

8: Unsupervised Learning Mini-Project

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Principle Component Analysis (PCA)

It is important to consider scalling your data before analysis such as PCA

```
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

```
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)
```

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	

```
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)
```

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

Key-Point: It is usually always a good idea to scale your data before to PCA. . .

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)
```

```
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			

Omit the diagnosis column (M for malignant)

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

Separately store the diagnosis column

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

Q1. How many observations are in this dataset?

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

```
[1] 569
```

Q2. How many of the observations have a malignant diagnosis? (M for malignant, B for benign)

```
table(diagnosis)
```

```
diagnosis
  B    M
357 212
```

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

```
sum(grepl("_mean", names(wisc.data)))
```

```
[1] 10
```

2. Principle 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
wisc.pr <- prcomp(wisc.data, scale. = T)
```

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

Importance of components:

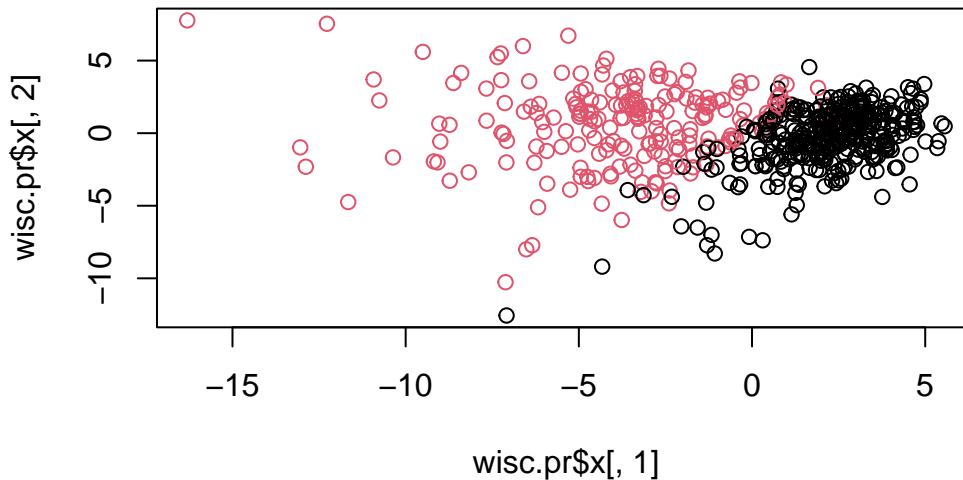
	PC1	PC2	PC3	PC4	PC5	PC6	PC7
Standard deviation	3.6444	2.3857	1.67867	1.40735	1.28403	1.09880	0.82172
Proportion of Variance	0.4427	0.1897	0.09393	0.06602	0.05496	0.04025	0.02251
Cumulative Proportion	0.4427	0.6324	0.72636	0.79239	0.84734	0.88759	0.91010
	PC8	PC9	PC10	PC11	PC12	PC13	PC14
Standard deviation	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					

Main “PC score plot”, “PC1 v. PC2 plot”

```
attributes(wisc.pr)
```

```
$names  
[1] "sdev"      "rotation" "center"    "scale"     "x"  
  
$class  
[1] "prcomp"
```

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



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

0.4427; 44.27%

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

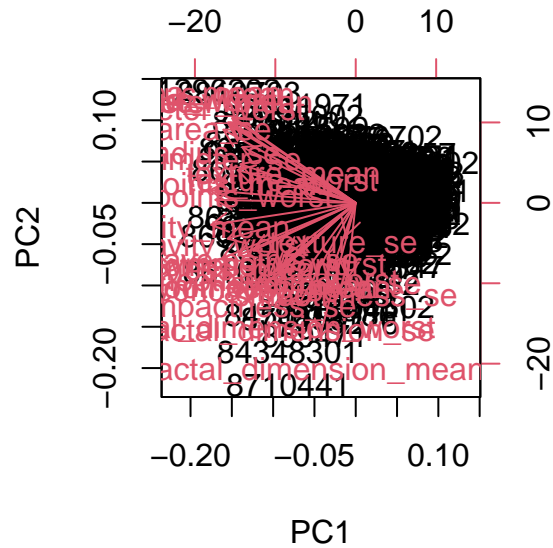
3 PCs

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

7 PCs

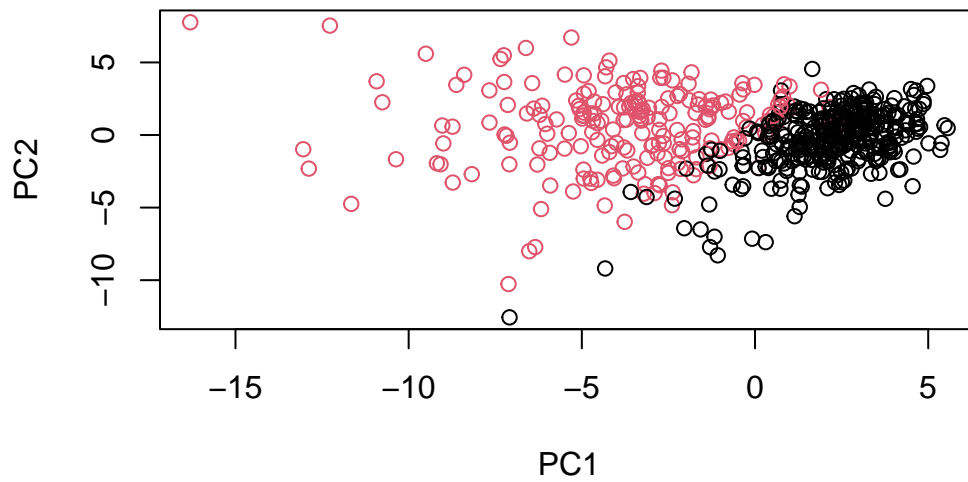
Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

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



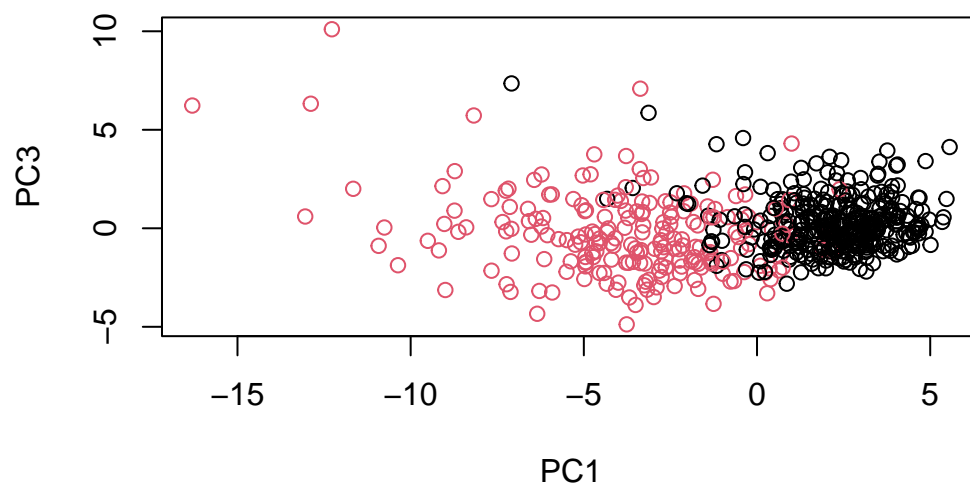
There are very few readable column names that are shown in red on the outer edge of the plot with lines attaching them to the origin of the plot. The black numbers that are clumped together around the origin seem to be the data.

```
plot(wisc.pr$x[,1], wisc.pr$x[,2], col = as.factor(diagnosis), xlab = "PC1", ylab = "PC2")
```

Q8. Cluster 1 (Benign; Black) is at lot more clumped up than Cluster 2 (Malignant; Red). Black is also more prevalent on the positive side of PC1 and Red is prevalent on the negative side of PC1

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

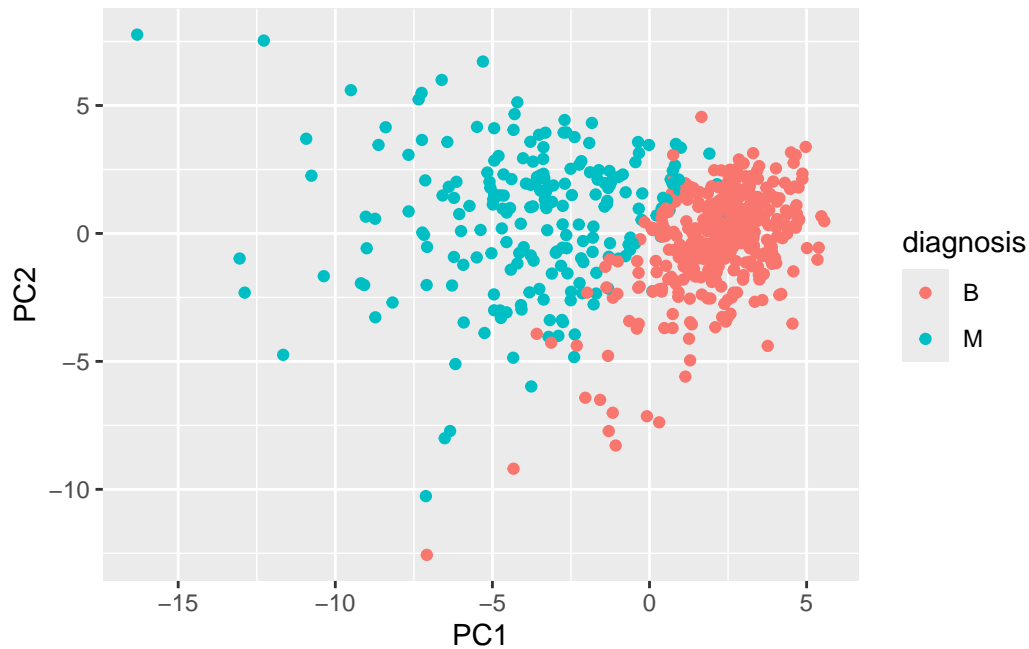


Using ggplot

```
# 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()
```



Explaining the Variance Calculate the variance of each principal component by squaring the `sdev` component of `wisc.pr` (i.e. `wisc.pr$sdev^2`). Save the result as an object called `pr.var`.

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

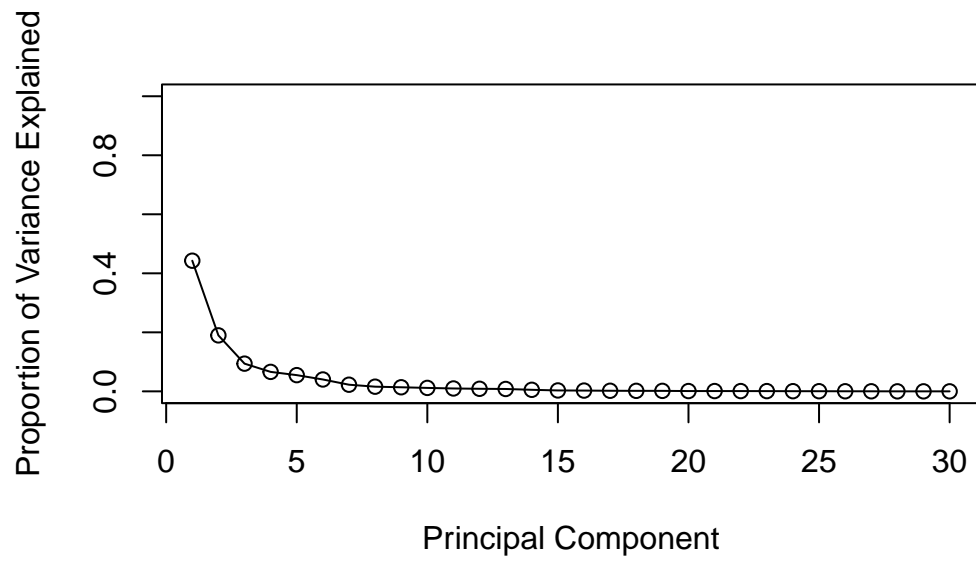
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
sum(pr.var)
```

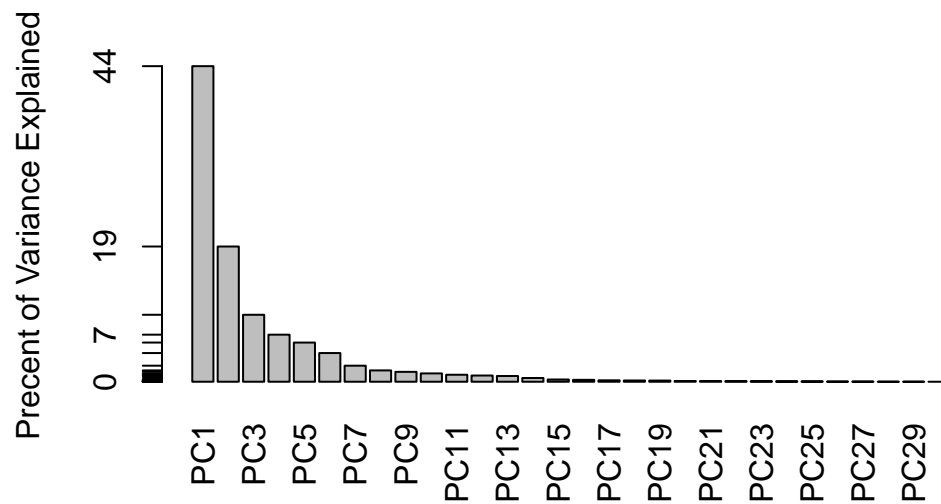
```
[1] 30
```

```
# 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")
```



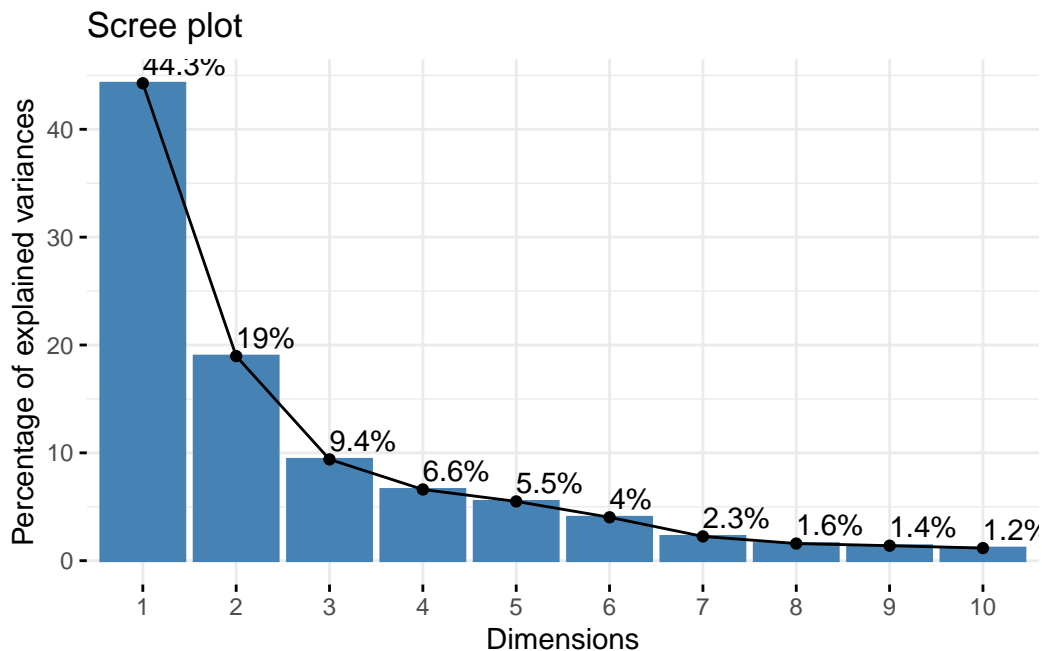
```
barplot(pve, ylab = "Precent of Variance Explained",
        names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```



```
## 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`?

```
# Get the loading for concave.points_mean from the first PC
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?

5 PCs

```
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

Hierarchical Clustering

Scale the data-set

```
data.scaled <- scale(wisc.data)
```

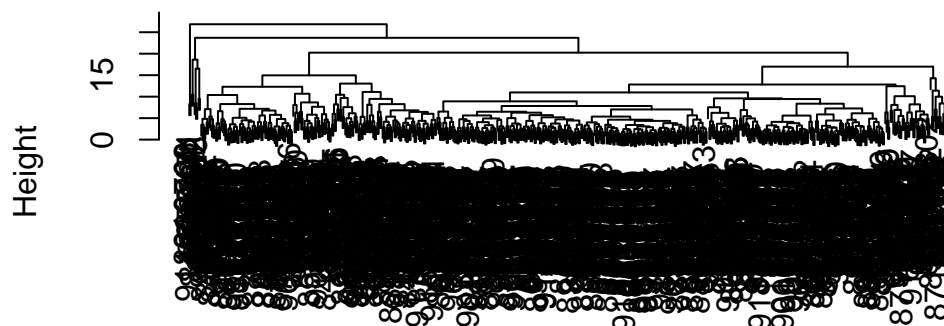
Calculate the distance between all pairs of observation in the new scaled data-set

```
# method = "euclidean" is default  
data.dist <- dist(data.scaled)
```

Create a hierarchical clustering model using complete linkage. Manually specify the method argument to `hclust()` and assign the results to `wisc.hclust`.

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

Cluster Dendrogram

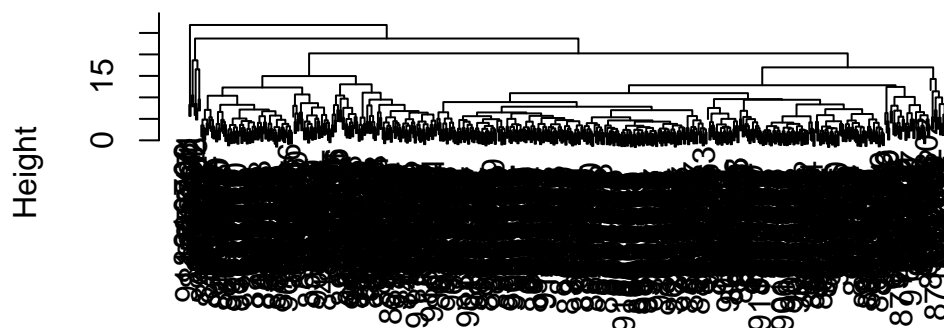


```
data.dist  
hclust (*, "complete")
```

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

```
x <- plot(wisc.hclust)
```

Cluster Dendrogram



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

Selecting Number of Clusters

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

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

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

```
wisc.hclust.clusters.test <- cutree(wisc.hclust, k = 8)
table(wisc.hclust.clusters.test, diagnosis)
```

	diagnosis	
wisc.hclust.clusters.test	B	M
1	12	86
2	0	79
3	0	3
4	331	39
5	2	0
6	12	1
7	0	2
8	0	2

Although a cluster of 2 appears to be cleaner in cutting the cluster v. diagnoses match, it is less clear as most of the data is on row 1. From group 8, the row 1 grouped M splits, so it seems that groups 4 to 7 seem to be the best split.

Using different Methods

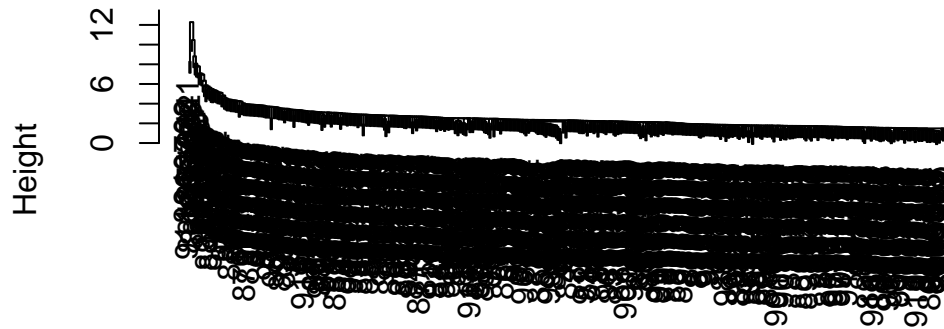
Q13. Which method gives your favorite results for the same data.dist dataset?
Explain your reasoning.

ward.D2 gives my favorite results for the same data.dist data-set because it gives 2 clear clusters, or a clear cut that can split the data-set into 2 clear clusters.

Single


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

Cluster Dendrogram

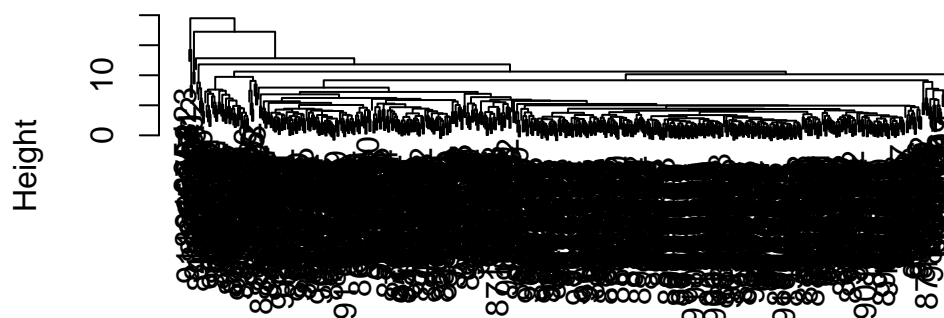


data.dist
hclust (*, "single")

Average

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

Cluster Dendrogram

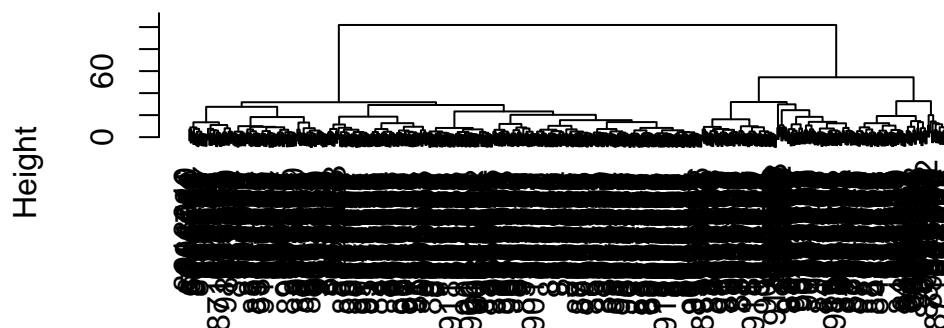


```
data.dist  
hclust (*, "average")
```

ward.D2

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

Cluster Dendrogram



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

Optional: K-means Clustering

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

```
diagnosis
  B    M
1 343  37
2  14 175
```

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

On the surface, the table shown by k-means seems to be a better separation of the 2 diagnoses than the table from the hclust results.

Compare the 2 tables

```
table(wisc.km$cluster, wisc.hclust.clusters)
```

```
wisc.hclust.clusters
  1    2    3    4
1 17    0 363    0
2 160    7  20    2
```