Class 8: Breast Cancer Mini Project

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

Data input

The data is supplied on CSV format:

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

	diagnosis radi	us_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	М	19.69	21.25	130.00	1203.0	
84348301	М	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	oncavity_mean c	oncave.poi	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	an radius_se te	xture_se p	erimeter_se
842302	0.2419		0.0787	71 1.0950	0.9053	8.589
842517	0.1812		0.0566	0.5435	0.7339	3.398
84300903	0.2069		0.0599	99 0.7456	0.7869	4.585
84348301	0.2597		0.0974	14 0.4956	1.1560	3.445
84358402	0.1809		0.0588	33 0.7572	0.7813	5.438

843786	(0.2087	0.07613	0.3345	0.8902	2.217
	area_se	smoothness_s	e compactness_se	concavity_se	e concave.po	oints_se
842302	153.40	0.006399	0.04904	0.05373	3	0.01587
842517	74.08	0.00522	0.01308	0.01860)	0.01340
84300903	94.03	0.00615	0.04006	0.03832	2	0.02058
84348301	27.23	0.00911	0.07458	0.05661	L	0.01867
84358402	94.44	0.01149	0.02461	0.05688	3	0.01885
843786	27.19	0.00751	0.03345	0.03672	2	0.01137
	symmetry	y_se fractal_d	dimension_se rad	lius_worst tex	ture_worst	
842302	0.03	3003	0.006193	25.38	17.33	
842517	0.0	1389	0.003532	24.99	23.41	
84300903	0.02	2250	0.004571	23.57	25.53	
84348301	0.05	5963	0.009208	14.91	26.50	
84358402	0.03	1756	0.005115	22.54	16.67	
843786	0.02	2165	0.005082	15.47	23.75	
	perimete	er_worst area	worst smoothnes	s_worst compa	actness_wors	st
842302		184.60	2019.0	0.1622	0.66	56
842517		158.80	1956.0	0.1238	0.186	66
84300903		152.50	1709.0	0.1444	0.424	45
84348301		98.87	567.7	0.2098	0.866	63
84358402		152.20	1575.0	0.1374	0.20	50
843786		103.40	741.6	0.1791	0.524	49
	concavit	• –	ave.points_worst	symmetry_wor	rst	
842302		0.7119	0.2654			
842517		0.2416	0.1860			
84300903		0.4504	0.2430			
84348301		0.6869	0.2575	0.66	38	
84358402		0.4000	0.1625		364	
843786		0.5355	0.1741	0.39	985	
	fractal_	_dimension_wo				
842302		0.118				
842517		0.089				
84300903		0.08				
84348301		0.173				
84358402		0.07				
843786		0.12	140			

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'

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

```
Q1 How many people are in this data set?
  nrow(wisc.df)
Γ17 569
    Q2 How many of the observations have a malignant diagnosis?
  table( wisc.df$diagnosis )
 В
      М
357 212
  sum ( wisc.df$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"
                                 "concavity_mean"
 [7] "compactness_mean"
 [9] "concave.points_mean"
                                 "symmetry_mean"
[11] "fractal_dimension_mean"
                                 "radius_se"
[13] "texture_se"
                                 "perimeter_se"
[15] "area_se"
                                 "smoothness_se"
                                 "concavity_se"
[17] "compactness_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"
```

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()'.

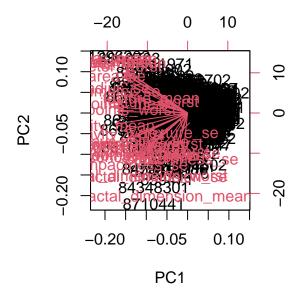
```
wisc.pr <- prcomp( wisc.data, scale= TRUE )
summary (wisc.pr)</pre>
```

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
                       0.92598 0.9399 0.95157 0.9614 0.97007 0.97812 0.98335
Cumulative Proportion
                          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
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
```

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

```
proportion_PC1 <- summary(wisc.pr)$importance["Proportion of Variance", "PC1"]</pre>
  proportion_PC1
[1] 0.44272
     Q5. How many principal components (PCs) are required to describe at least 70%
     of the original variance in the data?
  cumulative_proportions <- summary(wisc.pr)$importance["Cumulative Proportion",]</pre>
  pcs_70 <- which(cumulative_proportions >= 0.70)[1]
  pcs_70
PC3
  3
     Q6. How many principal components (PCs) are required to describe at least 90%
     of the original variance in the data?
  pcs_90 <- which(cumulative_proportions >= 0.90)[1]
  pcs_90
PC7
  7
     Q7. What stands out to you about this plot? Is it easy or difficult to understand?
     Why?
  biplot(wisc.pr)
```

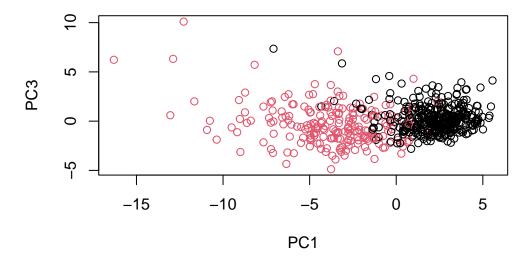


What strikes me about this plot is the confusion. The graph is very hard to understand. Because too many variables are plotted at the same time, the labels become overlapping, making the visualization difficult to interpret.

Generate one of our main result figures= the PC plot (a.k.a "score plot", "orientation plot", "PC1 vs PC2 plot", "PC plot", "projection plot", etc.) It is known by different names in different fields.

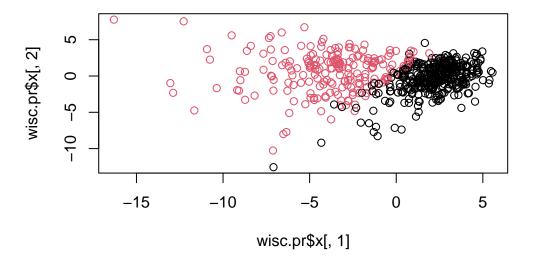
Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

Scatter plot of PC1 vs PC3



I noticed two clusters for P1 and P3, and the clusters can distinguish where P1 and P3 are. However, there is also some overlap, and there may not be enough PC1 and PC3 to make a completely clear distinction.

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

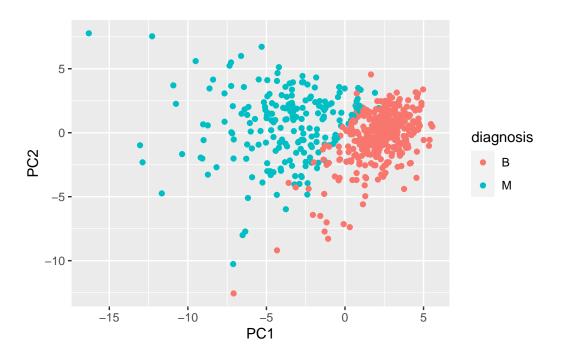


And a ggplot version

```
# Create a data.frame for ggplot
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()</pre>
```

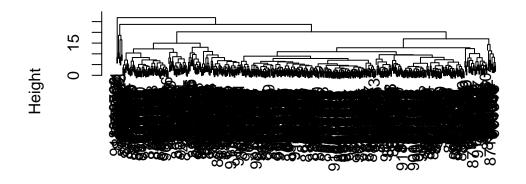


Hierarchical clustering

Can we just use clustering on the original data and get some insight into M vs B? It is rather difficult, this "tree" looks like a hot mess...

```
#distance matrix needed for hclust
data.dist <- dist( scale(wisc.data) )
wisc.hclust <- hclust(data.dist)
plot(wisc.hclust)</pre>
```

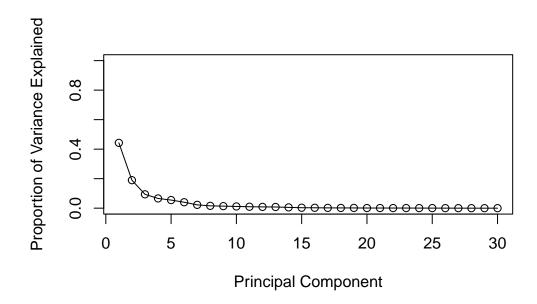
Cluster Dendrogram



data.dist hclust (*, "complete")

```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)</pre>
```

[1] 13.281608 5.691355 2.817949 1.980640 1.648731 1.207357

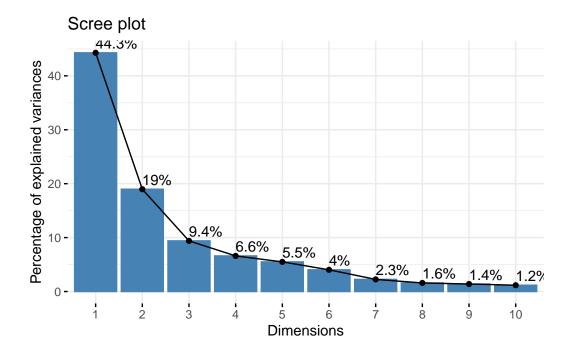




```
## ggplot based graph
#install.packages("factoextra")
library(factoextra)
```

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?

```
loading_value <- wisc.pr$rotation["concave.points_mean", 1]
loading_value</pre>
```

[1] -0.2608538

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

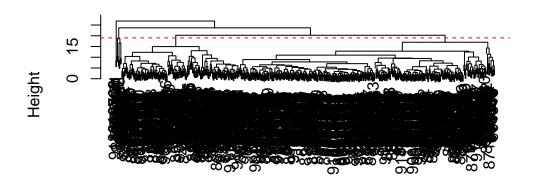
```
cumulative_pve <- cumsum(pve)
min_pc <- which(cumulative_pve >= 0.80)[1]
min_pc
```

[1] 5

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

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

Cluster Dendrogram



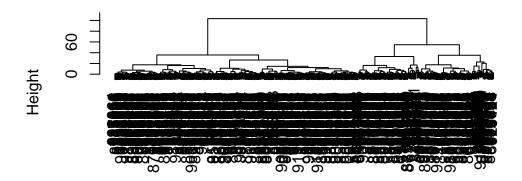
data.dist hclust (*, "complete")

5. Combining methods

This apprach will take not original data but our PCA results and work with them.

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

Cluster Dendrogram



d hclust (*, "ward.D2")

Generate 2 cluster groups from this helust object.

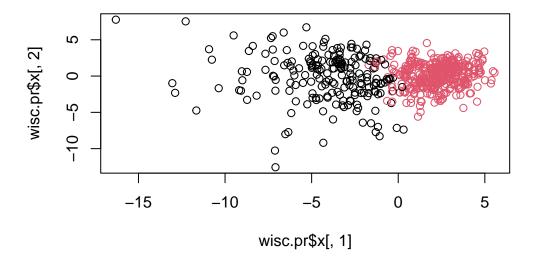
```
grps <- cutree(wisc.pr.hclust, k=2)
grps</pre>
```

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

1	1	2	2	1	2	1	1
859717	859983				8610637		8610908
1	2	2	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
1	1	2	1	1	2	1	2
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
2	1	1	2	1	2	2	2
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			881094802	8810955	8810987
1	2	1	2	1	1	1	1
8811523	8811779	8811842	88119002	8812816	8812818	8812844	8812877
2	2	1	1	2	2	2	1
8813129	88143502	88147101	88147102	88147202	881861	881972	88199202
		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	1	2	1	2	2	1
88466802	884689	884948	88518501	885429	8860702	886226	886452
2	2	1	2	1	1	1	1
88649001	886776	887181	88725602	887549	888264	888570	889403
1	1	1	1	1	2	1	2
889719	88995002	8910251	8910499	8910506	8910720	8910721	8910748
1	1	2	2	2	2	2	2
8910988	8910996	8911163	8911164	8911230	8911670	8911800	8911834
1	2	2	2	2	2	2	2
8912049	8912055	89122	8912280	8912284	8912521	8912909	8913
1	2	1	1	2	2	2	2
8913049	89143601	89143602	8915	891670	891703	891716	891923
1	2	1	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	1	2
894604	894618	894855	895100	89511501	89511502	89524	895299
2	1	2	1	2	2	2	
8953902	895633	896839	896864	897132	897137	897374	89742801
1	1	1	2	2	2	2	
897604	897630				898143		
2	1	2	1		2		1
89864002	898677		89869		899147	899187	899667
2	2	2	2	2	2	2	
899987					901028	9010333	901034301
1	1	2			2		
901034302					901088		
2	2	2	2	2	1		
9011971	9012000	9012315	9012568	9012795	901288		
1	1	1	2	1	1	2	2
							90251
1	2	2	1		2	2	
_					90312		
2	2	2	2		1		
					90401602		
1	1	2	2	2	2	2	
					904971		
1	2	2	2			2	
_					905557		
90524101	900001	905502	900020	905539	905551	905680	900000

1	2	2	2	2	2	2	2
	90602302						
2	1	2	2	2	1	2	2
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		2		1			
911384	9113846	911391	911408	911654	911673	911685	911916
2	2	2	2	2	2	2	1
912193	91227						
2	2	2	2	2	1	2	1
913512	913535	91376701				914102	914333
2	_	2	2		2	2	
914366	914580	914769	91485		91504	91505	915143
1		1					
915186	915276	91544001			915460	91550	915664
1	_	2				2	2
915691	915940						917080
1	-	2	2		1		
917092	91762702	91789				91813701	91813702
2	_	2				2	_
					91930402		
2		2		2			
91979701	919812						
1			2		1	2	
	922576						
2		2	2				
	924342						
2	_	2					
	925311						927241
2		1	1	1	1	2	1
92751							
2							



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

No, I cannot find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10. if I cut it below 4, one cluster would have both malignant cells and benign cells. if I cut it above 4, the data stratification becomes less distinct.

```
wisc.hclust.clusters <- cutree(wisc.hclust, k=4)
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.clusters <- cutree(wisc.hclust, k=3)
table(wisc.hclust.clusters, diagnosis)</pre>
```

```
diagnosis
wisc.hclust.clusters B M
1 355 205
2 2 5
3 0 2
```

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

My personal favorite method is "ward.D2", especially for this dataset where the inherent cluster structures are not very clear-cut. The Ward's method provides a good balance between the shape and size of clusters. It has the ability to search for clusters that are coherent internally, but distinct from each other.

Q14. How well does k-means separate the two diagnoses? How does it compare to your helust results?

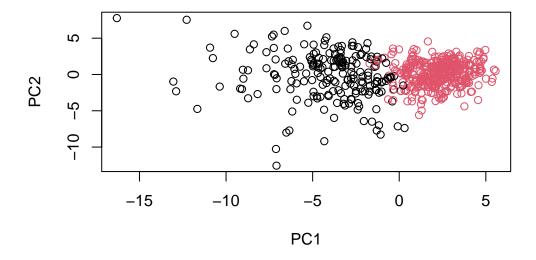
With the given data and the interpretation, it seems that both clustering methods have their strengths. The k-means algorithm seems to be providing a simpler split with two clusters, while the hierarchical method offers more granularity with its four clusters, potentially capturing subgroups within the data.

```
scaled_data <- scale(wisc.data)
wisc.km <- kmeans(scaled_data, centers=2, nstart=20)
comparison_table <- table(wisc.km$cluster, diagnosis)
print(comparison_table)

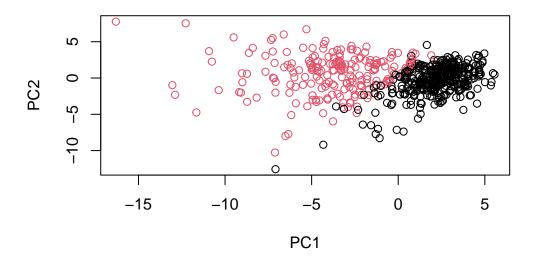
diagnosis
    B     M
1     343     37
2     14     175</pre>
```

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

The newly created model effectively distinguishes between the two diagnoses: benign (B) and malignant (M). The table shows that cluster 1 has 28 benign samples; 188 malignant samples. Most of the malignant samples are clustered in this cluster. Cluster 2 has 329 benign samples; 24 malignant samples and most of the benign samples are clustered in this cluster. In an ideal scenario, each cluster would exclusively represent one type of diagnosis, either benign or malignant. Despite this, the current model offers a clear categorization and remains a valuable tool.



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



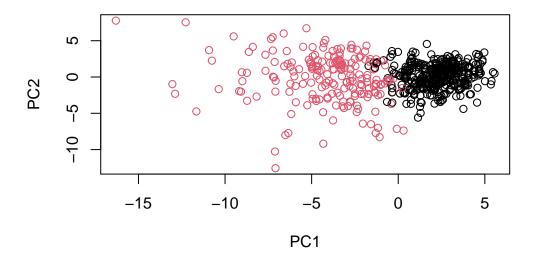
```
g <- as.factor(grps)
levels(g)

[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>
```



```
library(rgl)
plot3d(wisc.pr$x[,1:3], xlab="PC 1", ylab="PC 2", zlab="PC 3", cex=1.5, size=1, type="s",

dist.matrix <- dist(wisc.pr$x[, 1:7])

wisc.pr.hclust <- hclust(dist.matrix, method="ward.D2")

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

comparison.table <- table(wisc.pr.hclust.clusters, diagnosis)
print(comparison.table)

diagnosis
wisc.pr.hclust.clusters B M</pre>
```

Q16. How well do the k-means and 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

28 188

24

2 329

wisc.hclust.clusters) with the vector containing the actual diagnoses.

The k-mean clustering model distinguishes between two different diagnoses, with Cluster 1 grouping primarily malignant samples but still having 28 benign samples present. Cluster 2 groups mainly benign samples, but 24 malignant samples are still present. The hierarchical clustering model, on the other hand, uses four clusters, which is more detailed in comparison. Cluster 1 is predominantly malignant samples, but there are still a few benign samples present. Cluster 2 is mixed with a very small overall number, Cluster 3 is predominantly benign but a small number of malignant samples are present, and Cluster 4 is completely malignant but has a sample size of only two. Although neither sample is perfect, it is still possible to distinguish the separation of the two samples and be able to analyze the data in a valuable way.

```
table(wisc.km$cluster, diagnosis)
   diagnosis
      В
          Μ
  1 343
         37
    14 175
  table(wisc.hclust.clusters, diagnosis)
                     diagnosis
wisc.hclust.clusters
                        В
                             M
                    1 355 205
                        2
                             5
                    3
                        0
                             2
```

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

The best specificity:K-means clustering model The best sensitivity: hierarchical clustering model

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

Patient 1 was prioritized for follow-up. This is because patient 1 appears to be closer to dense clusters of dots based on the PCA plot, which may represent that the patient is a malignant sample and requires faster treatment.

```
#url <- "new_samples.csv"</pre>
  url <- "https://tinyurl.com/new-samples-CSV"</pre>
  new <- read.csv(url)</pre>
  npc <- predict(wisc.pr, newdata=new)</pre>
  npc
          PC1
                    PC2
                              PC3
                                         PC4
                                                   PC5
                                                             PC6
                                                                        PC7
[1,] 2.576616 -3.135913 1.3990492 -0.7631950 2.781648 -0.8150185 -0.3959098
[2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698 -1.2189945 0.8193031
           PC8
                     PC9
                              PC10
                                        PC11
                                                  PC12
                                                           PC13
                                                                    PC14
[1,] -0.2307350 0.1029569 -0.9272861 0.3411457 0.375921 0.1610764 1.187882
[2,] -0.3307423 0.5281896 -0.4855301 0.7173233 -1.185917 0.5893856 0.303029
         PC15
                    PC16
                               PC17
                                           PC18
                                                      PC19
                                                                 PC20
[1,] 0.3216974 -0.1743616 -0.07875393 -0.11207028 -0.08802955 -0.2495216
PC22
                               PC23
          PC21
                                          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=g)
  points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
  text(npc[,1], npc[,2], c(1,2), col="white")
```

