Class 8: Unsupervised Learning Mini-Project

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Introductionary Lecture

Scaling

```
data(mtcars)
head(mtcars)
```

```
mpg cyl disp hp drat
                                       wt qsec vs am gear carb
Mazda RX4
                         160 110 3.90 2.620 16.46 0
                21.0
Mazda RX4 Wag
                21.0
                       6 160 110 3.90 2.875 17.02 0 1
Datsun 710
                22.8 4 108 93 3.85 2.320 18.61 1 1
                                                             1
Hornet 4 Drive
                21.4 6 258 110 3.08 3.215 19.44 1 0
Hornet Sportabout 18.7
                       8 360 175 3.15 3.440 17.02 0 0
Valiant
                18.1
                       6 225 105 2.76 3.460 20.22 1 0
```

colMeans(mtcars)

```
cyl
                           disp
                                                  drat
                                                                         qsec
                                         hp
                                                                wt
      mpg
20.090625
            6.187500 230.721875 146.687500
                                              3.596563
                                                          3.217250 17.848750
                  am
                            gear
                                       carb
0.437500
            0.406250
                       3.687500
                                   2.812500
```

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

```
drat
      mpg
                  cyl
                             disp
                                            hp
                                                                    wt
6.0269481
            1.7859216 123.9386938 68.5628685
                                                 0.5346787
                                                             0.9784574
     qsec
                                                      carb
                   ٧s
                                          gear
1.7869432
            0.5040161
                        0.4989909
                                    0.7378041
                                                 1.6152000
```

It is important to scale your data: This will cause all of the data to be in more appropritate units

```
x <- scale(mtcars)
head(x)</pre>
```

```
disp
                                    cyl
                                                                     drat
                         mpg
                                                            hp
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
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
                                                  ٧s
                                                             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
```

round(colMeans(x),2)

```
mpg cyl disp hp drat wt qsec vs am gear carb 0 0 0 0 0 0 0 0 0 0
```

In-class Lab Section

Explanatory Data Analysis

Preparing the data

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

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

head(wisc.df)

	diagnosis radi	us_mean	texture_mean	perimeter_mean	area_mean	
842302	М	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_mea	n compa	ctness_mean co	ncavity_mean co	oncave.poir	nts_mean
842302	0.1184	0	0.27760	0.3001		0.14710
842517	0.0847	4	0.07864	0.0869		0.07017
84300903	0.1096	0	0.15990	0.1974		0.12790
84348301	0.1425	0	0.28390	0.2414		0.10520
84358402	0.1003	0	0.13280	0.1980		0.10430
843786	0.1278	0	0.17000	0.1578		0.08089
	symmetry_mean	fractal	_dimension_mea	n radius_se te	kture_se pe	erimeter_se
842302	0.2419		0.0787	1 1.0950	0.9053	8.589
842517	0.1812		0.0566	7 0.5435	0.7339	3.398
84300903	0.2069		0.0599	0.7456	0.7869	4.585
84348301	0.2597		0.0974	1 0.4956	1.1560	3.445
84358402	0.1809		0.0588	3 0.7572	0.7813	5.438
843786	0.2087		0.0761	3 0.3345	0.8902	2.217
	area_se smooth	_	-	• –	concave.po	oints_se
842302		.006399	0.0490			0.01587
842517	74.08 0	.005225	0.0130	0.01860		0.01340
84300903	94.03 0	.006150	0.0400	0.03832		0.02058
84348301	27.23 0	.009110	0.0745	0.05661		0.01867
84358402	94.44 0	.011490	0.0246	0.05688		0.01885
843786		.007510	0.0334			0.01137
	symmetry_se fr	actal_d:	_	-	_	
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	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	s_worst	compactne	ess_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.po	ints_worst	symmeti	ry_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	on_worst				
842302		0.11890				
842517		0.08902				
84300903		0.08758				
84348301		0.17300				
84358402		0.07678				
843786		0.12440				

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"	

Remove this first diagnosis coulmn from the dataset as I don't want to pass this PCA etc. It is essentially the experet "answer" that we will compare our analysis results to

```
# We can use -1 here to remove the first column
wisc.data <- wisc.df[,-1]
head(wisc.data)</pre>
```

	radius_mean	texture mean	n perimet	er mean	area mea	an smoothi	ness mean
842302	17.99	10.38	_	122.80	1001		0.11840
842517	20.57	17.77	7	132.90	1326	. 0	0.08474
84300903	19.69	21.25	5	130.00	1203	. 0	0.10960
84348301	11.42	20.38	3	77.58	386	. 1	0.14250
84358402	20.29	14.34	1	135.10	1297	. 0	0.10030
843786	12.45	15.70)	82.57	477	. 1	0.12780
	compactness_	mean concav	ity_mean	concave.	points_r	nean symme	etry_mean
842302	0.2	7760	0.3001		0.14	4710	0.2419
842517	0.0	7864	0.0869		0.0	7017	0.1812
84300903	0.1	.5990	0.1974		0.1	2790	0.2069
84348301	0.2	8390	0.2414		0.10	0520	0.2597
84358402	0.1	.3280	0.1980		0.10	0430	0.1809
843786	0.1	.7000	0.1578		0.08	3089	0.2087
	fractal_dime	nsion_mean n	radius_se	texture	e_se per	imeter_se	area_se
842302		0.07871	1.0950	0.9	9053	8.589	153.40
842517		0.05667	0.5435		7339	3.398	74.08
84300903		0.05999	0.7456	0.7	7869	4.585	94.03
84348301		0.09744	0.4956		1560	3.445	27.23
84358402		0.05883	0.7572		7813	5.438	94.44
843786		0.07613	0.3345		3902	2.217	27.19
	smoothness_s	_		-		_	
842302	0.00639		04904	0.0537		0.01	
842517	0.00522		01308	0.0186		0.013	
84300903	0.00615		04006	0.0383		0.020	
84348301	0.00911)7458	0.0566		0.018	
84358402	0.01149		02461	0.0568		0.018	
843786	0.00751		3345	0.0367		0.013	
	symmetry_se	fractal_dime	_	radius_	=	_	
842302	0.03003		0.006193		25.38		. 33
842517	0.01389		0.003532		24.99		.41
84300903	0.02250		0.004571		23.57		. 53
84348301	0.05963		0.009208		14.91		.50
84358402	0.01756		0.005115		22.54		. 67
843786	0.02165		0.005082		15.47	23	.75

	perimeter_worst	area_worst	smoothness	s_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.po	ints_worst	symmeti	ry_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	on_worst				
842302		0.11890				
842517		0.08902				
84300903		0.08758				
84348301		0.17300				
84358402		0.07678				
843786		0.12440				

colnames(wisc.data)

"radius_mean"	"texture_mean"
"perimeter_mean"	"area_mean"
"smoothness_mean"	"compactness_mean"
"concavity_mean"	"concave.points_mean"
"symmetry_mean"	"fractal_dimension_mean"
"radius_se"	"texture_se"
"perimeter_se"	"area_se"
"smoothness_se"	"compactness_se"
"concavity_se"	"concave.points_se"
"symmetry_se"	"fractal_dimension_se"
"radius_worst"	"texture_worst"
"perimeter_worst"	"area_worst"
"smoothness_worst"	"compactness_worst"
"concavity_worst"	"concave.points_worst"
"symmetry_worst"	"fractal_dimension_worst"
	"radius_mean" "perimeter_mean" "smoothness_mean" "concavity_mean" "radius_se" "perimeter_se" "smoothness_se" "concavity_se" "symmetry_se" "radius_worst" "perimeter_worst" "smoothness_worst" "concavity_worst" "symmetry_worst"

Takes a subset of the data of the first column

diagnosis <- wisc.df\$diagnosis diagnosis</pre>

```
[1] ייאוי ייאוי
```

Q1. How many observations are in this dataset?

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

```
[1] 569
```

There are 569 observations in this data set(

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

```
table(diagnosis)

diagnosis
B M
357 212
```

There are 212 observations of the malignant diagnosis

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

```
col_mean <- grep('_mean', colnames(wisc.df))
length(col_mean)</pre>
```

[1] 10

There are 10 variables/features in the data that are suffixed with _mean

Principal Component Analysis

Performing PCA on the wisc.df

- Always want to scale
- Different means and SDs so we want to treat the entire data set equally

```
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp( wisc.data, scale=T )
summary(wisc.pr)</pre>
```

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 0.30681 0.28260 0.24372 0.22939 0.22244 0.17652 0.1731 Standard deviation 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

See what is in our PCA result object -> List of 5 "things"

attributes(wisc.pr)

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

Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)?

44% of the variance is captured in PC1

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

You need 3 PCAs

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

You need 7 PCAs

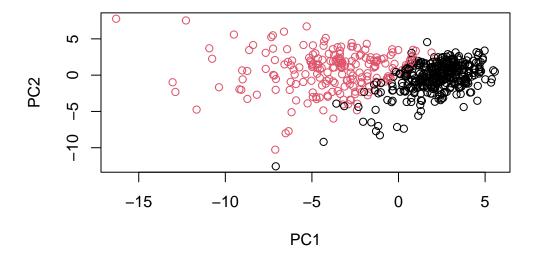
Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

Should use the first 2 columns to make the highest percentage.

head(wisc.pr\$x)

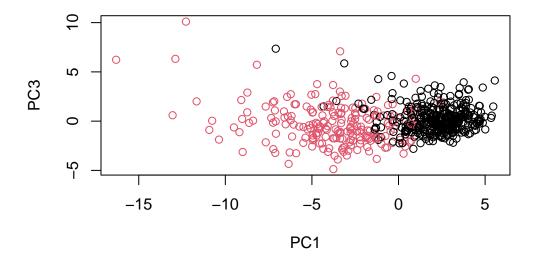
```
PC2
                                    PC3
              PC1
                                              PC4
                                                         PC5
                                                                     PC6
842302
        -9.184755
                   -1.946870 -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
                            PC8
                                        PC9
                                                  PC10
                                                             PC11
                PC7
                                                                        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 \quad 0.16529843 \quad -0.13335576 \quad -0.5299649 \quad -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
                                                           0.19671335
               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
```



There is a stark difference in clustering between the red and black cells showing the diagnosis of the individual

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



The cells are moving closer together and show less amount of clustering. But there are still levels of separation to allow for prediction

Q9. For the first principal component, what is the component of the loading vector (i.e.wisc.pr\$rotation[,1]) for the featureconcave.points_mean?

```
wisc.pr$rotation['concave.points_mean', 1]
```

[1] -0.2608538

-0.26085376 is the component of the loading vector

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

```
y <- summary(wisc.pr)
y$importance[2,]</pre>
```

```
PC1
            PC2
                    PC3
                             PC4
                                     PC5
                                             PC6
                                                      PC7
                                                              PC8
                                                                      PC9
                                                                              PC10
0.44272 0.18971 0.09393 0.06602 0.05496 0.04025 0.02251 0.01589 0.01390 0.01169
   PC11
           PC12
                   PC13
                           PC14
                                    PC15
                                            PC16
                                                     PC17
                                                             PC18
                                                                     PC19
                                                                              PC20
0.00980 0.00871 0.00805 0.00523 0.00314 0.00266 0.00198 0.00175 0.00165 0.00104
   PC21
           PC22
                   PC23
                           PC24
                                    PC25
                                            PC26
                                                     PC27
                                                             PC28
                                                                     PC29
                                                                              PC30
0.00100 0.00091 0.00081 0.00060 0.00052 0.00027 0.00023 0.00005 0.00002 0.00000
```

You need 5 principle components

Hierarchical Clustering

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

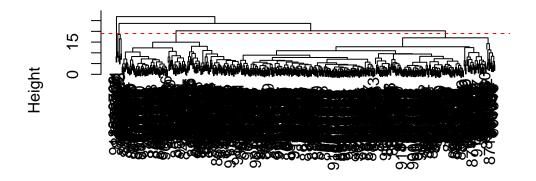
data.dist <- dist(data.scaled)

wisc.hclust <- hclust(data.dist, method='complete')</pre>
```

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

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

Cluster Dendrogram



data.dist hclust (*, "complete")

After scaling the data the height that has 4 clusters is 19

Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

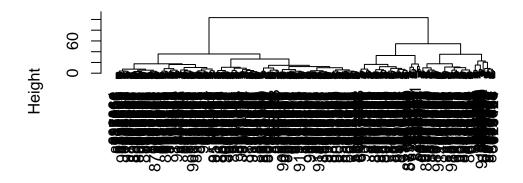
```
wisc.hclust.clusters <- cutree(wisc.hclust, h=19)
```

Our PCA results were in wisc.pr\$x

```
# Distance matrix from PCA result
d <- dist(wisc.pr$x[,1:3])

#
hc <- hclust(d, method='ward.D2')
plot(hc)</pre>
```

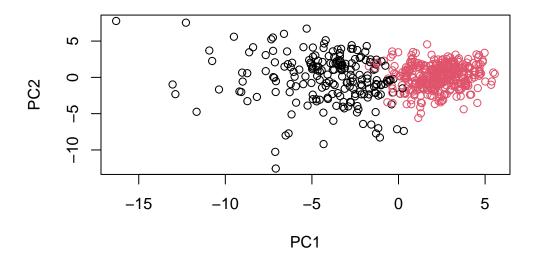
Cluster Dendrogram



d hclust (*, "ward.D2")

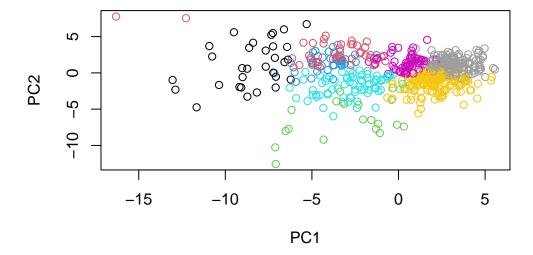
Cut tree into two groups/clusters

```
grps2 <- cutree(hc, k=2)
plot(wisc.pr$x, col=grps2)</pre>
```



Cut tree into ten groups/clusters

```
grps10 <- cutree(hc, k=10)
plot(wisc.pr$x, col=grps10)</pre>
```



Compare my clustering result (my grps) to the expert diagnosis

table(diagnosis)

diagnosis B M 357 212

table(grps2)

grps2 1 2 203 366

Cross table w/2 groups:

table(diagnosis, grps2)

```
grps2
diagnosis 1 2
B 24 333
M 179 33
```

In all of cluster 1 there are 24 benign points and 179 malignant point. In all of cluster 2 there are 333 benign points and 33 malignant points.

Cross table w/10 groups:

table(diagnosis, grps10)

It is really hard to tell the clusters of whether one is particularly benign or malignant. However this is helpful for solving false positives.