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R Notebook

Code **▼**

Hide

```
library(ggplot2)
```

Hide

```
setwd("C:/Users/Veeru/Desktop/ML/week 2")
getwd()
```

```
[1] "C:/Users/Veeru/Desktop/ML/week 2"
```

Hide

```
df1 <- read.csv("KMeansData_Group1.csv", header=FALSE, sep = ",")
df1 <- na.omit(df1)
str(df1)</pre>
```

```
'data.frame': 533 obs. of 2 variables:

$ V1: num 0.443 0.351 0.498 0.45 0.594 ...

$ V2: num 0.707 0.443 0.8 0.827 0.3 ...
```

The thumb rule for considering number of clusters: sqrt(2/# observations)

https://www.guru99.com/r-k-means-clustering.html#2 (https://www.guru99.com/r-k-means-clustering.html#2)

Hide

```
k <- round(sqrt(2/nrow(df1)))
k # this does not work.</pre>
```

```
[1] 0
```

Initialize a vector of length 10 for the scree plot, "nstart" is the number of times R will restart with different centroids(thumb rule nstart>10). "i" is the number of centers

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```
scree <- rep(0,10) #initializing empty vector
for (i in 1:10) {
   df1_kmeans <- kmeans(df1,i,nstart=20)
   scree[i] <- df1_kmeans$tot.withinss/df1_kmeans$totss # the ratio is as per da tacamp
}</pre>
```

Hide

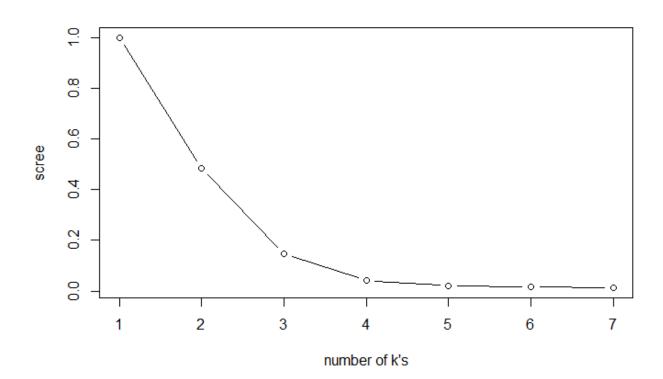
scree # 10 possible values for centroids of clusters

```
[1] 1.00000000 0.48297636 0.14583938 0.04195236 0.02054716 0.01714282 0.015554 99 [8] 0.01215065 0.01156906 0.01043754
```

scree plot, the points below 0.2 or elbow point is best for clustering.

Hide

```
plot(scree, type="b", xlab="number of k's")
```



choosing arbitary number of centroid/clusters: 3 (from scree plot)

Hide

k=3

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Empty vector called cluster_group is created. The motive is to store the assignment values in it.Each observation's distance from the 3 centroids will be calculated, the one which is the minimum is selected and that centroid is assigned to the observation.

3 of the cluster centers are choosed randomly and will be used as centroids. Euclidean distance formula will be used to compute the distance of each observation from three of these centroids

```
Hide

xcen <- sample(df$V1,k)
xcen

[1] 2.127337 6.279980 9.615745

Hide

ycen <- sample(df$V2,k)
ycen

[1] 0.8721779 9.0285042 7.6167140
```

In the above chunk, xcen and ycen are the vectors, which has randomly chosen values from the variables in dataframe df. Three values are chosen which represents the number of centroids from which the distance from rest of the observations will be calculated using euclidean distance formula and the same observations will be assigned to the centroid which is nearest(smaller distance) to them.

create random cluster centers

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```
# this is just for reference or future use.
#xcen <- runif(k, min = min(df$V1), max = max(df$V1))
#ycen <- runif(k, min = min(df$V2), max = max(df$V2))</pre>
```

cluster centroids choosed randomly from df variables are stored in seperate data-frame

```
#xcen <- runif(k, min = min(df$V1), max = max(df$V1))
#ycen <- runif(k, min = min(df$V2), max = max(df$V2))</pre>
```

assign cluster with minimum distance to each observation

```
for(i in 1:nrow(df)) {
   dist <- sqrt((df$V1[i]-centroid_df$xcen)^2 + (df$V2[i]-centroid_df$ycen)^2) #e
   uclidean
   df$cluster_group[i] <- which.min(dist)
#filling the cluster_group variable with the assignments, i.e observations assi
   ned to the one of the three cluster.
}</pre>
```

(df $V1[i]-centroid_df$ xcen)^2 this produces vector of 3 elements

[1] 71.701515767 9.889352276 0.004103784

The first observation of ${\rm df}V1 and df$ V2 subtracting the vector of the sample selected i.e 3 centroids. The distance which is the minimum is selected and is assigned with the respective cluster number.

head(df)# each obervation is now assigned with their cluster numbers

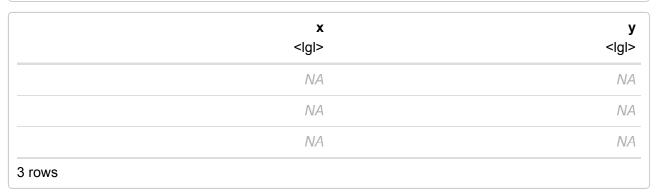
	V1	V2	cluster_group
	<dbl></dbl>	<dbl></dbl>	<int></int>
1	0.4429445	0.7071066	1
2	0.3514473	0.4426592	1
3	0.4975926	0.7999334	1
4	0.4501654	0.8270090	1
5	0.5940498	0.3003777	1
6	0.6268217	0.7995863	1

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making another data frame ready for another set of centroids from the same dataframe

```
Hide

x <- rep(NA,k)
y <- rep(NA,k)
centroid_upt <- data.frame(x,y)
centroid_upt</pre>
```



updating the centroids values

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```
for(i in 1:k) {
  centroid_upt[i,1] <- mean(subset(df$V1, df$cluster_group == i)) #xcen obs upda
te
  centroid_upt[i,2] <- mean(subset(df$V2, df$cluster_group == i)) #ycen obs upda
te
}</pre>
```

when i = 1, for 1st loop, the subset of observations which are assigned to cluster 1 are chosen from both the variables/columns i.e V1 and V2. mean for each variable's observations is calculated and is now the new centroid. Three such centroids are computed since we chose k=3 and stored in the new dataframe centroid_upt. This process will be continued untill there no change in the mean or in the centroids co-ordinates.

	Hide
centroid_upt	
x <dbl></dbl>	y <dbl></dbl>
1.805469	1.207068
4.650801	7.839537
8.594576	2.297604
3 rows	

Combining all together

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```
# Kmeans function
create clusters <- function(df,k) {</pre>
  xcen <- sample(df$V1,k)</pre>
  ycen <- sample(df$V2,k)</pre>
  centroid df <- data.frame(xcen = xcen, ycen = ycen)</pre>
  stop criteria <- FALSE
    while(stop criteria == FALSE) {
#filling the cluster group variable with the assignments, i.e observations assi
ned to the one of the three cluster.
      for(i in 1:nrow(df)) {
        dist <- sqrt((df$V1[i]-centroid df$xcen)^2 + (df$V2[i]-centroid df$yce
n)^2)
        df$cluster group[i] <- which.min(dist)# which will give index number</pre>
# storing the sample values computed for centroids, since we will be using to s
top the iteration at a point.
        xcen old <- centroid df$xcen
        ycen old <- centroid df$ycen
        # updating the centroids values
        for(i in 1:k) {
          centroid df[i,1] <- mean(subset(df$V1, df$cluster group == i))</pre>
          centroid df[i,2] <- mean(subset(df$V2, df$cluster group == i))</pre>
        # stop the loop if there is no change in cluster coordinates
        if(identical(xcen old, centroid df$xcen) & identical(ycen old, centroid
df$ycen))
          stop criteria <- TRUE
    } # while loop ends here
    the_list <- list(df, centroid_df)</pre>
    return(the list)
}# function ends here
```

Hide

```
df <- read.csv("KMeansData_Group1.csv",header=FALSE, sep = ",")
df <- na.omit(df)
#df <- scale(df)
df$cluster_group <- NA
str(df)</pre>
```

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k=3

Hide

df

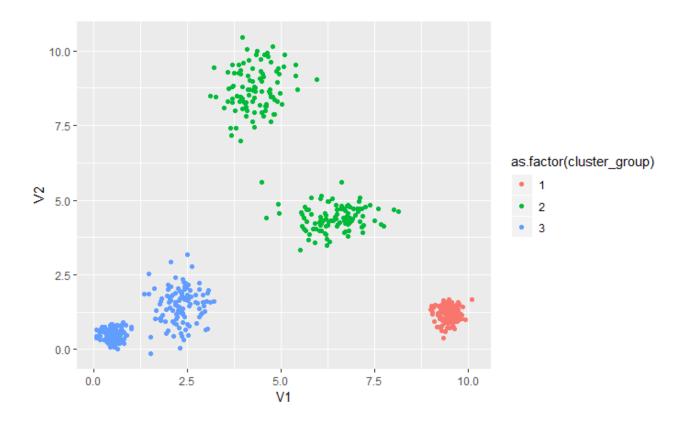
	V1 <dbl></dbl>	V2 <dbl></dbl>	cluster_group <lgl></lgl>
1	0.44294453	0.707106557	NA
2	0.35144735	0.442659199	NA
3	0.49759257	0.799933391	NA
4	0.45016541	0.827008997	NA
5	0.59404983	0.300377731	NA
6	0.62682167	0.799586314	NA
7	0.57155692	0.229410031	NA
8	0.57468328	0.570192935	NA
9	0.41352855	0.198721332	NA
10	0.21185378	0.698238836	NA
1-10 of 533 rows		Previous 1 2 3	4 5 6 54 Next

Hide

```
plot_cluster <- create_clusters(df,3)
data <- data.frame(plot_cluster[1])
centers <- data.frame(plot_cluster[2])</pre>
```

```
ggplot(data, aes(V1, V2, color = as.factor(cluster_group))) + geom_point()
```

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The above plot seems to be of 5 clusters not 3

```
Hide

pc <- create_clusters(df,5)
data <- data.frame(pc[1])
centers <- data.frame(pc[2])

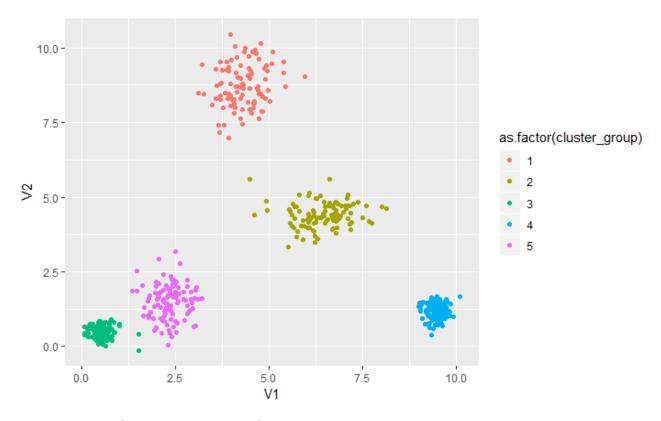
Hide

distinct_cluster <- ggplot(data, aes(V1, V2, color = as.factor(cluster_group)))
+ geom_point()

Hide

distinct_cluster</pre>
```

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Within sum of square is sum of summed up square distances between each point and the corresponding center of the cluster

"df" is the data-frame which has the observations assigned to their respective centroids

"centroid df" is the data-frame which have centers of each cluster

```
wss <- function(df,centroid_df) {
  wss_tot = 0
  for (i in 1:nrow(centroid_df)) {
    sub_set <- subset(df, df$cluster_group == i)
    for (s in 1:nrow(sub_set)) {
        sum_obs <- (sub_set$V1[s] - centroid_df$xcen[i])^2 + (sub_set$V2[s] - centroid_df$ycen[i])
        wss_tot = wss_tot + sum_obs
    }
  }
  wss_tot</pre>
```

for loop for clusters values varying from 1 to 10, so that wss is computed and by scree plot optimal clusters can be selected.

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```
scree <- rep(0,10)
for (k in 1:10) {
  clusters <- create_clusters(df,k)
  d <- data.frame(clusters[1])
  c <- data.frame(clusters[2])
  scree[k] <- wss(d, c)
}</pre>
```

```
Error in scree[k] <- wss(d, c) : replacement has length zero</pre>
```

wss for 1 to 7 clusters are calculated, but from 8 to 10 are not.

Hide

```
[1] 5517.09006 1754.49328 503.67285 269.57164 269.56429 98.15944 69.461 41 [8] 0.00000 0.00000
```

manually doing the for loop to check the error occurred

Hide

```
wss_df <- rep(0,10) \# i will be adding wss values from 1 to 10 clusters manuall y
```

Only 1 cluster

```
clusters <- create_clusters(df,1)
d <- data.frame(clusters[1])
c <- data.frame(clusters[2])
d</pre>
```

	V1	V2	cluster_group
	<dbl></dbl>	<dbl></dbl>	<int></int>
1	0.44294453	0.707106557	1
2	0.35144735	0.442659199	1
3	0.49759257	0.799933391	1
4	0.45016541	0.827008997	1
5	0.59404983	0.300377731	1

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	V1 <dbl></dbl>	V2 <dbl></dbl>	cluster_group <int></int>
6	0.62682167	0.799586314	1
7	0.57155692	0.229410031	1
8	0.57468328	0.570192935	1
9	0.41352855	0.198721332	1
10	0.21185378	0.698238836	1
1-10 of 533 rows		Previous 1 2 3	4 5 6 54 Next

Hide

С

 xcen
 ycen

 <dbl>
 <dbl>

 4.768795
 3.166096

 1 row

wss for one cluster

Hide

```
w <- wss(d,c)
w
```

[1] 5517.09

Hide

```
wss_df[1] <- w
wss_df</pre>
```

2 clusters

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```
clusters <- create_clusters(df,2)
d <- data.frame(clusters[1])
c <- data.frame(clusters[2])
d</pre>
```

	V1 <dbl></dbl>	V2 <dbl></dbl>	cluster_group <int></int>
1	0.44294453	0.707106557	1
2	0.35144735	0.442659199	1
3	0.49759257	0.799933391	1
4	0.45016541	0.827008997	1
5	0.59404983	0.300377731	1
6	0.62682167	0.799586314	1
7	0.57155692	0.229410031	1
8	0.57468328	0.570192935	1
9	0.41352855	0.198721332	1
10	0.21185378	0.698238836	1
1-10 of 533 rows		Previous 1 2 3	4 5 6 54 Next

Hide

С

xcen <dbl></dbl>	ycen <dbl></dbl>
2.413287	3.523559
8.120040	2.657524
2 rows	

wss for 2 clusters

```
wss_df[2] <- wss(d,c)
wss_df
```

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```
[1] 5517.090 1309.649 0.000 0.000 0.000 0.000 0.000 0.000 0.000 [10] 0.000
```

3 clusters

Hide

```
clusters <- create_clusters(df,3)
d <- data.frame(clusters[1])
c <- data.frame(clusters[2])
d</pre>
```

	V1 <dbl></dbl>	V2 <dbl></dbl>	cluster_group <int></int>
1	0.44294453	0.707106557	1
2	0.35144735	0.442659199	1
3	0.49759257	0.799933391	1
4	0.45016541	0.827008997	1
5	0.59404983	0.300377731	1
6	0.62682167	0.799586314	1
7	0.57155692	0.229410031	1
8	0.57468328	0.570192935	1
9	0.41352855	0.198721332	1
10	0.21185378	0.698238836	1
1-10 of 533 rows		Previous 1 2 3	4 5 6 54 Next

Hide

С

xcen <dbl></dbl>	ycen <dbl></dbl>
1.460688	1.008216
9.481592	1.190304
5.405729	6.513005
3 rows	

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wss for 3 clusters

```
Wss_df[3] <- wss(d,c)
wss_df
```

```
[1] 5517.0901 1309.6491 503.6728 0.0000 0.0000 0.0000 0.0000 0.0000 [9] 0.0000 0.0000
```

4 clusters

Hide

```
clusters <- create_clusters(df,4)
d <- data.frame(clusters[1])
c <- data.frame(clusters[2])
d</pre>
```

	V1 <dbl></dbl>	V2 <dbl></dbl>	cluster_group <int></int>
1	0.44294453	0.707106557	2
2	0.35144735	0.442659199	2
3	0.49759257	0.799933391	2
4	0.45016541	0.827008997	2
5	0.59404983	0.300377731	2
6	0.62682167	0.799586314	2
7	0.57155692	0.229410031	2
8	0.57468328	0.570192935	2
9	0.41352855	0.198721332	2
10	0.21185378	0.698238836	2
1-10 of 533 rows		Previous 1 2 3	4 5 6 54 Next

C Hide

xcen	ycen
<dbl></dbl>	<dbl></dbl>

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xcen <dbl></dbl>	ycen <dbl></dbl>
9.481592	1.190304
1.460688	1.008216
4.310716	8.727085
6.448599	4.404357
4 rows	

wss for 4 clusters

Hide

```
wss_df[4] <- wss(d,c)
wss_df

[11 5517 0901 1309 6491 503 6728 269 5716 0 0000 0 0000 0 0000
```

```
[1] 5517.0901 1309.6491 503.6728 269.5716 0.0000 0.0000 0.0000 0.0000 [9] 0.0000 0.0000
```

5 clusters

```
clusters <- create_clusters(df,5)
d <- data.frame(clusters[1])
c <- data.frame(clusters[2])
d</pre>
```

	V1	V2	cluster_group
	<dbl></dbl>	<dbl></dbl>	<int></int>
1	0.44294453	0.707106557	5
2	0.35144735	0.442659199	5
3	0.49759257	0.799933391	5
4	0.45016541	0.827008997	5
5	0.59404983	0.300377731	5
6	0.62682167	0.799586314	5
7	0.57155692	0.229410031	5
8	0.57468328	0.570192935	5

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	V1 <dbl></dbl>	V2 <dbl></dbl>	cluster_group <int></int>
9	0.41352855	0.198721332	5
10	0.21185378	0.698238836	5
1-10 of 533 rows		Previous 1 2 3	4 5 6 54 Next

Hide

С

xcen	ycen
<dbl></dbl>	<qpl></qpl>
2.3436601	1.4911035
6.4485995	4.4043567
9.4815923	1.1903036
4.3107156	8.7270851
0.5344319	0.5016579
5 rows	

wss for 5 clusters

Hide

```
wss_df[5] <- wss(d,c)
wss_df</pre>
```

```
[1] 5517.09006 1309.64915 503.67285 269.57164 98.63926 0.00000 0.000
00 0.00000
[9] 0.00000 0.00000
```

6 clusters

```
clusters <- create_clusters(df,6)
d <- data.frame(clusters[1])
c <- data.frame(clusters[2])
d</pre>
```

cluster_group	V2	V1
<int></int>	<dbl></dbl>	<dbl></dbl>
	<dbl></dbl>	<dbl></dbl>

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	V1 <dbl></dbl>	V2 <dbl></dbl>	cluster_group <int></int>
1	0.44294453	0.707106557	3
2	0.35144735	0.442659199	3
3	0.49759257	0.799933391	3
4	0.45016541	0.827008997	3
5	0.59404983	0.300377731	3
6	0.62682167	0.799586314	3
7	0.57155692	0.229410031	3
8	0.57468328	0.570192935	3
9	0.41352855	0.198721332	3
10	0.21185378	0.698238836	3
1-10 of 533 rows		Previous 1 2 3	4 5 6 54 Next

Hide

С

xcen <dbl></dbl>	ycen <dbl></dbl>
4.3107156	8.7270851
9.4815923	1.1903036
0.5344319	0.5016579
5.8626116	4.2814506
6.9054713	4.5001817
2.3436601	1.4911035
6 rows	

wss for 6 clusters

Hide

wss_df[6] <- wss(d,c)
wss_df</pre>

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```
[1] 5517.09006 1309.64915 503.67285 269.57164 98.63926 98.63926 0.000
00 0.00000
[9] 0.00000 0.00000
```

7 clusters gives out NAN as centoids, this is the reason the for loop above was producing error

```
clusters <- create_clusters(df,7)
d <- data.frame(clusters[1])
c <- data.frame(clusters[2])
d</pre>
```

	V1 <dbl></dbl>	V2 <dbl></dbl>	cluster_group <int></int>
1	0.44294453	0.707106557	6
2	0.35144735	0.442659199	6
3	0.49759257	0.799933391	6
4	0.45016541	0.827008997	6
5	0.59404983	0.300377731	6
6	0.62682167	0.799586314	6
7	0.57155692	0.229410031	6
8	0.57468328	0.570192935	6
9	0.41352855	0.198721332	6
10	0.21185378	0.698238836	6
1-10 of 533 rows		Previous 1 2 3	4 5 6 54 Next

| NaN | NaN | 4.310716 | 8.7270851 | 9.474428 | 1.3849314

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xcen <dbl></dbl>	ycen <dbl></dbl>
6.448599	4.4043567
9.490216	0.9560295
1.460688	1.0082162
NaN	NaN
7 rows	

The chunk of code is repeatedly re-runned for NAN to be removed.

```
clusters <- create_clusters(df,7)
d <- data.frame(clusters[1])
c <- data.frame(clusters[2])
d</pre>
```

	V1 <dbl></dbl>	V2 <dbl></dbl>	cluster_group <int></int>
1	0.44294453	0.707106557	5
2	0.35144735	0.442659199	5
3	0.49759257	0.799933391	5
4	0.45016541	0.827008997	5
5	0.59404983	0.300377731	5
6	0.62682167	0.799586314	5
7	0.57155692	0.229410031	5
8	0.57468328	0.570192935	5
9	0.41352855	0.198721332	5
10	0.21185378	0.698238836	5
1-10 of 533 rows		Previous 1 2 3	4 5 6 54 Next

xcen ycen <dbl>

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xcen <dbl></dbl>	ycen <dbl></dbl>
2.3436601	1.4911035
4.2123514	8.2519355
6.9369279	4.4873758
9.4815923	1.1903036
0.5344319	0.5016579
5.8905098	4.3094776
4.4582620	9.4398095
7 rows	

wss for 7 clusters

8 clusters after number of time re-running the chunk

clusters <- create_clusters(df,8)
d <- data.frame(clusters[1])
c <- data.frame(clusters[2])
d</pre>

	V1	V2	cluster_group
	<dbl></dbl>	<dbl></dbl>	<int></int>
1	0.44294453	0.707106557	8
2	0.35144735	0.442659199	8
3	0.49759257	0.799933391	8
4	0.45016541	0.827008997	8
5	0.59404983	0.300377731	8
6	0.62682167	0.799586314	8
7	0.57155692	0.229410031	8
8	0.57468328	0.570192935	8
9	0.41352855	0.198721332	8
10	0.21185378	0.698238836	8
1-10 of 533 rows		Previous 1 2 3	4 5 6 54 Next

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Hide C

xcen	ycen
<dbl></dbl>	<dbl></dbl>
9.4815923	1.1903036
2.2144108	0.8894687
5.8905098	4.3094776
2.6975626	1.6045346
6.9369279	4.4873758
2.1205750	2.0203725
4.3107156	8.7270851
0.5245982	0.5025811
8 rows	

wss for 8 clusters

```
wss_df[8] <- wss(d,c)
wss_df</pre>
```

```
[1] 5517.09006 1309.64915 503.67285 269.57164 98.63926 98.63926 68.572
17 63.04142
[9] 0.00000 0.00000
```

9 clusters(re-run chunk)

```
clusters <- create_clusters(df,9)
d <- data.frame(clusters[1])
c <- data.frame(clusters[2])
d</pre>
```

	V1 <dbl></dbl>	V2 <dbl></dbl>	cluster_group <int></int>
1	0.44294453	0.707106557	6
2	0.35144735	0.442659199	6

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	V1 <dbl></dbl>	V2 <dbl></dbl>	cluster_group <int></int>
3	0.49759257	0.799933391	6
4	0.45016541	0.827008997	6
5	0.59404983	0.300377731	6
6	0.62682167	0.799586314	6
7	0.57155692	0.229410031	6
8	0.57468328	0.570192935	6
9	0.41352855	0.198721332	6
10	0.21185378	0.698238836	6
1-10 of 533 rows		Previous 1 2 3	4 5 6 54 Next

Hide

С

xcen <dbl></dbl>	ycen <dbl></dbl>
5.862612	4.2814506
4.212351	8.2519355
2.100616	0.7881664
4.458262	9.4398095
6.905471	4.5001817
0.514492	0.5089155
2.695289	1.4366917
2.168817	1.9767393
9.481592	1.1903036
9 rows	

wss for 9 clusters

Hide

wss_df[9] <- wss(d,c)
wss_df</pre>

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```
[1] 5517.09006 1309.64915 503.67285 269.57164 98.63926 98.63926 68.572
17 63.04142
[9] 60.73801 0.00000
```

10 clusters

Hide

```
clusters <- create_clusters(df,10)
d <- data.frame(clusters[1])
c <- data.frame(clusters[2])
d</pre>
```

	V1 <dbl></dbl>	V2 <dbl></dbl>	cluster_group <int></int>
1	0.44294453	0.707106557	7
2	0.35144735	0.442659199	7
3	0.49759257	0.799933391	7
4	0.45016541	0.827008997	7
5	0.59404983	0.300377731	7
6	0.62682167	0.799586314	7
7	0.57155692	0.229410031	7
8	0.57468328	0.570192935	7
9	0.41352855	0.198721332	7
10	0.21185378	0.698238836	7
1-10 of 533 rows		Previous 1 2 3	4 5 6 54 Next

Hide

С

xcen <dbl></dbl>	ycen <dbl></dbl>
5.7886076	4.2224537
9.4815923	1.1903036
4.2123514	8.2519355
7.3329007	4.5311109

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	xcen <dbl></dbl>	ycen <dbl></dbl>
	6.5901073	4.4967582
	2.1269214	1.9956098
	0.5245982	0.5025811
	2.7837245	1.6376072
	2.2246254	0.9364170
	4.4582620	9.4398095
1-10 of 10 rows		

wss for 10 clusters.

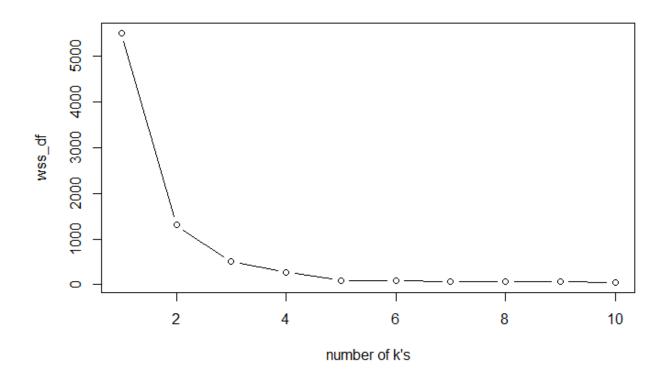
```
wss_df[10] <- wss(d,c)
wss_df</pre>
```

```
[1] 5517.09006 1309.64915 503.67285 269.57164 98.63926 98.63926 68.572
17 63.04142
[9] 60.73801 55.19255
```

elbow/scree plot is plotted for wss vs number of clusters and as per the elbow point which is 3 in this case, 3 should be choosed for computing kmeans for 3 number of clusters. In the scatter plot above we checked for both 3 and 5 clusters individually

```
number_of_clusters <- 1:10
plot(number_of_clusters,wss_df, type="b", xlab="number of k's")</pre>
```

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links referred:

http://dni-institute.in/blogs/k-means-clustering-algorithm-explained/ (http://dni-institute.in/blogs/k-means-clustering-algorithm-explained/) https://uc-r.github.io/kmeans_clustering#distance (https://uc-r.github.io/kmeans_clustering#distance)

http://enhancedatascience.com/2017/10/24/machine-learning-explained-kmeans/

(http://enhancedatascience.com/2017/10/24/machine-learning-explained-kmeans/)

https://github.com/mehdimo/K-Means/blob/master/kmeans mehdi.R

(https://github.com/mehdimo/K-Means/blob/master/kmeans_mehdi.R)

https://stackoverflow.com/questions/41912875/writing-own-kmeans-algorithm-in-r

(https://stackoverflow.com/questions/41912875/writing-own-kmeans-algorithm-in-r)

https://www.youtube.com/watch?v=j9ZPMIVHJVs (https://www.youtube.com/watch?v=j9ZPMIVHJVs)

within sum of square