Class08: Breast Cancer Mini Project

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About

In today's lab, we will work with fine need aspiration (FNA) of breast mass data from the University of Wisconsin.

Data Import

```
wisc.df <- read.csv("WisconsinCancer (1).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
```

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

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

```
[1] 569
```

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

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

```

  B   M 
357 212 
```

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

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

```
[1] 31
```

```r
colnames(wisc.df)
```

```
 [1] "diagnosis"               "radius_mean"            
 [3] "texture_mean"            "perimeter_mean"         
 [5] "area_mean"               "smoothness_mean"        
 [7] "compactness_mean"        "concavity_mean"         
 [9] "concave.points_mean"     "symmetry_mean"          
[11] "fractal_dimension_mean"  "radius_se"              
[13] "texture_se"              "perimeter_se"           
[15] "area_se"                 "smoothness_se"          
[17] "compactness_se"          "concavity_se"           
[19] "concave.points_se"       "symmetry_se"            
[21] "fractal_dimension_se"    "radius_worst"           
[23] "texture_worst"           "perimeter_worst"        
[25] "area_worst"              "smoothness_worst"       
[27] "compactness_worst"       "concavity_worst"        
[29] "concave.points_worst"    "symmetry_worst"         
[31] "fractal_dimension_worst"
```

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

# This tells us where in the column "_mean" suffices are located (position 2, 3, 4, etc...

length(inds)
```

```
[1] 10
```

```
grep("_mean", colnames(wisc.df), value=T)
```

```
 [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"
```

Initial Analysis

Before analysis, I want to remove the expert diagnoses column (aka the answer) from our dataset.

```
# This stores the diagonsis column as a factor. See bottom of printout for Levels: B M
diagnosis <- as.factor(wisc.df$diagnosis)
head(diagnosis)
```

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

```
#We can use -1 here to remove the first column
wisc.data <- wisc.df[,-1]
```

Clustering

We can try a kmeans() clustering first.

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

```
  842302    842517  84300903  84348301  84358402    843786    844359  84458202
       2         2         2         1         2         1         2         1
  844981  84501001    845636  84610002    846226    846381  84667401  84799002
       1         1         1         2         2         1         1         1
  848406  84862001    849014   8510426   8510653   8510824   8511133    851509
       1         2         2         1         1         1         1         2
  852552    852631    852763    852781    852973    853201    853401    853612
       2         2         1         2         2         2         2         1
85382601    854002    854039    854253    854268    854941    855133    855138
```

2	2	2	2	1	1	1	1
855167	855563	855625	856106	85638502	857010	85713702	85715
1	1	2	1	1	2	1	1
857155	857156	857343	857373	857374	857392	857438	85759902
1	1	1	1	1	2	1	1
857637	857793	857810	858477	858970	858981	858986	859196
2	1	1	1	1	1	1	1
85922302	859283	859464	859465	859471	859487	859575	859711
1	1	1	1	1	1	2	1
859717	859983	8610175	8610404	8610629	8610637	8610862	8610908
2	1	1	2	1	2	2	1
861103	8611161	8611555	8611792	8612080	8612399	86135501	86135502
1	1	2	2	1	2	1	2
861597	861598	861648	861799	861853	862009	862028	86208
1	1	1	1	1	1	1	2
86211	862261	862485	862548	862717	862722	862965	862980
1	1	1	1	1	1	1	1
862989	863030	863031	863270	86355	864018	864033	86408
1	1	1	1	2	1	1	1
86409	864292	864496	864685	864726	864729	864877	865128
1	1	1	1	1	1	2	2
865137	86517	865423	865432	865468	86561	866083	866203
1	2	2	1	1	1	1	2
866458	866674	866714	8670	86730502	867387	867739	868202
1	2	1	1	1	1	2	1
868223	868682	868826	868871	868999	869104	869218	869224
1	1	1	1	1	2	1	1
869254	869476	869691	86973701	86973702	869931	871001501	871001502
1	1	1	1	1	1	1	1
8710441	87106	8711002	8711003	8711202	8711216	871122	871149
1	1	1	1	2	1	1	1
8711561	8711803	871201	8712064	8712289	8712291	87127	8712729
1	2	2	1	2	1	1	2
8712766	8712853	87139402	87163	87164	871641	871642	872113
2	1	1	1	1	1	1	1
872608	87281702	873357	873586	873592	873593	873701	873843
1	1	1	1	2	2	2	1
873885	874158	874217	874373	874662	874839	874858	875093
1	1	2	1	1	1	1	1
875099	875263	87556202	875878	875938	877159	877486	877500
1	1	1	1	1	2	2	1
877501	877989	878796	87880	87930	879523	879804	879830
1	2	2	1	1	1	1	2

8810158	8810436	881046502	8810528	8810703	881094802	8810955	8810987
1	1	2	1	2	1	1	1
8811523	8811779	8811842	88119002	8812816	8812818	8812844	8812877
1	1	2	2	1	1	1	1
8813129	88143502	88147101	88147102	88147202	881861	881972	88199202
1	1	1	1	1	1	2	1
88203002	88206102	882488	88249602	88299702	883263	883270	88330202
1	2	1	1	2	2	1	2
88350402	883539	883852	88411702	884180	884437	884448	884626
1	1	1	1	2	1	1	1
88466802	884689	884948	88518501	885429	8860702	886226	886452
1	1	2	1	2	2	2	1
88649001	886776	887181	88725602	887549	888264	888570	889403
2	1	2	1	2	2	2	1
889719	88995002	8910251	8910499	8910506	8910720	8910721	8910748
2	2	1	1	1	1	1	1
8910988	8910996	8911163	8911164	8911230	8911670	8911800	8911834
2	1	2	1	1	2	1	1
8912049	8912055	89122	8912280	8912284	8912521	8912909	8913
2	1	2	1	1	1	1	1
8913049	89143601	89143602	8915	891670	891703	891716	891923
1	1	1	1	1	1	1	1
891936	892189	892214	892399	892438	892604	89263202	892657
1	1	1	1	2	1	2	1
89296	893061	89344	89346	893526	893548	893783	89382601
1	1	1	1	1	1	1	1
89382602	893988	894047	894089	894090	894326	894329	894335
1	1	1	1	1	2	1	1
894604	894618	894855	895100	89511501	89511502	89524	895299
1	2	1	2	1	1	1	1
8953902	895633	896839	896864	897132	897137	897374	89742801
1	1	1	1	1	1	1	2
897604	897630	897880	89812	89813	898143	89827	898431
1	2	1	2	1	1	1	2
89864002	898677	898678	89869	898690	899147	899187	899667
1	1	1	1	1	1	1	1
899987	9010018	901011	9010258	9010259	901028	9010333	901034301
2	1	1	1	1	1	1	1
901034302	901041	9010598	9010872	9010877	901088	9011494	9011495
1	1	1	1	1	2	2	1
9011971	9012000	9012315	9012568	9012795	901288	9013005	901303
2	2	1	1	2	2	1	1
901315	9013579	9013594	9013838	901549	901836	90250	90251

1	1	1	1	1	1	1	1
902727	90291	902975	902976	903011	90312	90317302	903483
1	1	1	1	1	2	1	1
903507	903516	903554	903811	90401601	90401602	904302	904357
2	2	1	1	1	1	1	1
90439701	904647	904689	9047	904969	904971	905189	905190
2	1	1	1	1	1	1	1
90524101	905501	905502	905520	905539	905557	905680	905686
2	1	1	1	1	1	1	1
905978	90602302	906024	906290	906539	906564	906616	906878
1	2	1	1	1	1	1	1
907145	907367	907409	90745	90769601	90769602	907914	907915
1	1	1	1	1	1	1	1
908194	908445	908469	908489	908916	909220	909231	909410
2	2	1	1	1	1	1	1
909411	909445	90944601	909777	9110127	9110720	9110732	9110944
1	2	1	1	2	1	2	1
911150	911157302	9111596	9111805	9111843	911201	911202	9112085
1	2	1	2	1	1	1	1
9112366	9112367	9112594	9112712	911296201	911296202	9113156	911320501
1	1	1	1	2	2	1	1
911320502	9113239	9113455	9113514	9113538	911366	9113778	9113816
1	1	1	1	2	1	1	1
911384	9113846	911391	911408	911654	911673	911685	911916
1	1	1	1	1	1	1	1
912193	91227	912519	912558	912600	913063	913102	913505
1	1	1	1	1	1	1	2
913512	913535	91376701	91376702	914062	914101	914102	914333
1	1	1	2	2	1	1	1
914366	914580	914769	91485	914862	91504	91505	915143
1	1	2	2	1	1	1	2
915186	915276	91544001	91544002	915452	915460	91550	915664
1	1	1	1	1	1	1	1
915691	915940	91594602	916221	916799	916838	917062	917080
1	1	1	1	2	2	1	1
917092	91762702	91789	917896	917897	91805	91813701	91813702
1	2	1	1	1	1	1	1
918192	918465	91858	91903901	91903902	91930402	919537	919555
1	1	1	1	1	2	1	2
91979701	919812	921092	921362	921385	921386	921644	922296
1	1	1	1	1	1	1	1
922297	922576	922577	922840	923169	923465	923748	923780
1	1	1	1	1	1	1	1

```
 924084  924342  924632  924934  924964  925236  925277  925291
      1       1       1       1       1       1       1       1
 925292  925311  925622  926125  926424  926682  926954  927241
      1       1       1       2       2       2       1       2
  92751
      1
```

```
table(km$cluster)
```

```

  1   2
438 131
```

Cross-table

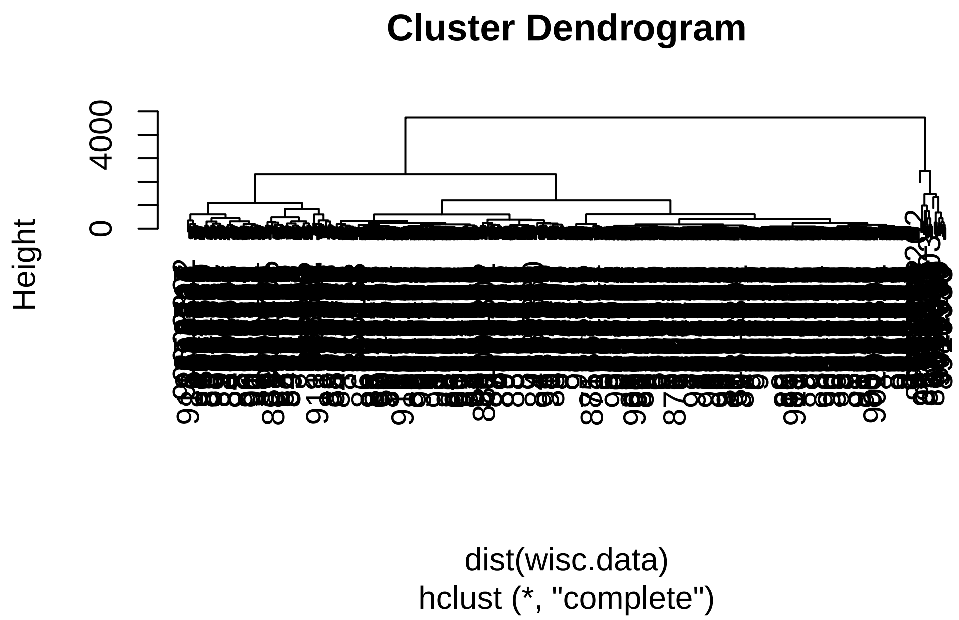
```
table(km$cluster, diagnosis)
```

```
   diagnosis
      B   M
  1 356  82
  2   1 130
```

```
# Shows that cluster 1 has 1 benign and 130 malignant. Cluster 2 has 356 benign and 82 mal
```

Let's try `hclust()`. The key input required for `hclust()` is a distance matrix as produced by the `dist()` function.

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




```
# We can't really tell which groups are malignant and benign. We can cut it at the top, bu
```

PCA

Do we need to scale the data?

We can look at the sd of each column (original variable).

```
round(apply(wisc.data, 2, sd),)
```

```
            radius_mean            texture_mean          perimeter_mean
                      4                       4                      24
              area_mean         smoothness_mean        compactness_mean
                    352                       0                       0
         concavity_mean     concave.points_mean           symmetry_mean
                      0                       0                       0
 fractal_dimension_mean               radius_se              texture_se
                      0                       0                       1
           perimeter_se                 area_se           smoothness_se
                      2                      45                       0
         compactness_se            concavity_se       concave.points_se
```

```
                      0                       0                       0
            symmetry_se    fractal_dimension_se            radius_worst
                      0                       0                       5
          texture_worst         perimeter_worst              area_worst
                      6                      34                     569
       smoothness_worst       compactness_worst         concavity_worst
                      0                       0                       0
   concave.points_worst          symmetry_worst fractal_dimension_worst
                      0                       0                       0
```

Yes, we need to scale. We will run `prcomp()` with `scale=TRUE`.

```r
wisc.pr <- prcomp(wisc.data, scale=TRUE)
summary(wisc.pr)
```

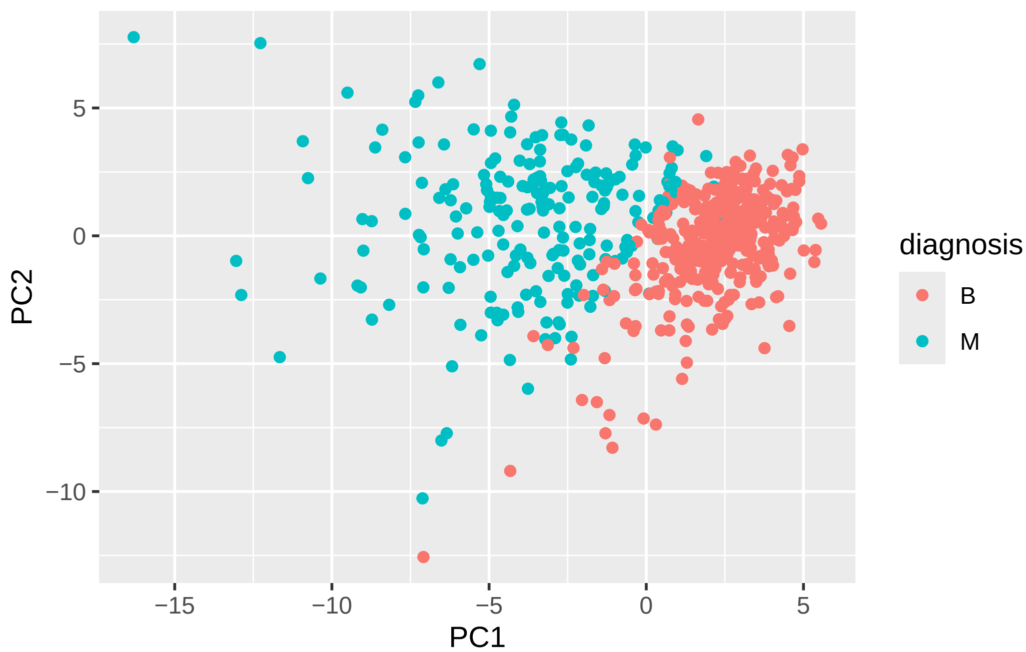
```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 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
```

Generate our main PCA plot (score plot, PC1 vs PC2 plot)…

```r
library(ggplot2)
```

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

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



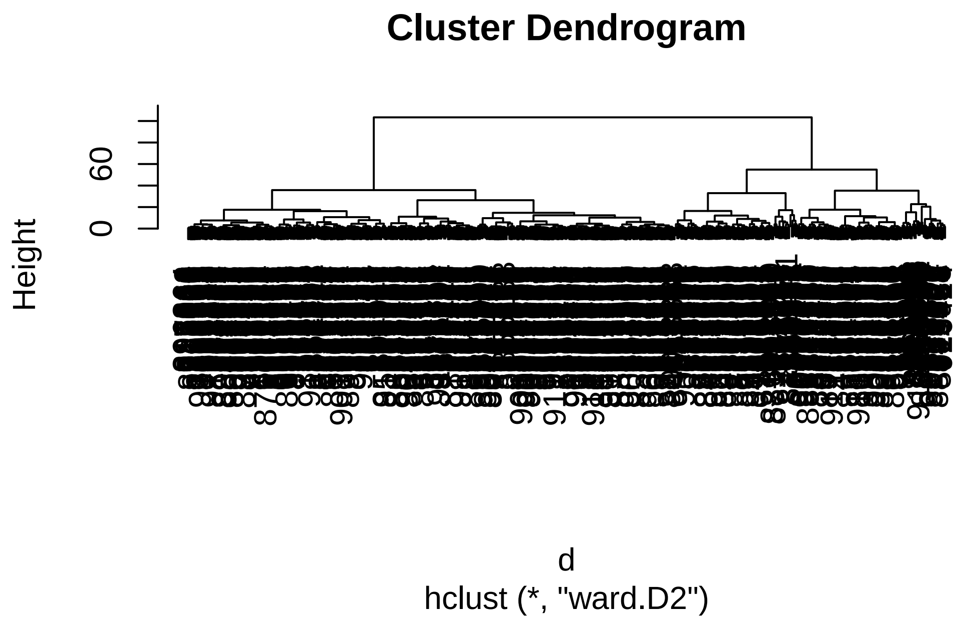
We can clearly see 2 clusters and can probably even draw a line to separate B and M.

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"`. We use Ward's criterion here because it is based on multidimensional variance like principal components analysis. Assign the results to `wisc.pr.hclust`.

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



To get my clustering result/membership vector, I need to "cut" the tree with the "cutree()‘' function.

```
grps <- cutree(hc, h=80)
```

> Q. How many patients are in each cluster group?

```
table(cutree(hc, h=80))
```

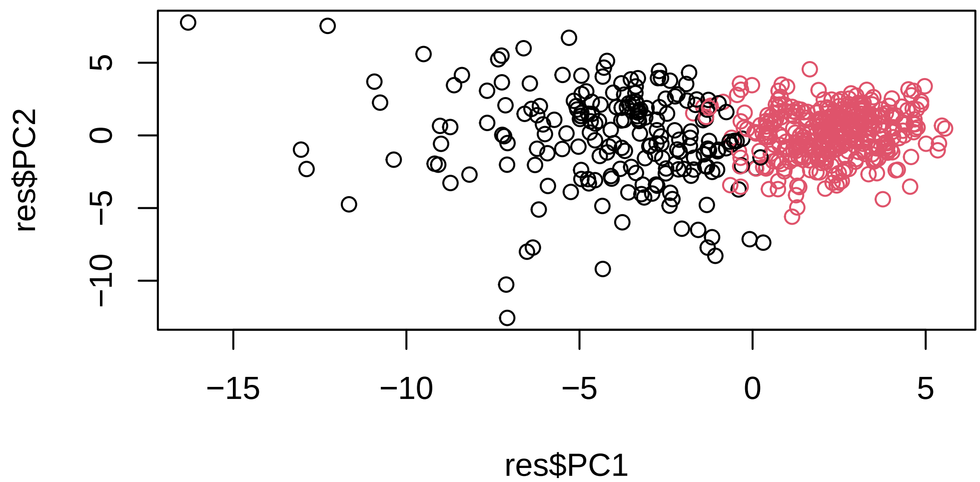
```

  1   2 
203 366 
```

```
table(grps)
```

```
grps
  1   2 
203 366 
```

```r
plot(res$PC1, res$PC2, col=grps)
```



Prediction

We can use our PCA result (model) to do predictions, i.e., taking new unseen data and projecting it onto our new PC variables.

```r
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
npc
```

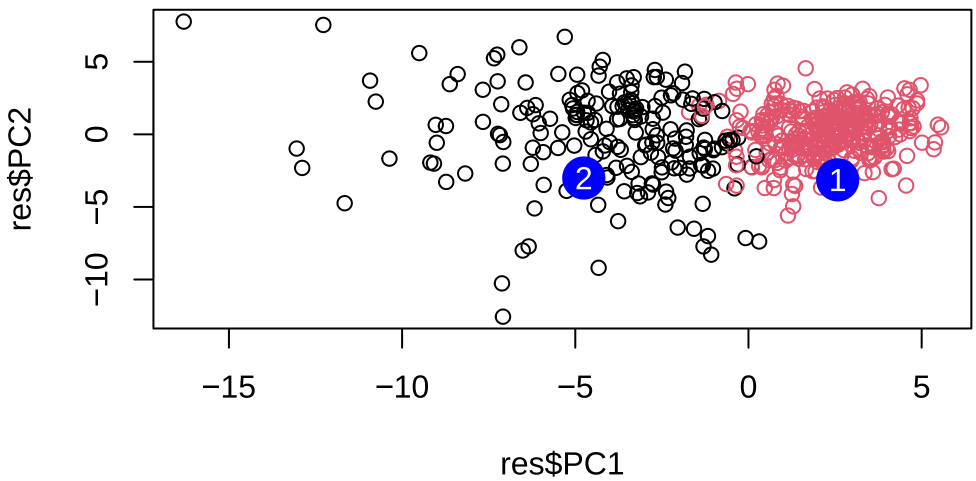
```
           PC1       PC2        PC3        PC4       PC5        PC6        PC7
[1,]  2.576616 -3.135913  1.3990492 -0.7631950  2.781648 -0.8150185 -0.3959098
[2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698 -1.2189945  0.8193031
            PC8       PC9       PC10      PC11      PC12      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(res$PC1, res$PC2, col=grps)

# This plots the 2 patients on the plot.
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)

#This labels the 2 points.
text(npc[,1], npc[,2], labels=c(1,2), col="white")
```



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

The hierarchical clustering of PCA resulted in the best sensitivity and specificity. The model with the best sensitivity should have the highest TP/(TP+FN). The model with the best sensitivity should have the highest TN/(TN+FN).

Q18. Which of these new patients should we prioritize for follow up based on your results?

We should prioritize a follow up for patient 2 because their diagnosis was malignant.

Summary

Principal Component Analysis (PCA) is a super useful method for analyzing large datasets. It works by finding new variables (PCs) that capture the most variance from the original variables in your dataset.