K-Means Clustering

Clustering is a unsupervised ML technique in which there is no target varible and unlabled data is generally grouped into different groups/ clusters.

We will study following clustering Algorithms

1) K-means clustering
2) DBscan clustering
3) Hierarchical clustering

Lets start with K-means

→ Here K is no. of pre-defined clusters that need to be created in order to initiate algorithm.

→ It is centroid-based Algorithm, where each cluster is associated with a centroid.

→ The main aim is to minimise the sum of distances b/w data point and their corresponding clusters.

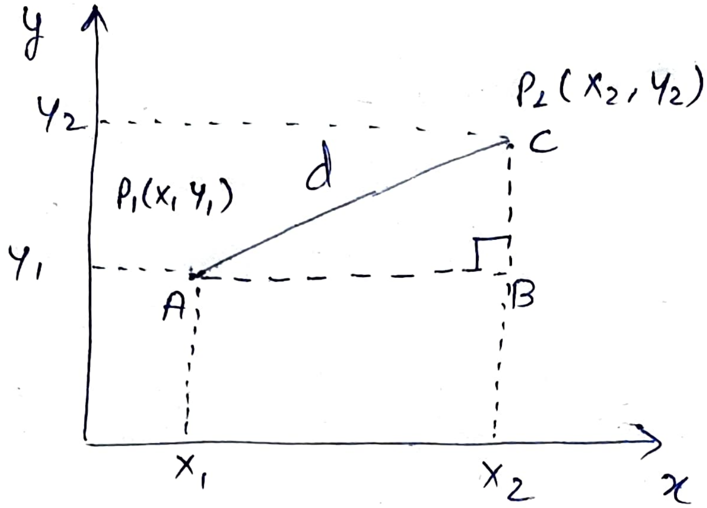
⇒ following distance methods are used.

1) Euclidean distance
2) Manhattan distance

] we will only see these two.

3) cosine distance
4) squared Euclidean distance
5) Tanimoto distance

① Euclidean distance



Pythagoras theorem in ΔABC

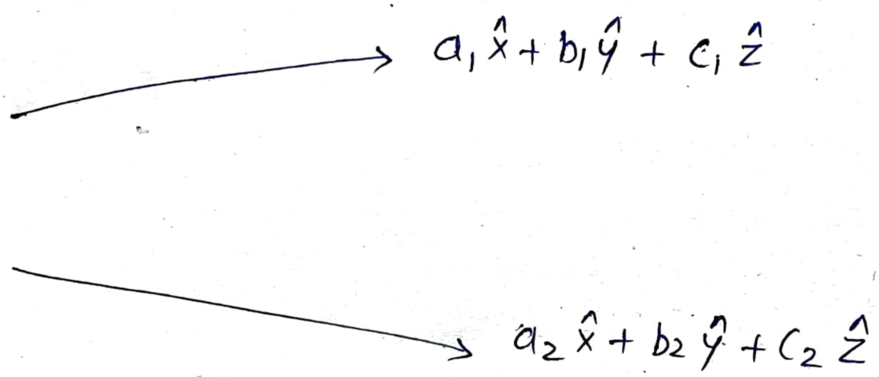
$$d^2 = AB^2 + BC^2$$

$$d = \sqrt{AB^2 + BC^2}$$

$$\boxed{d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}}$$

② Manhattan distance

It is calculated for two vectors.



$$\boxed{d = |(a_2 - a_1)| + |(b_2 - b_1)| + |(c_2 - c_1)|}$$

→ Steps to perform k-means Clustering

1) Decide No. of clusters. (k value)

2) Initialize centroids equal to No. of Clusters Randomly
say if you have 3 clusters so there will be 3 centroids and they will be selected randomly.

③ Assign cluster to each data point in dataset using distance similarity method (say Euclidean distance) ie calculate distance b/w centroids and all datapoint. Assign data point to that cluster whose dist is minimum.

⇒ Now we have distinct clusters.

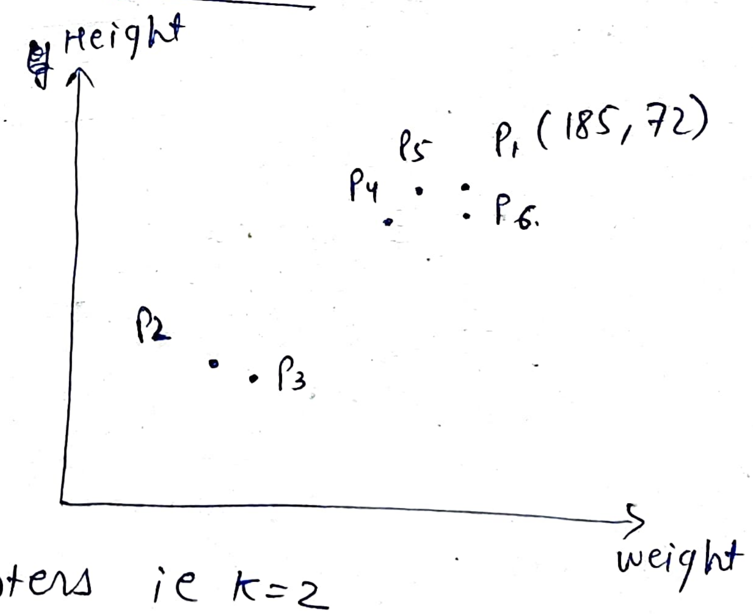
→ calculate New centroids for each cluster by taking mean of all the data point in that cluster.

④ ⇒ calculate distances b/w all the points wrt new ~~clusters~~ centroids and again assign the data points to clusters using minimum distance b/w centroid and datapoint.

⇒ Repeat 3rd and 4th step until there is no further change in centroid.

* lets see above with an example

	Height	weight
P_1	185	72
P_2	170	56
P_3	168	60
P_4	179	68
P_5	180	71
P_6	182	72



1) lets consider two clusters ie $k=2$

2) Randomly selecting 2 points

P_4 ⇒ (179, 68) and P_6 ⇒ (182, 72)

as two centroids

	Height	weight	dwrt P_4 (A)	dwrt P_6 (B)	cluster(A/B)
P_1	185	72	7.2	3	B
P_2	170	56	15	20	A
P_3	168	60	13.6	18.43	A
P_5	180	71	3.16	2.23	B

$P_4 = 179, 68$

$P_6 = 182, 72$

consider P_1 point

1) dist of P_1 from centroid A [P_4 (179, 68)]

$$d_{A_1} = \sqrt{(x_2-x_1)^2 + (y_2-y_1)^2}$$

$$= \sqrt{(72-68)^2 + (185-179)^2}$$

d_{A_1} = 7.2 units

2) dist of P_1 from centroid B, P_6 (182, 72).

$$d_{B_1} = \sqrt{(x_2-x_1)^2 + (y_2-y_1)^2}$$

$$= \sqrt{(72-72)^2 + (185-182)^2}$$

d_{B_1} = 3 units.

∴ P_1 belongs to B cluster as distance b/w P_1 and B centroid is less as compared to distance b/w P_1 and A centroid.

Now similarly lets calculate All distances

Cluster A

$P_4 \Rightarrow 179, 68$

$P_2 \Rightarrow 170, 56$

$P_3 \Rightarrow 168, 60$

Cluster B

$P_6 \Rightarrow 182, 72$

$P_1 \Rightarrow 185, 72$

$P_5 \Rightarrow 180, 71$

New centroids

Cluster A

$$\left(\frac{179+170+168}{3}, \frac{68+56+60}{3}\right)$$

$$\Rightarrow (172.33, 61.33)$$

Cluster B

$$\left(\frac{182+185+180}{3}, \frac{72+72+71}{3}\right)$$

$$\Rightarrow (182.33, 71.67)$$

	Height	weight	dist A	dist B	Cluster A/B
P_1	185	72	16.56	2.69	B
P_2	170	56	5.82	19.94	A
P_3	168	60	4.53	18.48	A
P_4	179	68	9.43	4.95	B
P_5	180	71	12.34	2.42	B
P_6	182	72	14.4	0.47	B

Cluster A

$$\left(\frac{170+168}{2}\right), \left(\frac{56+60}{2}\right)$$

$$\Rightarrow (169, 58)$$

Cluster B

$$\left(\frac{185+179+180+182}{4}, \frac{72+68+71+72}{4}\right)$$

$$(181.5, 70.75)$$

Height	weight	dist A (169,58)	dist B (181.5, 70.75)	cluster A/B.
185	72	21.26	3.72	B
170	56	2.24	18.7	A
168	60	2.24	17.26	A
179	68	14.14	3.72	B
180	71	17.03	1.52	B
182	72	19.1	1.35	B

New centroids

cluster A

$$\left(\frac{170+168}{2}, \frac{56+60}{2}\right)$$

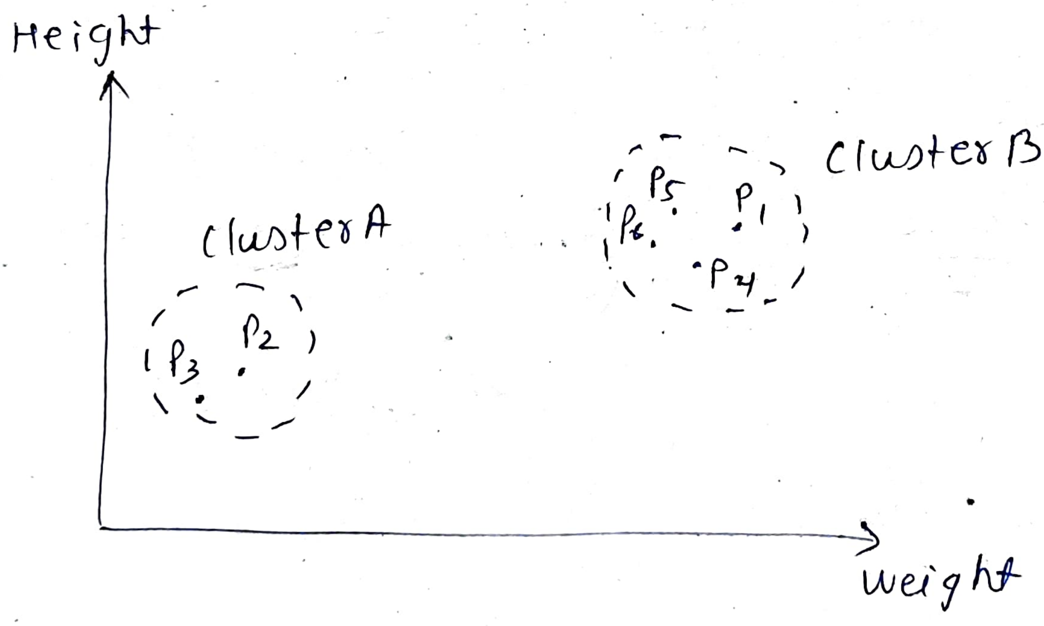
$(169, 58)$

cluster B

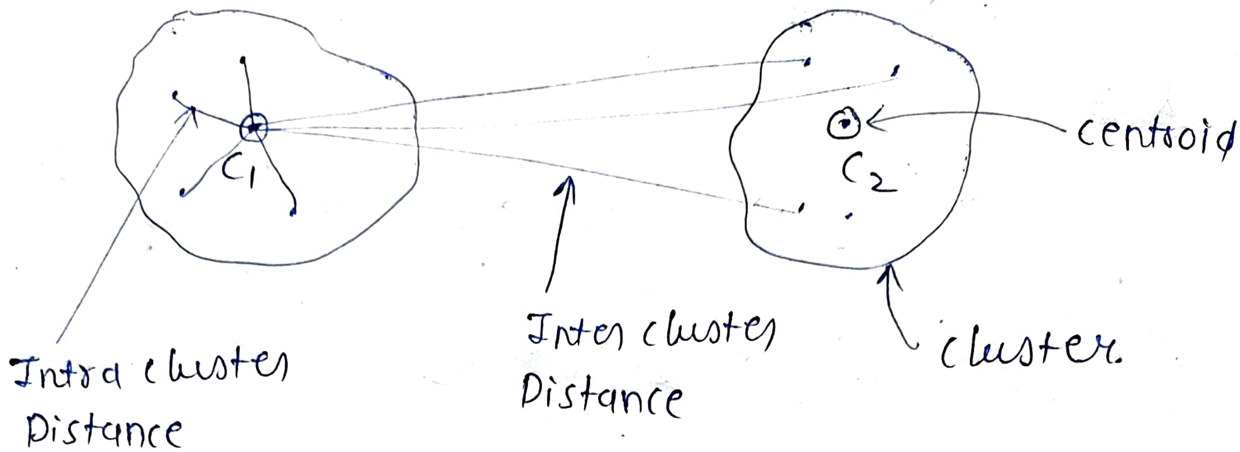
$$\left(\frac{185+179+180+182}{4}, \frac{72+68+71+72}{4}\right)$$

$(181.5, 70.75)$

$\because$ centroids in previous step and this step are same we have successfully clustered our data points



Terminology Related to clusters



Here $k = 2$, and 2 centroids

Que: How to decide No. of clusters in Step 1

⇒ For that we have Elbow method

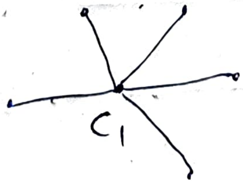
→ In elbow method we plot graph b/w WCSS and k value

→ Here we take $k = 1, 2, 3, 4, \ldots$ max 20, and for each k value we calculate WCSS. ie within ~~centroid~~ cluster sum of squares. and plot.

→ The k point at which there is no abrupt change in WCSS value is our optimum cluster value.

__For Example:__

$k = 1$



WCSS,

$K = 2$

$$WCSS_2 = (WCSS)_{C_1} + (WCSS)_{C_2}$$

C_1 C_2

$K = 3$

$$WCSS_3 = (WCSS)_{C_1} + (WCSS)_{C_2} + (WCSS)_{C_3}$$

C_1 C_2 C_3

Also $(WCSS)_1 > (WCSS)_2 > (WCSS)_3$.

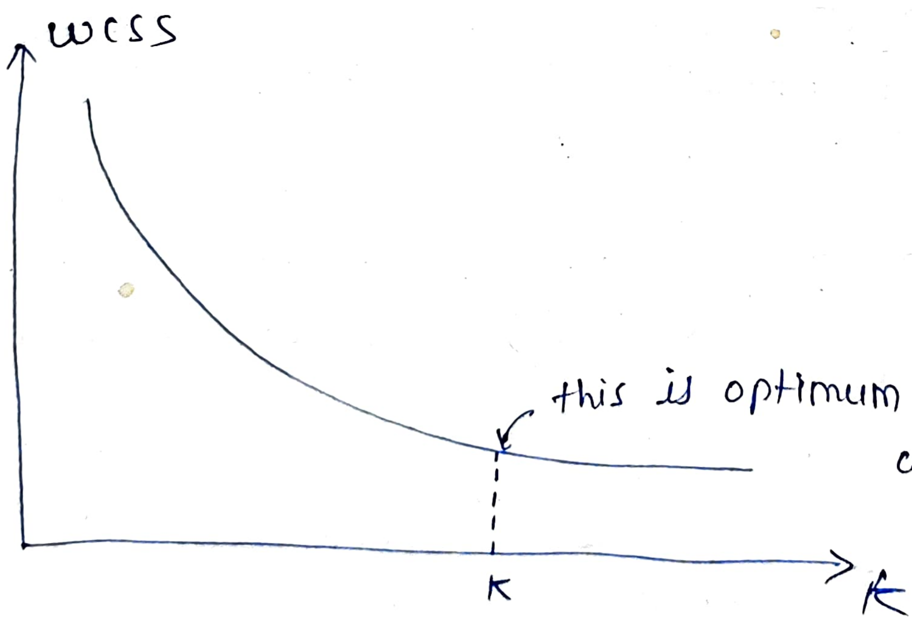
The above statement can be understood using below Argument:

consider 10 data points

→ for cluster $K = 1$ $(WCSS)_1$ will be maximum.

→ for K = No. of data points ie $K = 10$.
each point will act as centroid
ie WCSS will be zero.

So we can say that as K value increases WCSS value decreases.



this is optimum K value as further there is no abrupt change in WCSS value.

$$\boxed{WCSS = \sum_{i=1}^{n} d(c, x_i)^2}$$

where $n \equiv$ no. of points in c cluster.

$c \equiv$ centroid

$x_i \equiv$ i^{th} point in c cluster.

How to evaluate quality of clusters?

=> This is done using

1) dunn Index
2) silhoutte score.

1) Dunn index

$$\boxed{\text{Dunn index} = \frac{\min(\text{inter cluster distance})}{\max(\text{Intra cluster distance})}}$$

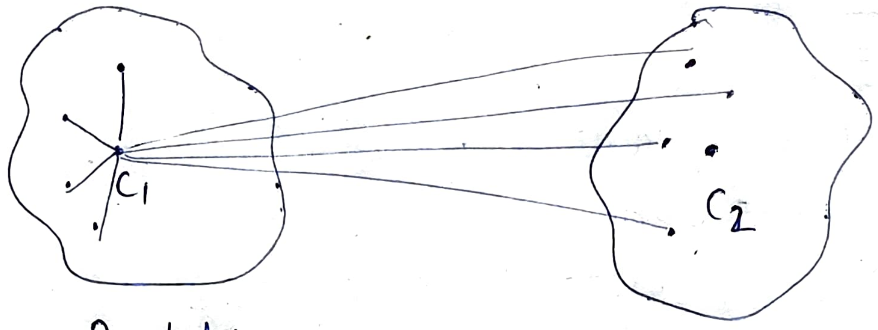
Dunn index ↑ quality of cluster ↑

2) silhoutte score

$$\boxed{\text{silhoute score} = \frac{b_i - a_i}{\max(b_i, a_i)}}$$

where $b_i \equiv$ (inter cluster distance) => mean

$a_i \equiv$ (intra cluster distance) => mean



n_1 data points

n_2 data points

$$\boxed{a_i = \frac{\sum_{i=1}^{n_1} d(C_1, x_{1i})}{n_1}}$$

⇒ mean of intra cluster distance

$$\boxed{b_i = \frac{\sum_{i=1}^{n_2} d(C_1, x_{2i})}{n_2}}$$

where

x_{1i} ⇒ i^{th} point in 1^{st} cluster.

x_{2i} ⇒ i^{th} point in 2^{nd} cluster.

mean of Inter cluster distance.

silhoutte score ranges b/w -1 to 1
with -1 being worst
and 1 being best.

K-Means Clustering

1.0 Importing required libraries

In [26]:
```
import pandas as pd
import numpy as np

import matplotlib.pyplot as plt
%matplotlib inline

import plotly.express as px

from sklearn.cluster import KMeans
from sklearn.metrics import silhouette_score
from sklearn.datasets import make_blobs

import warnings
warnings.filterwarnings('ignore')
```

2.0 Importing 2 feature dataset for clustering

In [3]:
```
data=pd.read_csv("data.csv")
data.head()
```

Out[3]:

	x	y	color
0	516.012706	393.014514	0
1	436.211762	408.656585	0
2	512.052601	372.022014	0
3	489.140464	401.807159	0
4	446.207986	338.516682	0

In [4]:
```
### dropping label color feature
dataset=data.drop('color', axis=1)
dataset.head()
```

Out[4]:

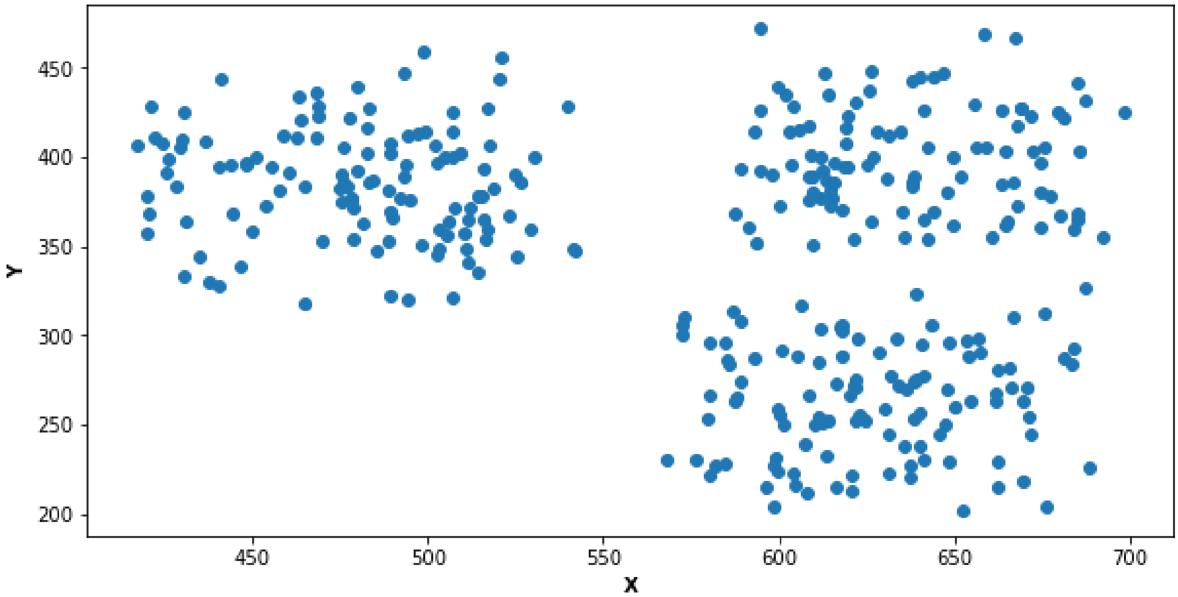
	x	y
0	516.012706	393.014514
1	436.211762	408.656585
2	512.052601	372.022014
3	489.140464	401.807159
4	446.207986	338.516682

In [7]:
```
dataset.shape
```

Out[7]:
```
(336, 2)
```

In [49]:
```
### Visualising dataset
plt.figure(figsize=(10,5))
plt.scatter(data= dataset, x='x', y='y')
plt.xlabel("X", fontsize=10, fontweight='bold')
plt.ylabel("Y", fontsize=10, fontweight='bold')
```

Out[49]: Text(0, 0.5, 'Y')

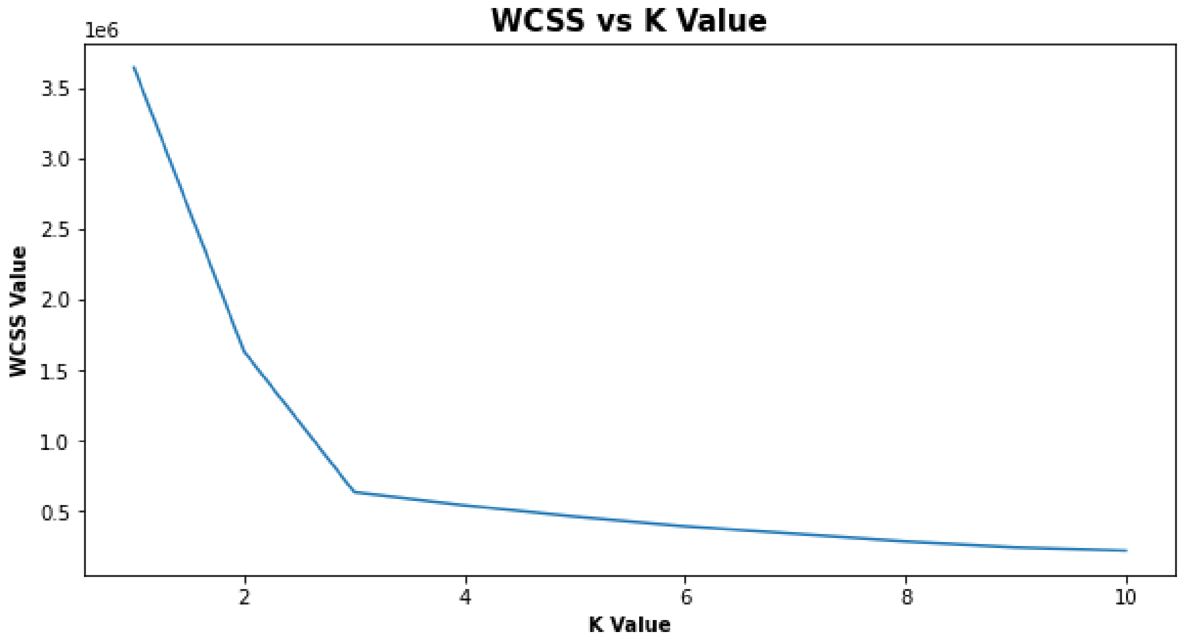


In [41]:
```
### Calculating WCSS for K=1 to K=11 clusters
wcss=[]


for i in range(2,11):
    km = KMeans(n_clusters=i)
    km.fit_predict(dataset)
    wcss.append(round(km.inertia_,2))

print(f"WCSS list: {wcss}")
```

```
WCSS list: [1634662.14, 637691.33, 544675.04, 467501.54, 401945.06, 338585.28, 287
823.43, 246019.25, 224975.35]
```

In [10]:
```
### Plotting WCSS with K
plt.figure(figsize=(10, 5))
plt.plot(range(1,11), wcss)
plt.xlabel("K Value", fontsize=10, fontweight='bold')
plt.ylabel("WCSS Value", fontsize=10, fontweight='bold')
plt.title("WCSS vs K Value", fontsize=15, fontweight='bold')
```

Out[10]: Text(0.5, 1.0, 'WCSS vs K Value')



In [12]:
```
### Getting labels of clustered records
X= dataset.iloc[:,:].values
km = KMeans(n_clusters=3)
y_means=km.fit_predict(X)
y_means
```

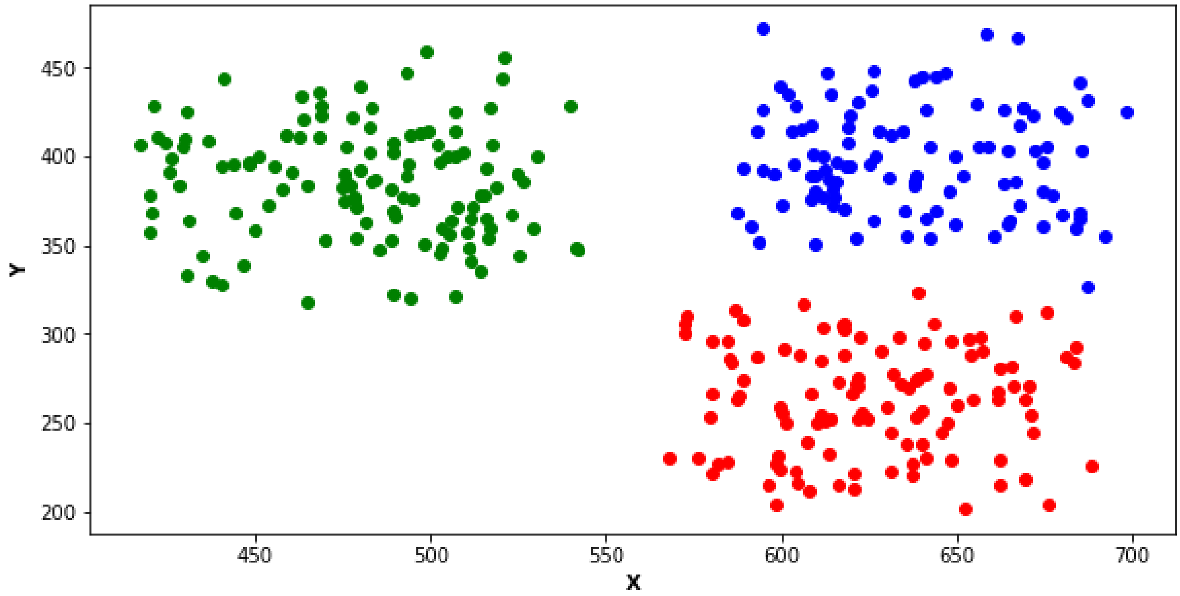
Out[12]:
```
array([2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 2, 2, 2, 0,
       0, 1, 2, 0, 2, 0])
```

In [30]:
```
### Silhoutte score
score= round(silhouette_score(X, km.labels_, metric='euclidean'),3)
score
```

Out[30]:
```
0.735
```

In [13]:
```
### Plotting different clusters after K-Means Clustering
plt.figure(figsize=(10,5))
plt.scatter(X[y_means==0,0], X[y_means==0,1], color='blue')
plt.scatter(X[y_means==1,0], X[y_means==1,1], color='red')
plt.scatter(X[y_means==2,0], X[y_means==2,1], color='green')
plt.xlabel("X", fontsize=10, fontweight='bold')
plt.ylabel("Y", fontsize=10, fontweight='bold')
```

Out[13]:
```
Text(0, 0.5, 'Y')
```



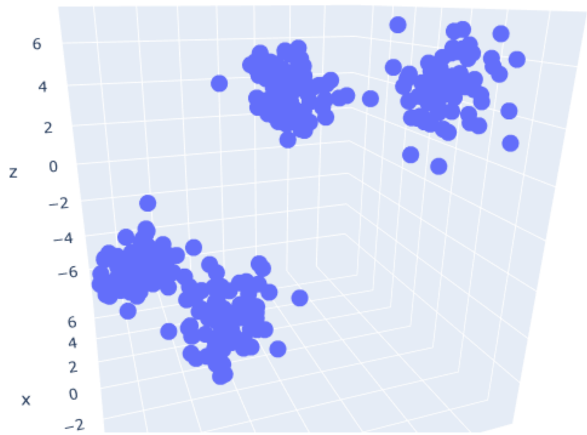
3.0 Creating 3-D dataset for clustering

In [43]:
```
### defining four centroid
centroids=[(-5,-5,5), (5,5,-5), (3.5,-2.5, 4), (-2.5, 2.5,-4)]

### standard deviation for cluster
cluster_std=[1,1,1,1]

### Creating 300 samples
X,y=make_blobs(n_samples=300, cluster_std=cluster_std, centers=centroids, n_featur
```

In [44]:
```
### Visualizing dataset
fig= px.scatter_3d(x=X[:,0], y=X[:,1], z=X[:,2])
fig.show();
```

In [51]:
```
from IPython import display
display.Image("wo_cluster.png")
```

Out[51]:



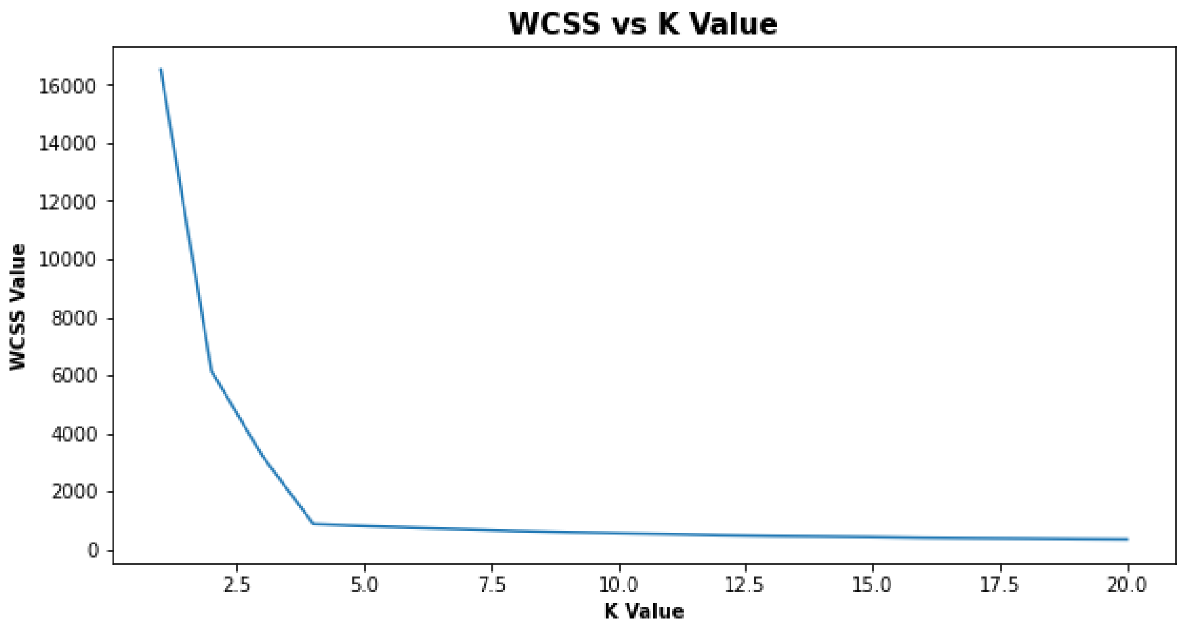
In [45]:
```
### Calculating WCSS for K=1 to K=21 clusters
wcss=[]

for i in range(1,21):
    km = KMeans(n_clusters=i)
    km.fit_predict(X)
```

```
    wcss.append(round(km.inertia_,2))
print(wcss)
```

```
[16520.33, 6135.27, 3215.25, 879.2, 810.02, 748.86, 693.28, 632.22, 587.3, 554.04,
525.92, 486.34, 461.4, 444.53, 424.88, 398.86, 384.19, 372.72, 357.65, 347.18]
```

In [46]:
```
### Plotting WCSS with K
plt.figure(figsize=(10, 5))
plt.plot(range(1,21), wcss)
plt.xlabel("K Value", fontsize=10, fontweight='bold')
plt.ylabel("WCSS Value", fontsize=10, fontweight='bold')
plt.title("WCSS vs K Value", fontsize=15, fontweight='bold')
```

Out[46]:
```
Text(0.5, 1.0, 'WCSS vs K Value')
```



In [47]:
```
### Getting labels of clustered records
km = KMeans(n_clusters=4)
y_pred=km.fit_predict(X)
y_pred
```

Out[47]:
```
array([0, 1, 1, 1, 0, 0, 1, 2, 0, 2, 3, 3, 3, 2, 3, 1, 2, 2, 1, 1, 0, 1,
       2, 1, 0, 2, 2, 1, 2, 0, 1, 0, 3, 3, 1, 1, 0, 2, 3, 0, 3, 1, 0, 2,
       2, 1, 2, 1, 3, 1, 0, 0, 1, 2, 0, 3, 0, 1, 0, 0, 3, 1, 1, 3, 0, 3,
       3, 0, 3, 0, 3, 3, 0, 3, 0, 3, 2, 3, 3, 2, 2, 1, 3, 3, 2, 2, 3, 3,
       3, 1, 0, 3, 2, 0, 0, 2, 1, 1, 1, 1, 0, 3, 2, 1, 3, 3, 2, 1, 0, 1,
       1, 1, 0, 0, 2, 1, 3, 2, 1, 1, 2, 2, 3, 0, 0, 3, 1, 1, 2, 2, 2, 3,
       2, 2, 0, 2, 3, 0, 3, 0, 0, 0, 1, 2, 1, 0, 0, 0, 0, 3, 3, 2, 2, 2,
       0, 1, 2, 1, 3, 1, 2, 0, 2, 2, 3, 0, 0, 1, 2, 3, 0, 3, 2, 3, 1, 1,
       3, 2, 1, 0, 0, 1, 2, 2, 3, 3, 1, 3, 2, 1, 1, 0, 2, 3, 1, 1, 3, 2,
       2, 1, 0, 2, 3, 1, 2, 2, 3, 2, 0, 0, 2, 0, 3, 2, 0, 3, 0, 3, 2, 0,
       0, 1, 2, 3, 2, 0, 0, 0, 3, 2, 1, 3, 3, 3, 1, 3, 2, 1, 2, 3, 3, 2,
       0, 1, 0, 3, 1, 1, 3, 1, 0, 0, 3, 3, 1, 0, 3, 0, 2, 2, 1, 1, 1, 2,
       3, 0, 0, 3, 0, 1, 2, 3, 2, 2, 1, 2, 2, 0, 2, 3, 3, 0, 2, 2, 1, 1,
       0, 1, 3, 1, 3, 0, 0, 2, 0, 1, 3, 0, 1, 1])
```

In [48]:
```
### Silhoutte score
score= round(silhouette_score(X, km.labels_, metric='euclidean'),3)
score
```

Out[48]:
```
0.735
```

In [23]:
```
### Creating dataset with labels and clustered data
df = pd.DataFrame()
```

```
df['col1']= X[:,0]
df['col2']= X[:,1]
df['col3']= X[:,2]
df['label']= y_pred

df.head()
```

Out[23]:

	col1	col2	col3	label
0	-4.470535	-4.862299	5.077821	1
1	-4.576802	3.447501	-4.503974	0
2	-2.349984	2.963534	-3.602120	0
3	-1.481448	3.730558	-5.181103	0
4	-4.801700	-4.880991	4.329338	1

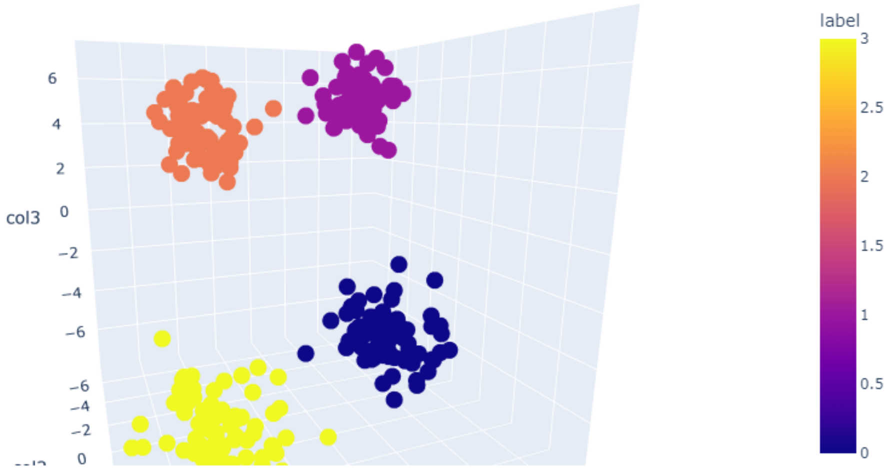
In [24]:

```
### Visualizing the clustered data
fig= px.scatter_3d(df, x='col1', y='col2', z='col3', color='label')
fig.show()
```

In [52]:

```
from IPython import display
display.Image("w_cluster.png")
```

Out[52]:



In [ ]: