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In [1]:
```
from IPython.core.interactiveshell import InteractiveShell
InteractiveShell.ast_node_interactivity = 'all'
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
%config InlineBackend.figure_format = 'svg'
import seaborn as sns
sns.set(style = "whitegrid")

# Clustering methods
from sklearn.cluster import KMeans, AgglomerativeClustering
from scipy.cluster.hierarchy import dendrogram

# Evaluation metrics
from sklearn import metrics
```

Task1

In [2]:
```
df1 = pd.read_csv('Data1.csv', index_col=0)
df2 = pd.read_csv('Data2.csv', index_col=0)
df3 = pd.read_csv('Data3.csv', index_col=0)
df4 = pd.read_csv('Data4.csv', index_col=0)
df5 = pd.read_csv('Data5.csv', index_col=0)
df1.head()
df2.head()
df3.head()
df4.head()
df5.head()
```

Out[2]:

	X1	X2	X3	Class
1	-0.063274	0.027734	0.022683	1
2	-0.000731	0.048211	0.069198	1
3	-0.060767	-0.009080	0.053085	1
4	0.013252	-0.011876	0.055324	1
5	-0.054508	-0.003813	0.001738	1

Out[2]:

	X	Y	C	Class
X1	3.277701	0.814082	0.326574	1
X2	0.387577	0.176780	0.888046	1
X3	0.268546	0.582963	0.080981	1
X4	2.031145	0.244597	0.643921	1
X5	0.188677	0.461280	0.496633	1

Out[2]:

	X1	X2	X3	Class
1	1.295428	0.050829	-0.385217	1
2	1.409178	-0.035191	-0.251980	1
3	1.096803	0.246365	-0.415011	1
4	1.463328	0.265354	-0.513488	1
5	1.603284	0.080577	-0.470257	1

Out[2]:

	X1	X2	X3	Class
1	-0.4530	-0.891	0.02300	1
2	0.6530	-0.846	0.02110	1
3	0.3980	0.913	-0.00139	1
4	0.0952	1.050	0.00628	1
5	0.5240	-0.941	0.03780	1

Out[2]:

	X1	X2	X3	Class
1	-4.822490	-50.402170	4.020861	1
2	-44.460120	20.964670	-11.492060	1
3	50.001020	0.780748	9.134460	1
4	-41.699080	-22.310060	16.314120	1
5	4.425242	-4.666664	50.223740	1

In [3]:
```
# uniform format for further analysis
df2 = df2.rename(columns={'X':'X1', 'Y':'X2', 'C':'X3'})
df2.index = pd.Series(np.arange(1, len(df2)+1))
```

1. Clustering

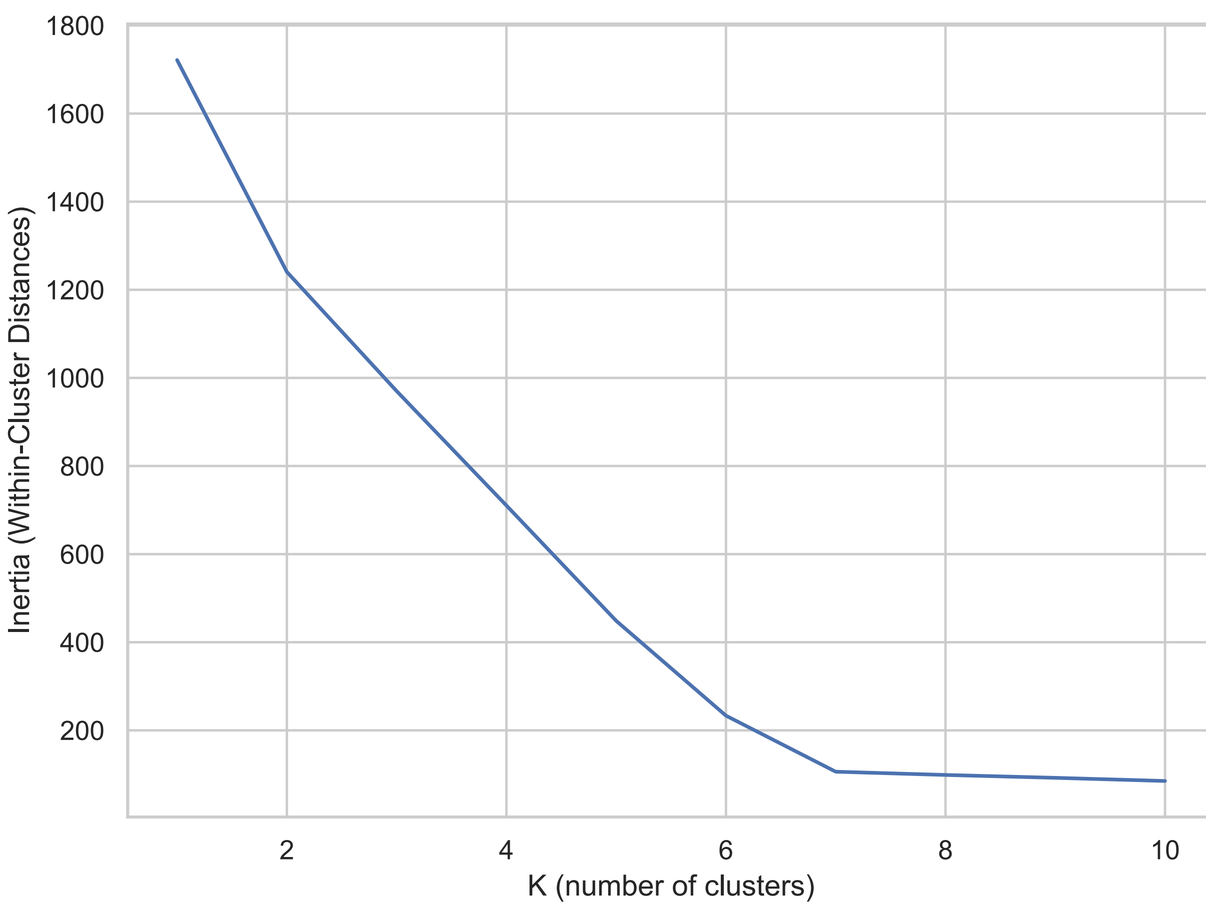
1-1 K-Means

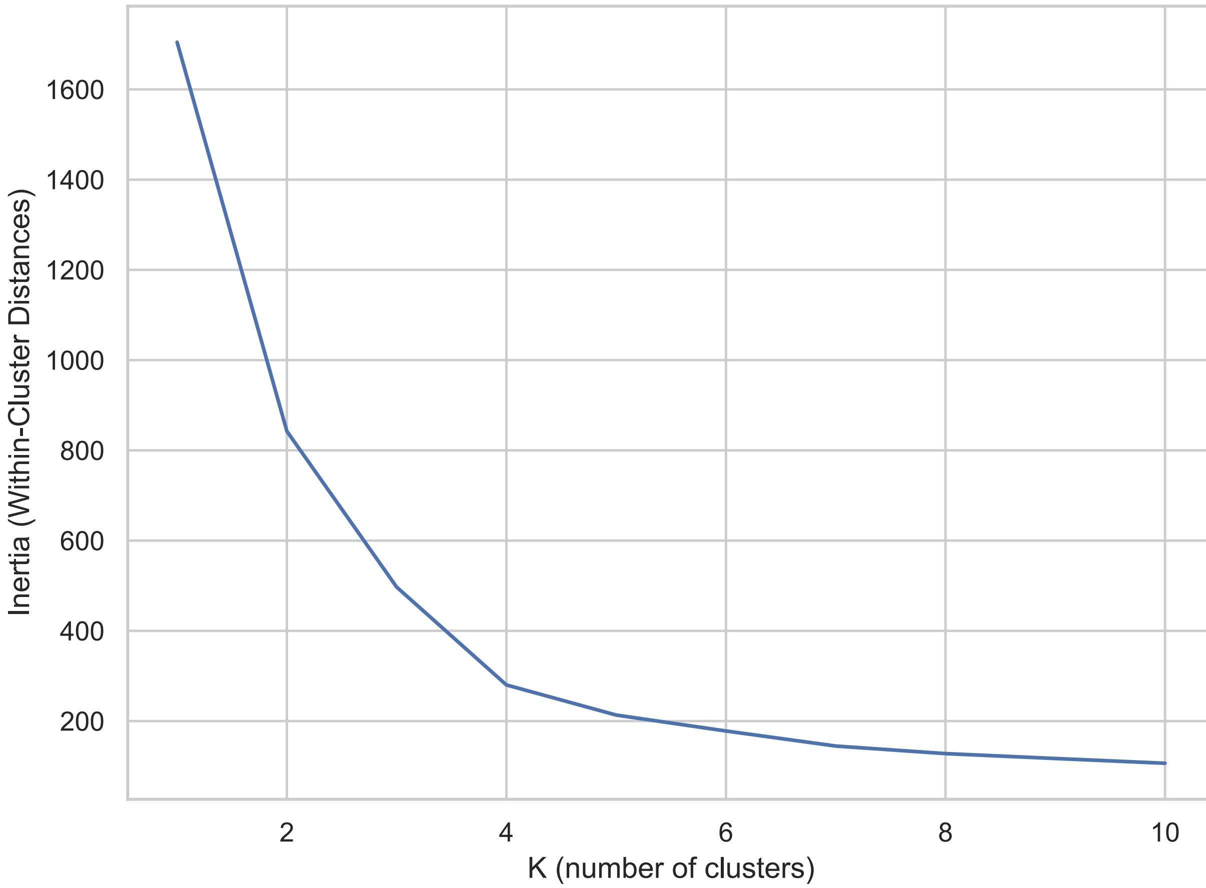
When we use K-Means algorithm, we need to find K first.
The function below will loop through 1-10 clusters, running K-Means for each. This will give us our "inertia" values, which we can plot against K to make an elbow plot.

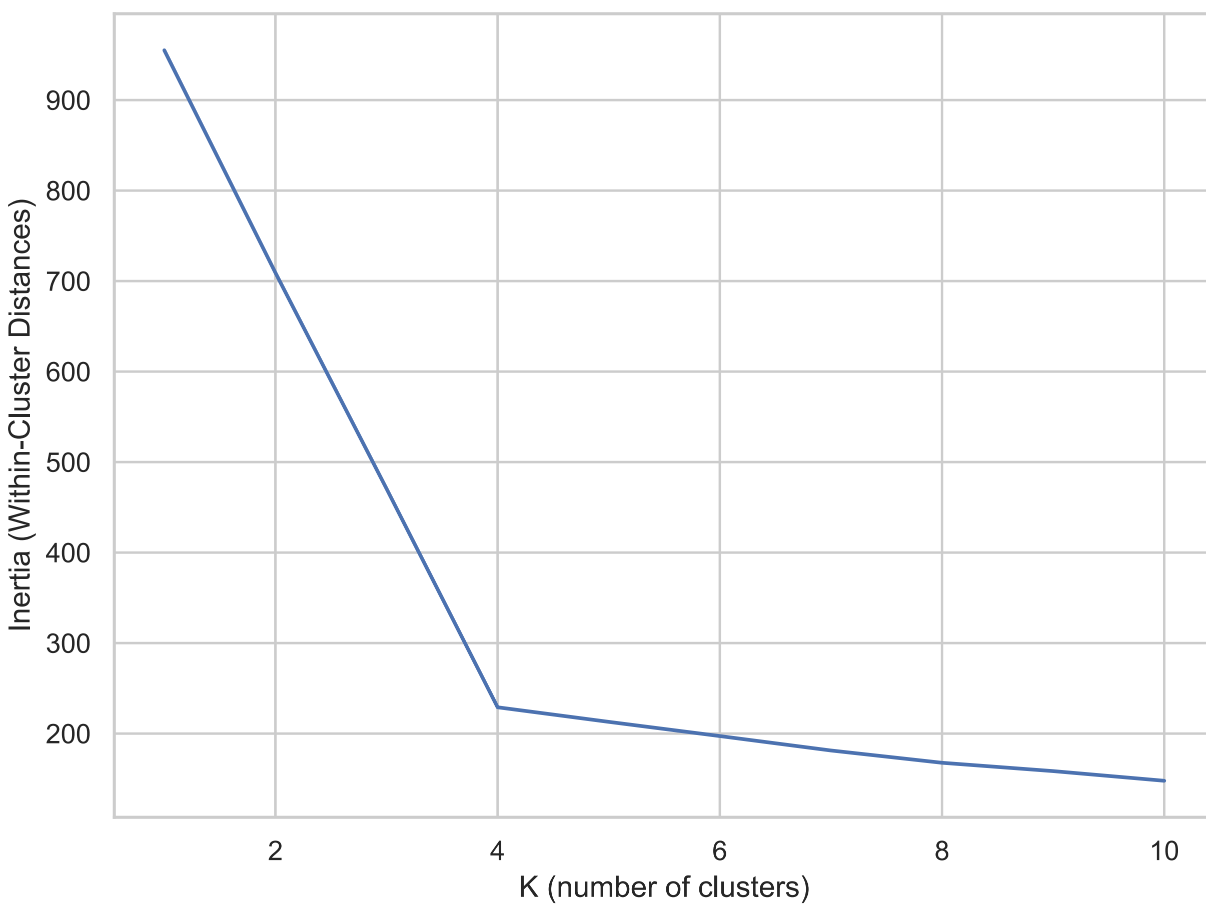
In [4]:
```
def kmfindk(df):
    inertias = []
    ds = df[['X1','X2','X3']]
    for k in range(1,11):
        kmeans = KMeans(n_clusters=k, random_state = 7)
        kmeans.fit(ds)
        inertias.append(kmeans.inertia_)

    plt.figure(figsize=(8,6))
    plt.plot(range(1,11), inertias)
    plt.xlabel("K (number of clusters)")
    plt.ylabel("Inertia (Within-Cluster Distances)")
    plt.show()
```

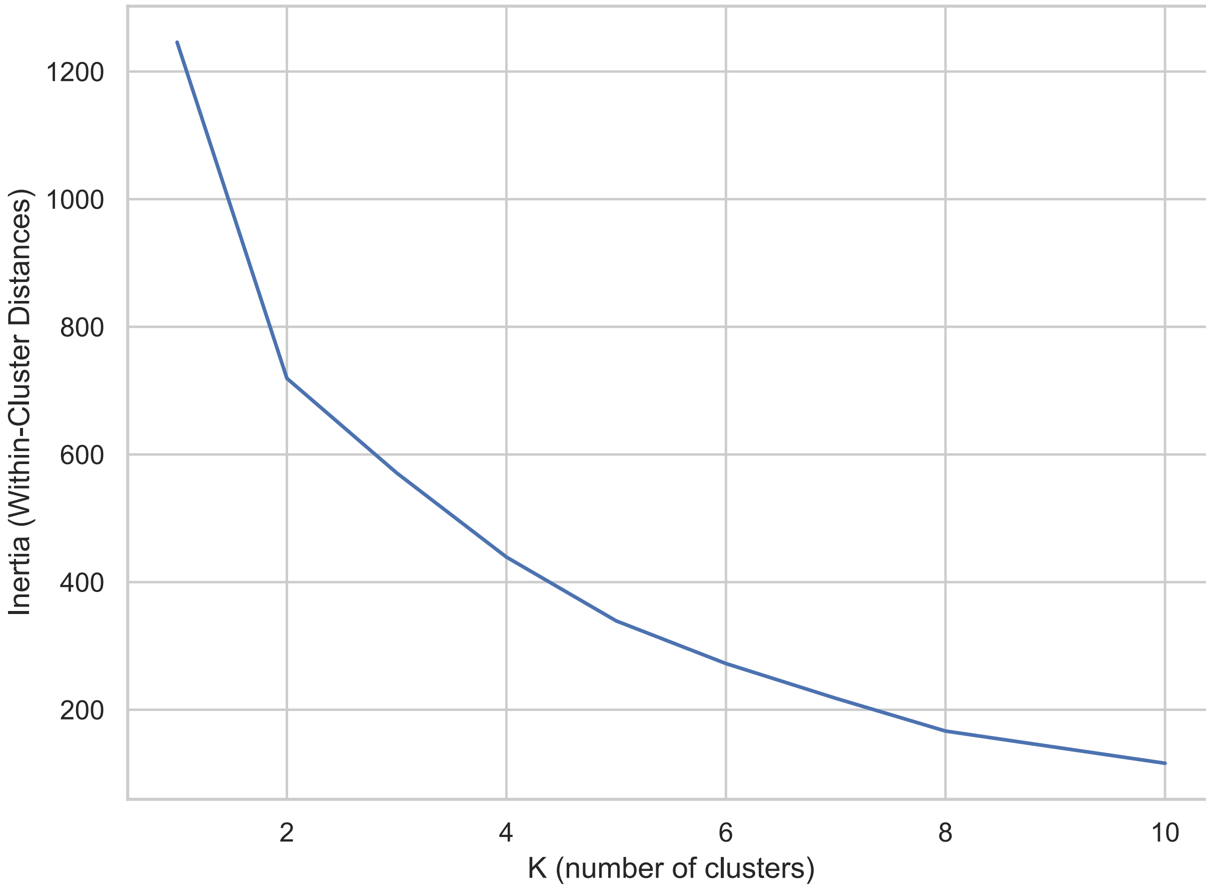
Run the function for each dataset, choose the K where we can see a pronounced change in slope.

In [5]:
```
kmfindk(df1)
kmfindk(df2)
kmfindk(df3)
kmfindk(df4)
kmfindk(df5)
```




Inertia (Within-Cluster Distances)
K (number of clusters)
1600
1400
1200
1000
800
600
400
200
2
4
6
8
10


Inertia (Within-Cluster Distances)
K (number of clusters)
900
800
700
600
500
400
300
200
2
4
6
8
10



Obviously, for data1, after k=7, the plot flattens out substantially. Therefore 7 is our "elbow" and we should probably choose k=7.

Similarly,

data2, k2 = 4;

data3, k3 = 4;

data4, k4 = 2;

data5, k5 = 2.

In [6]:
```
# define K of each dataset
k1 = 7
k2 = 4
k3 = 4
k4 = 2
k5 = 2
```

Then write a function to apply K-Means method on each datasets to generate clusters.

In [7]:
```
def kmeans(k, df):
    ds = df.copy()
    y_KMeans = KMeans(n_clusters = k, random_state = 7)
    y_pred = y_KMeans.fit_predict(ds[['X1', 'X2', 'X3']])

    # get the labels
    ds['labels'] = y_KMeans.labels_
    display(ds.head())
    display(ds['labels'].value_counts())
    return ds
```

In [8]:
```
# get the clustered dataframes
ds1 = kmeans(k1, df1)
ds2 = kmeans(k2, df2)
ds3 = kmeans(k3, df3)
ds4 = kmeans(k4, df4)
ds5 = kmeans(k5, df5)
```

	X1	X2	X3	Class	labels
1	-0.063274	0.027734	0.022683	1	3
2	-0.000731	0.048211	0.069198	1	3
3	-0.060767	-0.009080	0.053085	1	3
4	0.013252	-0.011876	0.055324	1	3
5	-0.054508	-0.003813	0.001738	1	3

```
3    32
2    30
5    30
4    30
6    30
0    30
1    30
Name: labels, dtype: int64
```

	X1	X2	X3	Class	labels
1	3.277701	0.814082	0.326574	1	0
2	0.387577	0.176780	0.888046	1	3
3	0.268546	0.582963	0.080981	1	3
4	2.031145	0.244597	0.643921	1	0
5	0.188677	0.461280	0.496633	1	3

```
3    141
1    100
0     83
2     80
Name: labels, dtype: int64
```

	X1	X2	X3	Class	labels
1	1.295428	0.050829	-0.385217	1	2
2	1.409178	-0.035191	-0.251980	1	2
3	1.096803	0.246365	-0.415011	1	2
4	1.463328	0.265354	-0.513488	1	2
5	1.603284	0.080577	-0.470257	1	2

```
2    100
0    100
3    100
1    100
Name: labels, dtype: int64
```

	X1	X2	X3	Class	labels
1	-0.4530	-0.891	0.02300	1	0
2	0.6530	-0.846	0.02110	1	0
3	0.3980	0.913	-0.00139	1	1
4	0.0952	1.050	0.00628	1	1
5	0.5240	-0.941	0.03780	1	0

```
0    500
1    500
Name: labels, dtype: int64
```

	X1	X2	X3	Class	labels
1	-4.822490	-50.402170	4.020861	1	0
2	-44.460120	20.964670	-11.492060	1	0
3	50.001020	0.780748	9.134460	1	0
4	-41.699080	-22.310060	16.314120	1	1
5	4.425242	-4.666664	50.223740	1	1

```
0    629
1    171
Name: labels, dtype: int64
```

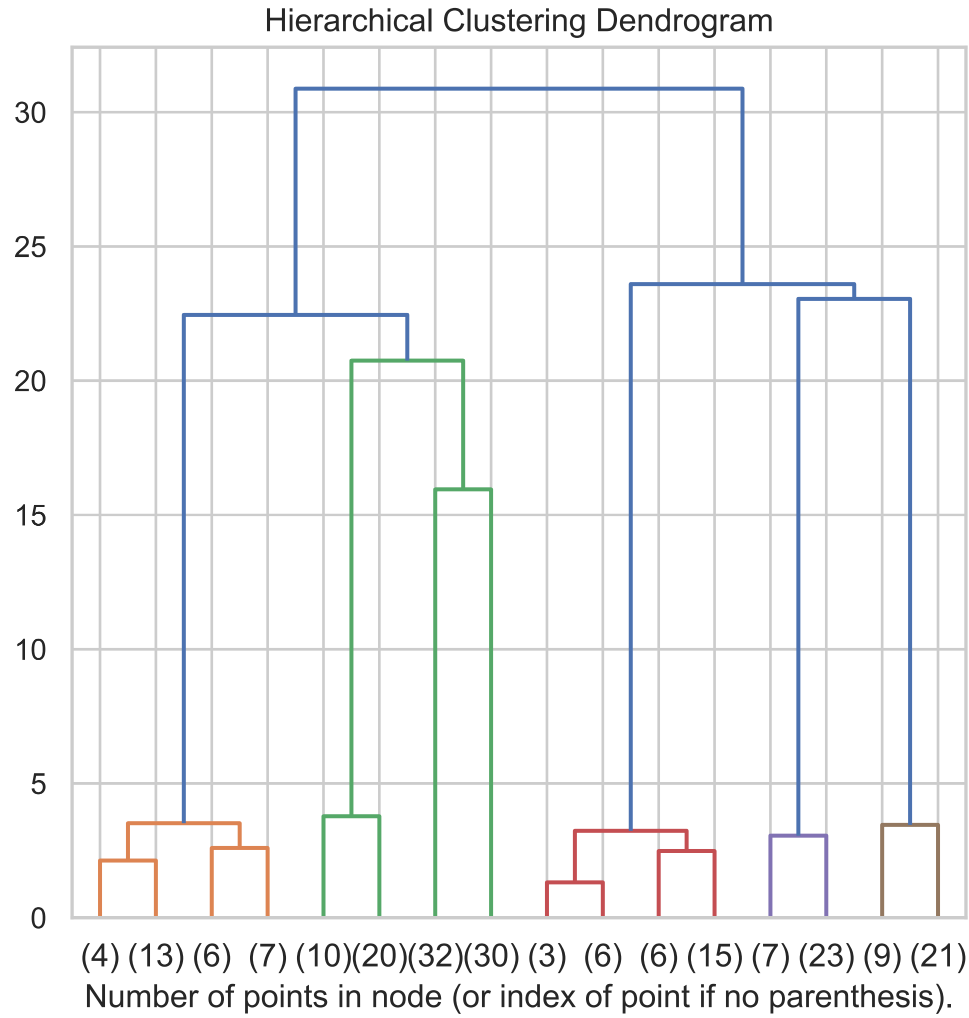
1-2 Hierarchical Clustering

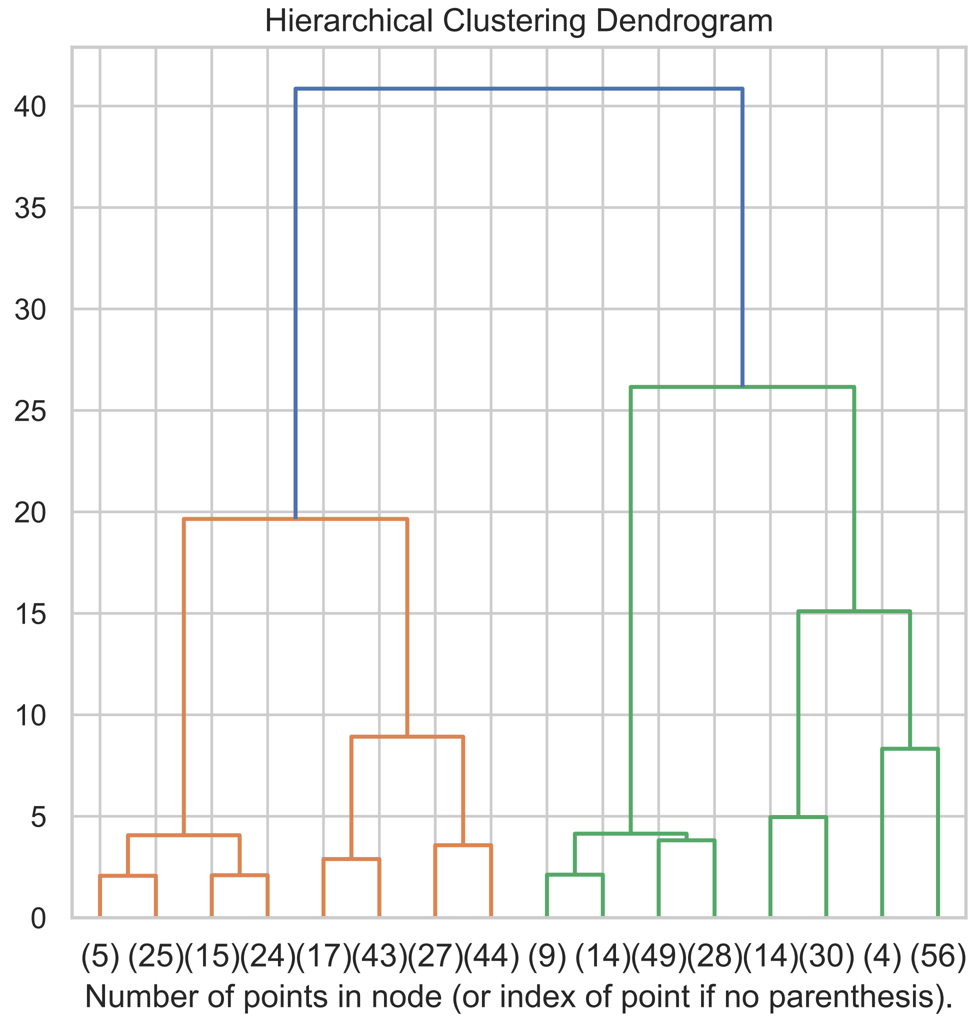
When we use Hierarchical method to generate clusters, we can plot a full dendrogram and choose the correct number of clusters.
The below function will plot the full dendrogram.

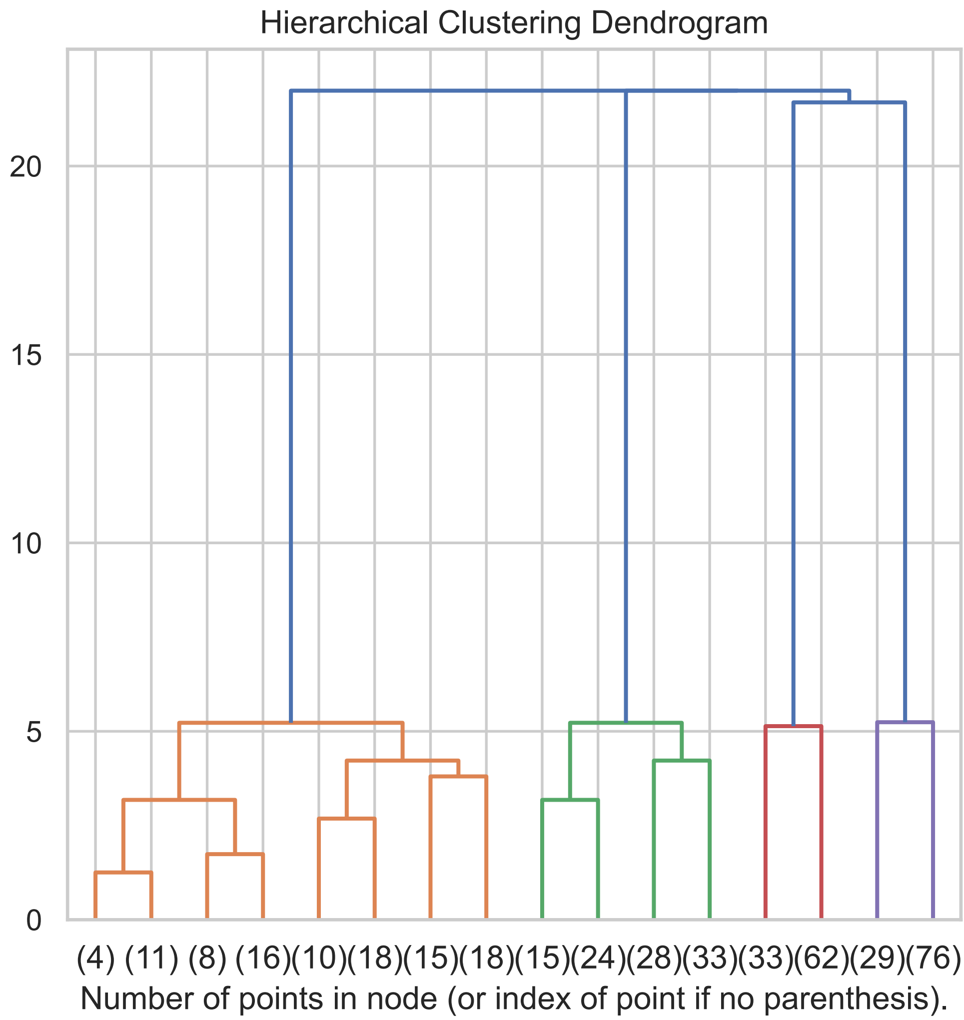
In [9]:
```
def plot_dendrogram(df, **kwargs):
    plt.figure(figsize=(6,6))
    plt.title("Hierarchical Clustering Dendrogram")
    plt.xlabel("Number of points in node (or index of point if no parenthesis).

    ds = df.copy()
    # setting distance_threshold=0 ensures we compute the full tree.
    model = AgglomerativeClustering(distance_threshold=0, n_clusters=None)
    model = model.fit(ds.drop(columns=["Class"]))

    # Create linkage matrix and then plot the dendrogram
    # create the counts of samples under each node
    counts = np.zeros(model.children_.shape[0])
    n_samples = len(model.labels_)
    for i, merge in enumerate(model.children_):
        current_count = 0
        for child_idx in merge:
            if child_idx < n_samples:
                current_count += 1  # leaf node
            else:
                current_count += counts[child_idx - n_samples]
        counts[i] = current_count

    linkage_matrix = np.column_stack(
        [model.children_, model.distances_, counts]
    ).astype(float)

    # Plot the corresponding dendrogram
    dendrogram(linkage_matrix, **kwargs)

    plt.show()
```

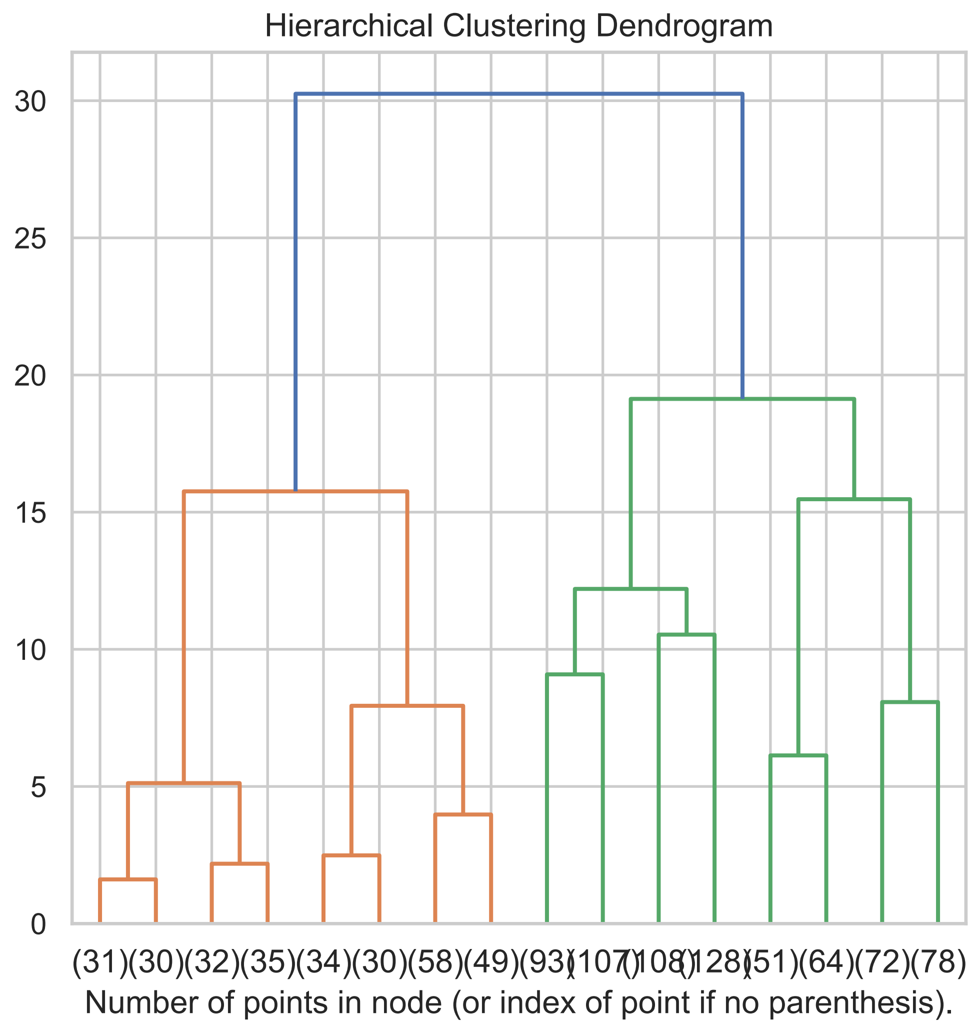
Run the function for each data set, use the dendrogram to examine the distances between clusters and find the meaningful K.

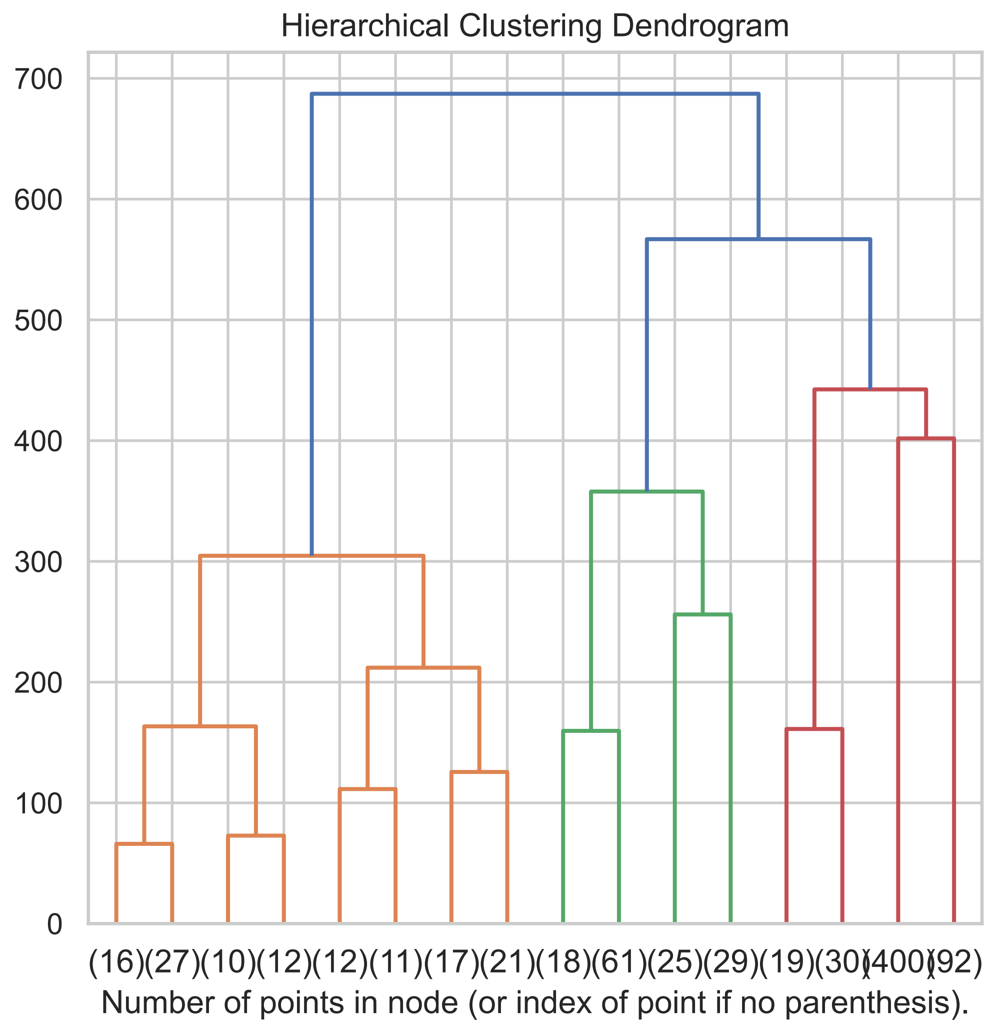
In [10]:
```
# plot the top three levels of the dendrogram for each data set
plot_dendrogram(df1, truncate_mode="level", p=3)
plot_dendrogram(df2, truncate_mode="level", p=3)
plot_dendrogram(df3, truncate_mode="level", p=3)
plot_dendrogram(df4, truncate_mode="level", p=3)
plot_dendrogram(df5, truncate_mode="level", p=3)
```


Hierarchical Clustering Dendrogram
30
25
20
15
10
5
0
(4) (13) (6) (7) (10)(20)(32)(30) (3) (6) (6) (15) (7) (23) (9) (21)
Number of points in node (or index of point if no parenthesis).


Hierarchical Clustering Dendrogram
40
35
30
25
20
15
10
5
0
(5) (25)(15)(24)(17)(43)(27)(44) (9) (14)(49)(28)(14)(30) (4) (56)
Number of points in node (or index of point if no parenthesis).


Hierarchical Clustering Dendrogram
20
15
10
5
0
(4) (11) (8) (16)(10)(18)(15)(18)(15)(24)(28)(33)(33)(62)(29)(76)
Number of points in node (or index of point if no parenthesis).


Hierarchical Clustering Dendrogram
30
25
20
15
10
5
0
(31)(30)(32)(35)(34)(30)(58)(49)(93)(107)(108)(128)(51)(64)(72)(78)
Number of points in node (or index of point if no parenthesis).



As shown above, for data set 1, we can see a huge decrease in the distance metric when going from 1 to 2, 2 to 3...and 6 to 7. After 7 clusters, the decrease trend becomes quite smooth, so K=7 should be answer.
Therefore, for data1, K1 = 7;
Similarly,
data2, K2 = 4;
data3, K3 = 4;
data4, K4 = 2;
data5, K5 = 2.

In [11]:
```
# define K of each dataset
K1 = 7
K2 = 4
K3 = 4
K4 = 2
K5 = 2
```

Write a function to apply Hierarchical method on each datasets to generate clusters.

In [12]:
```
def hierarchical(K, df):
    ds = df.copy()
    y_HC = AgglomerativeClustering(n_clusters = K)
```

```
    y_pred = y_HC.fit_predict(ds[['X1', 'X2', 'X3']])

    ds['labels'] = y_HC.labels_
    display(ds.head())
    display(ds['labels'].value_counts())
    return ds
```

In [13]:
```
# Get the clustered dataframes
DS1 = hierarchical(K1, df1)
DS2 = hierarchical(K2, df2)
DS3 = hierarchical(K3, df3)
DS4 = hierarchical(K4, df4)
DS5 = hierarchical(K5, df5)
```

	X1	X2	X3	Class	labels
1	-0.063274	0.027734	0.022683	1	6
2	-0.000731	0.048211	0.069198	1	6
3	-0.060767	-0.009080	0.053085	1	6
4	0.013252	-0.011876	0.055324	1	6
5	-0.054508	-0.003813	0.001738	1	6

```
6    32
4    30
2    30
5    30
1    30
0    30
3    30
Name: labels, dtype: int64
```

	X1	X2	X3	Class	labels
1	3.277701	0.814082	0.326574	1	3
2	0.387577	0.176780	0.888046	1	1
3	0.268546	0.582963	0.080981	1	1
4	2.031145	0.244597	0.643921	1	1
5	0.188677	0.461280	0.496633	1	1

```
1    131
0    104
2    100
3     69
Name: labels, dtype: int64
```

	X1	X2	X3	Class	labels
1	1.295428	0.050829	-0.385217	1	1
2	1.409178	-0.035191	-0.251980	1	1
3	1.096803	0.246365	-0.415011	1	1
4	1.463328	0.265354	-0.513488	1	1
5	1.603284	0.080577	-0.470257	1	1

```
0    105
1    100
2    100
3     95
Name: labels, dtype: int64
```

	X1	X2	X3	Class	labels
1	-0.4530	-0.891	0.02300	1	1
2	0.6530	-0.846	0.02110	1	1
3	0.3980	0.913	-0.00139	1	0
4	0.0952	1.050	0.00628	1	0
5	0.5240	-0.941	0.03780	1	1

```
0    701
1    299
Name: labels, dtype: int64
```

	X1	X2	X3	Class	labels
1	-4.822490	-50.402170	4.020861	1	1
2	-44.460120	20.964670	-11.492060	1	0
3	50.001020	0.780748	9.134460	1	0
4	-41.699080	-22.310060	16.314120	1	0
5	4.425242	-4.666664	50.223740	1	0

```
0    674
1    126
Name: labels, dtype: int64
```

2. Plot (3D)

Then write a function to plot(3D) the data points for each dataset and color them according to the class allocated by 2 clustering algorithms.

In [14]:

```
import matplotlib.colors as mcolors
color = list(mcolors.BASE_COLORS)

def hcplot(method, k, ds):
    fig = plt.figure(figsize = (8,8))
    ax = fig.add_subplot(projection = '3d')

    # For each set of style and range settings
    i = 0
    for c in color[:k]:
        xs = ds.loc[ds['labels'] == i]['X1']
        ys = ds.loc[ds['labels'] == i]['X2']
        zs = ds.loc[ds['labels'] == i]['X3']
        ax.scatter(xs, ys, zs, color = c, s = 50)
        i = i + 1

    ax.set_xlabel('X1')
    ax.set_ylabel('X2')
    ax.set_zlabel('X3')
```

```
    ax.set_title(f'{method} clustering, clusters = {k}')
    ax.set_xlim(xmin = min(ds['X1'])-0.1, xmax = max(ds['X1'])+0.1)
    ax.set_ylim(ymin = min(ds['X2'])-0.1, ymax = max(ds['X2'])+0.1)
    ax.set_zlim(zmin = min(ds['X3'])-0.1, zmax = max(ds['X3'])+0.1)

    plt.show()
```

This is the function to plot(3D) the data points for each dataset and color them according to the original class.

In [15]:
```
def plotori(df):
    ds = df.copy()
    kclass = len(ds['Class'].unique())
    Class = np.arange(1, kclass+1)
    Class = np.vstack((Class, color[:kclass]))

    # plot
    fig = plt.figure(figsize = (8,8))
    ax = fig.add_subplot(projection = '3d')

    # For each set of style and range settings
    for i, c in Class.T:
        xs = ds.loc[ds['Class'] == int(i)]['X1']
        ys = ds.loc[ds['Class'] == int(i)]['X2']
        zs = ds.loc[ds['Class'] == int(i)]['X3']
        ax.scatter(xs, ys, zs, color = c, s = 50)

    ax.set_xlabel('X1')
    ax.set_ylabel('X2')
    ax.set_zlabel('X3')
    ax.set_title(f'Original classes, class = {kclass}')
    ax.set_xlim(xmin = min(ds['X1'])-0.1, xmax = max(ds['X1'])+0.1)
    ax.set_ylim(ymin = min(ds['X2'])-0.1, ymax = max(ds['X2'])+0.1)
    ax.set_zlim(zmin = min(ds['X3'])-0.1, zmax = max(ds['X3'])+0.1)

    plt.show()
```

3. External validation

Compare these 2 clustering algorithms results C to the given classes P and use several external validation methods to to evaluate the algorithm performance.

Purity

Calculate the Purity to evaluate the matching accurancy.

$$U = \sum_i p_i(max_j \frac{p_{ij}}{p_i}) = \frac{1}{n} \sum_i n_i(max_j \frac{n_{ij}}{n_i})$$

where $p_i = \frac{n_i}{n}$, $p_j = \frac{n_j}{n}$, $p_{ij} = \frac{n_{ij}}{n}$, n_{ij} is the number of examples belonging to the class i found in the cluster j and $n_i(n_j)$ is the number of examples in the cluster $i(j)$. $max_j \frac{n_{ij}}{n_i}$ indicates the maximum overlap fraction between each cluster i and class j.

If U is close to 1, the clustering algorithm performs perfectly.

In [16]:
```
# Purity
def purity(method, df):
    Labels = df['labels']
    Classes = df['Class']
    nol = Labels.unique()
    noc = Classes.unique()

    maxoverlaps = []

    for i in nol:
        indices_l = [ii for ii in range(1, len(Labels)+1) if Labels[ii]==i]
        overlap=[]

        # count overlaps of each j on i
        for j in noc:
            indices_c = [jj for jj in range(1, len(Classes)+1) if Classes[jj]==
            overlap.append(len(set(indices_l).intersection(indices_c)))

        maxoverlaps.append(max(overlap))

    purity = sum(maxoverlaps)/len(Labels)
    print(f'{method} clustering, Purity = {purity}')
```

Rand coefficient

We have the knowledge of truth classes, we can use the Rand coefficient to evaluate the performance against the total data set based on peer-to-peer correlation.

$$Rand = \frac{TP + TN}{M}$$

where TP is the number of data pairs found in the same cluster, both in C and in P, TN is the number of data pairs found in different clusters, both in C and in P.

If Rand coefficient is close to 1, the clustering algorithm performs perfectly.

In [17]:
```
def rand(method, df):
    labels_true = df['Class']
    labels_pred = df['labels']
    score = metrics.adjusted_rand_score(labels_true, labels_pred)
    print(f'{method} clustering, Rand = {score}')
```

Mutual information

Based on information theory.
Mutual Information measures the agreement of C and P. If the score is close to 1, the clustering algorithm performs perfectly.
If Mutual information is close to 1, the clustering algorithm performs perfectly.

In [18]:
```
def mutualinfo(method, df):
```

```
    labels_true = df['Class']
    labels_pred = df['labels']
    score = metrics.adjusted_mutual_info_score(labels_true, labels_pred)
    print(f'{method} clustering, Mutual information score = {score}')
```

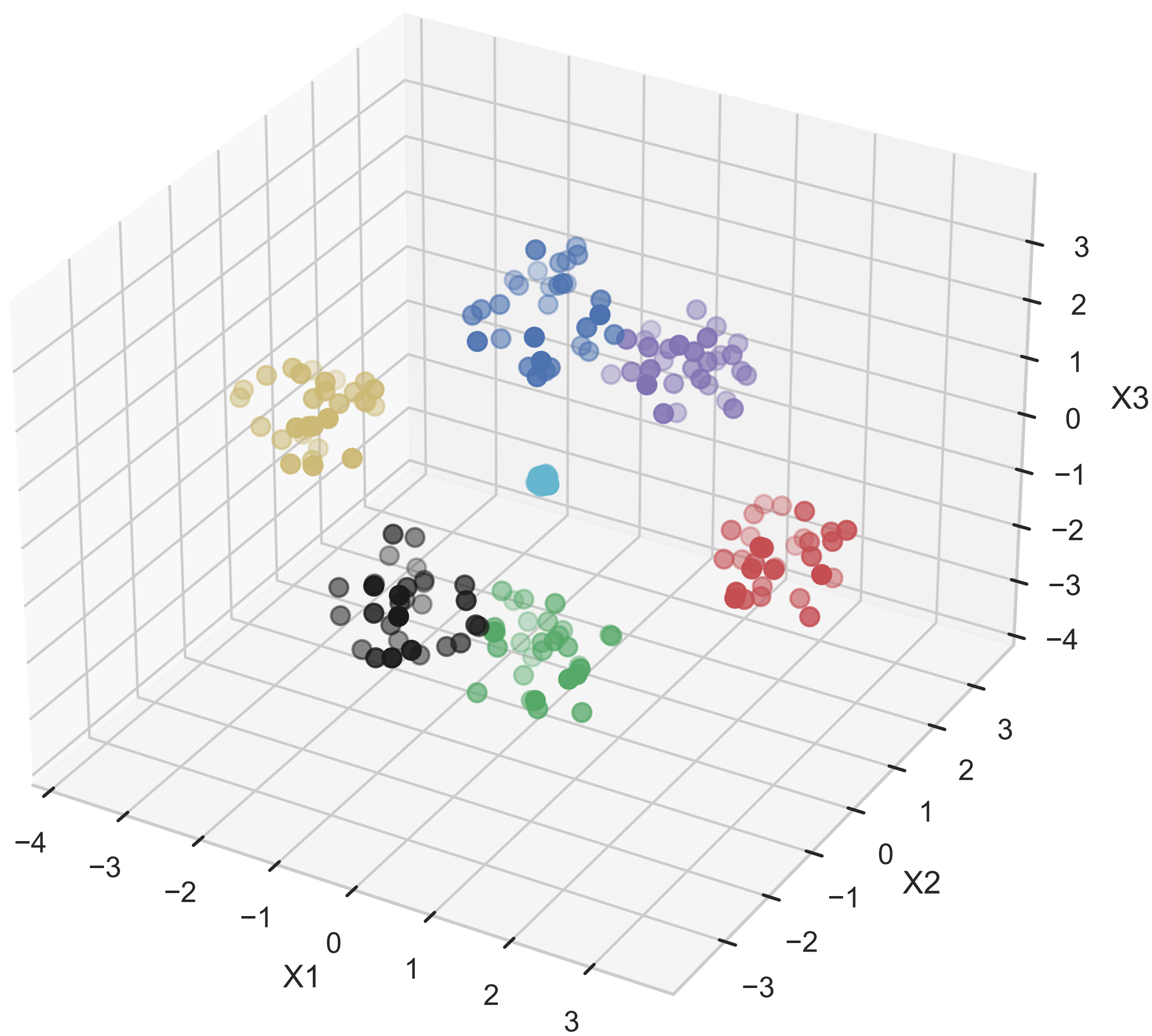
4. Compare and conclusion

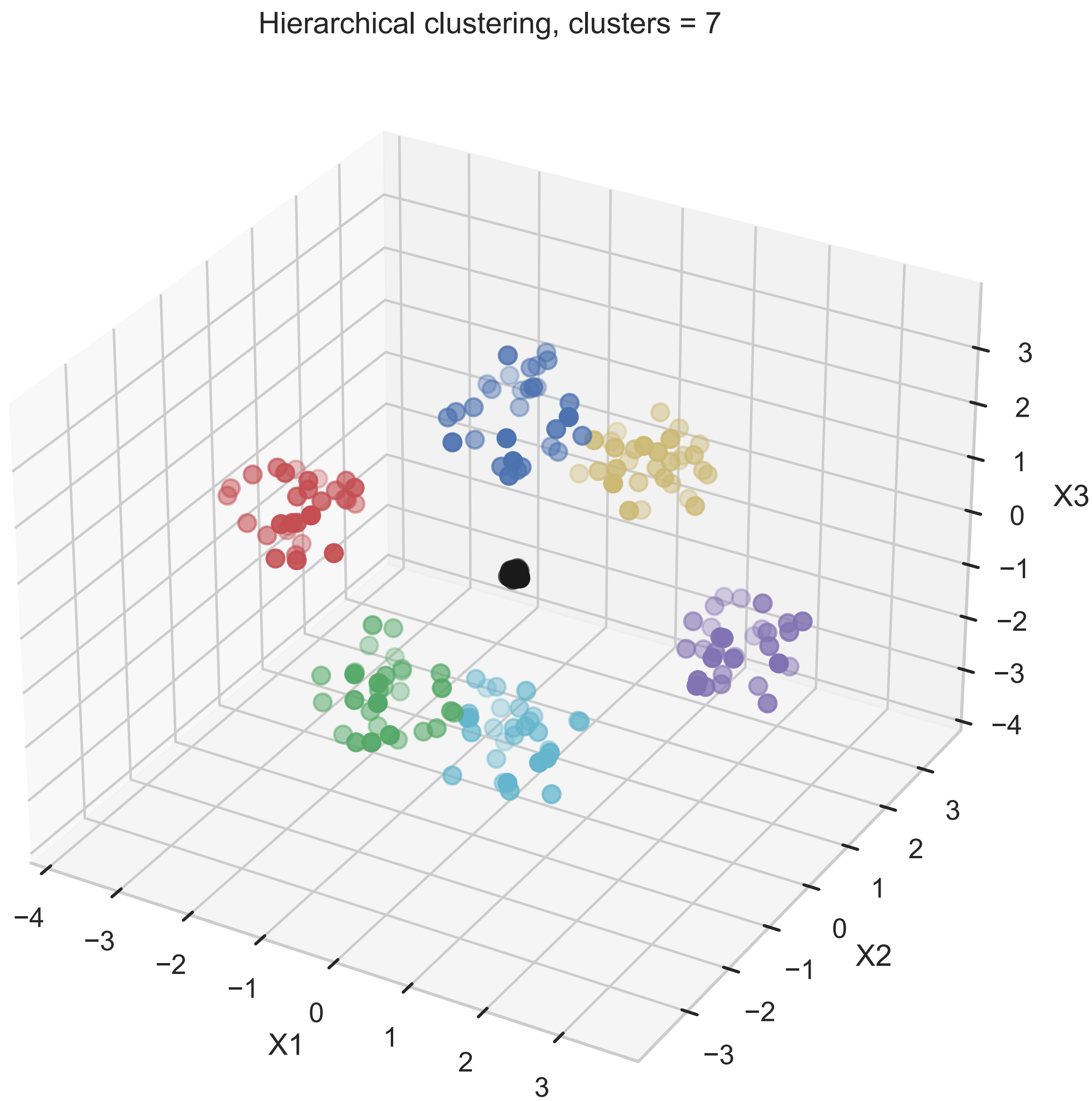
Now we can showing the data points of the original class and the class allocated by each clustering algorithm for each data and evaluate the performance.

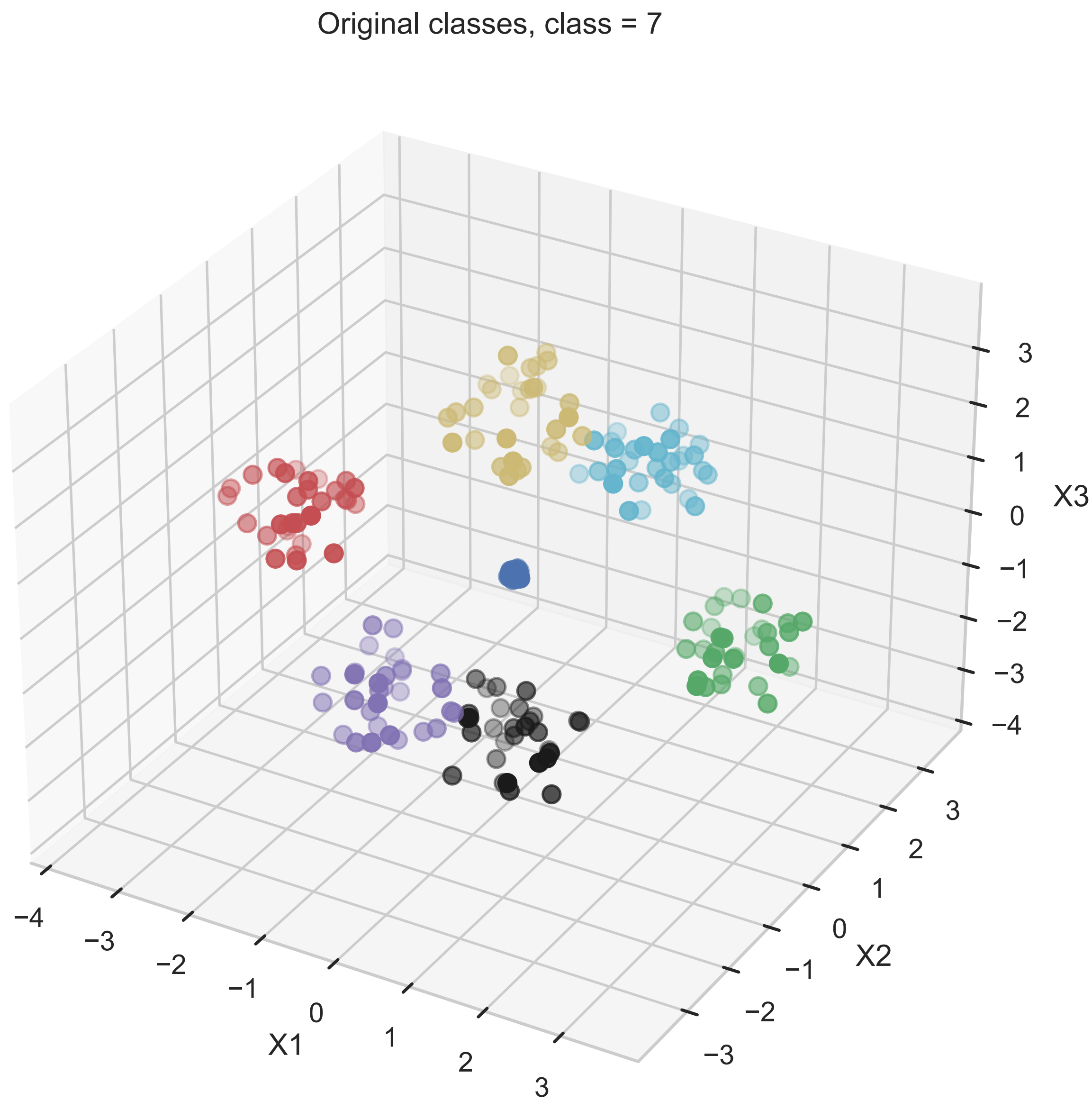
In [19]:
```
print('For Data set 1:')
hcplot('K-Means', k1, ds1)
hcplot('Hierarchical', K1, DS1)
plotori(df1)
purity('K-Means', ds1)
purity('Hierarchical', DS1)
rand('K-Means', ds1)
rand('Hierarchical', DS1)
mutualinfo('K-Means', ds1)
mutualinfo('Hierarchical', DS1)
```

```
For Data set 1:
```

K-Means clustering, clusters = 7




Hierarchical clustering, clusters = 7
X1
X2
X3
−4
−3
−2
−1
0
1
2
3

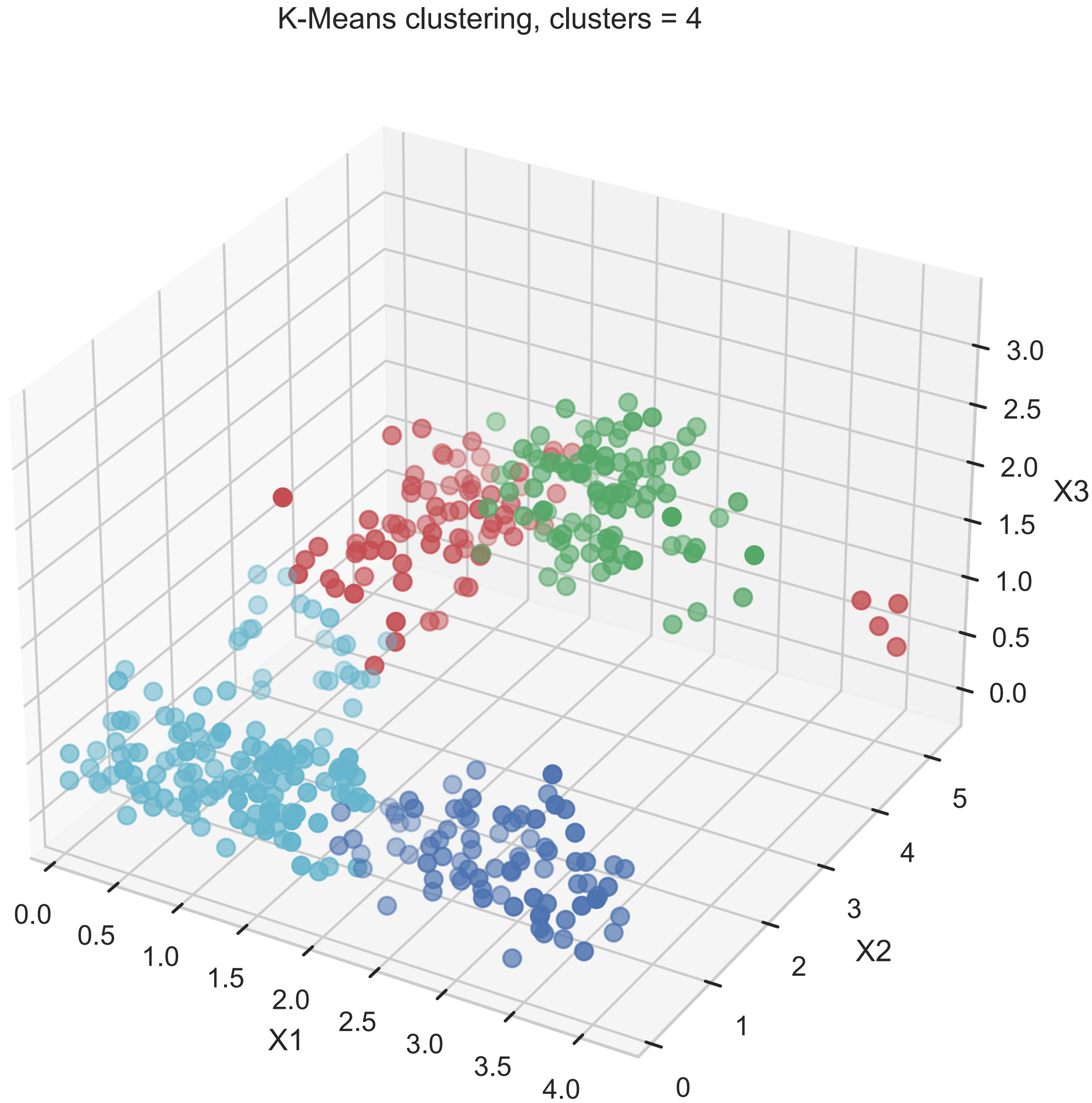


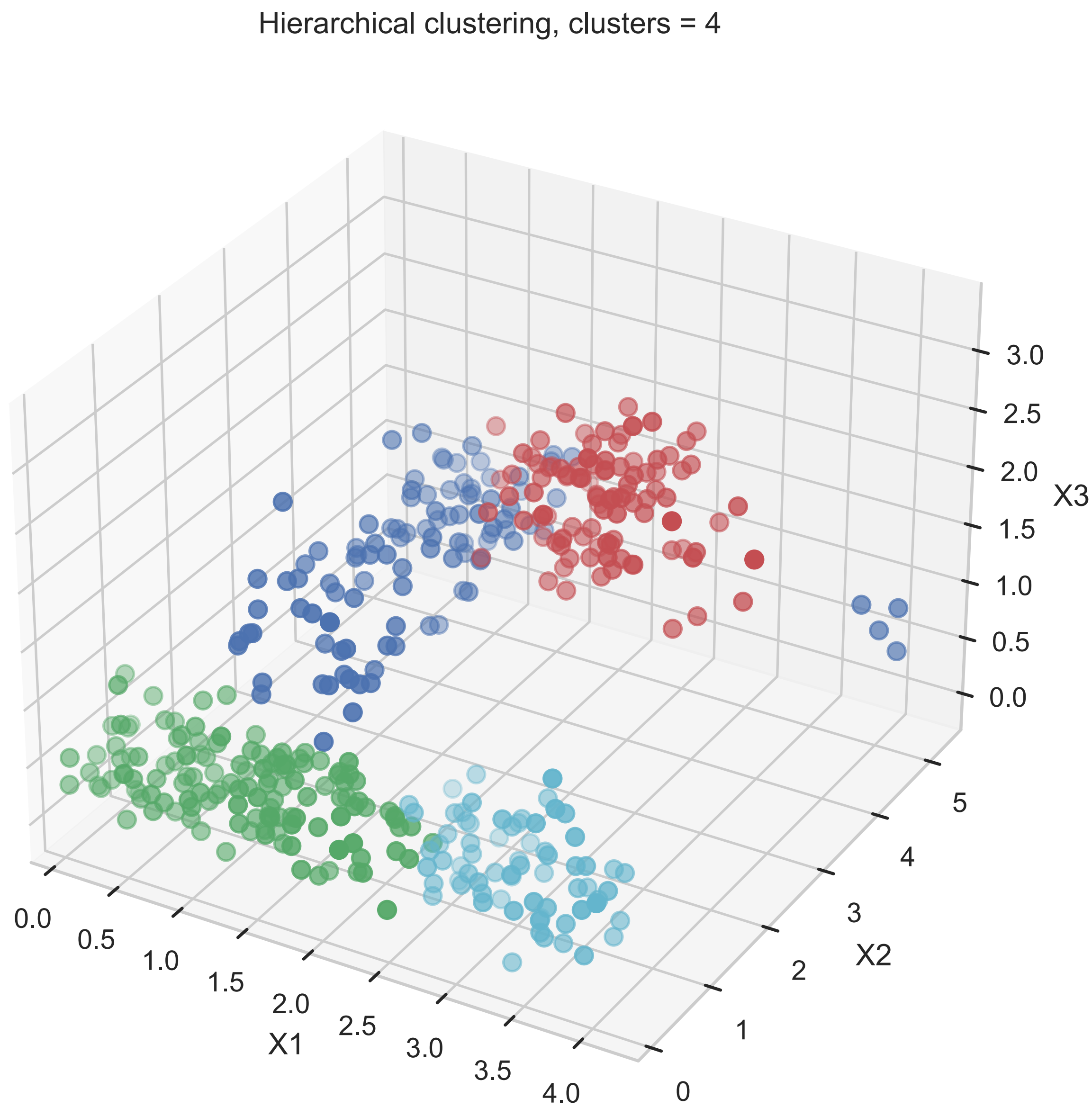

```
K-Means clustering, Purity = 1.0
Hierarchical clustering, Purity = 1.0
K-Means clustering, Rand = 1.0
Hierarchical clustering, Rand = 1.0
K-Means clustering, Mutual information score = 1.0
Hierarchical clustering, Mutual information score = 1.0
```

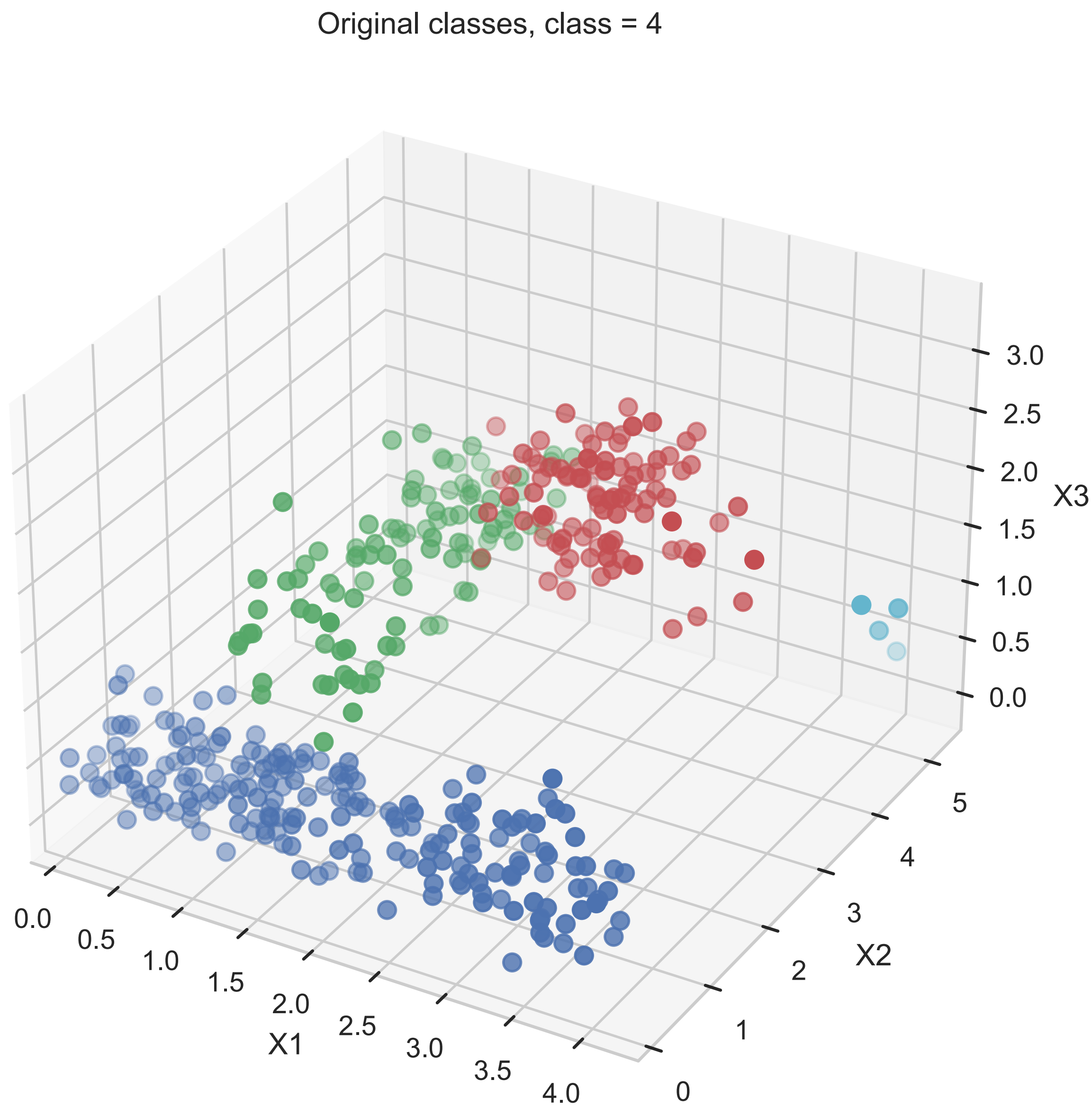
Obviously, for data set 1, metrics are equal to 1. Both K-Means and Hierarchical algorithms perform perfectly, the clustering results are the same as the original classes.

In [20]:
```
print('For Data set 2:')
hcplot('K-Means', k2, ds2)
hcplot('Hierarchical', K2, DS2)
plotori(df2)
purity('K-Means', ds2)
purity('Hierarchical', DS2)
rand('K-Means', ds2)
rand('Hierarchical', DS2)
mutualinfo('K-Means', ds2)
mutualinfo('Hierarchical', DS2)
```

```
For Data set 2:
```


K-Means clustering, clusters = 4
X1
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
X2
0
1
2
3
4
5
X3
0.0
0.5
1.0
1.5
2.0
2.5
3.0


Hierarchical clustering, clusters = 4
X1
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
X2
0
1
2
3
4
5
X3
0.0
0.5
1.0
1.5
2.0
2.5
3.0

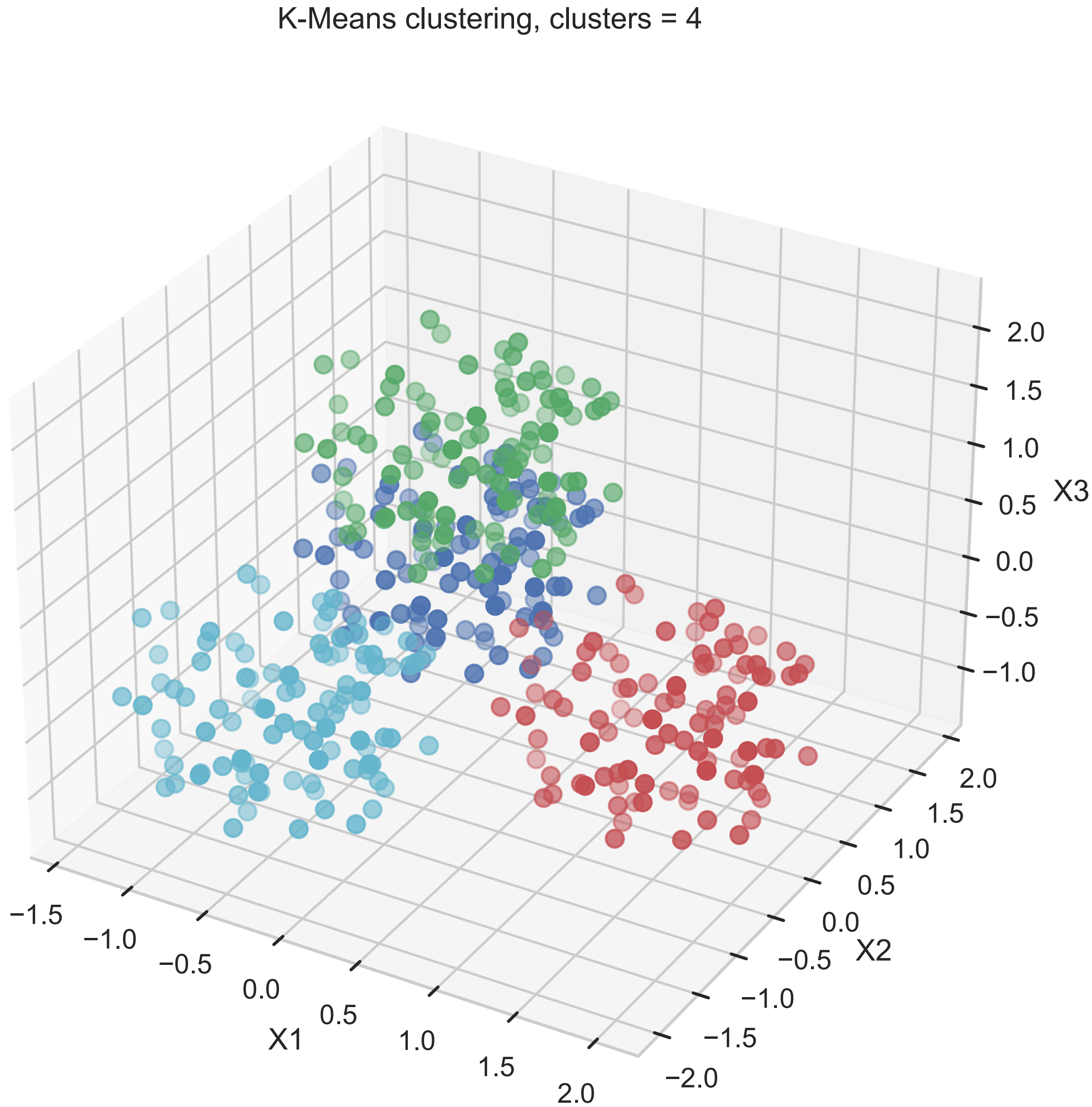


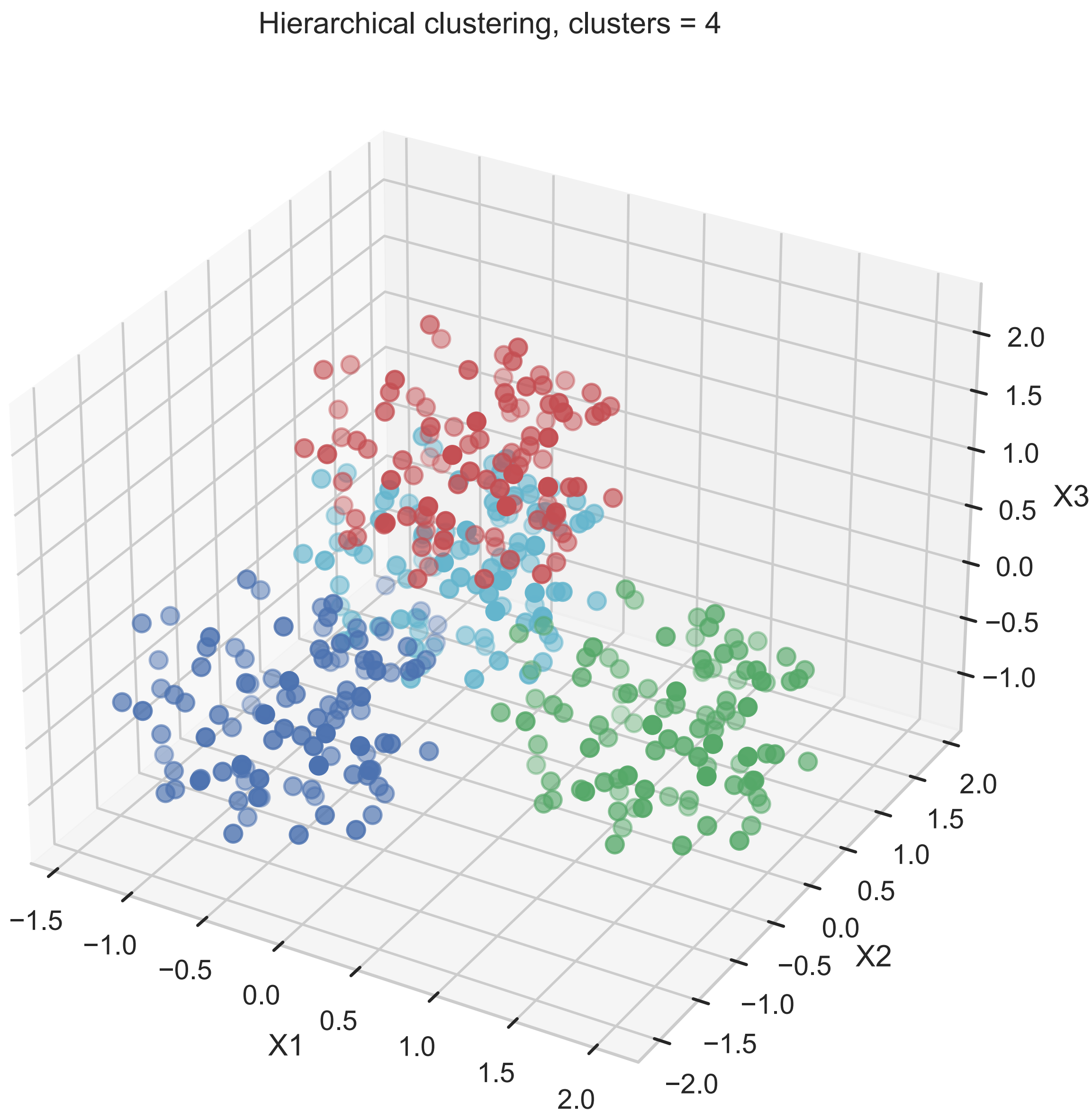

```
K-Means clustering, Purity = 0.9306930693069307
Hierarchical clustering, Purity = 0.9900990099009901
K-Means clustering, Rand = 0.5877644016112638
Hierarchical clustering, Rand = 0.7339089891331867
K-Means clustering, Mutual information score = 0.7227234211971405
Hierarchical clustering, Mutual information score = 0.8510276117074035
```

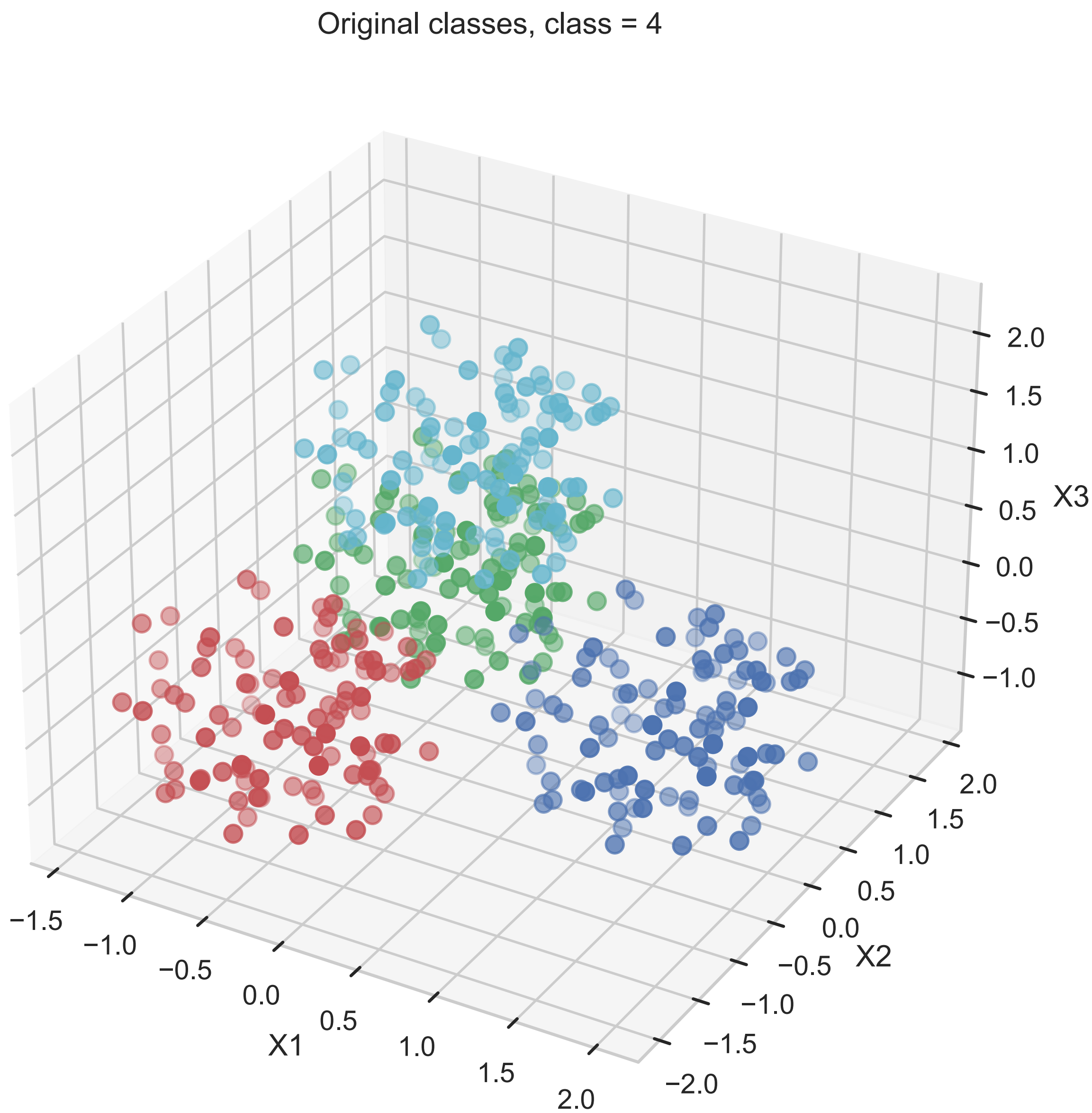
For data set 2, the metrics are all near 1, both of the algorithms perform well. Hierarchical metrics are lager than K-Means. Hierarchical performs better than K-Means.

In [21]:
```
print('For Data set 3:')
hcplot('K-Means', k3, ds3)
hcplot('Hierarchical', K3, DS3)
plotori(df3)
purity('K-Means', ds3)
purity('Hierarchical', DS3)
rand('K-Means', ds3)
rand('Hierarchical', DS3)
mutualinfo('K-Means', ds3)
mutualinfo('Hierarchical', DS3)
```

```
For Data set 3:
```


K-Means clustering, clusters = 4
X1
X2
X3
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0


Hierarchical clustering, clusters = 4
X1
X2
X3
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

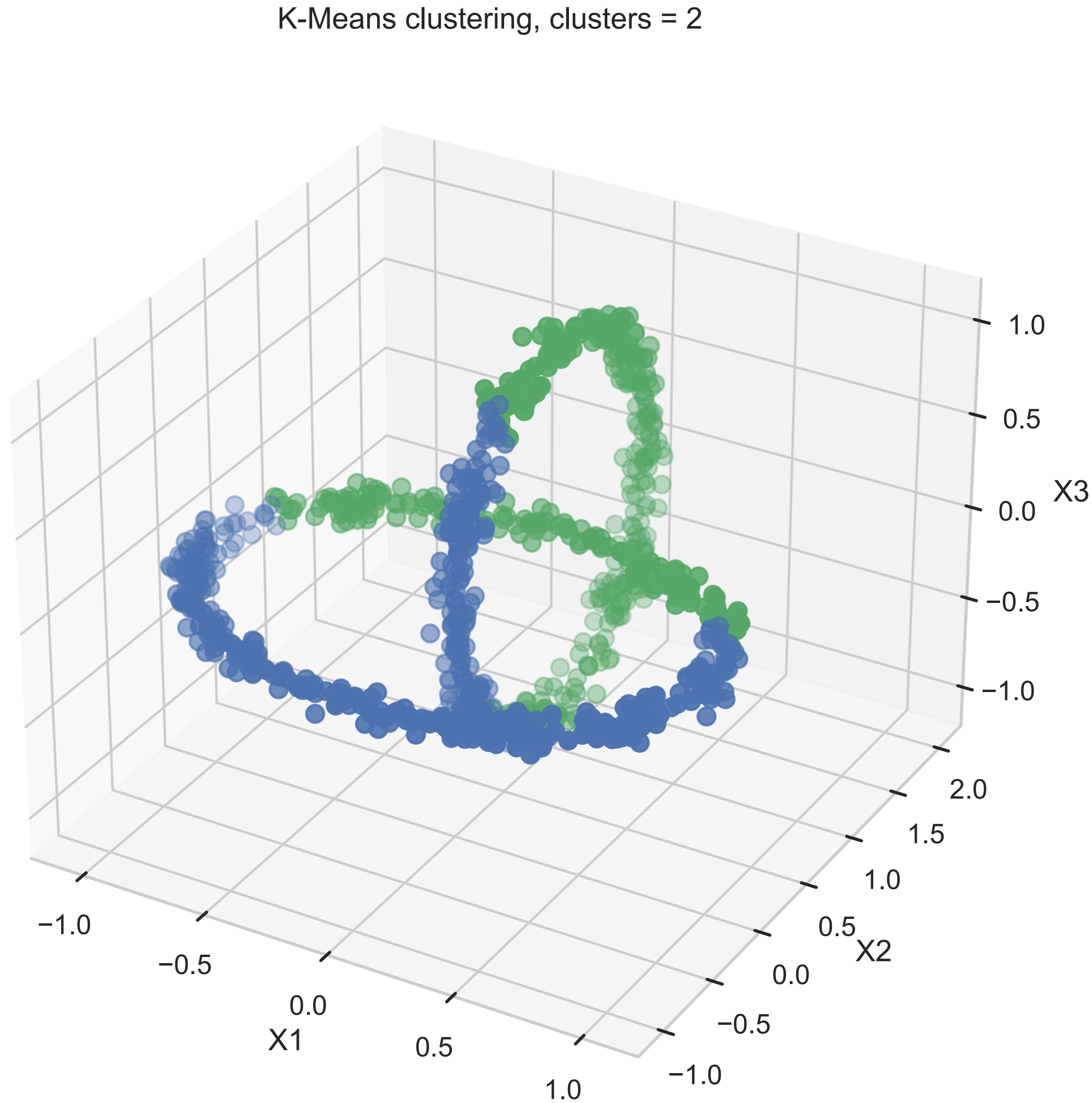


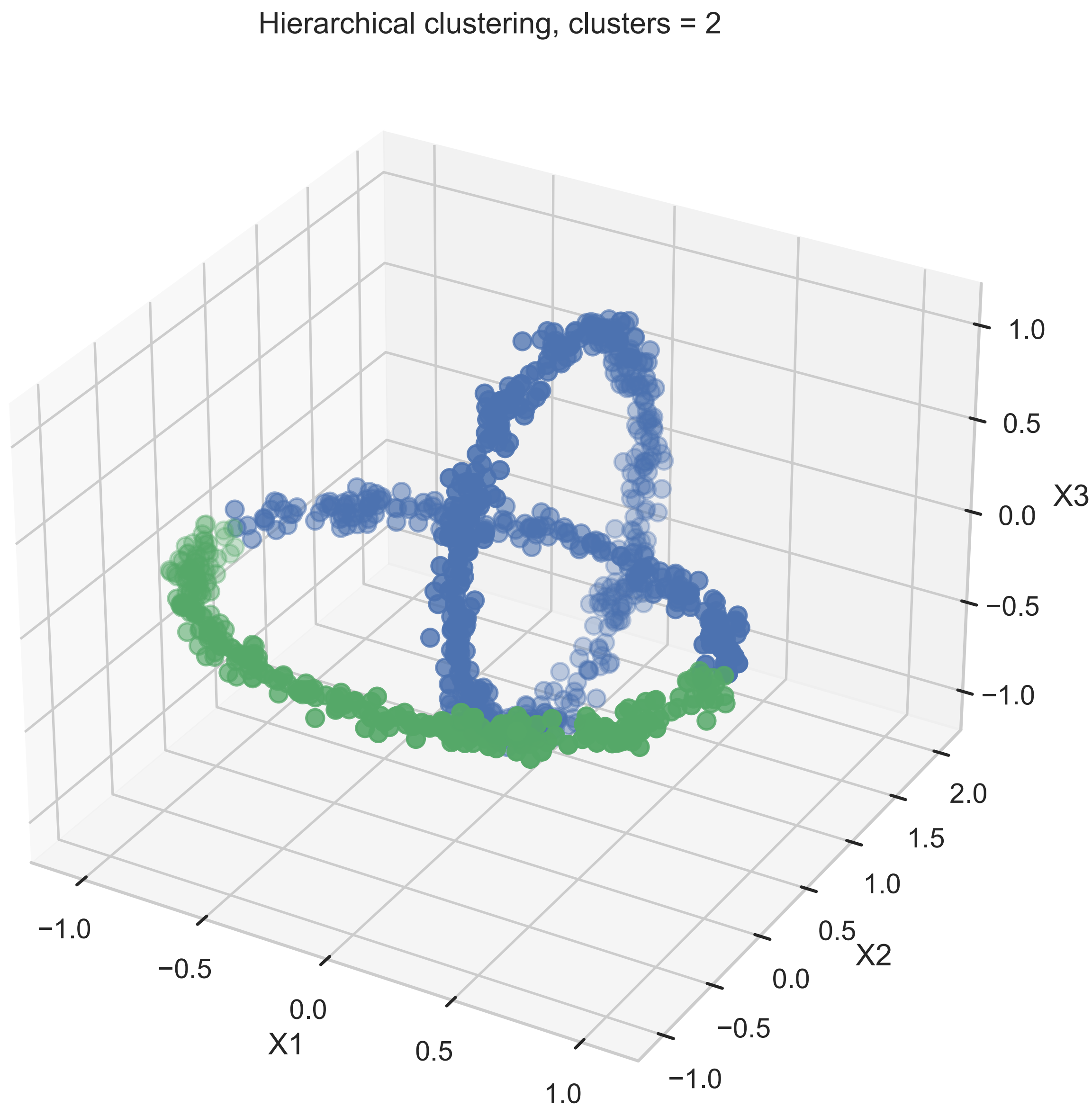

```
K-Means clustering, Purity = 1.0
Hierarchical clustering, Purity = 0.9875
K-Means clustering, Rand = 1.0
Hierarchical clustering, Rand = 0.9672676330087653
K-Means clustering, Mutual information score = 1.0
Hierarchical clustering, Mutual information score = 0.9636686786293007
```

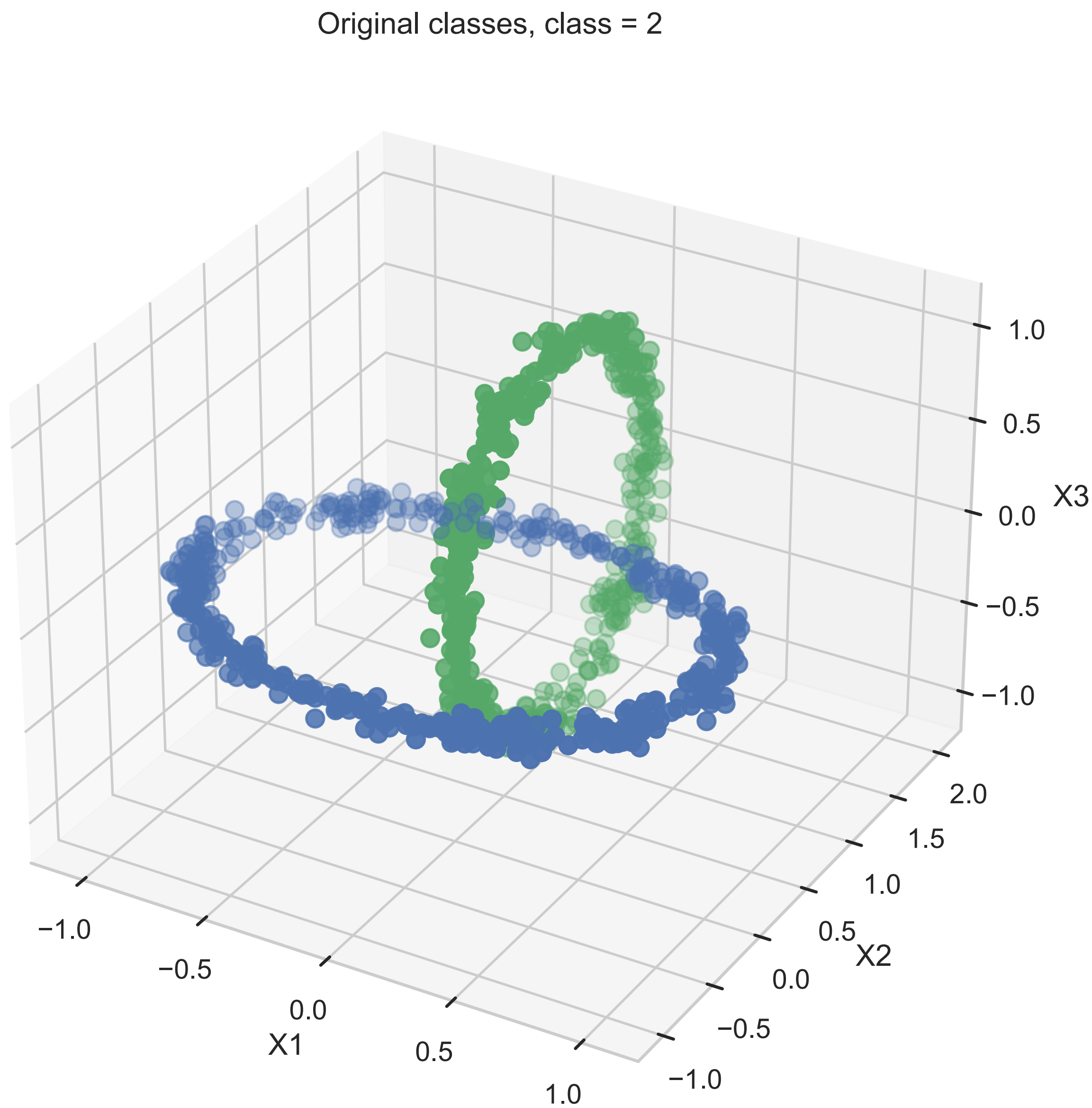
For data set 3, K-Means metrics are all 1 which means K-Means clusters are the same as the original. Hierarchical metrics are all near 1 showing an excellent performance.

In [22]:
```
print('For Data set 4:')
hcplot('K-Means', k4, ds4)
hcplot('Hierarchical', K4, DS4)
plotori(df4)
purity('K-Means', ds4)
purity('Hierarchical', DS4)
rand('K-Means', ds4)
rand('Hierarchical', DS4)
mutualinfo('K-Means', ds4)
mutualinfo('Hierarchical', DS4)
```

```
For Data set 4:
```


K-Means clustering, clusters = 2
X1
X2
X3
−1.0
−0.5
0.0
0.5
1.0
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
1.0
0.5
0.0
−0.5
−1.0


Hierarchical clustering, clusters = 2
X1
X2
X3
−1.0
−0.5
0.0
0.5
1.0
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
−1.0
−0.5
0.0
0.5
1.0



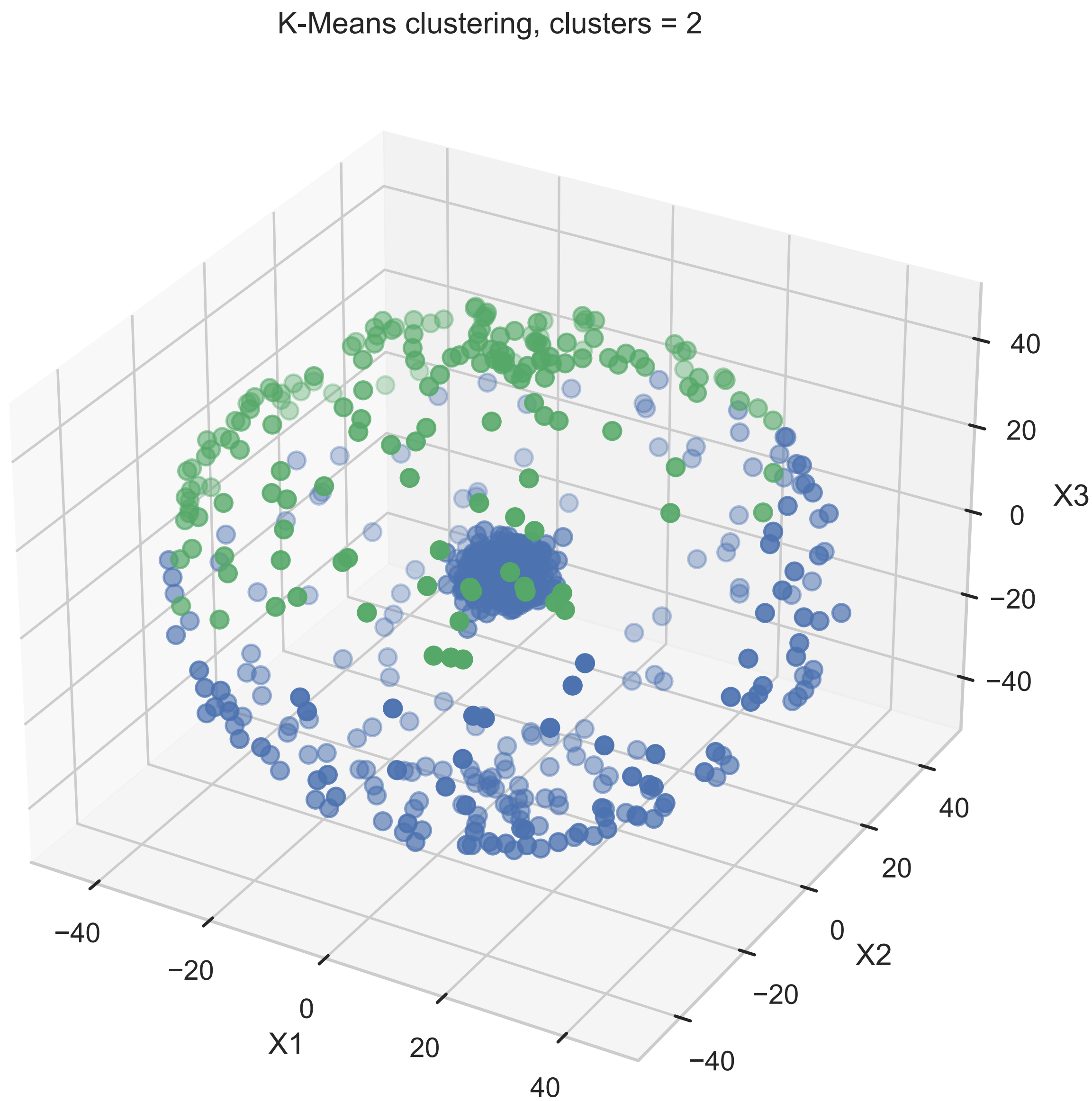

```
K-Means clustering, Purity = 0.654
Hierarchical clustering, Purity = 0.799
K-Means clustering, Rand = 0.0939570501002004
Hierarchical clustering, Rand = 0.35706442581215536
K-Means clustering, Mutual information score = 0.0688824373461325
Hierarchical clustering, Mutual information score = 0.41869902393117836
```

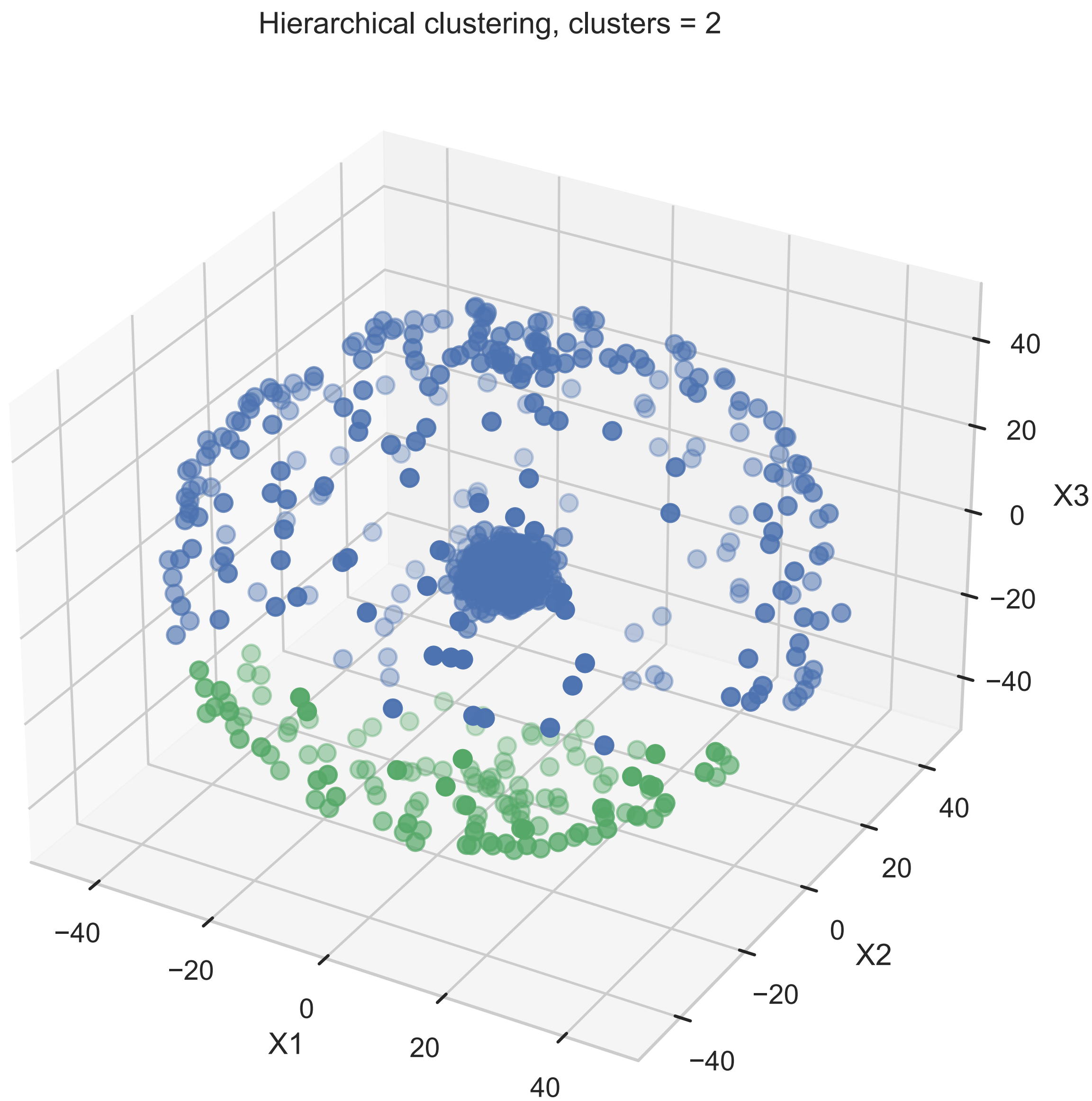
For data set 4, by the plots, we can find that neither of them perform well. The matching accuracy is low. Hierarchical is better than K-Means.

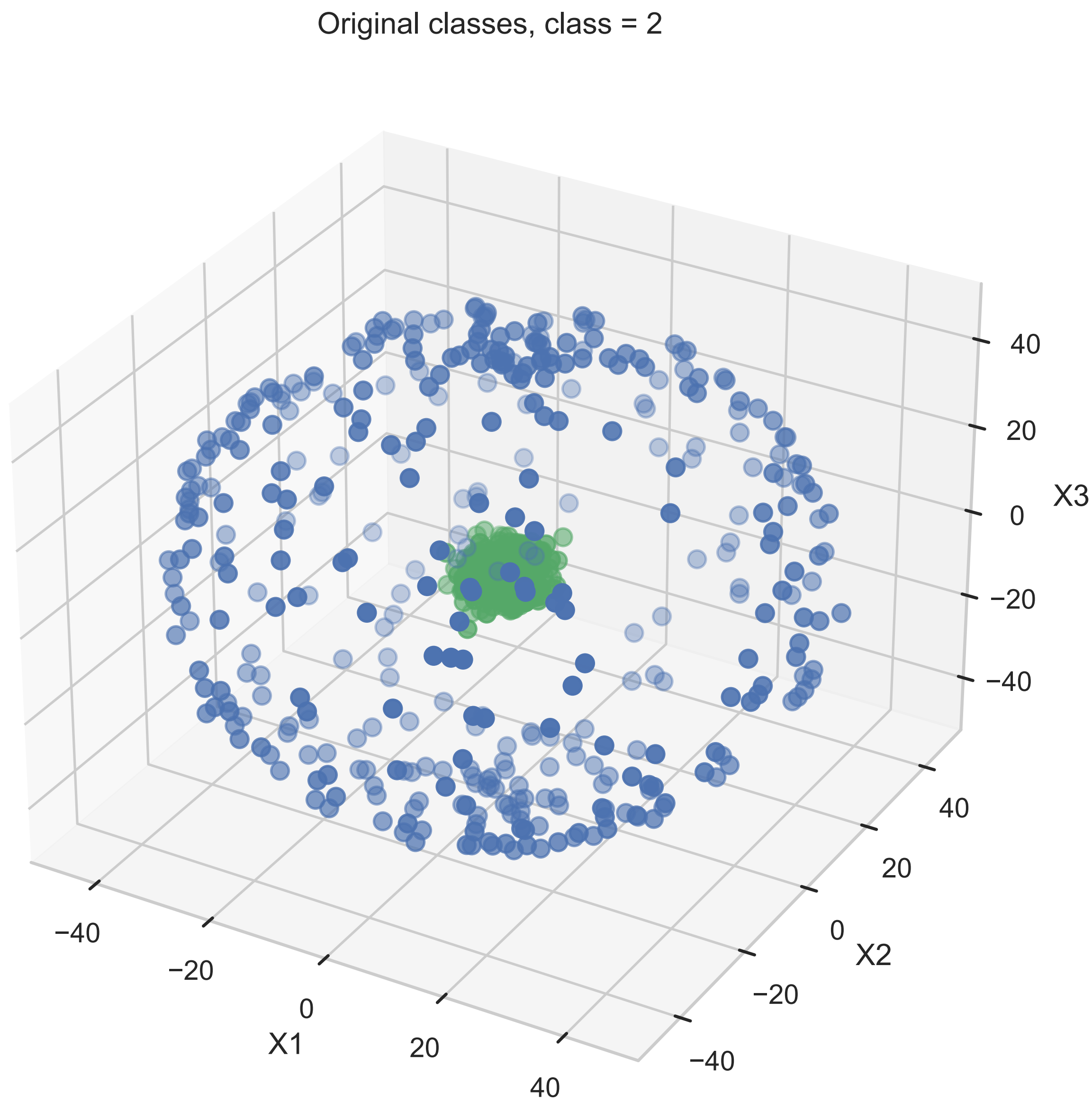
In [23]:

```
print('For Data set 5:')
hcplot('K-Means', k5, ds5)
hcplot('Hierarchical', K5, DS5)
plotori(df5)
purity('K-Means', ds5)
purity('Hierarchical', DS5)
rand('K-Means', ds5)
rand('Hierarchical', DS5)
mutualinfo('K-Means', ds5)
mutualinfo('Hierarchical', DS5)
```

```
For Data set 5:
```


K-Means clustering, clusters = 2
X1
X2
X3
−40
−20
0
20
40
−40
−20
0
20
40
40
20
0
−20
−40


Hierarchical clustering, clusters = 2
X1
X2
X3
−40
−20
0
20
40




```
K-Means clustering, Purity = 0.71375
Hierarchical clustering, Purity = 0.6575
K-Means clustering, Rand = 0.18206807775637826
Hierarchical clustering, Rand = 0.09862621818643041
K-Means clustering, Mutual information score = 0.2923037752676178
Hierarchical clustering, Mutual information score = 0.21882677576382464
```

For data set 5, by the plots, the data points around the origin are in the same class in original calsses, the others in another class. The clustering results are different from it. K-Means perform better than Hierarchical.

Task 2

Preprocess data set

In [24]:
```
df_worldindicators = pd.read_csv('World Indicators.csv')
```

In [25]:
```
sum(df_worldindicators.isnull().T.any())
len(df_worldindicators)
```

Out[25]:
```
121
```

Out[25]:
```
208
```

Find the number of empty data rows. 121 of 208 has empty data, so we fill the empty.

In [26]:
```
df_worldindicators.fillna(0,inplace=True)
```

In [27]:
```
df_worldindicators.head()
```

Out[27]:

	Birth Rate	Business Tax Rate	Days to Start Business	Energy Usage	GDP	Health Exp % GDP	Health Exp/Capita	Hours to do Tax	Infant Mortality Rate
0	0.025	72.0%	25.0	41852.0	$199,070,864,638	0.044	$233	451.0	0.023
1	0.046	52.1%	66.0	13576.0	$104,115,863,405	0.034	$178	282.0	0.107
2	0.037	65.9%	29.0	3761.0	$7,294,900,431	0.045	$34	270.0	0.060
3	0.024	19.5%	60.0	2215.0	$15,292,424,757	0.052	$404	152.0	0.039
4	0.042	43.5%	13.0	0.0	$10,395,757,480	0.064	$39	270.0	0.068

In [28]:
```
# Clean Data: convert datatype from object to float ( remove'$',',' from the da
df_worldindicators.loc[:,'Business Tax Rate'] = df_worldindicators['Business Ta
df_worldindicators.loc[:,'GDP']=df_worldindicators['GDP'].str.replace('$','').s
df_worldindicators.loc[:,'Health Exp/Capita']=df_worldindicators['Health Exp/Ca

df_worldindicators.head()
```

```
/var/folders/8n/53__nr295cb0k9fmzrhgslsh0000gn/T/ipykernel_88919/1237162006.p
y:3: FutureWarning: The default value of regex will change from True to False
in a future version. In addition, single character regular expressions will *n
ot* be treated as literal strings when regex=True.
  df_worldindicators.loc[:,'GDP']=df_worldindicators['GDP'].str.replace
('$','').str.replace(',','').astype(float)
/var/folders/8n/53__nr295cb0k9fmzrhgslsh0000gn/T/ipykernel_88919/1237162006.p
y:4: FutureWarning: The default value of regex will change from True to False
in a future version. In addition, single character regular expressions will *n
ot* be treated as literal strings when regex=True.
  df_worldindicators.loc[:,'Health Exp/Capita']=df_worldindicators['Health Ex
p/Capita'].str.replace('$','').str.replace(',','').astype(float)
```

Out[28]:

	Birth Rate	Business Tax Rate	Days to Start Business	Energy Usage	GDP	Health Exp % GDP	Health Exp/Capita	Hours to do Tax	Infant Mortality Rate	In
0	0.025	0.720	25.0	41852.0	1.990709e+11	0.044	233.0	451.0	0.023	
1	0.046	0.521	66.0	13576.0	1.041159e+11	0.034	178.0	282.0	0.107	
2	0.037	0.659	29.0	3761.0	7.294900e+09	0.045	34.0	270.0	0.060	
3	0.024	0.195	60.0	2215.0	1.529242e+10	0.052	404.0	152.0	0.039	
4	0.042	0.435	13.0	0.0	1.039576e+10	0.064	39.0	270.0	0.068	

In [29]:

```
# apply integer 1-6 to stand for 6 different regions in order to make every col
df_worldindicators.loc[df_worldindicators['Region']=='Africa','Region']=1
df_worldindicators.loc[df_worldindicators['Region']=='Europe','Region']=2
df_worldindicators.loc[df_worldindicators['Region']=='The Americas','Region']=3
df_worldindicators.loc[df_worldindicators['Region']=='Asia','Region']=4
df_worldindicators.loc[df_worldindicators['Region']=='Oceania','Region']=5
df_worldindicators.loc[df_worldindicators['Region']=='Middle East','Region']=6
```

In [30]:

```
# make several df_worldindicators(already cleaned) copies for using on later qu
df_worldindicators.fillna(0,inplace=True)
df_worldindicators_copy1 = df_worldindicators.copy()
df_worldindicators_copy2 = df_worldindicators.copy()
df_worldindicators_copy3 = df_worldindicators.copy()
```

1. Clustering

1-1 K-Means

When we use K-Means algorithm, we need to find the appropriate K value first. We plot against K to make an elbow plot to find our "inertia" values.

In [31]:

```
inertias = []
for k in range(1,15):
    kmeans = KMeans(n_clusters=k)
    kmeans.fit(df_worldindicators_copy1.drop(columns=['Country']))
    inertias.append(kmeans.inertia_)

plt.figure(figsize=(8,6))
plt.plot(range(1,15), inertias)
plt.title('Elbow method for optimal k',fontsize=20)
plt.xlabel("K (number of clusters)",fontsize=15)
plt.ylabel("SSE (Within-Cluster Distances)",fontsize=15)
plt.show()
```

Out[31]: KMeans(n_clusters=1)

Out[31]: KMeans(n_clusters=2)

Out[31]: KMeans(n_clusters=3)

Out[31]: KMeans(n_clusters=4)

Out[31]: KMeans(n_clusters=5)

Out[31]: KMeans(n_clusters=6)

Out[31]: KMeans(n_clusters=7)

Out[31]: KMeans()

Out[31]: KMeans(n_clusters=9)

Out[31]: KMeans(n_clusters=10)

Out[31]: KMeans(n_clusters=11)

Out[31]: KMeans(n_clusters=12)

Out[31]: KMeans(n_clusters=13)

Out[31]: KMeans(n_clusters=14)

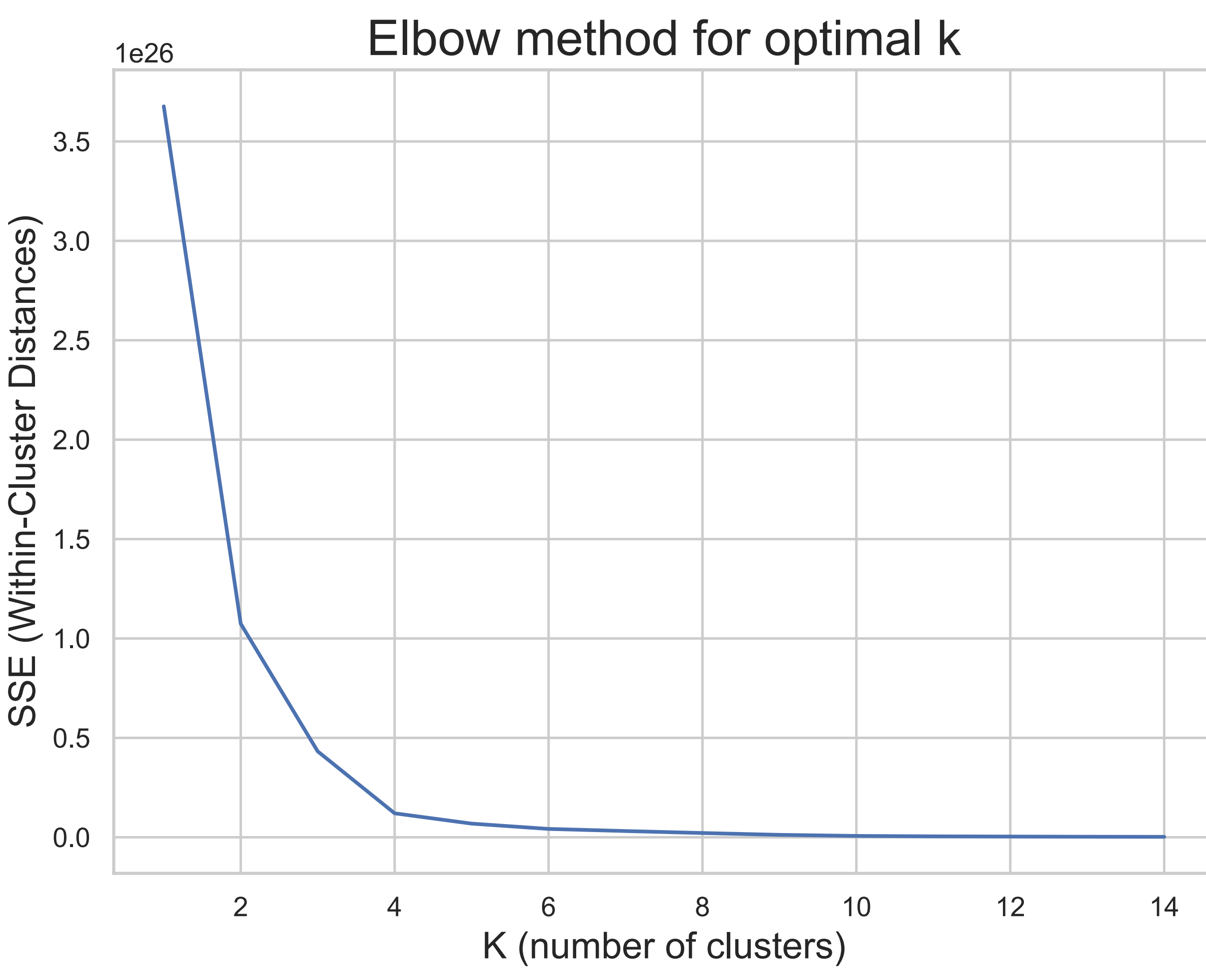
Out[31]: <Figure size 576x432 with 0 Axes>

Out[31]: [<matplotlib.lines.Line2D at 0x7ff0f2f1d970>]

Out[31]: Text(0.5, 1.0, 'Elbow method for optimal k')

Out[31]: Text(0.5, 0, 'K (number of clusters)')

Out[31]: Text(0, 0.5, 'SSE (Within-Cluster Distances)')



Looking at the plot, we can see that after K=4, the plot flattens out substantially. Therefore

4 is our "elbow" and we should probably choose K=4.

In [32]:
```
kmeans = KMeans(n_clusters=4)
pred = kmeans.fit_predict(df_worldindicators_copy1.drop(columns=['Country']))
df_worldindicators_copy1['pred']=kmeans.labels_
display(df_worldindicators_copy1.head())
display(df_worldindicators_copy1['pred'].value_counts())
```

	Birth Rate	Business Tax Rate	Days to Start Business	Energy Usage	GDP	Health Exp % GDP	Health Exp/Capita	Hours to do Tax	Infant Mortality Rate	In
0	0.025	0.720	25.0	41852.0	1.990709e+11	0.044	233.0	451.0	0.023	
1	0.046	0.521	66.0	13576.0	1.041159e+11	0.034	178.0	282.0	0.107	
2	0.037	0.659	29.0	3761.0	7.294900e+09	0.045	34.0	270.0	0.060	
3	0.024	0.195	60.0	2215.0	1.529242e+10	0.052	404.0	152.0	0.039	
4	0.042	0.435	13.0	0.0	1.039576e+10	0.064	39.0	270.0	0.068	

5 rows × 21 columns

```
0    193
2     12
3      2
1      1
Name: pred, dtype: int64
```

1-2 Hierarchical clustering

In [33]:
```
def plot_dendrogram(model, **kwargs):
    # Create linkage matrix and then plot the dendrogram

    # create the counts of samples under each node
    counts = np.zeros(model.children_.shape[0])
    n_samples = len(model.labels_)
    for i, merge in enumerate(model.children_):
        current_count = 0
        for child_idx in merge:
            if child_idx < n_samples:
                current_count += 1  # leaf node
            else:
                current_count += counts[child_idx - n_samples]
        counts[i] = current_count

    linkage_matrix = np.column_stack(
        [model.children_, model.distances_, counts]
    ).astype(float)

    # Plot the corresponding dendrogram
    dendrogram(linkage_matrix, **kwargs)
```

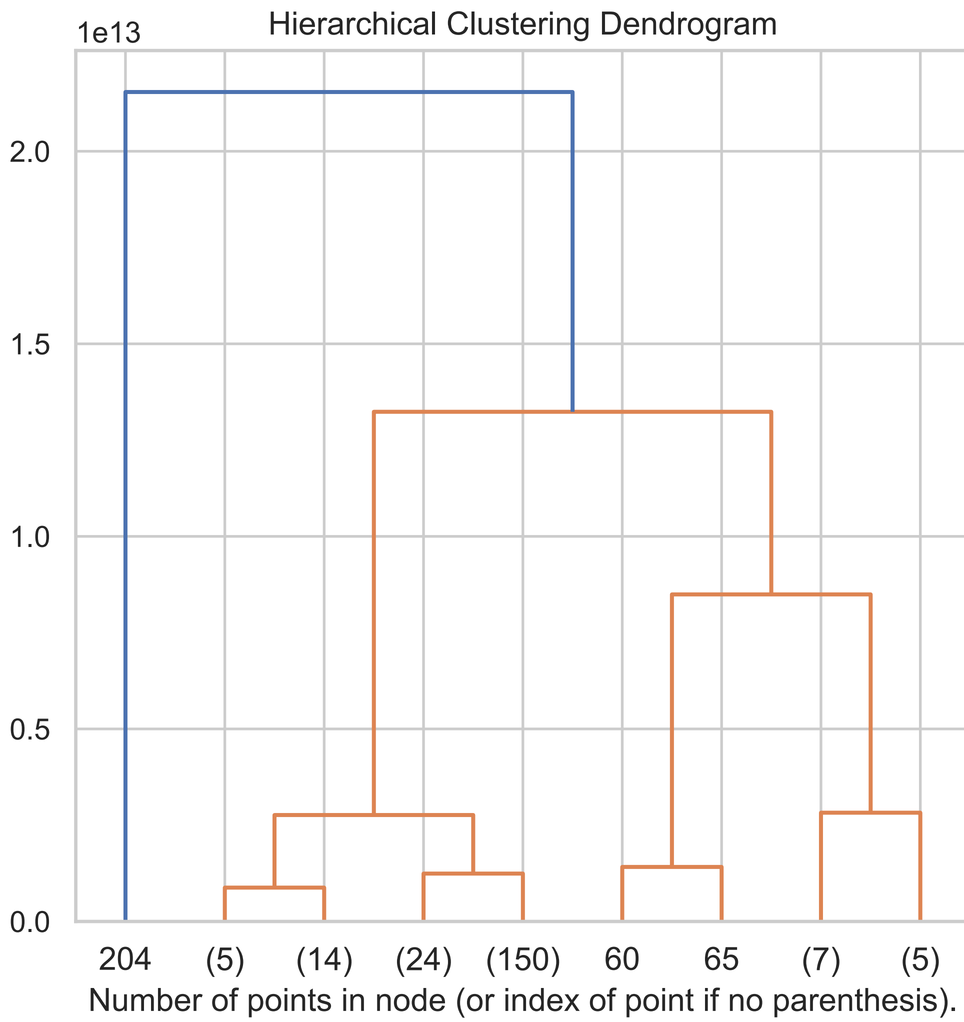
In [34]:
```
model = AgglomerativeClustering(distance_threshold=0, n_clusters=None)
model = model.fit(df_worldindicators_copy2.drop(columns=['Country']))
plt.figure(figsize=(6,6))
plt.title("Hierarchical Clustering Dendrogram")
```

```
# plot the top three levels of the dendrogram
plot_dendrogram(model, truncate_mode="level", p=3)
plt.xlabel("Number of points in node (or index of point if no parenthesis).")
plt.show()
```

Out[34]: <Figure size 432x432 with 0 Axes>

Out[34]: Text(0.5, 1.0, 'Hierarchical Clustering Dendrogram')

Out[34]: Text(0.5, 0, 'Number of points in node (or index of point if no parenthesis).')



As shown in the K-Means approach as well, we can see a huge decrease in the distance metric when going from 1 to 2, 2 to 3 and 3 to 4. After 4 clusters, the decrease trend becomes quite smooth, so k=4 should be answer.

In [35]:
```
model = AgglomerativeClustering(distance_threshold=None, n_clusters=4)
pred = model.fit_predict(df_worldindicators_copy2.drop(columns=['Country']))
```

In [36]:
```
df_worldindicators_copy2['pred'] = pred
display(df_worldindicators_copy2.head())
display(df_worldindicators_copy2['pred'].value_counts())
```

	Birth Rate	Business Tax Rate	Days to Start Business	Energy Usage	GDP	Health Exp % GDP	Health Exp/Capita	Hours to do Tax	Infant Mortality Rate	In
0	0.025	0.720	25.0	41852.0	1.990709e+11	0.044	233.0	451.0	0.023	
1	0.046	0.521	66.0	13576.0	1.041159e+11	0.034	178.0	282.0	0.107	
2	0.037	0.659	29.0	3761.0	7.294900e+09	0.045	34.0	270.0	0.060	
3	0.024	0.195	60.0	2215.0	1.529242e+10	0.052	404.0	152.0	0.039	
4	0.042	0.435	13.0	0.0	1.039576e+10	0.064	39.0	270.0	0.068	

5 rows × 21 columns

```
2    193
0     12
1      2
3      1
Name: pred, dtype: int64
```

2. Internal validation

SSE

$$SSE(C_i) = \sum_{x \in C_i} d(c_i, x)^2 = \frac{1}{2m_i} \sum_{x \in C_i} \sum_{y \in C_i} d(x, y)^2$$

where x is an example in the cluster, c_i is a cluster representative, m_i is the number of examples in cluster C_i.
Smaller SSE indicates better performance.

In [37]:
```
kmeans = KMeans(n_clusters=4)
kmeans.fit(df_worldindicators_copy3.drop(columns=['Country']))
kmeans.inertia_
```

Out[37]:
```
KMeans(n_clusters=4)
```

Out[37]:
```
1.2056190641452904e+25
```

Silhouetter Coefficient

the average distance a_i:

$$a(i) = \frac{1}{|C_a|} \sum_{j \in C_a, i \neq j} d(i, j)$$

the minimum average distance b_i:

$$b(i) = \min_{C_b \neq C_a} \frac{1}{|C_b|} \sum_{j \in C_b} d(i, j)$$

Sihouette Coefficient:

$$s(i) = \frac{b(i) - a(i)}{max\{a(i), b(i)\}}$$

In [38]:
```
metrics.silhouette_score(df_worldindicators_copy3.drop(columns=['Country']),kme
```

Out[38]:
```
0.8910544567101041
```

the SHC metric(0.89) is close to 1, so the quality of this cluster method is excellent!

Dunn Index

The lowest intercluster distance divided by the highest intracluster distance:

$$DI_m = \frac{min_{1 \le i < j \le m} \delta(C_i, C_j)}{\max_{1 \le k \le m} \Delta k}$$

In [39]:
```
from validclust import dunn
dunn(metrics.pairwise_distances(df_worldindicators_copy3.drop(columns=['Country
```

Out[39]:
```
0.1318757876803419
```

3. Clustering solutions and detailed list

In [40]:
```
country_list = df_worldindicators_copy1['Country']
pred_list = df_worldindicators_copy1['pred']
```

In [41]:
```
# set 4 lists to store 4 kinds of countries
list1 = []
list2 = []
list3 = []
list4 = []
```

In [42]:
```
def detailed_list(country_list,pred_list):
    dict_report = {'cat1':list1,'cat2':list2,'cat3':list3,'cat4':list4}
    for i,pred in enumerate(pred_list):
        if pred==0:
            list1.append(country_list[i])
        if pred==1:
            list2.append(country_list[i])
        if pred==2:
            list3.append(country_list[i])
        if pred==3:
            list4.append(country_list[i])
    return dict_report
```

In [43]:
```
detailed = detailed_list(country_list,pred_list)
len(detailed)
```

Out[43]:
```
4
```

In [44]:
```
cat1 = detailed['cat1']
cat2 = detailed['cat2']
cat3 = detailed['cat3']
cat4 = detailed['cat4']
print(f'Cluster 1 contains {cat1}\n')
print(f'Cluster 2 contains {cat2}\n')
print(f'Cluster 3 contains {cat3}\n')
print(f'Cluster 4 contains {cat4}\n')
```

```
Cluster 1 contains ['Algeria', 'Angola', 'Benin', 'Botswana', 'Burkina Faso',
'Burundi', 'Cameroon', 'Central African Republic', 'Chad', 'Comoros', 'Congo,
Dem. Rep.', 'Congo, Rep.', "Cote d'Ivoire", 'Djibouti', 'Egypt, Arab Rep.', 'E
quatorial Guinea', 'Eritrea', 'Ethiopia', 'Gabon', 'Gambia, The', 'Ghana', 'Gu
inea', 'Guinea-Bissau', 'Kenya', 'Lesotho', 'Liberia', 'Libya', 'Madagascar',
'Malawi', 'Mali', 'Mauritania', 'Mauritius', 'Morocco', 'Mozambique', 'Namibi
a', 'Niger', 'Nigeria', 'Rwanda', 'Sao Tome and Principe', 'Senegal', 'Seychel
les', 'Sierra Leone', 'Somalia', 'South Africa', 'South Sudan', 'Sudan', 'Swaz
iland', 'Tanzania', 'Togo', 'Tunisia', 'Uganda', 'Zambia', 'Zimbabwe', 'Afghan
istan', 'Armenia', 'Azerbaijan', 'Bangladesh', 'Bhutan', 'Brunei Darussalam',
'Cambodia', 'Georgia', 'Hong Kong SAR, China', 'Indonesia', 'Kazakhstan', 'Kor
ea, Dem. Rep.', 'Kyrgyz Republic', 'Lao PDR', 'Macao SAR, China', 'Malaysia',
'Maldives', 'Mongolia', 'Myanmar', 'Nepal', 'Pakistan', 'Philippines', 'Singap
ore', 'Sri Lanka', 'Tajikistan', 'Thailand', 'Timor-Leste', 'Turkmenistan', 'U
zbekistan', 'Vietnam', 'Albania', 'Andorra', 'Austria', 'Belarus', 'Belgium',
'Bosnia and Herzegovina', 'Bulgaria', 'Croatia', 'Cyprus', 'Czech Republic',
'Denmark', 'Estonia', 'Faeroe Islands', 'Finland', 'Greece', 'Hungary', 'Icela
nd', 'Ireland', 'Isle of Man', 'Kosovo', 'Latvia', 'Liechtenstein', 'Lithuani
a', 'Luxembourg', 'Macedonia, FYR', 'Malta', 'Moldova', 'Monaco', 'Montenegr
o', 'Netherlands', 'Norway', 'Poland', 'Portugal', 'Romania', 'San Marino', 'S
erbia', 'Slovak Republic', 'Slovenia', 'Sweden', 'Switzerland', 'Turkey', 'Ukr
aine', 'Bahrain', 'Iran, Islamic Rep.', 'Iraq', 'Israel', 'Jordan', 'Kuwait',
'Lebanon', 'Oman', 'Qatar', 'Saudi Arabia', 'Syrian Arab Republic', 'United Ar
ab Emirates', 'Yemen, Rep.', 'American Samoa', 'Fiji', 'French Polynesia', 'Gu
am', 'Kiribati', 'Marshall Islands', 'Micronesia, Fed. Sts.', 'New Caledonia',
'New Zealand', 'Papua New Guinea', 'Samoa', 'Solomon Islands', 'Tonga', 'Vanua
tu', 'Antigua and Barbuda', 'Argentina', 'Aruba', 'Bahamas, The', 'Barbados',
'Belize', 'Bermuda', 'Bolivia', 'Cayman Islands', 'Chile', 'Colombia', 'Costa
Rica', 'Cuba', 'Curacao', 'Dominica', 'Dominican Republic', 'Ecuador', 'El Sal
vador', 'Greenland', 'Grenada', 'Guatemala', 'Guyana', 'Haiti', 'Honduras', 'J
amaica', 'Nicaragua', 'Panama', 'Paraguay', 'Peru', 'Puerto Rico', 'Sint Maart
en (Dutch part)', 'St. Kitts and Nevis', 'St. Lucia', 'St. Martin (French par
t)', 'St. Vincent and the Grenadines', 'Suriname', 'Trinidad and Tobago', 'Tur
ks and Caicos Islands', 'Uruguay', 'Venezuela, RB', 'Virgin Islands (U.S.)']

Cluster 2 contains ['United States']

Cluster 3 contains ['India', 'Korea, Rep.', 'France', 'Germany', 'Italy', 'Rus
sian Federation', 'Spain', 'United Kingdom', 'Australia', 'Brazil', 'Canada',
'Mexico']

Cluster 4 contains ['China', 'Japan']
```

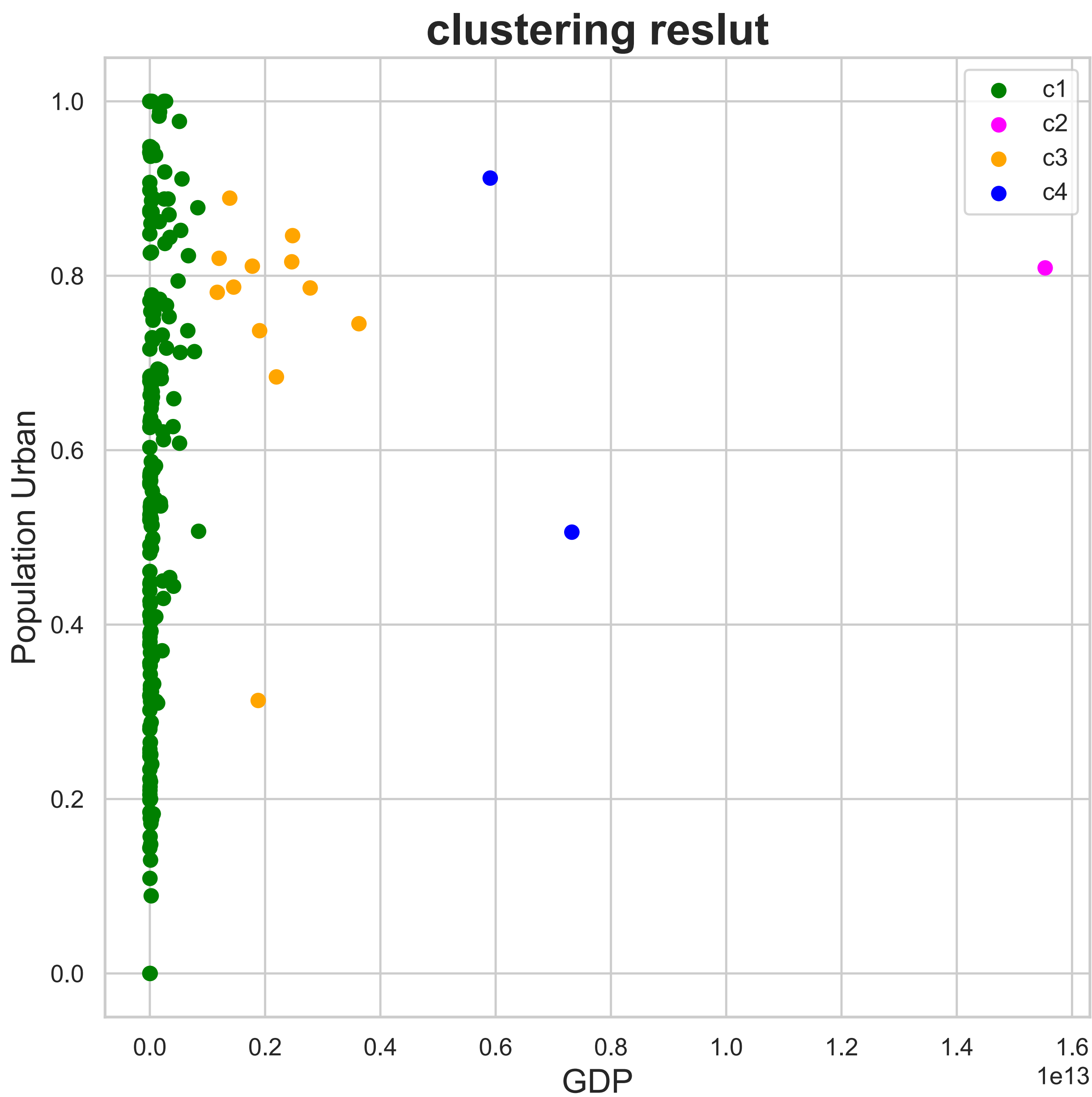
Scatter plot

In [45]:
```
def vsplot(column1,column2):
    plt.figure(figsize=(8,8))
    df1 = df_worldindicators_copy1[df_worldindicators_copy1['pred']==0]
```

```
    df2 = df_worldindicators_copy1[df_worldindicators_copy1['pred']==1]
    df3 = df_worldindicators_copy1[df_worldindicators_copy1['pred']==2]
    df4 = df_worldindicators_copy1[df_worldindicators_copy1['pred']==3]
    plt.scatter(df1[column1],df1[column2],color='green')
    plt.scatter(df2[column1],df2[column2],color='magenta')
    plt.scatter(df3[column1],df3[column2],color='orange')
    plt.scatter(df4[column1],df4[column2],color='blue')
    plt.title("clustering reslut",fontweight='bold',fontsize=20)
    plt.xlabel(column1,fontsize=15)
    plt.ylabel(column2,fontsize=15)
    plt.legend(('c1','c2','c3','c4'),loc='best')
    plt.show()
```

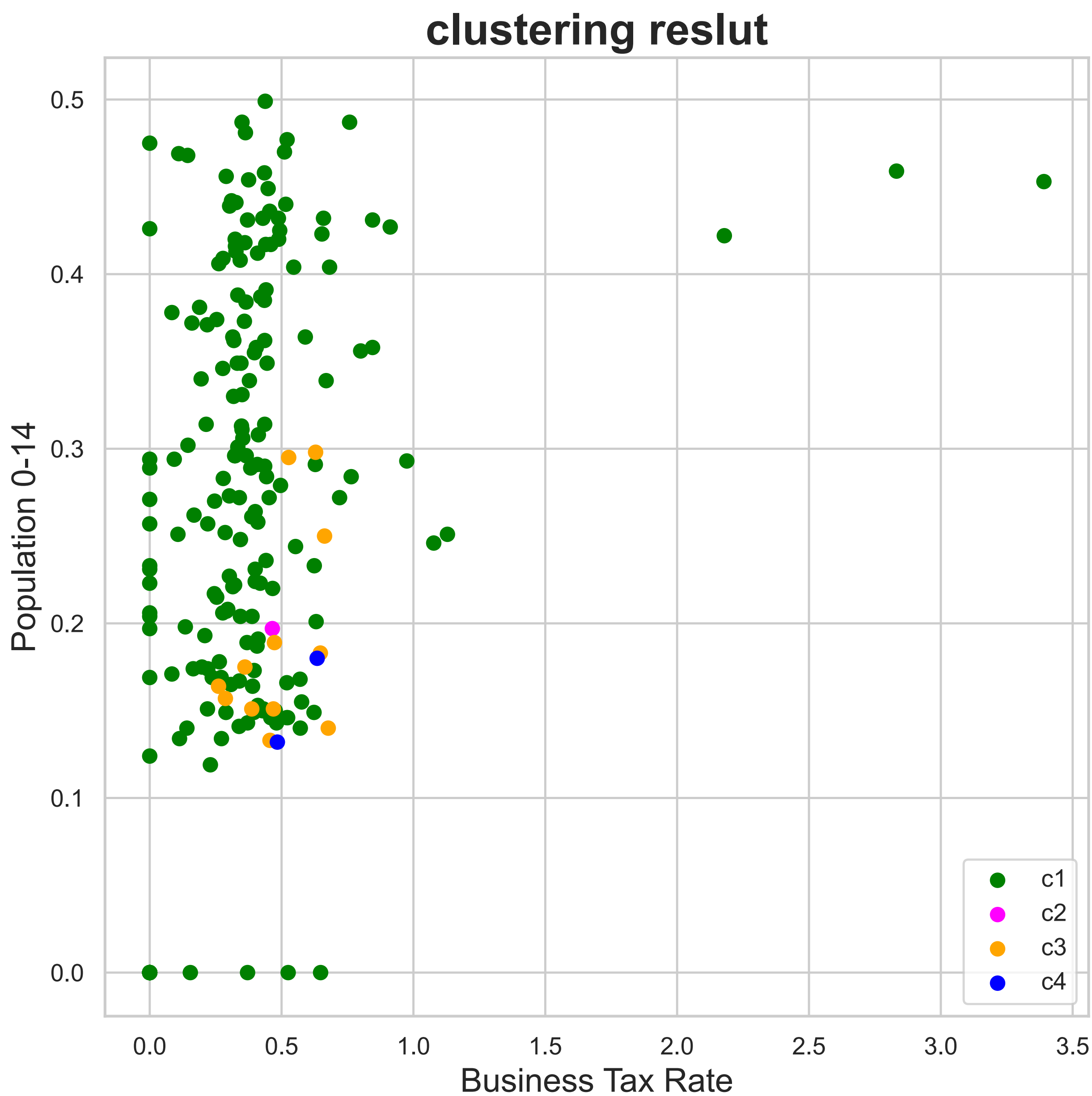
Population urban VS GDP

In [46]:
```
vsplot('GDP','Population Urban')
```



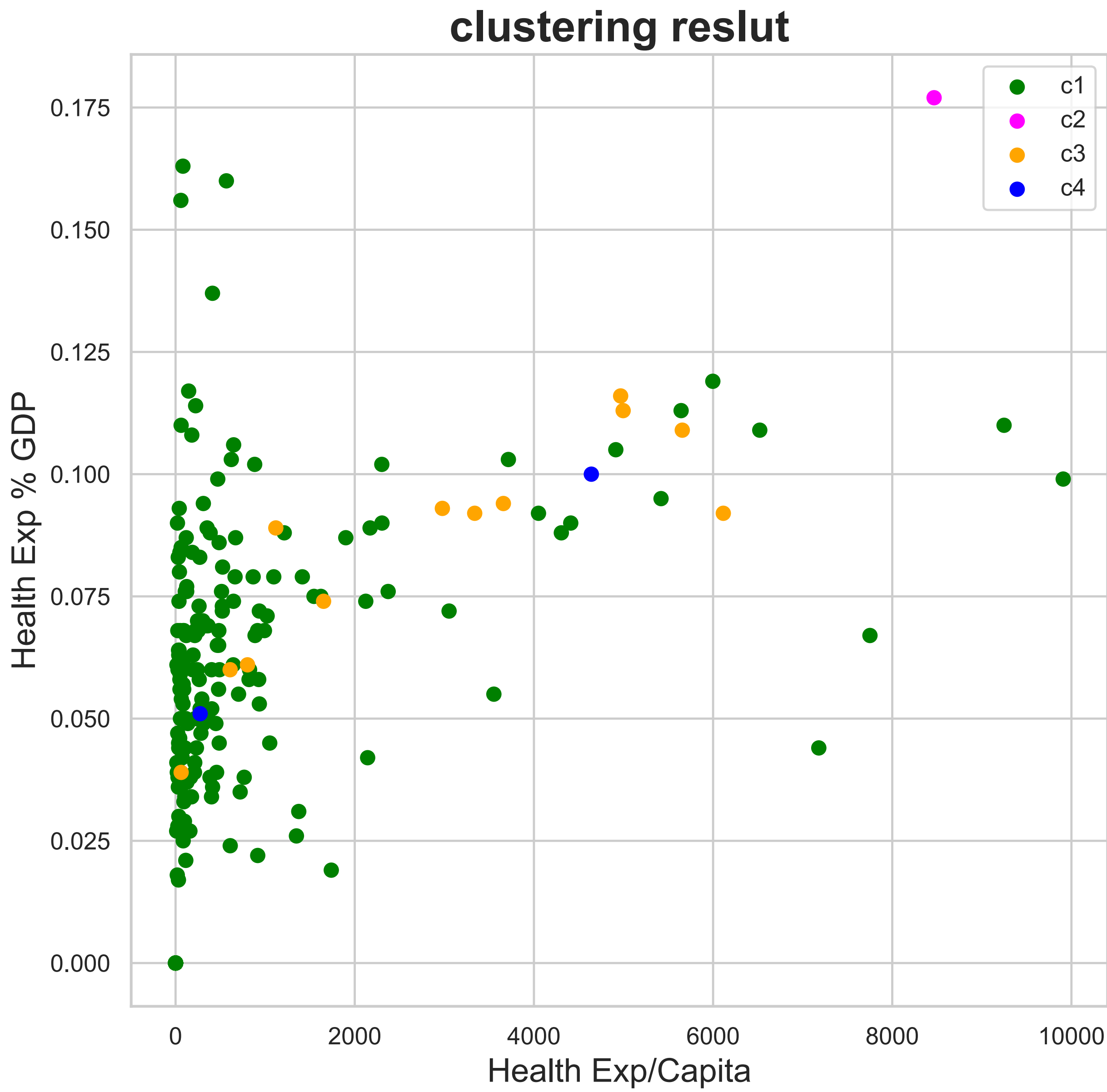
Business Tax Rate vs Population 0-14

In [47]:
```
vsplot('Business Tax Rate','Population 0-14')
```



Health Exp/Capita vs Health Exp % GDP

In [48]:
```
vsplot('Health Exp/Capita','Health Exp % GDP')
```


clustering reslut
Health Exp % GDP
Health Exp/Capita
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
0
2000
4000
6000
8000
10000
c1
c2
c3
c4

In [ ]: