

Class09

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1

```
# 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)
```

lets look at the dataframe

```
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				

```
# We can use -1 here to remove the first column
wisc.data <- wisc.df[,-1]
#here is the diagnosis vector to use in the questions
```

```
diagnosis <- as.factor(wisc.df$diagnosis)
```

```
diagnosis
```

```
[1] M M M M M M M M M M M M M M M M M M B B B M M M M M M M M M M M M M
[38] B M M M M M M M B M B B B B B M M B M M B B B B M B M M B B B B M B M M
[75] B M B M M B B B M M B M M M B B B M B B M M B B B B M M B B B B M B B M B B
[112] B B B B B B M M M B M M B B B M M B M B M M B M M B B M B B M B B B B M B
[149] B B B B B B B M B B B B M M B M B B M M B B M M B B B B M B B M M M B M
[186] B M B B B M B B M M B M M M M B M M M B M B B M B M M M M B B M M B B
[223] B M B B B B B M M B B M B B M M B M B B B B B M B B B B B M B M M M M M M
[260] M M M M M M M B B B B B B M B M B B M B B M B M M B B B B B B B B B B B
[297] B M B B M B M B B B B B B B B B B B B B B M B B B M B M B B B B M M M B B
[334] B B M B M B M B B B M B B B B B B B M M M B B B B B B B B B B M M B M M
[371] M B M M B B B B B M B B B B B M B B B M B B M M B B B B B B M B B B B B B
[408] B M B B B B B M B B M B B B B B B B B B B B M B M M B M B B B B B M B B
[445] M B M B B M B M B B B B B B B B M M B B B B B B M B B B B B B B B B M B
[482] B B B B B B M B M B B M B B B B B M M B M B M B B B B B M B B M B M B M M
[519] B B B M B B B B B B B B B B B M B M M B B B B B B B B B B B B B B B B B
[556] B B B B B B B M M M M M M B
Levels: B M
```

Q1. How many observations are in this dataset?

The number of rows is the number of observations

```
nrow(wisc.data)
```

```
[1] 569
```

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

```
table(diagnosis)
```

```
diagnosis
  B    M
357 212
```

there's 212 malignant

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

```
grep("_mean", colnames(wisc.data))
```

```
[1] 1 2 3 4 5 6 7 8 9 10
```

there are 10 variables suffixed by `_mean`

2. PCA

```
# 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, scale=T)
```

```
# 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)?

```
v <- summary(wisc.pr)
pcvar <- v$importance[3,]
pcvar["PC1"]
```

```
PC1
0.44272
```

```
44.27%
```

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

```
which(pcvar >= 0.7)[1]
```

```
PC3
3
```

We need to use 3 PCs to reach 70%+

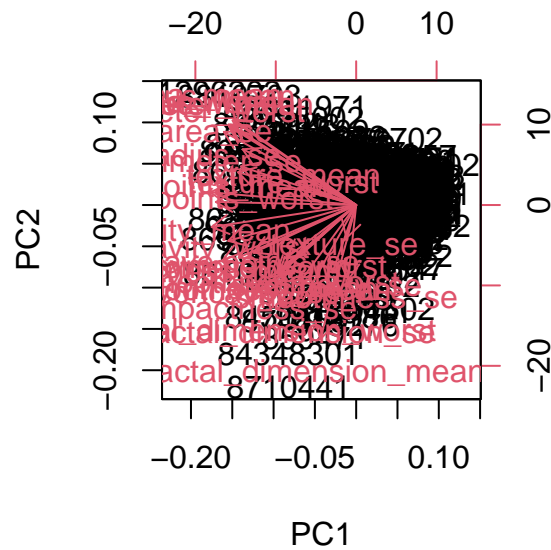
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

```
which(pcvar >= 0.9)[1]
```

```
PC7
7
```

We need to use 7 PCs to reach 90%+

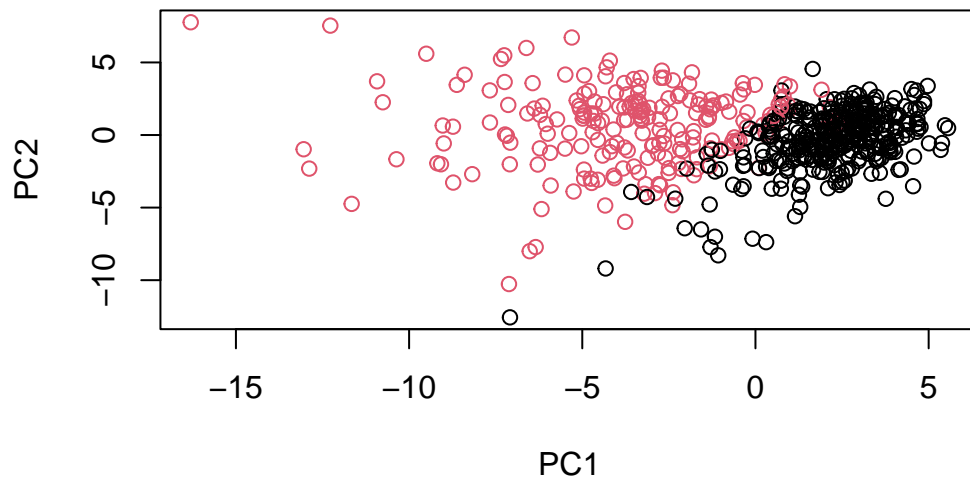
```
biplot(wisc.pr)
```



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

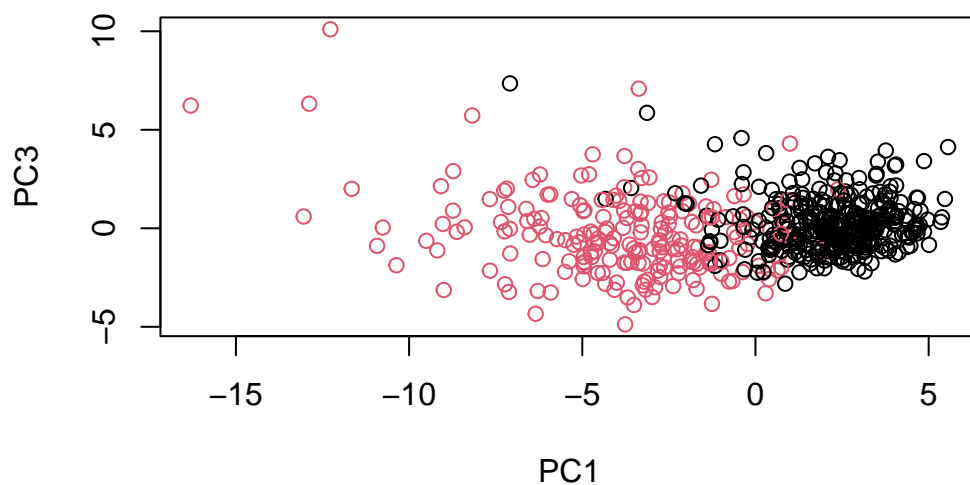
There is WAY too much on this plot to understand it. It's covered in labels for all of the different observations.

```
# Scatter plot observations by components 1 and 2
plot(wisc.pr$x[,1], wisc.pr$x[,2], col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



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

```
# Repeat for components 1 and 3
plot(wisc.pr$x[,1], wisc.pr$x[,3], col = as.factor(diagnosis),
     xlab = "PC1", ylab = "PC3")
```

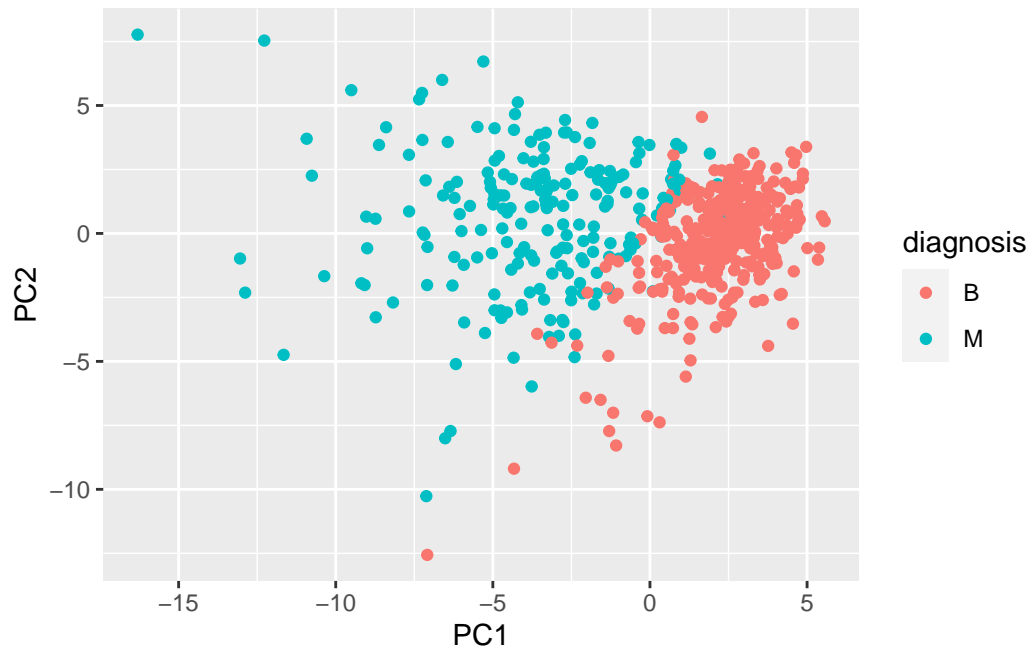



It looks very similar to the previous graph but the variance seems slightly greater in the plot using PC2.

```
# 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()
```



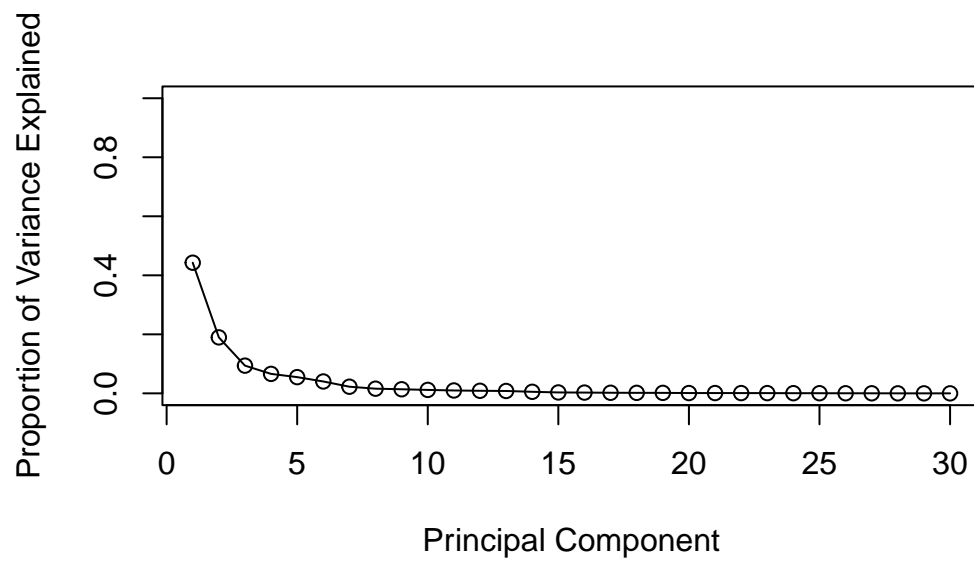
3 variance

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

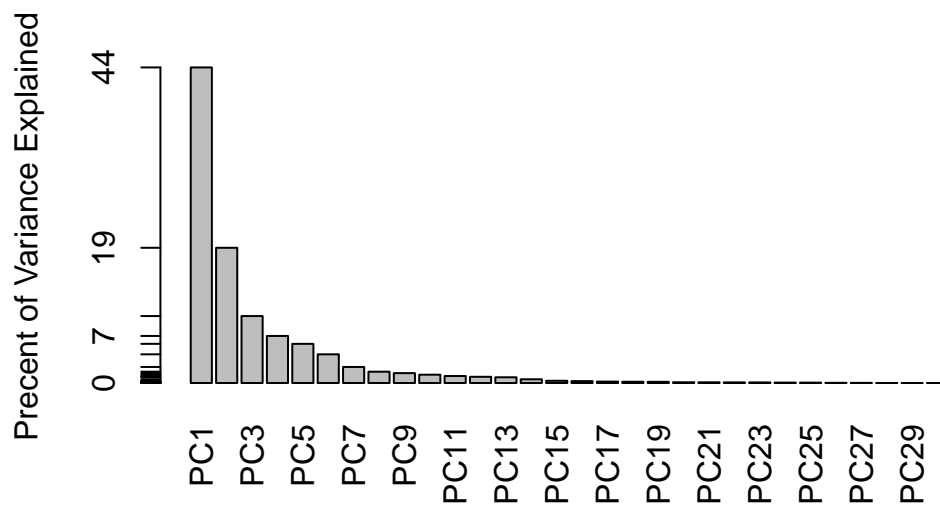
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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")
```



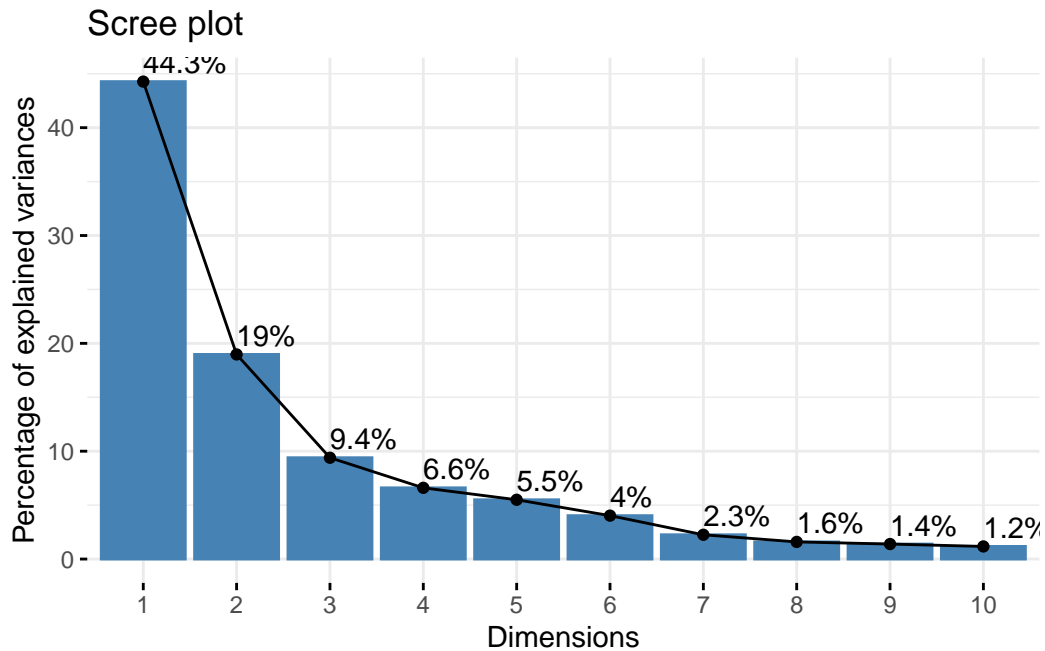
```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
        names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```



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

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

```
[1] -0.2608538
```

the feature “concave.points” negatively contributes to the PC1, meaning that the

Hierarchical clustering

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

```
data.dist <- dist(data.scaled)
```

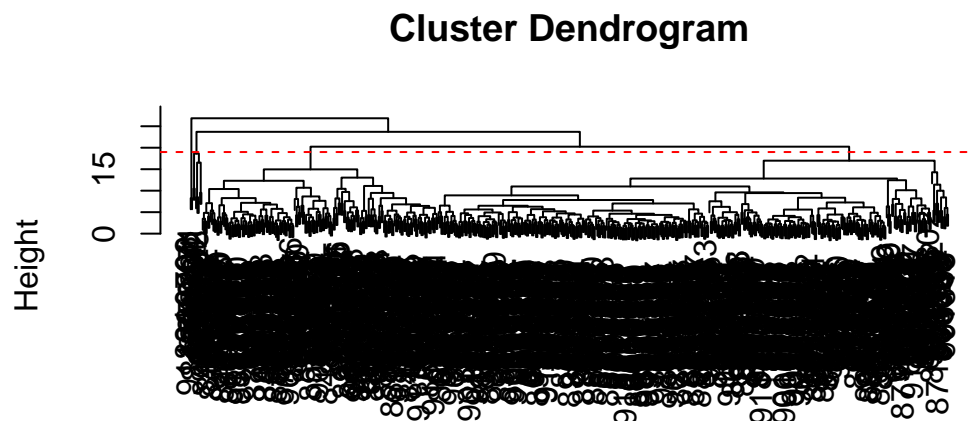
```
wisc.hclust <- hclust(data.dist,)
wisc.hclust
```

```
Call:
hclust(d = data.dist)
```

```
Cluster method   : complete
Distance         : euclidean
Number of objects: 569
```

Q10. 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)
```



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

at a height of about 19 the model has 4 clusters

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

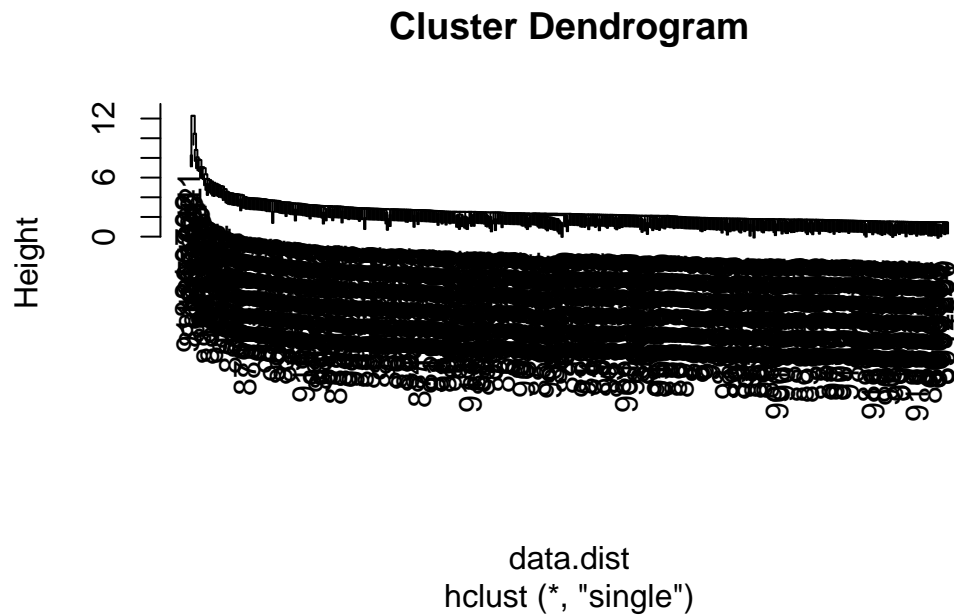
```
diagnosis
wisc.hclust.clusters  B  M
```

1	12	165
2	2	5
3	343	40
4	0	2

different methods

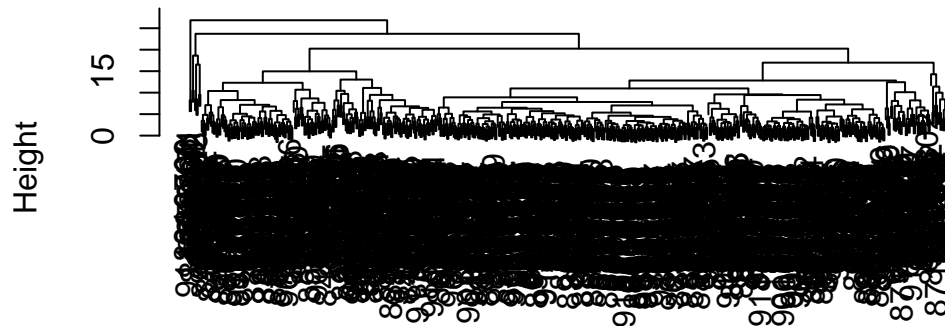
Q12. Which method gives your favorite results for the same data.dist dataset?
Explain your reasoning.

```
wisc.hclust.single<- hclust(data.dist,method="single")
plot(wisc.hclust.single)
```



```
wisc.hclust.complete<- hclust(data.dist,method="complete")
plot(wisc.hclust.complete)
```

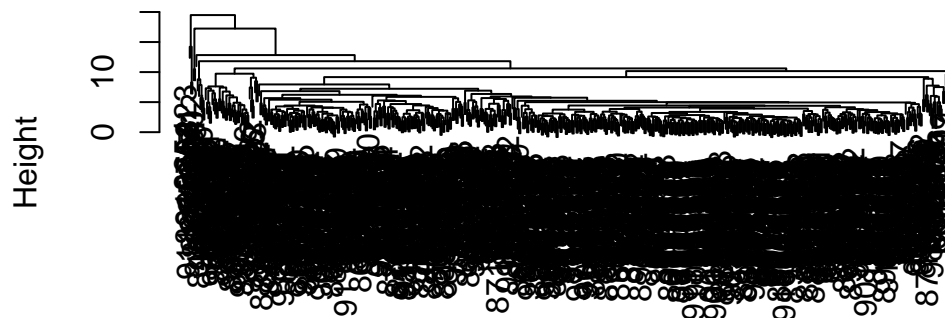
Cluster Dendrogram



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

```
wisc.hclust.average<- hclust(data.dist,method="average")  
plot(wisc.hclust.average)
```

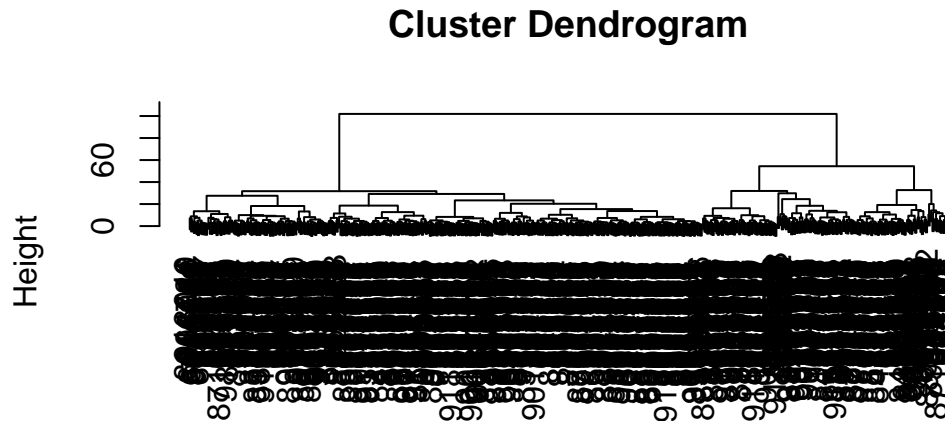
Cluster Dendrogram



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



```
wisc.hclust.wardd2<- hclust(data.dist,method="ward.D2")
plot(wisc.hclust.wardd2)
```

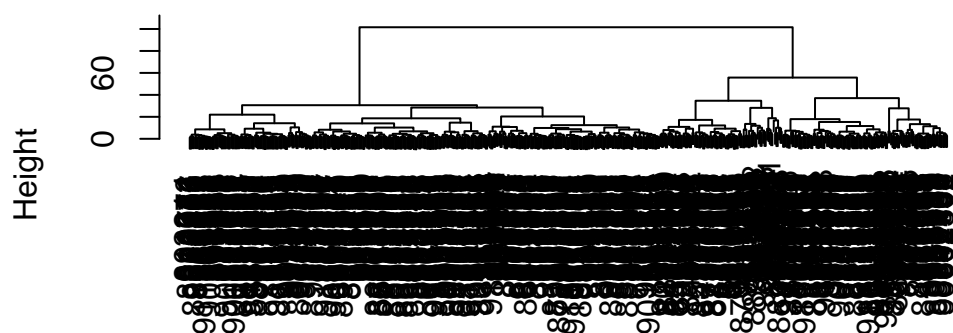


```
data.dist
hclust (*, "ward.D2")
```

I like ward.D2 the best. It looks a bit cleaner and it seems easier to cut the tree at meaningful places to separate the benign and malignant

```
data.dist.1 <- dist(wisc.pr$x[,1:7])
wisc.pr.hclust <- hclust(data.dist.1, method="ward.D2")
plot(wisc.pr.hclust)
```

Cluster Dendrogram



data.dist.1
hclust (*, "ward.D2")

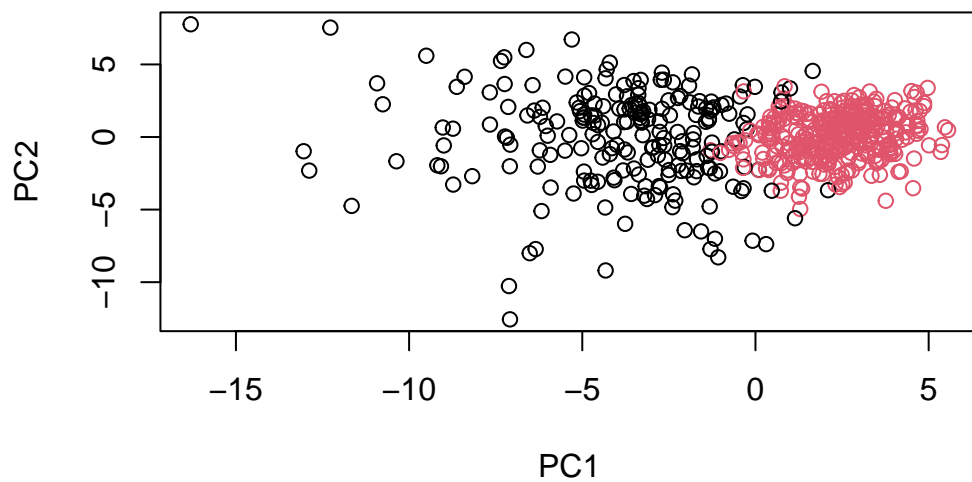
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
216 353
```

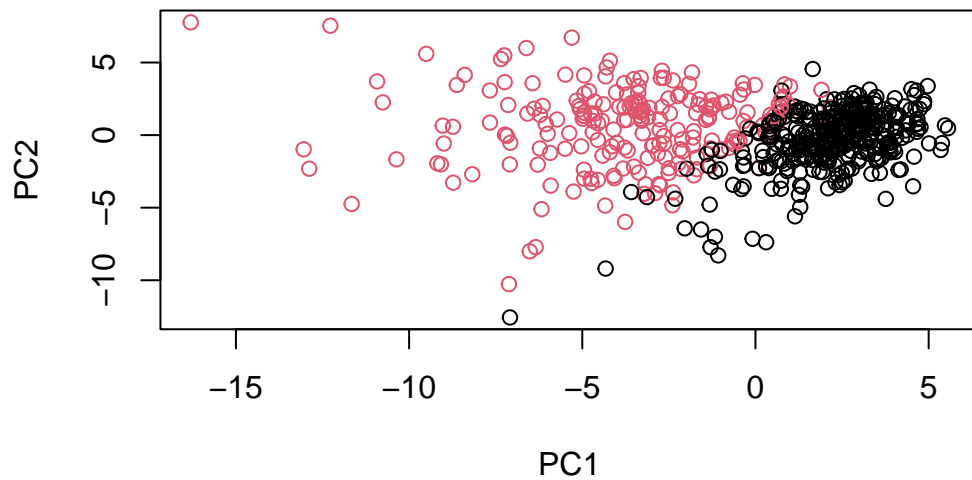
```
table(grps, diagnosis)
```

```
diagnosis
grps  B   M
  1  28 188
  2 329  24
```

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



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



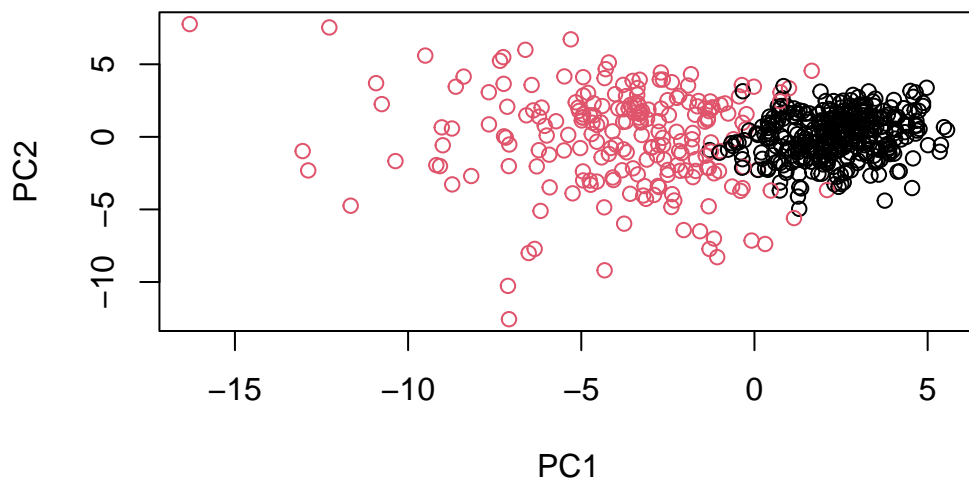
```
g <- as.factor(grps)
levels(g)
```

```
[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)
```



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

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

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

```
# Compare to actual diagnoses
table(wisc.pr.hclust.clusters, diagnosis)
```

```

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

looking at the first data set, the count for B and M is the same here. There's not many false positives (28) and false negatives (24).

Q14. 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.

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

```

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

```
wisc.pr.hclust.single <- hclust(data.dist.1, method="single")
wisc.pr.hclust.single.cut <- cutree(wisc.pr.hclust.single, k=4)
table(wisc.pr.hclust.single.cut, diagnosis)
```

```

              diagnosis
wisc.pr.hclust.single.cut  B   M
1     356 209
2       1   0
3       0   2
4       0   1
```

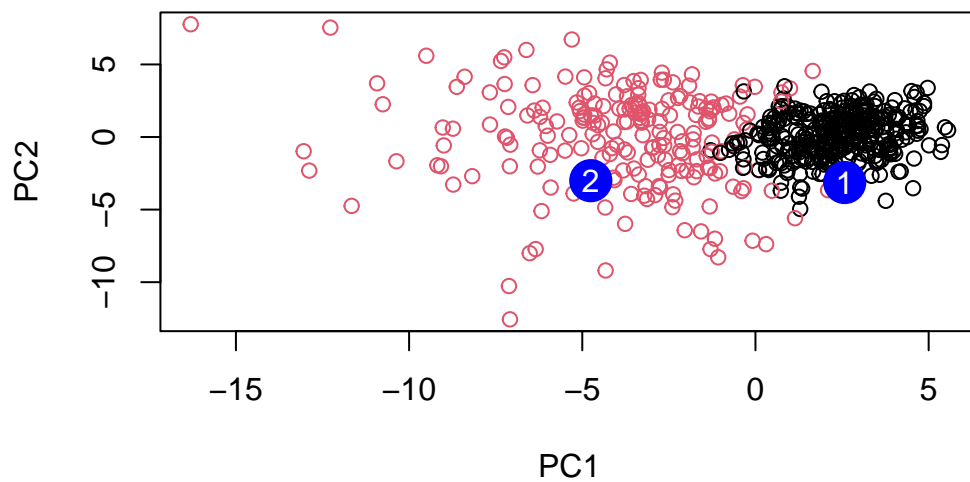
This is way harder to read/interpret than the first one. It's way tougher to use.

#Prediction

```
#url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
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			

```
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 would prioritize the second for follow up because they are likely to be malignant.