Class 8: Breast Cancer Mini Project

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Background

Data import

Our data come from the U. of Wisconsin Medical Center

```
wisc.df <- read.csv("WisconsinCancer.csv", row.names = 1)</pre>
```

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

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

[1] 569

How many of the observations have a malignant diagnosis?

```
wisc.df$diagnosis
```

table(wisc.df\$diagnosis)

B M 357 212

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

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"
```

```
length(grep("mean", colnames(wisc.df)))
```

[1] 10

There is a diagnosis column that is the clinician consensus that I want to exclude from any further analysis. We will come back later and compare our results to this diagnosis.

```
diagnosis <- as.factor(wisc.df$diagnosis)
head(diagnosis)</pre>
```

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

Now we can remove it from the wisc.df

```
wisc.data <- wisc.df[,-1]
```

Clustering

```
kmeans(wisc.data, centers=2)
```

K-means clustering with 2 clusters of sizes 131, 438

Cluster means:

```
radius_mean texture_mean perimeter_mean area_mean smoothness_mean
     19.37992
                  21.69458
                                128.23130 1185.9298
                                                           0.1012946
1
2
     12.55630
                  18.57037
                                 81.12347 496.0619
                                                           0.0948845
  compactness_mean concavity_mean concave.points_mean symmetry_mean
        0.14861298
                       0.17693947
                                           0.10069878
                                                           0.1915397
1
2
        0.09109982
                       0.06243776
                                                           0.1780580
                                           0.03343254
 fractal_dimension_mean radius_se texture_se perimeter_se area_se
```

0 00045400 0 0044000 4 045450 0 450004 00 70500										
2 0.06345402 0.3041909 1.215153 2.152881 23.78529										
smoothness_se compactness_se concavity_se concave.points_se symmetry_se										
	030397									
2 0.007173263 0.02347469 0.02874551 0.01063632 0.02061358										
fractal_dimension_se radius_worst texture_worst perimeter_worst area_worst										
1 0.003953389 23.70947 28.91267 158.49618 1753.0229										
2 0.003747503 14.04390 24.70954 91.93751 619.6479										
smoothness_worst compactness_worst concavity_worst concave.points_worst										
1 0.1404247 0.3577577 0.4493061 0.19243107										
2 0.1299591 0.2233118 0.2192149 0.09	132984									
symmetry_worst fractal_dimension_worst										
1 0.3118817 0.08616550										
2 0.2835537 0.08328194										
Clustering vector:										
842302 842517 84300903 84348301 84358402 843786 8443										
1 1 1 2 1 2	1 2									
844981 84501001 845636 84610002 846226 846381 846674										
2 2 2 1 1 2	2 2									
848406 84862001 849014 8510426 8510653 8510824 85111										
2 1 1 2 2 2	2 1									
852552 852631 852763 852781 852973 853201 8534	01 853612									
1 1 2 1 1 1	1 2									
85382601 854002 854039 854253 854268 854941 8551										
1 1 1 2 2	2 2									
855167 855563 855625 856106 85638502 857010 857137	02 85715									
2 2 1 2 2 1	2 2									
857155 857156 857343 857373 857374 857392 8574										
2 2 2 2 1	2 2									
857637 857793 857810 858477 858970 858981 8589	86 859196									
1 2 2 2 2 2	2 2									
85922302 859283 859464 859465 859471 859487 8595	75 859711									
2 2 2 2 2	1 2									
859717 859983 8610175 8610404 8610629 8610637 86108										
1 2 2 1 2 1										
861103 8611161 8611555 8611792 8612080 8612399 861355	01 86135502									
2 2 1 1 2 1										
861597 861598 861648 861799 861853 862009 8620										
2 2 2 2 2										
86211 862261 862485 862548 862717 862722 8629										
2 2 2 2 2 2	2 2									
862989 863030 863031 863270 86355 864018 8640										

2	2	2	2	1	2	2	2
86409	864292	864496	864685	864726	864729	864877	865128
2	2	2	2	2	2	1	1
865137	86517	865423	865432	865468	86561	866083	866203
2	1	1	2	2	2	2	1
866458	866674	866714	8670	86730502	867387	867739	868202
2	1						
868223	868682	868826	868871	868999	869104	869218	869224
2	2		2		1		2
869254		869691					
2	2						2
8710441		8711002					
2	2		2				2
		871201					
2	1			1			
8712766		87139402					
1	2		2				2
872608		873357					873843 2
2	2						
873885		874217	8/43/3				
2	975063	87556202			2		_
015099	015265			010930			
		878796					
2	1				2		1
	_	881046502					
2	2				2		
8811523	_	8811842					
2	2		1		2		2
8813129	88143502	88147101					
2	2		2	2			
88203002	88206102	882488	88249602	88299702	883263	883270	88330202
2	1	2	2	1	1	2	1
88350402	883539	883852	88411702	884180	884437	884448	884626
2	2	2	2	1	2	2	2
88466802	884689	884948	88518501	885429	8860702	886226	886452
		1					
88649001	886776	887181	88725602	887549	888264	888570	889403
	2						2
889719	88995002	8910251	8910499				
1		2			2		2
8910988		8911163					
1	2	1	2	2	1	2	2

8912049	8912055					8912909	
1	-		2			_	2
8913049	89143601	89143602					
2	2	2	2	2	2	2	2
891936	892189	892214	892399	892438	892604	89263202	892657
2	2	2	2	1	2	1	2
89296	893061	89344	89346	893526	893548	893783	89382601
2	2	2	2	2	2	2	2
89382602	893988	894047	894089	894090	894326	894329	894335
2	2	2	2	2	1	2	2
894604	894618	894855	895100	89511501	89511502	89524	895299
2	1	2	1	2	2	2	2
8953902	895633	896839	896864	897132	897137	897374	89742801
2	2	2	2	2	2	2	1
897604	897630	897880	89812	89813	898143	89827	898431
2	1	2	1	2	2	2	1
89864002	898677	898678	89869	898690	899147	899187	899667
2	2	2	2	2	2	2	2
899987	9010018	901011	9010258	9010259	901028	9010333	901034301
1	2	2	2	2	2	2	2
901034302	901041	9010598	9010872	9010877	901088	9011494	9011495
2	2	2	2	2	1	1	2
9011971	9012000	9012315	9012568	9012795	901288	9013005	901303
1	1	2	2	1	1	2	2
901315	9013579	9013594	9013838	901549	901836	90250	90251
2	2	2	2	2	2	2	2
902727	90291	902975	902976	903011	90312	90317302	903483
2	2	2	2	2	1	2	2
903507	903516	903554	903811	90401601	90401602	904302	904357
1	1	2	2	2	2	2	2
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
2		2	2			2	
907145	907367	907409	90745	90769601	90769602	907914	907915
2	2	2	2	2	2	2	2
908194	908445	908469	908489	908916	909220	909231	909410
1	1	2	2	2	2	2	
909411	_						
	1			1			
	911157302						
511100		0 1 0 0 0	5500	0 1 0 1 0	U-1201	511252	52000

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	2	2	2	1	2	2	2
911384	9113846	911391	911408	911654	911673	911685	911916
2	2	2	2	2	2	2	2
912193	91227	912519	912558	912600	913063	913102	913505
2	2	2	2	2	2	2	1
913512	913535	91376701	91376702	914062	914101	914102	914333
2	2	2	1	1	2	2	2
914366	914580	914769	91485	914862	91504	91505	915143
2	2	1	1	2	2	2	1
915186	915276	91544001	91544002	915452	915460	91550	915664
2	2	2	2	2	2	2	2
915691	915940	91594602	916221	916799	916838	917062	917080
2	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
2	2	2	2	2	2	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	2	1	1	1	2	1
92751							
2							

Within cluster sum of squares by cluster:

[1] 49383423 28559677

(between_SS / total_SS = 69.6 %)

Available components:

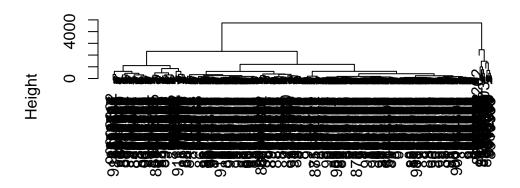
[1] "cluster" "centers" "totss" "withinss" "tot.withinss"

[6] "betweenss" "size" "iter" "ifault"

Let's try a hclust

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

Cluster Dendrogram



dist(wisc.data) hclust (*, "complete")

We can extract clusters from this rather poor dendrogram/tree with the cutree()

```
grps <- cutree(hc, k=2)</pre>
```

How many individuals in each cluster

table(grps)

grps 1 2 549 20

table(diagnosis)

diagnosis B M 357 212 We can generate a cross-table that compares our cluster grps vector without diagnosis vector values

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

```
grps
diagnosis 1 2
B 357 0
M 192 20
```

Principal Component Analysis

The importance of data scaling

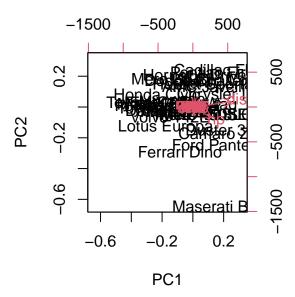
The main functiom for PCA in base R is prcomp() it has a default input parameter of scale=F

```
#prcomp()
head(mtcars)
```

	mpg	cyl	disp	hp	drat	wt	qsec	٧s	\mathtt{am}	gear	carb
Mazda RX4	21.0	6	160	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag	21.0	6	160	110	3.90	2.875	17.02	0	1	4	4
Datsun 710	22.8	4	108	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive	21.4	6	258	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout	18.7	8	360	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225	105	2.76	3.460	20.22	1	0	3	1

We could do a PCA of this data as is and it could be misleading...

```
pc <- prcomp(mtcars)
biplot(pc)</pre>
```



Let's look at the ean values of each column and their standard deviation.

colMeans(mtcars)

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

apply(mtcars, 2, sd)

```
disp
                                                         drat
                                                                        wt
      mpg
                   cyl
                                              hp
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
```

We can "scale" this data before PCA to get a much better representation and analysis of all the columns.

mtscale <- scale(mtcars)</pre>

round(colMeans(mtscale))

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

        0
        0
        0
        0
        0
        0
        0
        0
```

```
apply(mtscale, 2, sd)
```

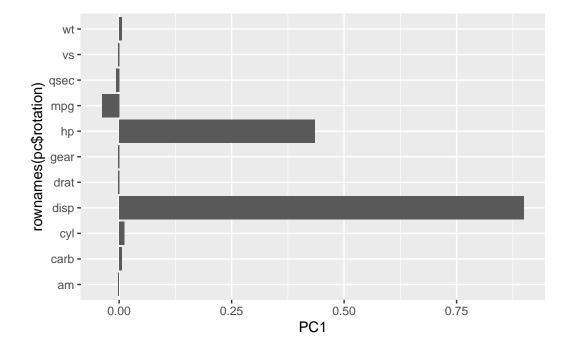
```
mpg cyl disp hp drat wt qsec vs am gear carb
1 1 1 1 1 1 1 1 1 1 1
```

```
pr.scale <- prcomp(mtscale)</pre>
```

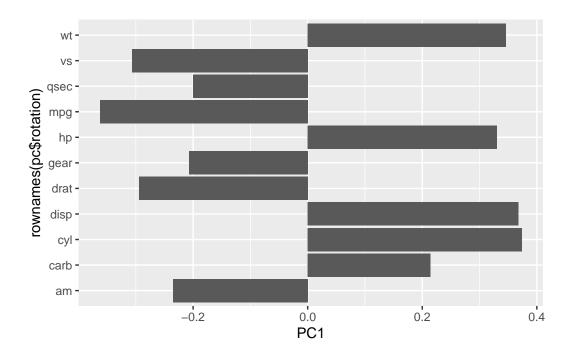
We can look at the two main results figures from PCA- the "PC plot" (a.k.a. score plot, ordienation plot, or PC1 vs PC2 plot). The "loadings plot" how the original variables contribute to the new PCs.

A loadings plot of the unscaled PCA results

```
library(ggplot2)
ggplot(pc$rotation) +
  aes(PC1, rownames(pc$rotation)) +
  geom_col()
```

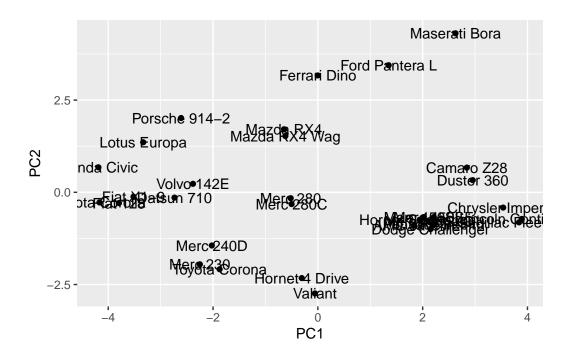


```
ggplot(pr.scale$rotation) +
  aes(PC1, rownames(pc$rotation)) +
  geom_col()
```



PC plot of scaled PCA results

```
ggplot(pr.scale$x) +
  aes(PC1, PC2, label=rownames(pr.scale$x)) +
  geom_point() +
  geom_text()
```



Key point: In general, we will set scale=TRUE when we do PCA. This is not the default but probably should be...

We can check the SD and mean of the different columns in wisc.data to see if we need to scale - hint, we do!

PCA of wisc data

```
wisc.pr <- prcomp(wisc.data, scale=TRUE)</pre>
```

To see how well PCA is doing here in terms capturing the variance (or spread) in the data, we can use the 'summary() function.

```
summary(wisc.pr)
```

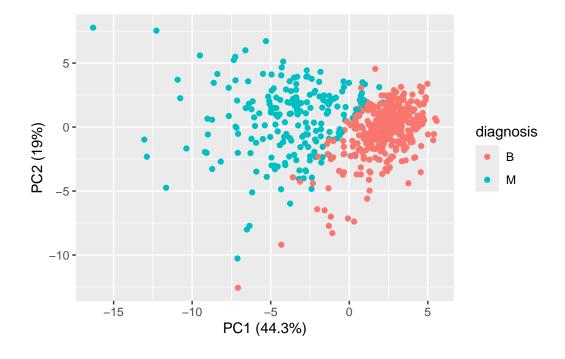
Importance of components:

```
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
```

```
0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 0.39624
Standard deviation
Proportion of Variance 0.01589 0.0139 0.01169 0.0098 0.00871 0.00805 0.00523
                       0.92598\ 0.9399\ 0.95157\ 0.9614\ 0.97007\ 0.97812\ 0.98335
Cumulative Proportion
                          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
                       0.98649\ 0.98915\ 0.99113\ 0.99288\ 0.99453\ 0.99557\ 0.9966
Cumulative Proportion
                                          PC24
                                                          PC26
                          PC22
                                   PC23
                                                  PC25
                                                                   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
                       0.99749\ 0.99830\ 0.9989\ 0.99942\ 0.99969\ 0.99992\ 0.99997
Cumulative Proportion
                          PC29
                                   PC30
Standard deviation
                       0.02736 0.01153
Proportion of Variance 0.00002 0.00000
Cumulative Proportion 1.00000 1.00000
```

Let's make the main PC1 vs PC2

```
ggplot(wisc.pr$x) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point() +
  xlab("PC1 (44.3%)") +
  ylab("PC2 (19%)")
```



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

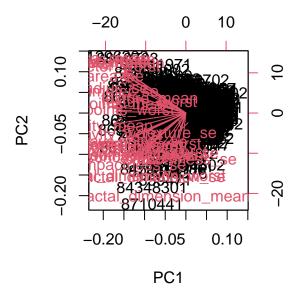
0.4427 or 44.27%.

- Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?
- 3 PCs are required to get to 70%.
 - Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

You need about 7 principal components to reach 90% of the original variance.

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

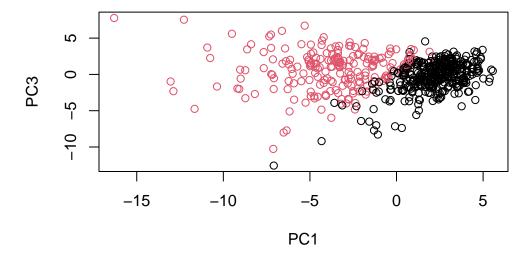
biplot(wisc.pr)



What stands out to me about this plot is the fact that it is a massive mess. This plot seems very difficult to understand, as everything is very unorganized.

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

```
plot(wisc.pr$x[, 1:3], col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```



What I can notice about this graph is that it is much cleaner than the previous. This plot shows two clumps of data, separating the two groups by diagnosis.

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?

The minimum number of principal components to explain 80% of variance is five principal components.

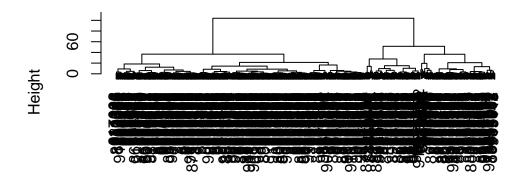
5. Combining methods

We can take our PCA results and use them as a basis set for other analysis such as clustering.

Clustering on PCA Results

```
wisc.pr.hclust <- hclust( dist(wisc.pr$x[,1:2]), method="ward.D2" )
plot(wisc.pr.hclust)</pre>
```

Cluster Dendrogram



dist(wisc.pr\$x[, 1:2]) hclust (*, "ward.D2")

We can "cut" this tree to yield our cluster (groups):

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

pc.grps
 1 2
195 374

How do my cluster grps compare to the expert diagnosis

```
table(diagnosis, pc.grps)
```

```
pc.grps
diagnosis 1 2
B 18 339
M 177 35
```

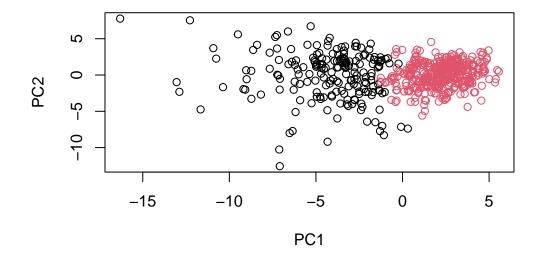
table(diagnosis)

```
diagnosis
B M
357 212
```

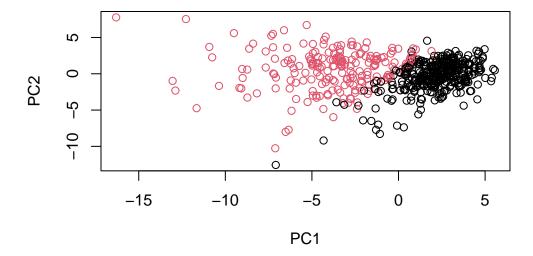
q15. How well does the newly created model with four clusters separate out the two diagnoses?

The newly created model with four clusters separates the diagnosis well. It helps visualize how the benign groups and metastacized groups differ across the different groups.

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



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



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

```
table(wisc.pr.hclust.clusters, diagnosis)
```

```
diagnosis
wisc.pr.hclust.clusters B M
1 18 177
2 339 35
```

Q16. How well do the hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.km\$cluster and wisc.hclust.clusters) with the vector containing the actual diagnoses.

I think they do a good job at separating the models well, as you could see the two groups separated well. However, it could be better, as it could be in much more detail.

They did really poorly, we do much better after PCA- the new PCA variables give us much better separation of M and B.

7. Prediction

We can use our model PCA model for the analysis of new "unseen" data. In this case fro, U. Mich.

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

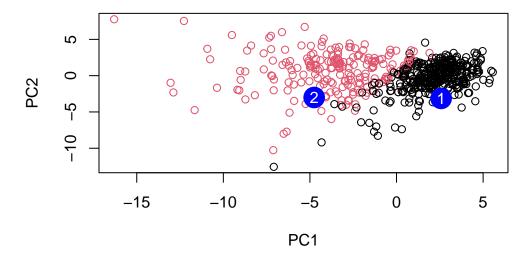
```
PC1
                     PC2
                                PC3
                                           PC4
                                                      PC5
                                                                 PC6
                                                                            PC7
                          1.3990492 -0.7631950 2.781648 -0.8150185 -0.3959098
     2.576616 -3.135913
[2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698 -1.2189945
                                                                      0.8193031
            PC8
                      PC9
                                PC10
                                          PC11
                                                     PC12
                                                               PC13
[1,] -0.2307350 0.1029569 -0.9272861 0.3411457
                                                0.375921 0.1610764 1.187882
[2,] -0.3307423 0.5281896 -0.4855301 0.7173233 -1.185917 0.5893856 0.303029
          PC15
                     PC16
                                 PC17
                                              PC18
                                                          PC19
                                                                     PC20
[1,] 0.3216974 -0.1743616 -0.07875393 -0.11207028 -0.08802955 -0.2495216
[2,] 0.1299153 0.1448061 -0.40509706 0.06565549 0.25591230 -0.4289500
           PC21
                      PC22
                                 PC23
                                             PC24
                                                         PC25
                                                                      PC26
```

```
[1,] 0.1228233 0.09358453 0.08347651 0.1223396 0.02124121 0.078884581 [2,] -0.1224776 0.01732146 0.06316631 -0.2338618 -0.20755948 -0.009833238 PC27 PC28 PC29 PC30
```

[1,] 0.220199544 -0.02946023 -0.015620933 0.005269029

[2,] -0.001134152 0.09638361 0.002795349 -0.019015820

```
plot(wisc.pr$x[,1:2], col=diagnosis)
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



For follow-up, patients in group 2 should be asked for a follow-up.