BIMM143class08

##Outline Today we will apply the machine learning methods we introduced in the last class on breast cancer biopsy data from the fine needle aspiration (FNA)

##Data input The data is supplied on CSV format:

```
# Save your input data file into your Project directory
fna.data <- "WisconsinCancer.csv"

# input the data and store as wisc.df
wisc.df <- read.csv(fna.data, row.names=1)
head(wisc.df)</pre>
```

	diagnosis	radius_mean	texture_mean	perimeter_mean	n area_mea	n
842302	М	17.99	10.38	122.80	0 1001.	0
842517	M	20.57	17.77	132.9	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	82.5	7 477.	1
	smoothness	s_mean compa	ctness_mean co	ncavity_mean	concave.po	ints_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_r	mean fractal	_dimension_mea	n radius_se to	exture_se	perimeter_se
842302	0.2	2419	0.0787	1.0950	0.9053	8.589
842517	0.1	1812	0.0566	0.5435	0.7339	3.398
84300903	0.2	2069	0.0599	0.7456	0.7869	4.585
84348301	0.2	2597	0.0974	14 0.4956	1.1560	3.445
84358402	0.1	1809	0.0588	33 0.7572	0.7813	5.438

```
843786
                0.2087
                                       0.07613
                                                  0.3345
                                                              0.8902
         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
                                                                       0.01867
                                                    0.05661
84358402
           94.44
                      0.011490
                                       0.02461
                                                    0.05688
                                                                       0.01885
           27.19
843786
                      0.007510
                                       0.03345
                                                    0.03672
                                                                       0.01137
         symmetry_se fractal_dimension_se radius_worst texture_worst
                                  0.006193
                                                  25.38
842302
             0.03003
                                                                 17.33
             0.01389
                                  0.003532
                                                  24.99
                                                                 23.41
842517
84300903
             0.02250
                                                                 25.53
                                  0.004571
                                                  23.57
84348301
             0.05963
                                  0.009208
                                                  14.91
                                                                 26.50
                                  0.005115
                                                  22.54
84358402
             0.01756
                                                                 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
                  0.4504
84300903
                                        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
  ##Now I will store the diagnosis column for later
  ##and exclude it from the data set I will actually
  ##do things with that I will call `wisc.data()`
```

##-1 to remove first column
wisc.data<-wisc.df[,-1]</pre>

```
diagnosis<-as.factor(wisc.df$diagnosis)</pre>
    Q1 How many people are in this data set?
  nrow(wisc.df)
[1] 569
    Q2. How many of the observations have a malignant diagnosis?
  ##use table to figure out which type the patients fall under benign B or malignant M
  table(wisc.df$diagnosis)
 В
     Μ
357 212
  ##you can also do sum of the thing that equal to M
  ##which is inside the parentheses.
  ##Inside parentheses are true false. Remeber T=1, F=0
  sum(wisc.df$diagnosis=="M")
[1] 212
  ##So 212
    Q3. How many variables/features in the data are suffixed with _mean?
  ##use grep function to find the column that
  ##have character and then length to find the total
  x<-colnames(wisc.data)
```

[1] 10

length(grep("_mean", x))

##Principal Component Analysis

##We need to scale our input data before PCA
##as some of the columns ar emeasured in terms of
##very different units with different means and different variants.
##THe upshot is we set `scale=TRUE`

colMeans(wisc.data)

radius_mean	texture_mean	perimeter_mean	
1.412729e+01	1.928965e+01	9.196903e+01	
area_mean	${\tt smoothness_mean}$	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	
<pre>fractal_dimension_mean</pre>	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	${\tt compactness_worst}$	concavity_worst	
1.323686e-01	2.542650e-01	2.721885e-01	
concave.points_worst	symmetry_worst	${\tt fractal_dimension_worst}$	
1.146062e-01	2.900756e-01	8.394582e-02	

apply(wisc.data,2,sd)

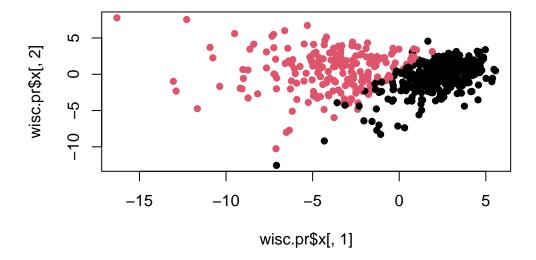
radius_mean 3.524049e+00	texture_mean 4.301036e+00	perimeter_mean 2.429898e+01
area_mean	smoothness_mean	compactness_mean
3.519141e+02	1.406413e-02	5.281276e-02
concavity_mean	concave.points_mean	$symmetry_mean$
7.971981e-02	3.880284e-02	2.741428e-02
fractal_dimension_mean	radius_se	texture_se
7.060363e-03	2.773127e-01	5.516484e-01

```
perimeter_se
                                                        smoothness_se
                                      area_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
```

```
wisc.pr <- prcomp( wisc.data, scale=TRUE )
##summary to get the percent variance and every important info we want
summary(wisc.pr)</pre>
```

Importance of components:

PC1 PC2 PC3 PC4 PC5 PC6 PC7 3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172 Standard deviation 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 PC10 PC11 PC12 PC8 PC9 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 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 0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 0.03987 Standard deviation 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)?

around 44.27%

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

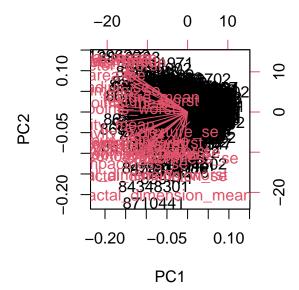
Three

##proportion of variance tells you how much each PC represents. Cumulative proportion adds them all up

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

Seven

biplot(wisc.pr)



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

It is very dense and confusing. Cannot identify each and every element, difficult to understand.

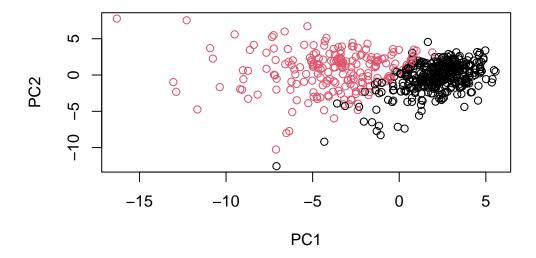
head(wisc.pr\$x)

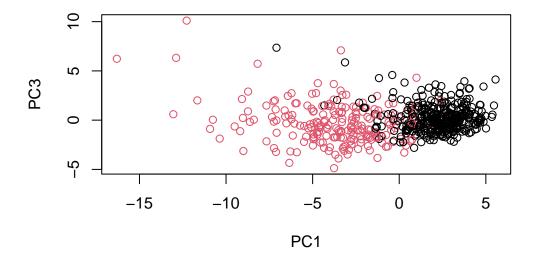
```
PC1
                           PC2
                                      PC3
                                                PC4
                                                            PC5
                                                                        PC6
842302
         -9.184755
                    -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
                    -3.946456 -2.9322967 0.9402096
                                                     1.0551135 -0.45064213
         -2.378155
                              PC8
                 PC7
                                          PC9
                                                     PC10
                                                                PC11
                                                                            PC12
842302
                      0.39805698 -0.15698023 -0.8766305 -0.2627243 -0.8582593
          2.15747152
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
          1.42865363 -1.05863376 -1.40420412 -1.1159933
84348301
                                                           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
```

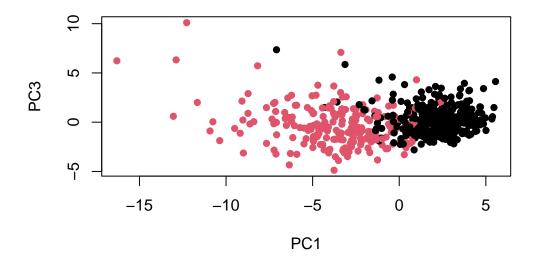
```
842302
         0.10329677 -0.690196797 0.601264078 0.74446075 -0.26523740
842517 -0.94269981 -0.652900844 -0.008966977 -0.64823831 -0.01719707
84300903 -0.41026561 0.016665095 -0.482994760 0.32482472 0.19075064
84348301 -0.93245070 -0.486988399 0.168699395 0.05132509 0.48220960
84358402 0.38760691 -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
       -0.29727706 -0.1297265 -0.07117453 -0.002400178 0.10108043
843786
               PC23
                           PC24
                                        PC25
                                                     PC26
                                                                PC27
         0.08444429 0.175102213 0.150887294 -0.201326305 -0.25236294
842302
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
         0.0007296587 -0.019703996 -0.0034564331
843786
```

Scatter plot observations by PC 1 and 2 help us see better

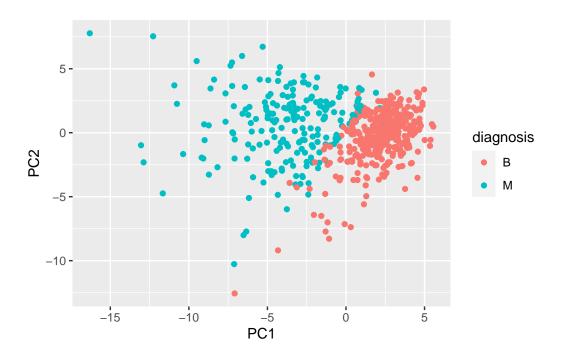
##you can either do column 1, column two like
##before or just set the column and then the
##PC1 and PC2 becomes x and y lab respectively
##so note it later if that makes sense. But as
##can be seen later this only works for default PC1/PC2
plot(wisc.pr\$x, col=diagnosis, xlab="PC1",ylab="PC2")







```
##i quess you can either do
\#\#wisc.pr\$x[,c(1,3)]
 ##wisc.pr$x[,1], wisc.pr$x[,3]
## Repeat for components 1 and 3
##plot(wisc.pr$x[,], col = diagnosis,
##xlab = "PC1", ylab = "PC3")
##this is wrong. You need to tell it that it
##is column 1 or 3 otherwise they will default to column 1 and 2
##also the [] part does not seem to matter as much i guess
##Anyhow to answer question 8, it seems that compared to
##PC1 vs PC2, the black concentration part location
##is now ##slighly lower compared to before?
##Also because PC2 contributed to more variance,
##the separation is more clear than when compared
##to PC3??
# Create a data.frame for ggplot because that is the input
df <- as.data.frame(wisc.pr$x)</pre>
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()
```



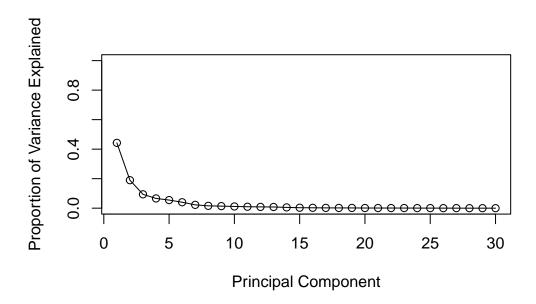
```
##calculating variance
pr.var<-wisc.pr$sdev^2
head(pr.var)</pre>
```

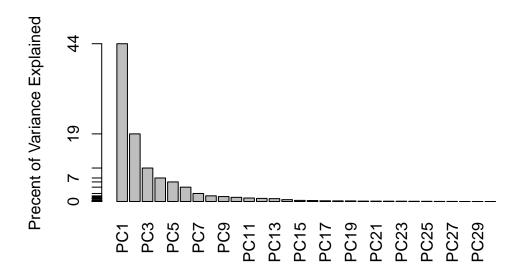
[1] 13.281608 5.691355 2.817949 1.980640 1.648731 1.207357

```
## 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")</pre>
```





library(factoextra)

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

```
fviz_eig(wisc.pr, addlabels = TRUE)
```



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?

-0.26085376

```
##it is one of the columns of wisc.df
wisc.pr$rotation[,1]
```

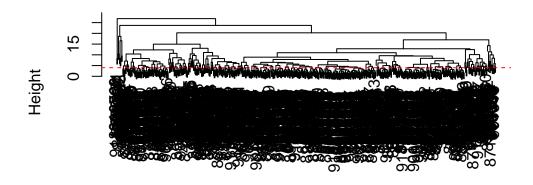
perimeter_mean	texture_mean	radius_mean
-0.22753729	-0.10372458	-0.21890244
compactness_mean	${\tt smoothness_mean}$	area_mean
-0.23928535	-0.14258969	-0.22099499
symmetry_mean	concave.points_mean	concavity_mean
-0.13816696	-0.26085376	-0.25840048
texture_se	radius_se	fractal_dimension_mean
-0.01742803	-0.20597878	-0.06436335
smoothness_se	area_se	perimeter_se
-0.01453145	-0.20286964	-0.21132592
concave.points_se	concavity_se	compactness_se
-0.18341740	-0.15358979	-0.17039345
radius_worst	fractal_dimension_se	symmetry_se
-0.22799663	-0.10256832	-0.04249842
area_worst	perimeter_worst	texture_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
                                 -0.12290456
         -0.25088597
                                                          -0.13178394
```

Q10. What is the minimum number of principal components required to explain

```
80% of the variance of the data?
5
At least to section #5 question 15
  data.scaled<-scale(wisc.data)</pre>
  data.dist <- dist(data.scaled)</pre>
  head(data.dist)
[1] 10.309426 6.771675 10.463467 8.663413 8.402233 9.843286
  wisc.hclust <- hclust(data.dist, method="complete")</pre>
  wisc.hclust
Call:
hclust(d = data.dist, method = "complete")
Cluster method
                 : complete
Distance
                  : euclidean
Number of objects: 569
  ## Q.11 Using the plot() and abline() functions,
  ##what is the height at which the clustering model
  ##has 4 clusters?
  plot(wisc.hclust)
```

abline(h=4, col="red", lty=2)



data.dist hclust (*, "complete")

```
##Answer is around 20??

##here it also shows that you can choose two columns
##with [1:3]

wisc.hclust.clusters <- cutree(wisc.hclust, k=4)
##to compare just (,)
table(wisc.hclust.clusters, diagnosis)</pre>
```

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

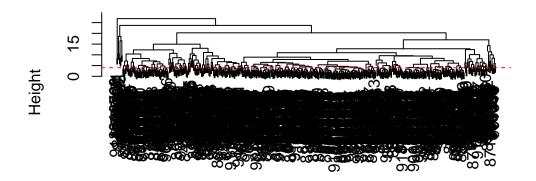
```
wisc.hclust.clusters2 <- cutree(wisc.hclust, k=2)
table(wisc.hclust.clusters2, diagnosis)</pre>
```

diagnosis

diagnosis wisc.hclust.clusters3 В М 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

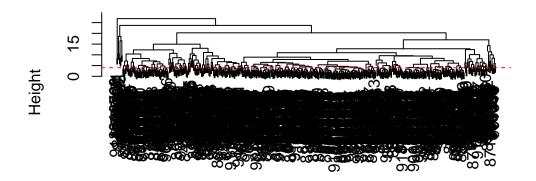
```
##Q12. Can you find a better cluster vs diagnoses
##match by cutting into a different number of clusters between 2 and 10?
##Yes it seems the k value increases the more certain
##the difference or gap in value between the two BM i
##ncreases

plot(wisc.hclust)
abline(h = 4, col = "red", lty = 2, method = "ward.D2")
```



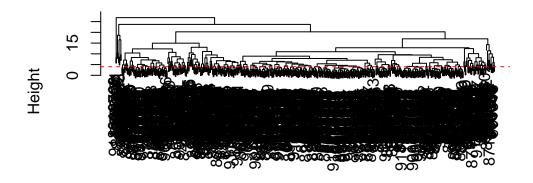
data.dist hclust (*, "complete")

```
plot(wisc.hclust)
abline(h = 4, col = "red", lty = 2, method = "single")
```



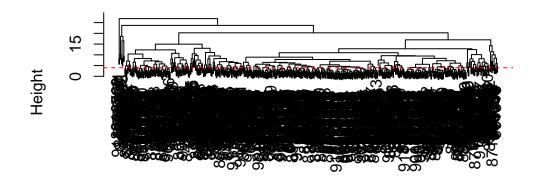
data.dist hclust (*, "complete")

```
plot(wisc.hclust)
abline(h = 4, col = "red", lty = 2, method = "complete")
```



data.dist hclust (*, "complete")

```
plot(wisc.hclust)
abline(h = 4, col = "red", lty = 2, method = "average")
```

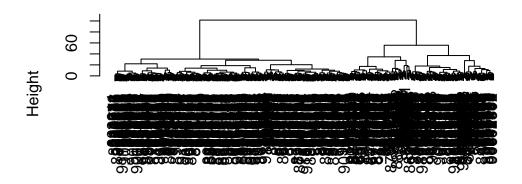


data.dist hclust (*, "complete")

```
##they all look the same to me
x<-scale(wisc.data)</pre>
wisc.km<-kmeans(x,centers=2,nstart=20)</pre>
table(wisc.km$cluster, diagnosis)
diagnosis
    В
        Μ
1 343 37
2 14 175
\#\#Q14. How well does k-means separate the two diagnoses?
##How does it compare to your hclust results?
table(wisc.km$cluster, wisc.hclust.clusters)
wisc.hclust.clusters
      2
           3
        0 363
  17
2 160
       7 20
```

```
##well it seems both get the job done well
##at least in this case not a whole difference

d<-dist(wisc.pr$x[,1:7])
wisc.pr.hclust<-hclust(d, method="ward.D2")
plot(wisc.pr.hclust)</pre>
```



d hclust (*, "ward.D2")

```
##wisc.hclust.clusters <- c
```

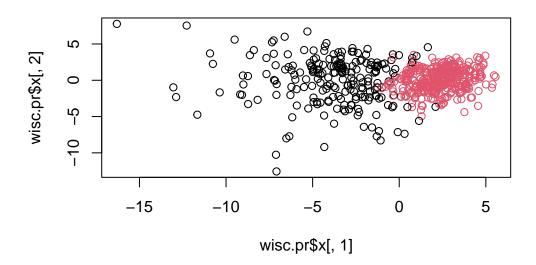
Generate 2 cluster groups from this helust object

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

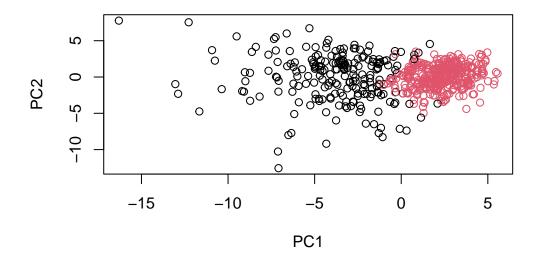
```
diagnosis
grps B M
1 28 188
2 329 24

##these two gets you the same graph
```

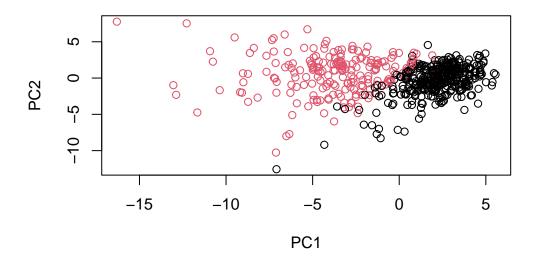
plot(wisc.pr\$x[,1], wisc.pr\$x[,2], col=grps)



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



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



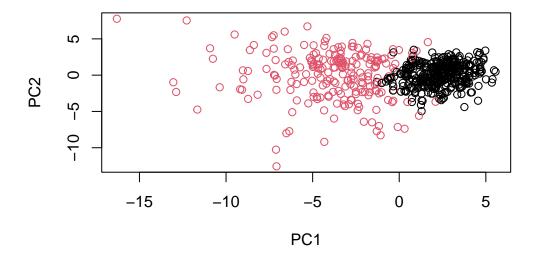
```
##swap colors by making it as factor
g <- as.factor(grps)
levels(g)

[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)</pre>
```



```
##Q.15
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
table(wisc.pr.hclust.clusters, diagnosis)</pre>
```

diagnosis

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