

Class 8 mini project

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PCA practical issue: larger range and values in a column of the data set are given more importance, but we need to make sure each feature contributes equally to the —> do this with scaling inside `prcomp()`

```
head(mtcars)
```

	mpg	cyl	disp	hp	drat	wt	qsec	vs	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

```
apply(mtcars,2,sd)
```

mpg	cyl	disp	hp	drat	wt
6.0269481	1.7859216	123.9386938	68.5628685	0.5346787	0.9784574
qsec	vs	am	gear	carb	
1.7869432	0.5040161	0.4989909	0.7378041	1.6152000	

Scale our data

```
x <- scale(mtcars)
head(x)
```

	mpg	cyl	disp	hp	drat
Mazda RX4	0.1508848	-0.1049878	-0.57061982	-0.5350928	0.5675137
Mazda RX4 Wag	0.1508848	-0.1049878	-0.57061982	-0.5350928	0.5675137
Datsun 710	0.4495434	-1.2248578	-0.99018209	-0.7830405	0.4739996

Hornet 4 Drive	0.2172534	-0.1049878	0.22009369	-0.5350928	-0.9661175
Hornet Sportabout	-0.2307345	1.0148821	1.04308123	0.4129422	-0.8351978
Valiant	-0.3302874	-0.1049878	-0.04616698	-0.6080186	-1.5646078
	wt	qsec	vs	am	gear
Mazda RX4	-0.610399567	-0.7771651	-0.8680278	1.1899014	0.4235542
Mazda RX4 Wag	-0.349785269	-0.4637808	-0.8680278	1.1899014	0.4235542
Datsun 710	-0.917004624	0.4260068	1.1160357	1.1899014	0.4235542
Hornet 4 Drive	-0.002299538	0.8904872	1.1160357	-0.8141431	-0.9318192
Hornet Sportabout	0.227654255	-0.4637808	-0.8680278	-0.8141431	-0.9318192
Valiant	0.248094592	1.3269868	1.1160357	-0.8141431	-0.9318192
	carb				
Mazda RX4	0.7352031				
Mazda RX4 Wag	0.7352031				
Datsun 710	-1.1221521				
Hornet 4 Drive	-1.1221521				
Hornet Sportabout	-0.5030337				
Valiant	-1.1221521				

```
round(colMeans(x),2) #mean = 0, st.dev = 1
```

mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
0	0	0	0	0	0	0	0	0	0	0

```
prcomp
```

```
function (x, ...)
UseMethod("prcomp")
<bytecode: 0x11aa2f988>
<environment: namespace:stats>
```

Using scale in prcomp usually passes values to the scale function - we always need to choose whether or not to scale data

1. Exploratory data analysis

```
# 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)
```

```
# We can use -1 here to remove the first column
wisc.data <- wisc.df[,-1]
# Create diagnosis vector for later
diagnosis <- as.factor(wisc.df[,1])
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 M M 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 B M B B B B M M B 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 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 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
[556] B B B B B B B M M M M M M M B
Levels: B M
```

QUESTION 1

Q1. How many observations are in this dataset?

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

```
[1] 569
```

```
# 569 observations
```

QUESTION 2

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

```
sum(diagnosis=="M")
```

```
[1] 212
```

```
table(diagnosis)
```

```
diagnosis
  B    M
357 212
```

```
# 212 malignant
```

Remove first column 'diagnosis' from data frame, this is the answer we need to compare to our analysis result

```
# Use -1 here to remove the first column
wisc.data <- wisc.df[,-1]
head(wisc.data)
```

	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean
842302	17.99	10.38	122.80	1001.0	0.11840
842517	20.57	17.77	132.90	1326.0	0.08474
84300903	19.69	21.25	130.00	1203.0	0.10960
84348301	11.42	20.38	77.58	386.1	0.14250
84358402	20.29	14.34	135.10	1297.0	0.10030
843786	12.45	15.70	82.57	477.1	0.12780
	compactness_mean	concavity_mean	concave.points_mean	symmetry_mean	
842302	0.27760	0.3001	0.14710	0.2419	
842517	0.07864	0.0869	0.07017	0.1812	
84300903	0.15990	0.1974	0.12790	0.2069	
84348301	0.28390	0.2414	0.10520	0.2597	
84358402	0.13280	0.1980	0.10430	0.1809	
843786	0.17000	0.1578	0.08089	0.2087	
	fractal_dimension_mean	radius_se	texture_se	perimeter_se	area_se
842302	0.07871	1.0950	0.9053	8.589	153.40
842517	0.05667	0.5435	0.7339	3.398	74.08
84300903	0.05999	0.7456	0.7869	4.585	94.03
84348301	0.09744	0.4956	1.1560	3.445	27.23
84358402	0.05883	0.7572	0.7813	5.438	94.44
843786	0.07613	0.3345	0.8902	2.217	27.19
	smoothness_se	compactness_se	concavity_se	concave.points_se	
842302	0.006399	0.04904	0.05373	0.01587	
842517	0.005225	0.01308	0.01860	0.01340	

84300903	0.006150	0.04006	0.03832	0.02058
84348301	0.009110	0.07458	0.05661	0.01867
84358402	0.011490	0.02461	0.05688	0.01885
843786	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			

QUESTION 3

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

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

```
[1] 10
```

```
# 10 variables are suffixed with _mean
```

2. Principal component analysis

```
# 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
# SCALE
wisc.pr <- prcomp(wisc.data, scale=T)
```

QUESTION 4

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

```
# Find proportion variance of each PC
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

```
# 44.27%
```

QUESTION 5

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

```
# 3 PCs
```

QUESTION 6

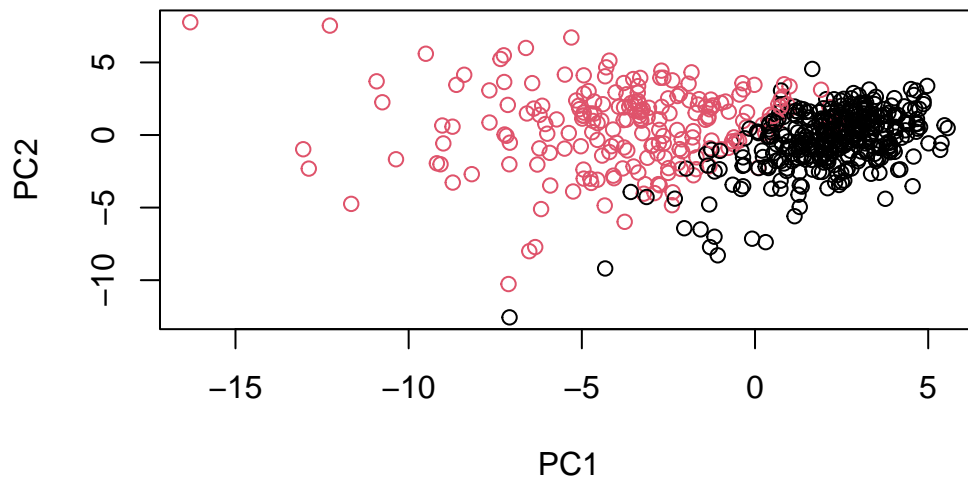
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

```
# 7 PCs
```

QUESTION 7

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

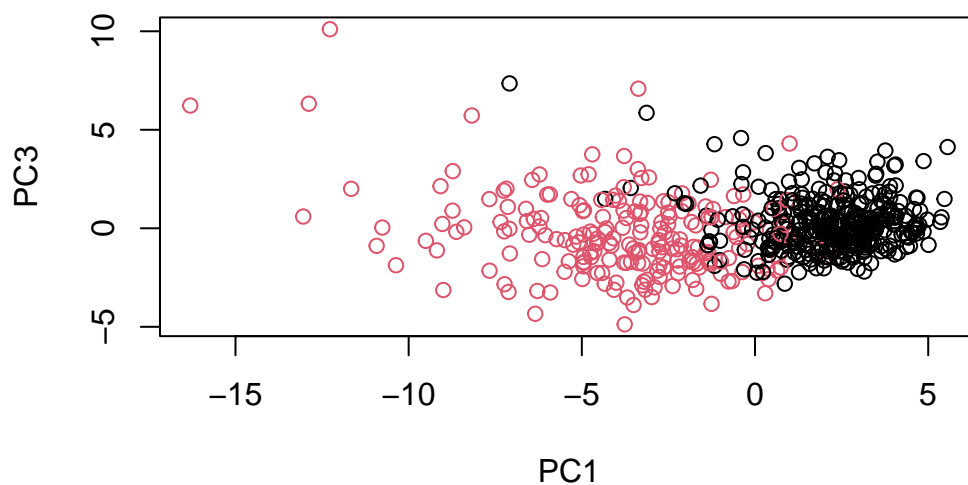
```
biplot(wisc.pr)
```

QUESTION 8

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

```
# Scatter plot observations by components 1 and 2
plot(wisc.pr$x[,1], wisc.pr$x[,3],
     col=diagnosis,xlab = "PC1", ylab = "PC3") #diagnosis shown by color
```



The PC axis are the most important axis for the data

PC1 is the axis with most variation, PC2 is the axis with second most variation, etc.

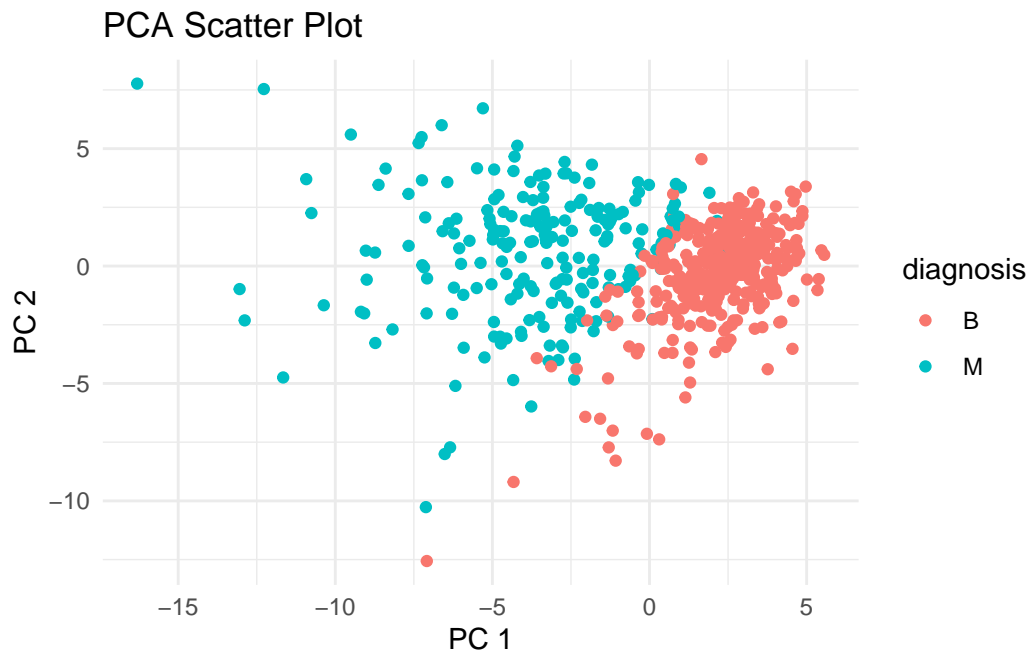
Find the middle of each PC axis and it is 0, then measure the points based on how far/close they are from it, this is the **influence** of the

ggplot

```
# 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() +
  labs(title = "PCA Scatter Plot", x = "PC 1", y = "PC 2") +
  theme_minimal()
```



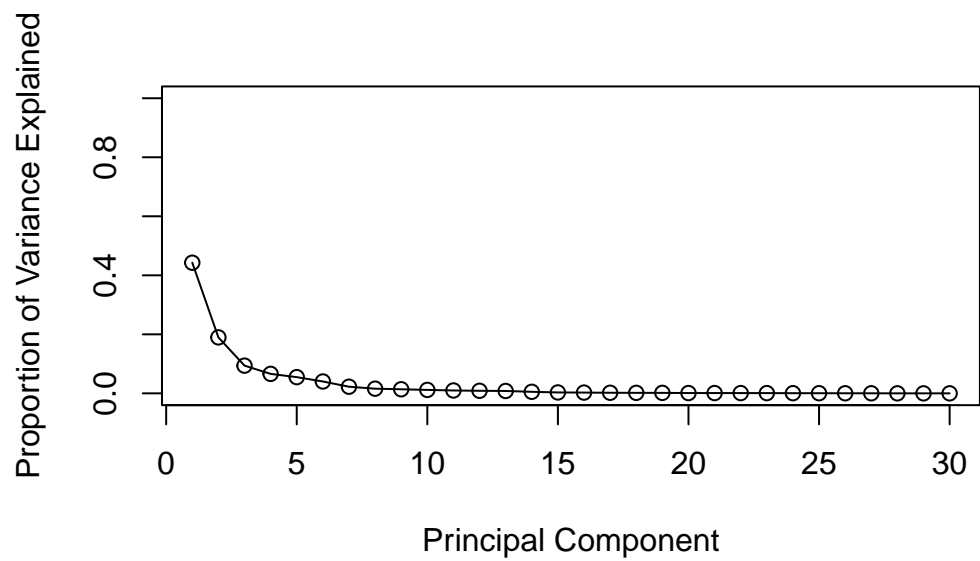
variance

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

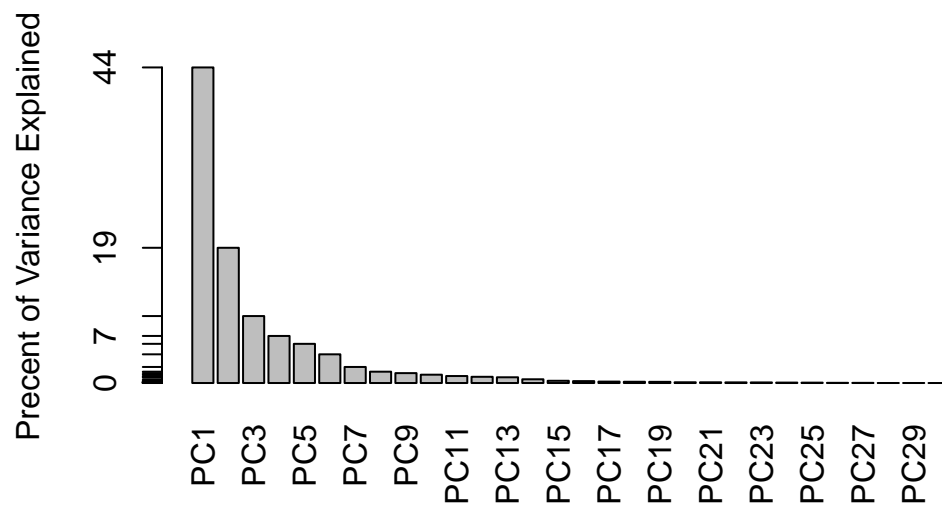
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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")
```



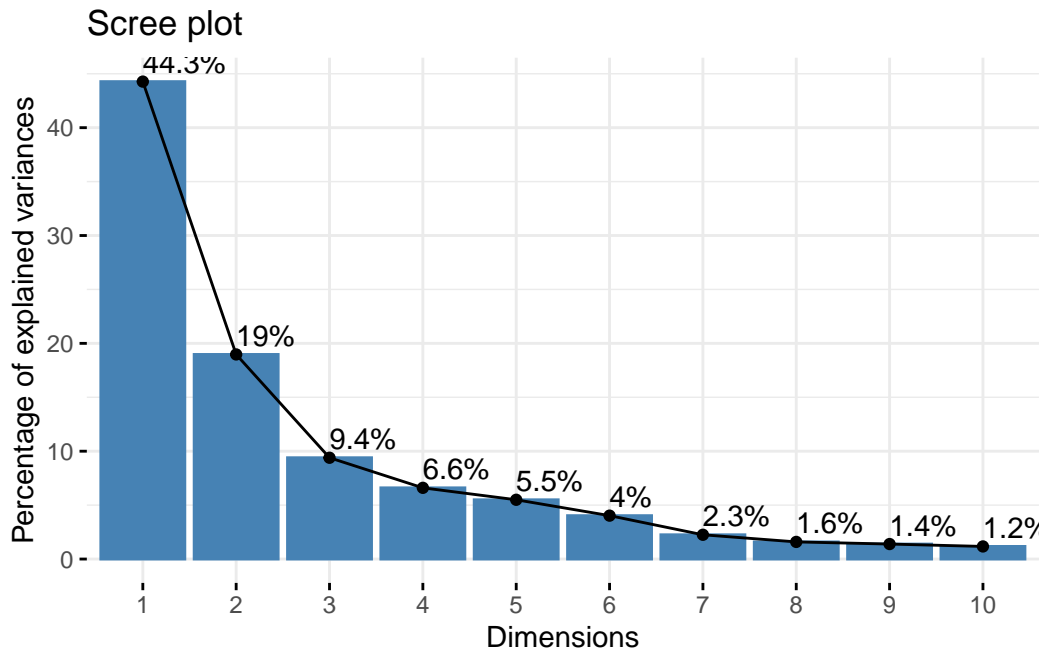
```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
        names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```



```
## 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)
```



QUESTION 9

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
```

QUESTION 10

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

```
# 5 PCs
```

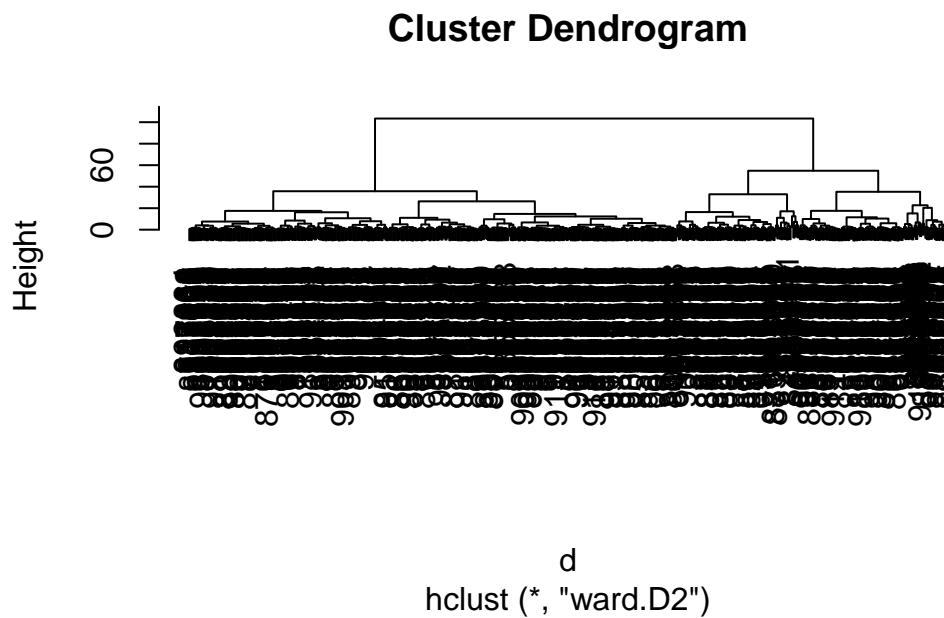
QUESTION 11

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

```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
# Get distance of data
data.dist <- dist(data.scaled)
# Make hierarchy tree
wisc.hclust <- hclust(data.dist, method="complete")
```

Class walk through

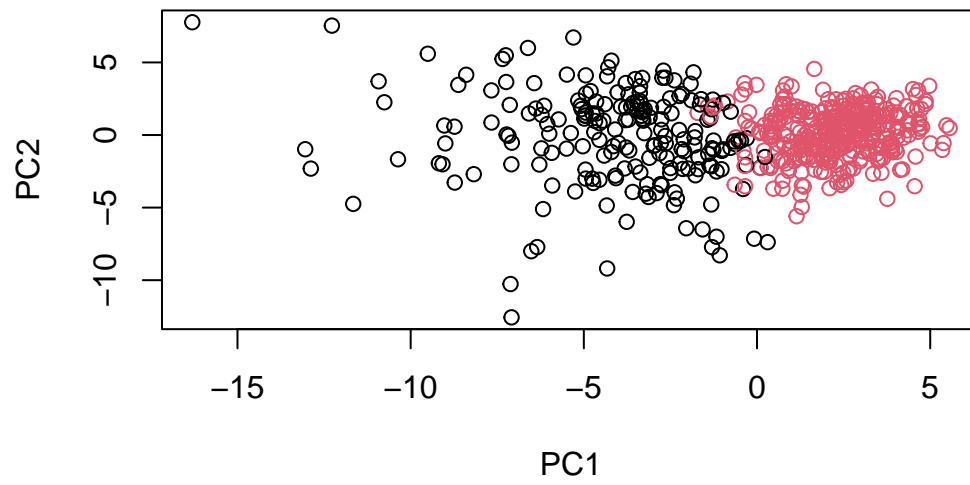
```
# distance matrix from PCA result
d <- dist(wisc.pr$x[,1:3])
hc <- hclust(d,method="ward.D2")
plot(hc)
```



Cut the tree into 2 groups/branches/clusters

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

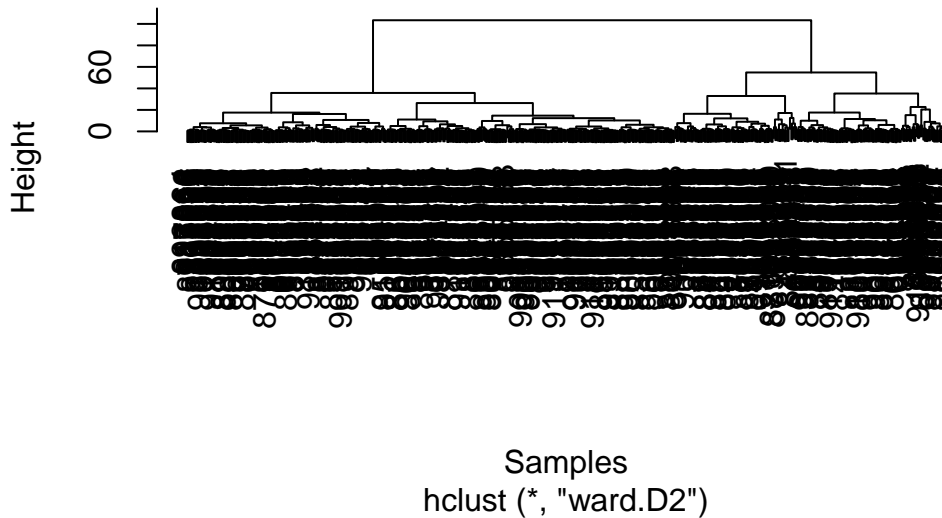
```
plot(wisc.pr$x,col=grps)
```

?abline

```
plot(hc, main = "Hierarchical Clustering Dendrogram",  
      xlab = "Samples", ylab = "Height")  
# Make line to get only 4 clusters  
abline(h=1800, col="red", lty=2)
```

Hierarchical Clustering Dendrogram



QUESTION 12

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

```
# The best cluster vs diagnoses is done by cutting 2 clusters
```

QUESTION 13

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

```
# The PCA scattter plot is my favorite representation of the data since it clearly shows the
```

QUESTION 14

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

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

```

      grps
diagnosis 1  2
B    24 333
M   179  33

```

```
# This table clearly shows how many benign and malignant tumors in each cluster
```

QUESTION 16

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

```

#table(wisc.km$cluster)
#table(wisc.hclust.clusters)
# I think k-means and hierarchical clustering models do not work well for separating diagnoses

```