

Class08 Breast Cancer PCA

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Background

The goal of this mini-project is for you to explore a complete analysis using the unsupervised learning techniques covered in class. You'll extend what you've learned by combining PCA as a preprocessing step to clustering using data that consist of measurements of cell nuclei of human breast masses.

The data itself comes from the Wisconsin Breast Cancer Diagnostic Data Set first reported by K. P. Benne and O. L. Mangasarian: "Robust Linear Programming Discrimination of Two Linearly Inseparable Sets".

Values in this data set describe characteristics of the cell nuclei present in digitized images of a fine needle aspiration (FNA) of a breast mass.

Exploratory data analysis

The data is available as a CSV from teh class website:

```
fna.data <- "WisconsinCancer.csv"  
wisc.df <- read.csv(fna.data, 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
842517	0.1812		0.05667	0.5435	0.7339
84300903	0.2069		0.05999	0.7456	0.7869
84348301	0.2597		0.09744	0.4956	1.1560
84358402	0.1809		0.05883	0.7572	0.7813
843786	0.2087		0.07613	0.3345	0.8902
	area_se	smoothness_se	compactness_se	concavity_se	concave.points_se
842302	153.40	0.006399	0.04904	0.05373	0.01587
842517	74.08	0.005225	0.01308	0.01860	0.01340
84300903	94.03	0.006150	0.04006	0.03832	0.02058
84348301	27.23	0.009110	0.07458	0.05661	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			

Separating the “answer” from the data

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

Q1. How many observations are in this dataset?

There are 569 observations in the data set.

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

There's 212 observations with a malignant diagnosis.

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

There's 10 features with “`_mean`” suffix.

Principal Component Analysis

Let's perform a PCA on our data using the base R function `prcomp()`. An optional argument `scale` should nearly always be switched to True (`scale = TRUE`) for this function.

```
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					

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

44.27% of the variance is captured by the first PC.

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

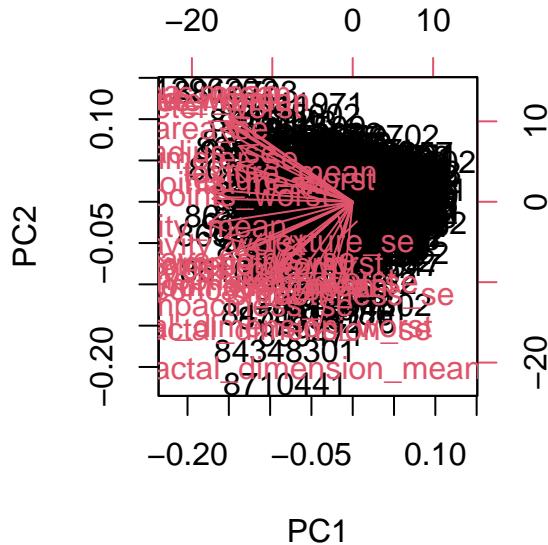
The first 3 PCs are required to describe at least 70% of the variance in the data.

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

The first 7 PCs are required to describe at least 90% of the variance in the data.

Let's start with a biplot of our PC analysis.

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

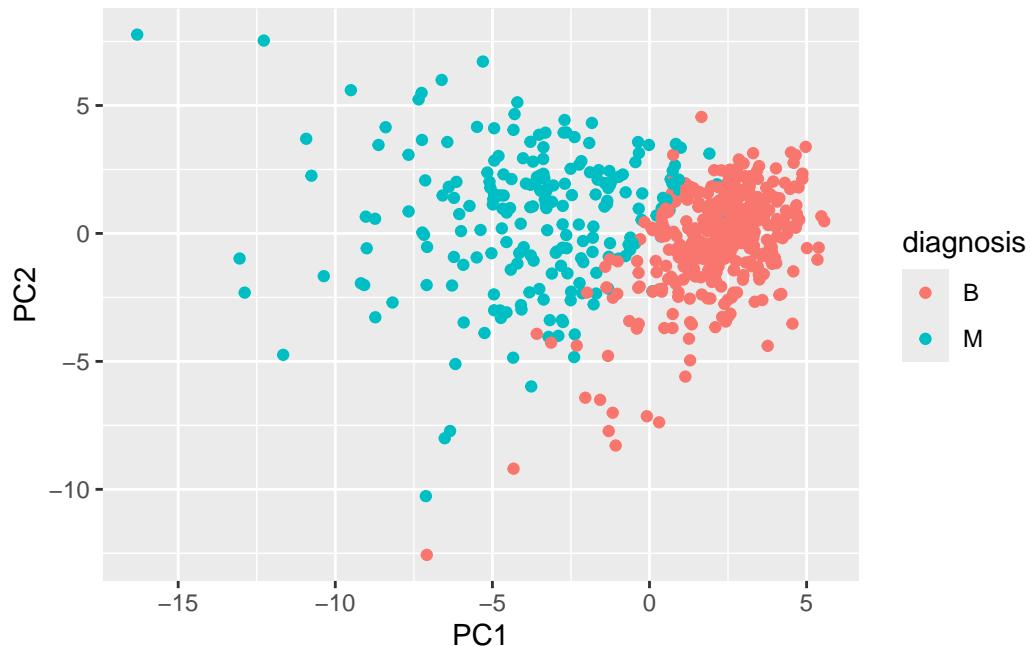


Q7. What stands out to you about this plot? Is it easy or difficult to understand?
Why?

Nothing really stands out, it's a blob of data and factors that is hard to interpret. Since rownames are being plotted, it is extremely messy. And since we are plotting 30 factors, the arrows don't tell us much either.

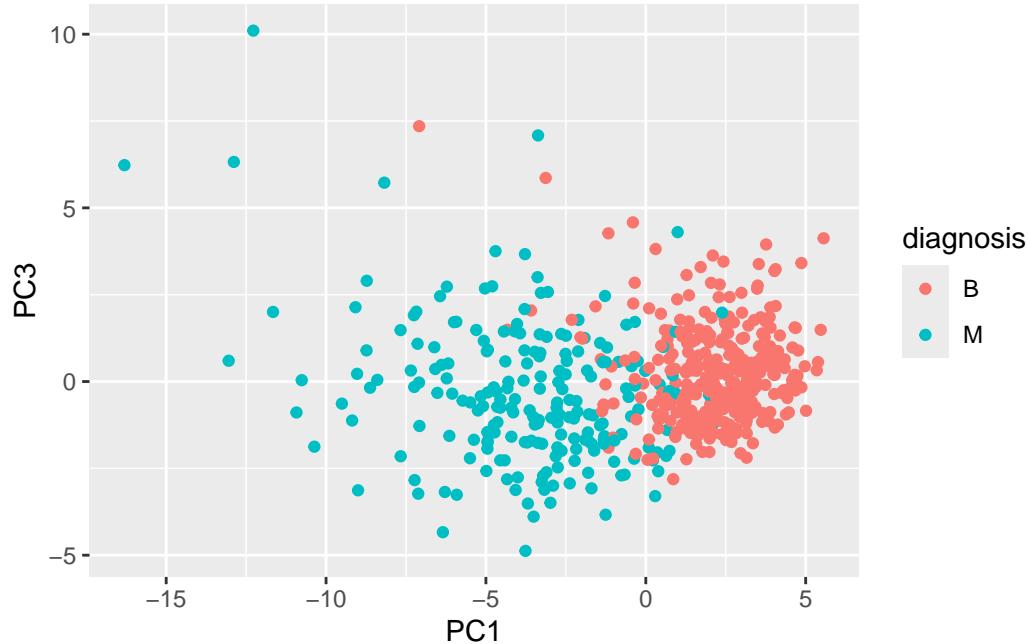
Let's make a scatterplot of PC1 and PC2

```
library(ggplot2)
ggplot(wisc.pr$x) +
  aes(PC1,PC2, col = diagnosis) +
  geom_point()
```



And now a scatterplot with PC1 and PC3

```
ggplot(wisc.pr$x) +
  aes(PC1,PC3, col = diagnosis) +
  geom_point()
```

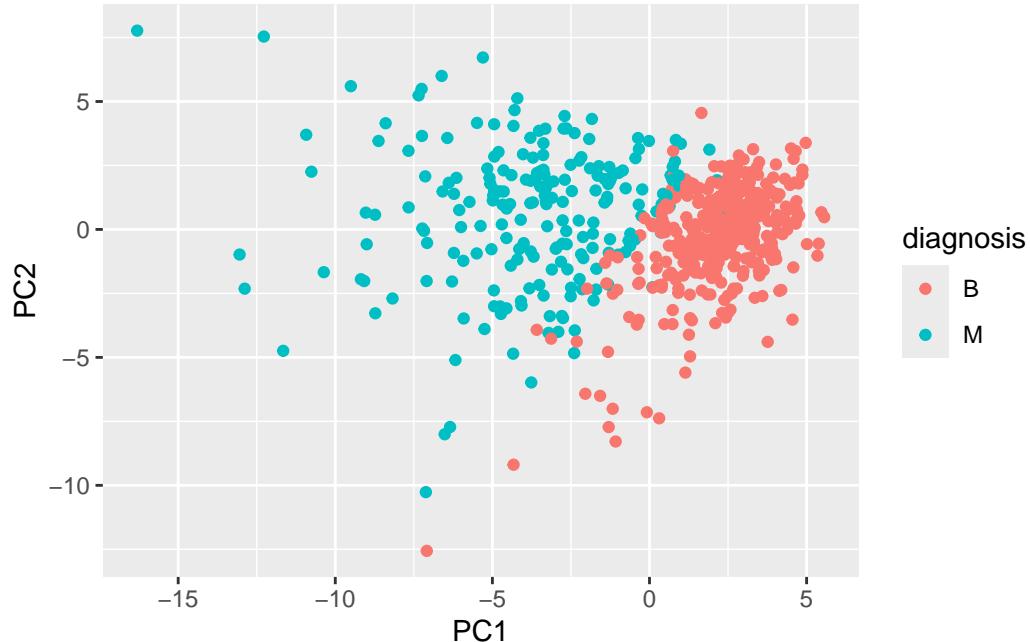


Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

There is less of a defined division of diagnosis with 1 and 3 as compared to 1 and 2.

Instead, let's make our main result figure - the "PC plot" or "score plot" or "ordination plot" colored by diagnosis.

```
ggplot(wisc.pr$x) +
  aes(PC1,PC2, col = diagnosis) +
  geom_point()
```



Variance explained

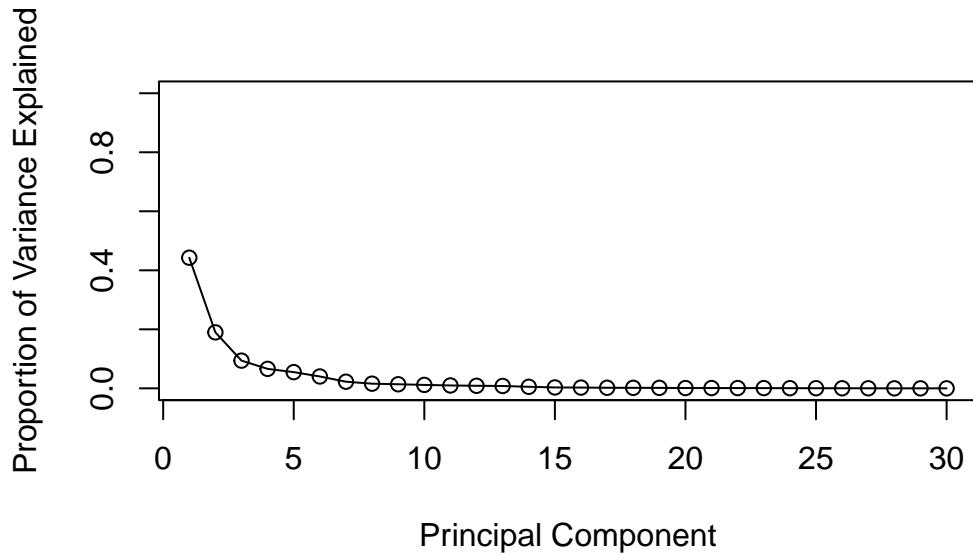
Let's plot variance by PCs

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

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

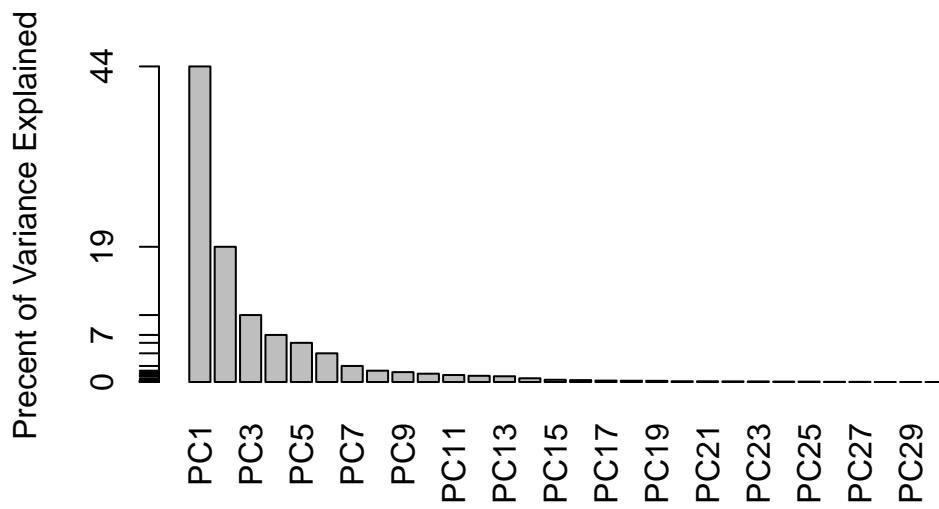
```
pve <- pr.var / sum(pr.var)

plot(pve, xlab = "Principal Component",
      ylab = "Proportion of Variance Explained",
      ylim = c(0, 1), type = "o")
```



Alternative scree plot of the same data

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



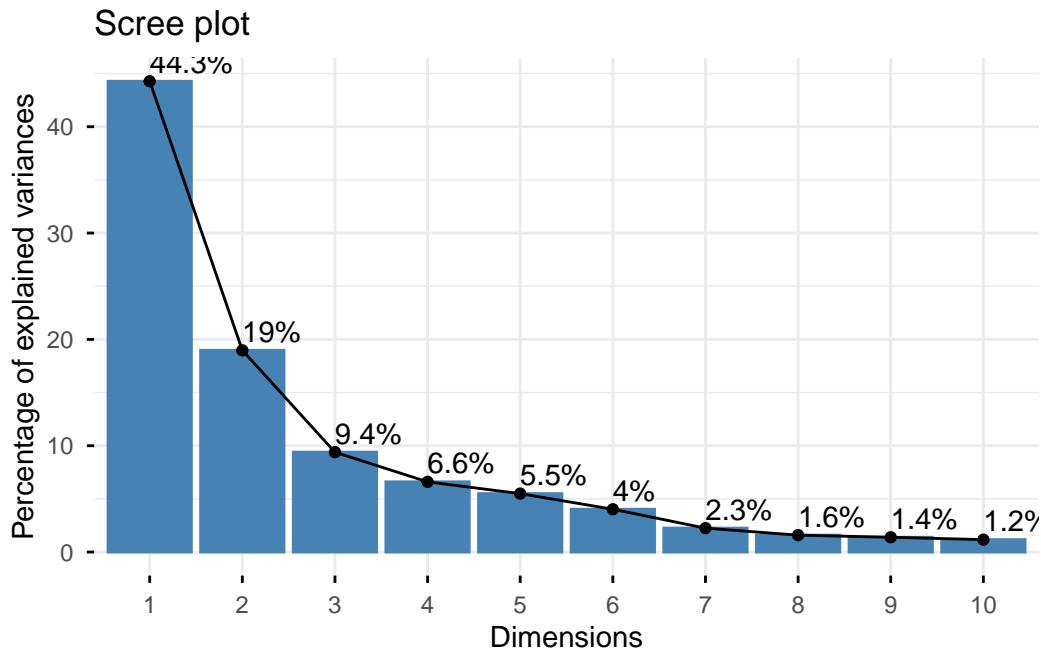
And now plotting with factoextra package

```
library(factoextra)
```

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

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

```
Warning in geom_bar(stat = "identity", fill = barfill, color = barcolor, :
  Ignoring empty aesthetic: `width`.
```



Communicating PCA results

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`? This tells us how much this original feature contributes to the first PC.

The component of the loading vector is -0.2608538

Hierarchical clustering

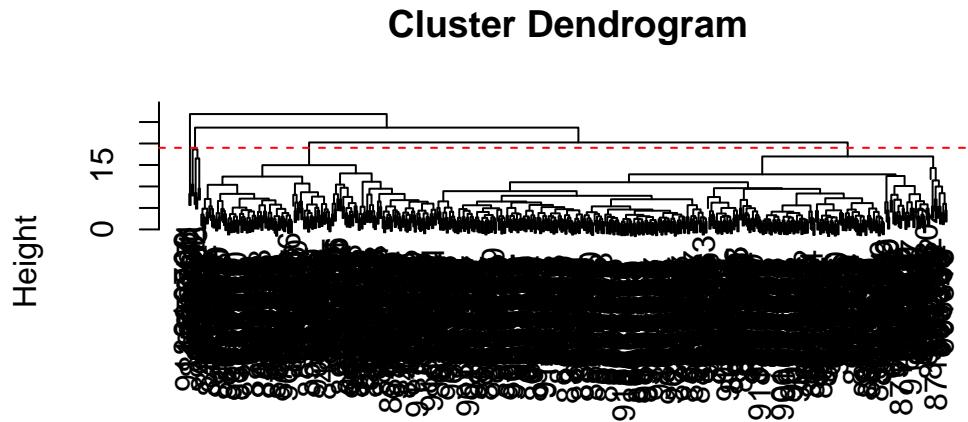
Scaling the data

```
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled, method = "euclidean")
wisc.hclust <- hclust(data.dist, method = "complete")
```

Results of hierarchical clustering

Let's make a cluster dendrogram

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



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

Q10. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

A height of 19 will cut the dendrogram into 4 clusters.

Selecting number of clusters

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

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

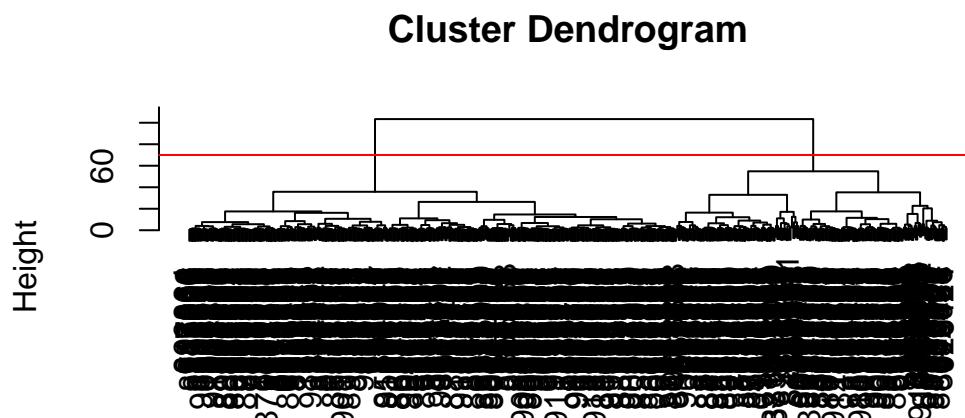
Using different methods.

Q12. Which method gives your favorite results for the same data.dist dataset?
Explain your reasoning.

Ward.D2 is my favorite method because it consistently yields the most compact, distinct, and statistically sound clusters by minimizing within-cluster variance.

Combining Methods

```
d <- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <- hclust(d, method = "ward.D2")
plot(wisc.pr.hclust)
abline(h=70, col="red")
```



```
d
hclust (*, "ward.D2")
```

Get my cluster membership vector

```
grps <- cutree(wisc.pr.hclust, h = 70)
table(grps)
```

```
grps
  1   2
203 366
```

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

make a “cross-table

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

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

TP: 179 FP: 24 TN: 333 FN: 33

Q13. How well does the newly created model with four clusters separate out the two diagnoses?

Pretty well, with around a 90% true negative rate and a 87% true positive rate.

Prediction

Using predict() on a new dataset.

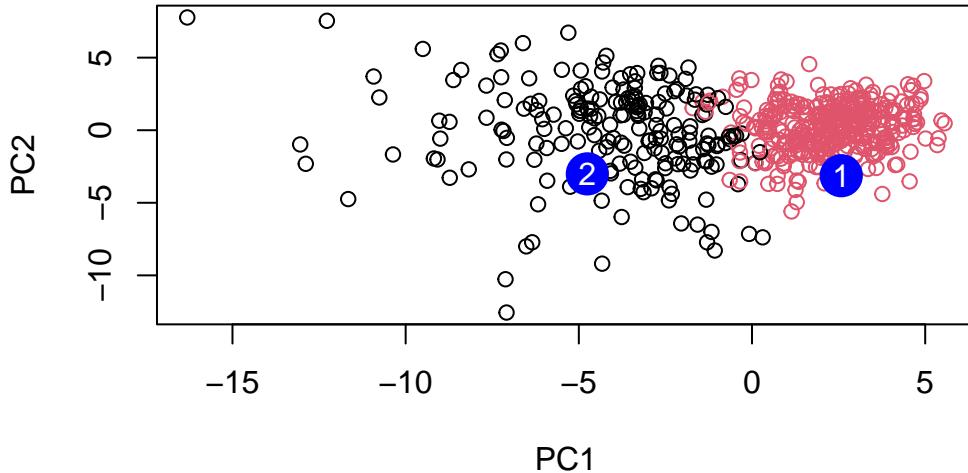
```
g <- as.factor(grps)
new <- read.csv("new_samples.csv")
npc <- predict(wisc.pr, newdata=new)
npc
```

	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
[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
```

Plotting our predictions

```
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")
```



Q16. Which of these new patients should we prioritize for follow up based on your results?

We should prioritize patient 1 for followup since they cluster with the Malignant group.