24
```

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

The model clearly separate benign and malignant into two clusters with small set of data being overlaped (less false positive and false negative).

> 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.

```
table(wisc.km$cluster, diagnosis)
```

```
##    diagnosis
##       B   M
##   1 343  37
##   2  14 175
```

```
wisc.hclust <- hclust(data.dist, method = "complete")
wisc.hclust.clusters <- cutree(wisc.hclust, k = 4)
table(wisc.hclust.clusters, diagnosis)
```

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

The k-mean gives a clear separation of cluster than hclust because hclust gives extra clusters contain small sets of data.

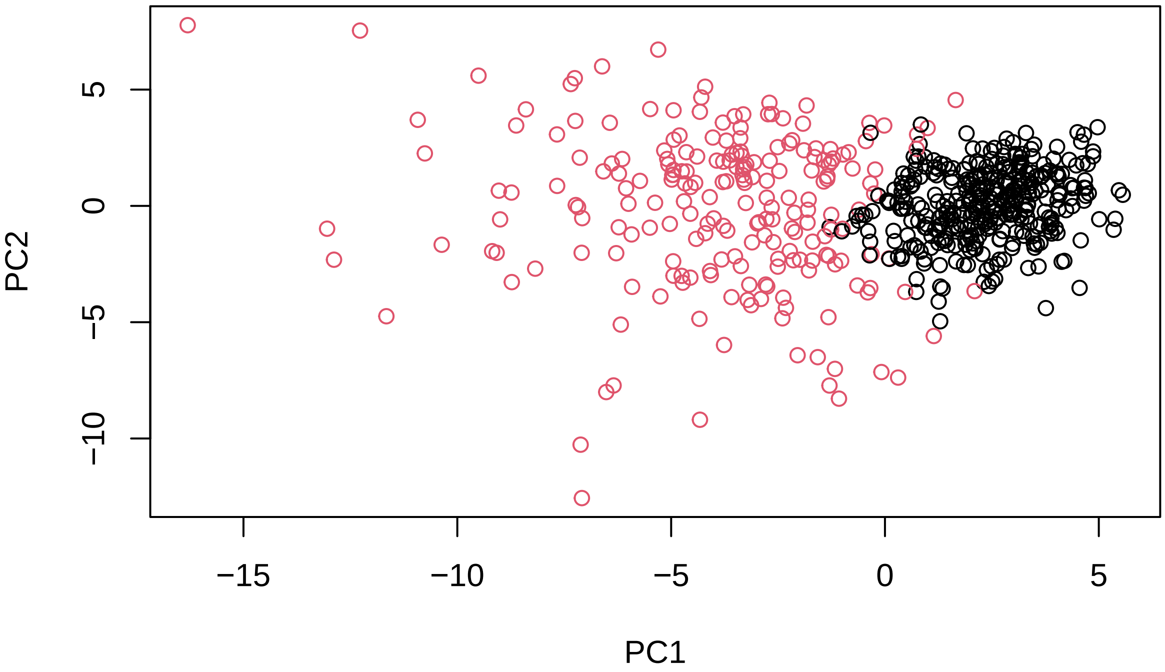
```
g <- as.factor(grps)
levels(g)
```

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

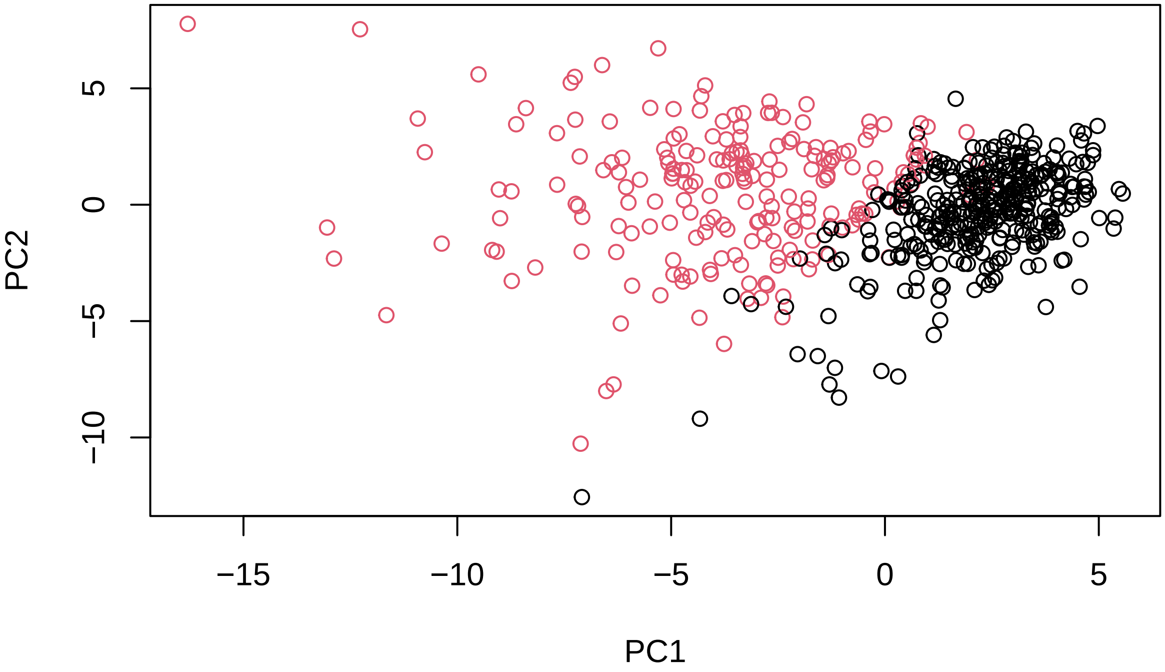
```
g <- relevel(g,2)
levels(g)
```

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

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



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



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

```
wisc.pr.hclust.ss <- c(188 / (188 + 24), 329 / (329 + 24))
wisc.km.ss <- c(175 / (175 + 37), 343 / (343 + 37))
wisc.hclust.ss <- c(165 / (165 + 40), 343 / (343 + 40))

ss.df <- data.frame(wisc.pr.hclust.ss, wisc.km.ss, wisc.hclust.ss,
                    row.names = c("Sensitivity", "Specificity"))
ss.df
```

```
##             wisc.pr.hclust.ss wisc.km.ss wisc.hclust.ss
## Sensitivity         0.8867925  0.8254717      0.8048780
## Specificity         0.9320113  0.9026316      0.8955614
```

PCR hclust produce for both sensitivity and specificity.

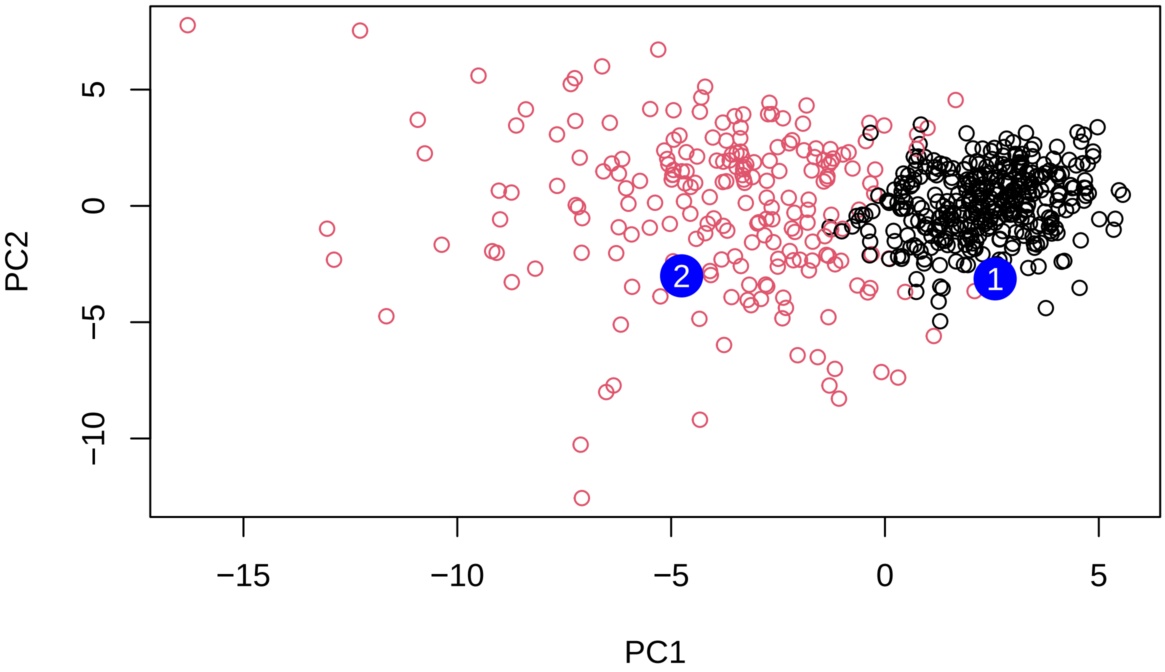
7. Prediction

We will use the `predict()` function that will take our PCA model from before and new cancer cell data and project that data onto our 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?

Patient 2 should be prioritize because the patient fall in tha maglignant cluster.