

class 8: Breast Cancer Mini Project

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Outline

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

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

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

Now I will store the diagnosis for later and exclude it from the data set I will actually do things with that I will call `wisc.data`

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

Q1 How many people are in this data set?

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

```
[1] 569
```

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

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

```
  B   M  
357 212
```

```
sum(wisc.df$diagnosis=="M")
```

```
[1] 212
```

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

```
x <- colnames(wisc.df)  
length(grep("_mean",x))
```

```
[1] 10
```

```
x
```

```
[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"
```

```
# Check column means and standard deviations
colMeans(wisc.data)
```

radius_mean	texture_mean	perimeter_mean
1.412729e+01	1.928965e+01	9.196903e+01
area_mean	smoothness_mean	compactness_mean
6.548891e+02	9.636028e-02	1.043410e-01
concavity_mean	concave.points_mean	symmetry_mean
8.879932e-02	4.891915e-02	1.811619e-01
fractal_dimension_mean	radius_se	texture_se
6.279761e-02	4.051721e-01	1.216853e+00
perimeter_se	area_se	smoothness_se
2.866059e+00	4.033708e+01	7.040979e-03
compactness_se	concavity_se	concave.points_se
2.547814e-02	3.189372e-02	1.179614e-02
symmetry_se	fractal_dimension_se	radius_worst
2.054230e-02	3.794904e-03	1.626919e+01
texture_worst	perimeter_worst	area_worst
2.567722e+01	1.072612e+02	8.805831e+02
smoothness_worst	compactness_worst	concavity_worst
1.323686e-01	2.542650e-01	2.721885e-01
concave.points_worst	symmetry_worst	fractal_dimension_worst
1.146062e-01	2.900756e-01	8.394582e-02

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

radius_mean	texture_mean	perimeter_mean
3.524049e+00	4.301036e+00	2.429898e+01
area_mean	smoothness_mean	compactness_mean
3.519141e+02	1.406413e-02	5.281276e-02
concavity_mean	concave.points_mean	symmetry_mean
7.971981e-02	3.880284e-02	2.741428e-02
fractal_dimension_mean	radius_se	texture_se
7.060363e-03	2.773127e-01	5.516484e-01
perimeter_se	area_se	smoothness_se
2.021855e+00	4.549101e+01	3.002518e-03

compactness_se	concavity_se	concave.points_se
1.790818e-02	3.018606e-02	6.170285e-03
symmetry_se	fractal_dimension_se	radius_worst
8.266372e-03	2.646071e-03	4.833242e+00
texture_worst	perimeter_worst	area_worst
6.146258e+00	3.360254e+01	5.693570e+02
smoothness_worst	compactness_worst	concavity_worst
2.283243e-02	1.573365e-01	2.086243e-01
concave.points_worst	symmetry_worst	fractal_dimension_worst
6.573234e-02	6.186747e-02	1.806127e-02

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

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

```
pc1_variance <- summary(wisc.pr)$importance[2, 1]
pc1_variance
```

```
[1] 0.44272
```

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

```
cum_var <- cumsum(summary(wisc.pr)$importance[2,])
num_pcs_70 <- which(cum_var >= 0.70)[1]
num_pcs_70
```

PC3

```
3
```

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

```
num_pcs_90 <- which(cum_var >= 0.90)[1]
num_pcs_90
```

PC7

```
7
```

Principal Component Analysis

We need to scale our input data before PCA as some of the columns are measured in terms of very different units with different means and different variances. The upshot here is we set `scale=TRUE` argument to `prcomp()`

```
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					

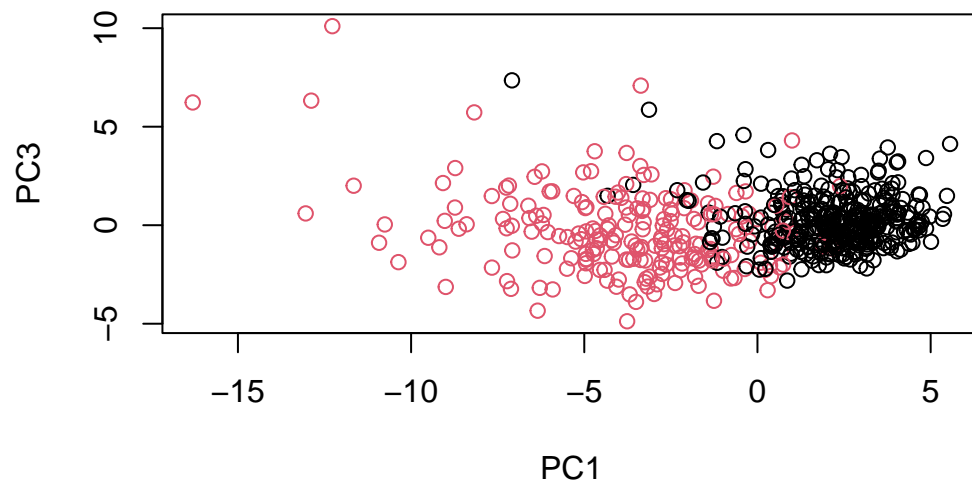
Generate one of our main result figures - the PC plot (a.k.a. “source plot”, “orientation plot”, “PC1 vs PC2 plot”, “PC plot”, “Projection plot”, etc.) It is known by different names in different fields.

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

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


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

```
# Scatter plot of PC1 vs PC3 colored by diagnosis
plot(wisc.pr$x[,1], wisc.pr$x[,3], col = diagnosis,
      xlab = "PC1", ylab = "PC3")
```

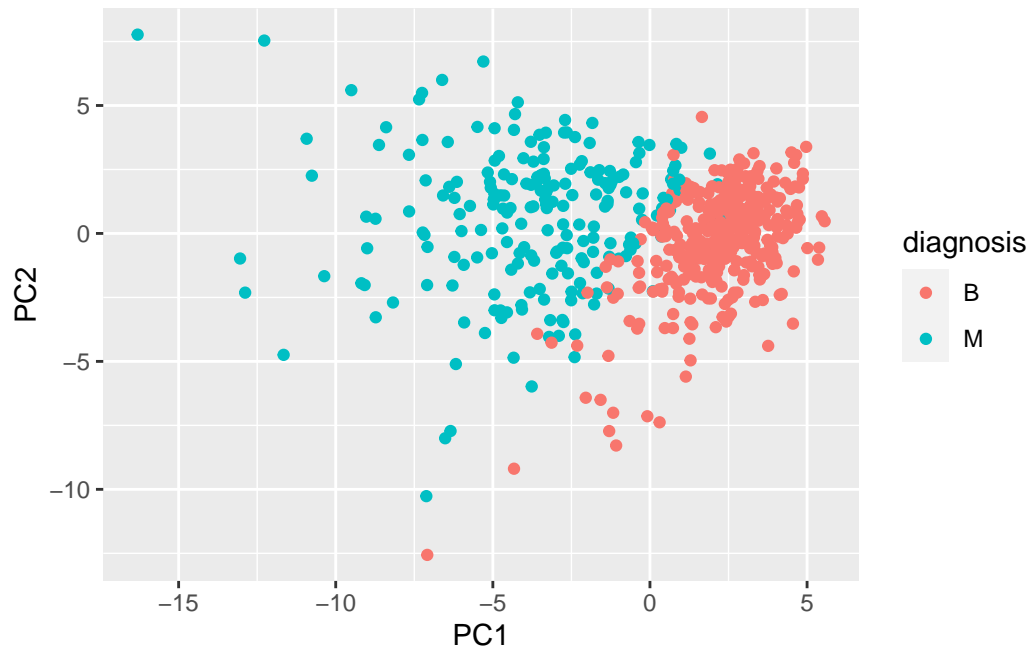


Add a ggplot version

```
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()
```



Calculate variance of each principal component

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

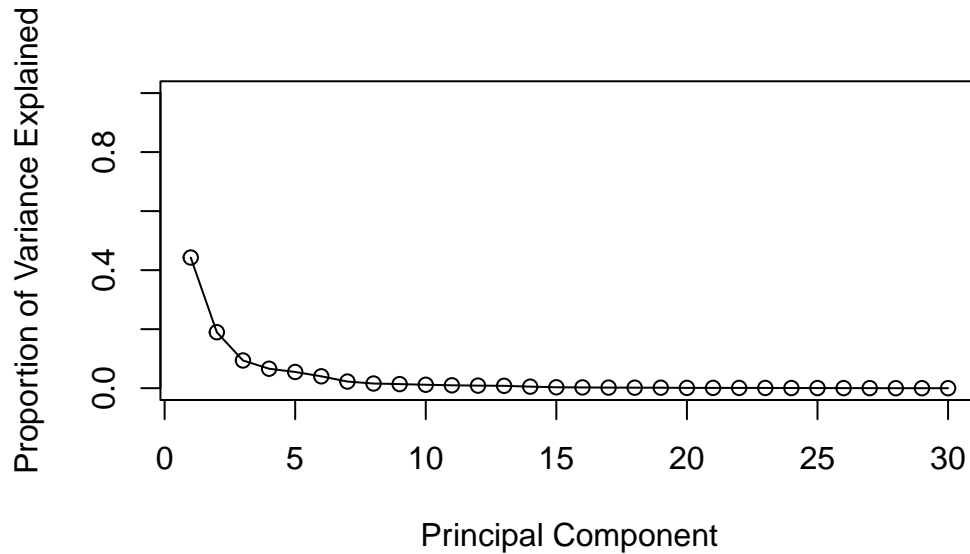
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

Variance explained by each principal component: pve

```
pve <- pr.var / sum(pr.var)
```

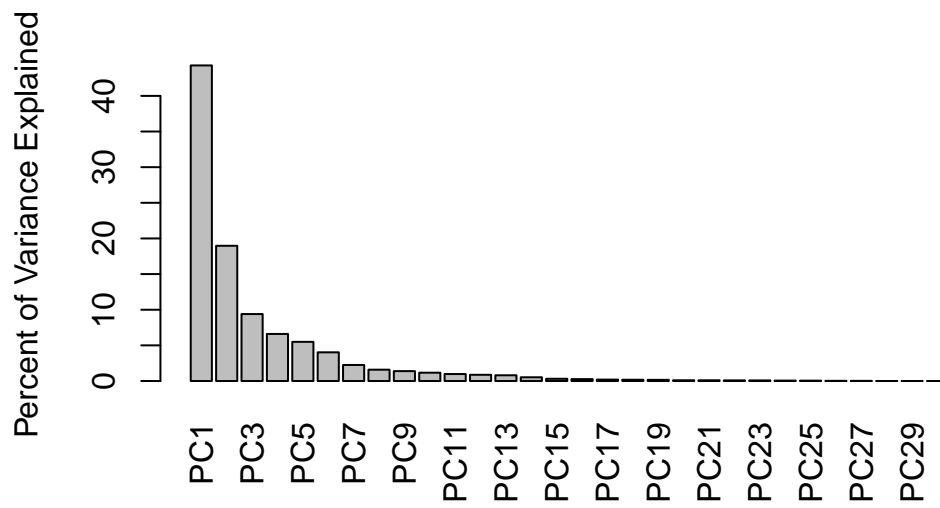
Plot variance explained for each principal component

```
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 = "Percent of Variance Explained",  
        names.arg = paste0("PC", 1:length(pve)), las = 2, axes = FALSE)  
axis(2, at = seq(0, max(pve), by = 0.05), labels = round(seq(0, max(pve), by = 0.05) * 100
```



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

```
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?

```
cumulative_pve <- cumsum(pve)
which(cumulative_pve >= 0.8)[1]
```

```
[1] 5
```

Hierarchical clustering

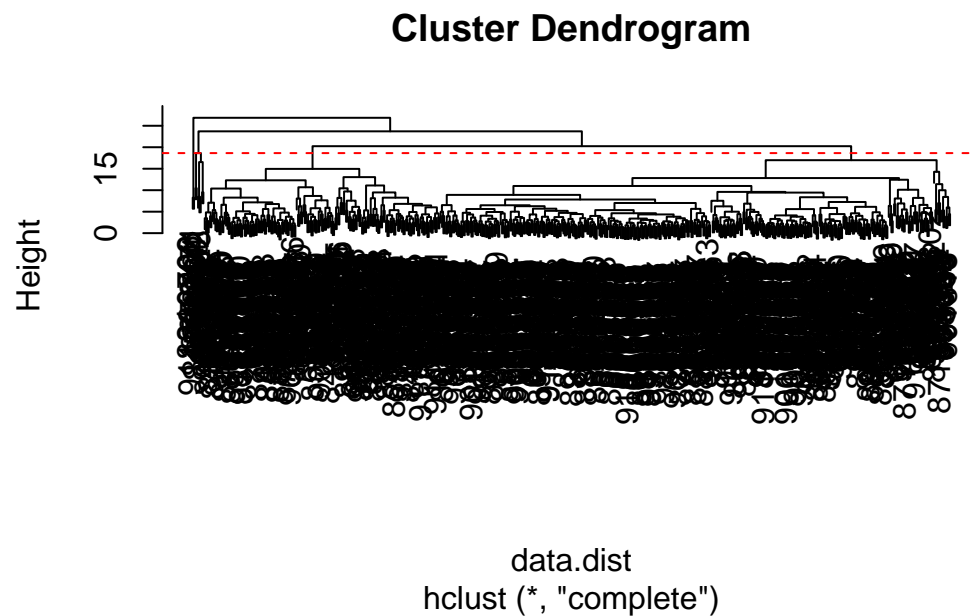
Can we just use clustering on the original data and get some insight into M vs B?

It is difficult, this “tree” looks like a hot mess...

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

```
#distance matrix needed for hclust

data.dist <- dist(scale(wisc.data))
wisc.hclust <- hclust(data.dist)
plot(wisc.hclust)
abline(h = wisc.hclust$height[length(wisc.hclust$height) - 4 + 1], col="red", lty=2)
```



```
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?

```
comparison_list <- list()

for(k in 2:10) {
  clusters <- cutree(wisc.hclust, k)
  comp_table <- table(clusters, diagnosis)
  comparison_list[[paste0("k=", k)]] <- comp_table
}

comparison_list
```

```
$`k=2`
      diagnosis
clusters  B   M
      1 357 210
      2   0   2
```

```
$`k=3`
      diagnosis
clusters  B   M
      1 355 205
      2   2   5
      3   0   2
```

```
$`k=4`
      diagnosis
clusters  B   M
      1  12 165
      2   2   5
      3 343  40
      4   0   2
```

```
$`k=5`
      diagnosis
clusters  B   M
      1  12 165
      2   0   5
      3 343  40
      4   2   0
      5   0   2
```

\$`k=6`

	diagnosis		
clusters	B	M	
1	12	165	
2	0	5	
3	331	39	
4	2	0	
5	12	1	
6	0	2	

\$`k=7`

	diagnosis		
clusters	B	M	
1	12	165	
2	0	3	
3	331	39	
4	2	0	
5	12	1	
6	0	2	
7	0	2	

\$`k=8`

	diagnosis		
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	

\$`k=9`

	diagnosis		
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

```
$`k=10`
      diagnosis
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
```

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

```
methods <- c("single", "complete", "average", "ward.D2")

results = list()

for(method in methods) {
  hclust_obj = hclust(data.dist, method = method)
  clusters = cutree(hclust_obj, k = 4)
  comp_table = table(clusters, diagnosis)
  results[[method]] = comp_table
}

results
```

```
$single
      diagnosis
clusters  B   M
1     356 209
2       1   0
3       0   2
4       0   1
```



```
$complete
      diagnosis
clusters  B   M
1      12 165
2       2   5
3     343  40
4       0   2
```

```
$average
      diagnosis
clusters  B   M
1     355 209
2       2   0
3       0   1
4       0   2
```

```
$ward.D2
      diagnosis
clusters  B   M
1       0 115
2       6  48
3     337  48
4      14   1
```

5. combining methods

This approach will take not original data but our PCA results and work with the.

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

Cluster Dendrogram



d
hclust (*, "ward.D2")

Generate 2 cluster groups from this hclust object.

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

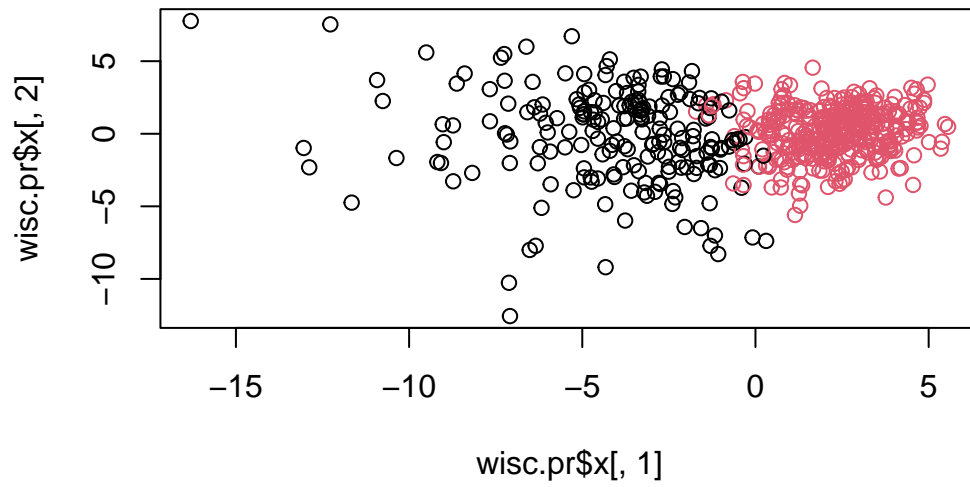
842302	842517	84300903	84348301	84358402	843786	844359	84458202
1	1	1	1	1	1	1	1
844981	84501001	845636	84610002	846226	846381	84667401	84799002
1	1	2	1	1	2	1	1
848406	84862001	849014	8510426	8510653	8510824	8511133	851509
2	1	1	2	2	2	1	1
852552	852631	852763	852781	852973	853201	853401	853612
1	1	1	1	1	2	1	1
85382601	854002	854039	854253	854268	854941	855133	855138
1	1	1	1	1	2	2	1
855167	855563	855625	856106	85638502	857010	85713702	85715
2	1	1	1	2	1	2	1
857155	857156	857343	857373	857374	857392	857438	85759902
2	2	2	2	2	1	2	2
857637	857793	857810	858477	858970	858981	858986	859196
1	1	2	2	2	2	1	2
85922302	859283	859464	859465	859471	859487	859575	859711

1	1	2	2	1	2	1	1
859717	859983	8610175	8610404	8610629	8610637	8610862	8610908
1	2	2	2	2	1	1	2
861103	8611161	8611555	8611792	8612080	8612399	86135501	86135502
2	1	1	1	2	1	2	1
861597	861598	861648	861799	861853	862009	862028	86208
2	1	2	2	2	2	1	1
86211	862261	862485	862548	862717	862722	862965	862980
2	2	2	1	2	2	2	2
862989	863030	863031	863270	86355	864018	864033	86408
2	1	2	2	1	2	2	2
86409	864292	864496	864685	864726	864729	864877	865128
1	2	2	2	2	1	1	2
865137	86517	865423	865432	865468	86561	866083	866203
2	1	1	2	2	2	2	1
866458	866674	866714	8670	86730502	867387	867739	868202
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868223	868682	868826	868871	868999	869104	869218	869224
2	2	1	2	2	2	2	2
869254	869476	869691	86973701	86973702	869931	871001501	871001502
2	2	1	2	2	2	2	1
8710441	87106	8711002	8711003	8711202	8711216	871122	871149
1	2	2	2	1	2	2	2
8711561	8711803	871201	8712064	8712289	8712291	87127	8712729
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8712766	8712853	87139402	87163	87164	871641	871642	872113
1	2	2	2	1	2	2	2
872608	87281702	873357	873586	873592	873593	873701	873843
1	1	2	2	1	1	1	2
873885	874158	874217	874373	874662	874839	874858	875093
2	2	2	2	2	2	1	2
875099	875263	87556202	875878	875938	877159	877486	877500
2	1	1	2	1	1	1	1
877501	877989	878796	87880	87930	879523	879804	879830
2	1	1	1	2	2	2	2
8810158	8810436	881046502	8810528	8810703	881094802	8810955	8810987
1	2	1	2	1	1	1	1
8811523	8811779	8811842	88119002	8812816	8812818	8812844	8812877
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8813129	88143502	88147101	88147102	88147202	881861	881972	88199202
2	2	2	2	2	1	1	2
88203002	88206102	882488	88249602	88299702	883263	883270	88330202
2	1	2	2	1	1	2	1

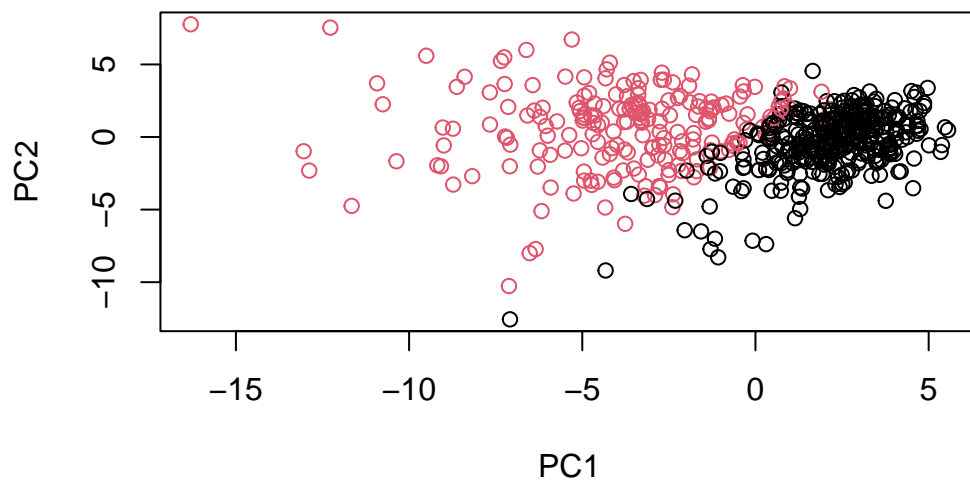
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894604	894618	894855	895100	89511501	89511502	89524	895299
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8953902	895633	896839	896864	897132	897137	897374	89742801
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89864002	898677	898678	89869	898690	899147	899187	899667
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899987	9010018	901011	9010258	9010259	901028	9010333	901034301
1	1	2	2	2	2	2	2
901034302	901041	9010598	9010872	9010877	901088	9011494	9011495
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90439701	904647	904689	9047	904969	904971	905189	905190
1	2	2	2	2	2	2	2
90524101	905501	905502	905520	905539	905557	905680	905686

1	2	2	2	2	2	2	2
905978	90602302	906024	906290	906539	906564	906616	906878
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907145	907367	907409	90745	90769601	90769602	907914	907915
2	2	2	2	2	2	1	2
908194	908445	908469	908489	908916	909220	909231	909410
1	1	2	1	2	2	2	2
909411	909445	90944601	909777	9110127	9110720	9110732	9110944
2	1	2	2	1	2	1	2
911150	911157302	9111596	9111805	9111843	911201	911202	9112085
2	1	2	1	2	2	2	2
9112366	9112367	9112594	9112712	911296201	911296202	9113156	911320501
2	2	2	2	1	1	2	2
911320502	9113239	9113455	9113514	9113538	911366	9113778	9113816
2	1	2	2	1	2	2	2
911384	9113846	911391	911408	911654	911673	911685	911916
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912193	91227	912519	912558	912600	913063	913102	913505
2	2	2	2	2	1	2	1
913512	913535	91376701	91376702	914062	914101	914102	914333
2	2	2	2	1	2	2	2
914366	914580	914769	91485	914862	91504	91505	915143
1	2	1	1	2	1	2	1
915186	915276	91544001	91544002	915452	915460	91550	915664
1	1	2	2	2	1	2	2
915691	915940	91594602	916221	916799	916838	917062	917080
1	2	2	2	1	1	2	2
917092	91762702	91789	917896	917897	91805	91813701	91813702
2	1	2	2	2	2	2	2
918192	918465	91858	91903901	91903902	91930402	919537	919555
2	2	2	2	2	1	2	1
91979701	919812	921092	921362	921385	921386	921644	922296
1	2	2	2	2	1	2	2
922297	922576	922577	922840	923169	923465	923748	923780
2	2	2	2	2	2	2	2
924084	924342	924632	924934	924964	925236	925277	925291
2	2	2	2	2	2	2	2
925292	925311	925622	926125	926424	926682	926954	927241
2	2	1	1	1	1	2	1
92751							
2							

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



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



```
table(grps)
```

```
grps
  1  2
203 366
```

```
table(diagnosis)
```

```
diagnosis
  B  M
357 212
```

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

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

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

```
d <- dist(wisc.pr$x[,1:7])
wisc.pr.hclust <- hclust(d, method = "ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
table( wisc.pr.hclust.clusters , diagnosis)
```

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