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Project Title - Understanding Ego Graph for Structural Profiling through Clustering

Introduction

The objective of this project is to use machine learning techniques to explore the complex world of graph analysis, with a focus on clustering based on the local properties of nodes. The primary goal is to analyze and cluster ego graphs obtained from a social network dataset. Ego graphs represent the neighborhood of individual users within a larger social network. The goal was to identify and group similar ego graphs based on their structural properties, hence uncovering cohorts of individuals with similar characteristics or interests. This project has great potential in a variety of domains, including targeted marketing campaigns, community detection initiatives, and a deeper comprehension of complex social dynamics.

This report summarizes the problem, our approach, experiments conducted, and conclusions drawn.

Data

Dataset Description

This dataset consists of 'circles' (or 'friends lists') from Facebook. Facebook data was collected from survey participants using this Facebook app.

- We utilized the "Facebook Combined" dataset from the Stanford SNAP repository. Link https://snap.stanford.edu/data/ego-Facebook.html
- The dataset contains ego graphs of Facebook users, representing their friends and connections.
- · Each ego graph is represented as an adjacency list.
- Facebook data has been anonymized by replacing the Facebook-internal ids for each user with a new value. Also, while feature vectors from this dataset have been provided, the interpretation of those features has been obscured.

```
# Installing dependency
!pip install networkx # Installing NetworkX library
!pip install pycaret --upgrade # Installing Pycaret
# Loading the dependencies
import numpy as np
import pandas as pd
import networkx as nx
import matplotlib.pyplot as plt
import seaborn as sns
%matplotlib inline
from sklearn.preprocessing import MinMaxScaler
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import silhouette score
from sklearn.cluster import KMeans, AgglomerativeClustering, DBSCAN
from sklearn.metrics import silhouette_score, calinski_harabasz_score, davies_bouldin_score
from sklearn.decomposition import PCA
from pycaret.clustering import *
import itertools
from itertools import combinations # Import the 'combinations' function
from sklearn.decomposition import PCA
from scipy import stats
def warn(*args, **kwargs):
   pass
import warnings
warnings.warn = warn
```

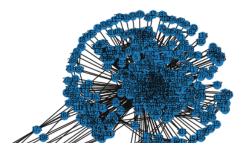
▼ EDA and Data Preprocessing

- · Load the dataset
- · Perform Exploratory Data Analyis on the loaded data
- · Handle missing data by removing nodes with incomplete information.
- Remove isolated nodes as they did not provide meaningful information for clustering.
- · Convert it into a ego graph for each node for analysis using NetworkX.

```
# Define the path to the dataset
#dataset_path = '/content/facebook_combined.txt'
# Load or create your social engineering graph (replace G with your data)
G = nx.Graph()
with open('/content/facebook_combined.txt','r') as file:
  for line in file:
   line = line.strip()
                            # Remove leading/trailing whitespace and new line characters
   line = line.split(' ')  #split the line up into a list - the first entry will be the node, the others his friends
                            #in case the node has no friends, we should still add him to the network
    if len(line)==1:
       if line[0] not in G:
               nx.add_node(int(line[0]))
    else:
                          #in case the node has friends, loop over all the entries in the list
        focal_node = int(line[0]) #pick your node
        for friend in line[1:]:
                                   #loop over the friends
            G.add edge(focal node,int(friend))
                                                               #add each edge to the graph
# Load the dataset into a NetworkX graph
#G = nx.read_edgelist(dataset_path)
# Basic data exploration
print(f"Number of nodes: {len(G.nodes)}")
print(f"Number of edges: {len(G.edges)}")
# Visualize a subset of the graph (e.g., first 500 nodes)
subset_nodes = list(G.nodes)[:500]
# Create a subgraph containing only the subset of nodes and their edges
subset graph = G.subgraph(subset nodes)
# Visualize the subset of the graph
pos = nx.spring_layout(subset_graph, seed=42) # Layout for visualization
nx.draw(subset_graph, pos, with_labels=True, node_size=100, font_size=8)
plt.title('Subset of the Graph')
plt.show()
```

Number of nodes: 4039 Number of edges: 88234

Subset of the Graph



→ Preprocessing:

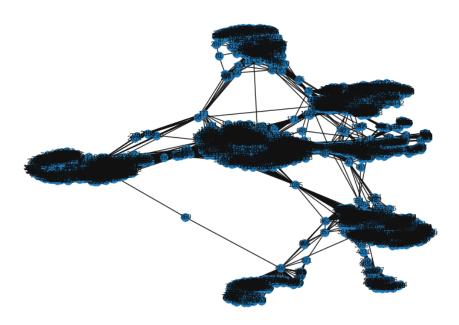


```
# 1. Removing isolated nodes (nodes with degree 0)
isolated_nodes = [node for node in G.nodes if G.degree(node) == 0]
G.remove_nodes_from(isolated_nodes)

# 2. Handling missing data
# Identify nodes with missing edges by checking if their neighbor list is empty.
# Remove nodes with missing edges using G.remove_nodes_from(missing_nodes).

missing_nodes = [node for node in G.nodes if len(list(G.neighbors(node))) == 0]
G.remove_nodes_from(missing_nodes)
```

Filtered Graph (Degree >= 5)



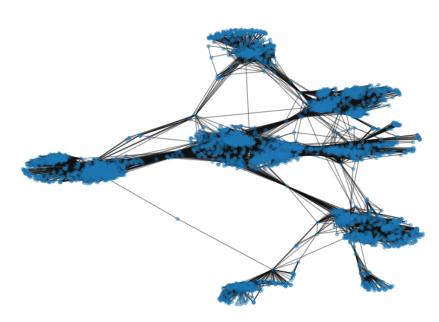
```
print(f"Number of nodes: {len(G.nodes)}")
print(f"Number of edges: {len(G.edges)}")
```

Number of nodes: 4039 Number of edges: 88234

Outlier Removal

```
# Calculate Z-scores for the graph data
z_scores = np.abs(stats.zscore(G))
# Define a threshold for identifying outliers (e.g., nodes with Z-scores > 3)
threshold = 3
# Identify outlier nodes based on Z-scores
outliers = [node for node, z_score in enumerate(z_scores) if np.any(z_score > threshold)]
# Create a scatter plot to visualize the outlier nodes
pos = nx.spring_layout(G, seed=42) # Layout for visualization
# Draw the entire graph
nx.draw(G, pos, with_labels=False, node_size=20, alpha=0.5)
# Highlight outlier nodes with a different color
nx.draw(G.subgraph(outliers), pos, with_labels=False, node_size=50, node_color='red')
plt.title('Visualization of Outlier Nodes')
plt.show()
# Remove outlier nodes and their edges from the original graph
filtered_G = G.copy()
filtered_G.remove_nodes_from(outliers)
# Now, 'filtered_G' contains the original graph with outlier nodes removed
```

Visualization of Outlier Nodes



```
print(f"Number of nodes: {len(filtered_G.nodes)}")
print(f"Number of edges: {len(filtered_G.edges)}")
```

Number of nodes: 4039 Number of edges: 88234

→ Create Ego Graph for all nodes

Definations

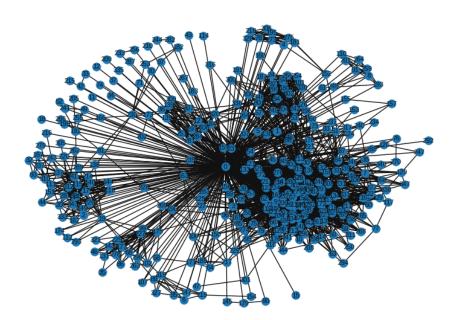
"**Ego**" is an individual "focal" node. A network has as many egos as it has nodes. Egos can be persons, groups, organizations, or whole societies

"Neighborhood" is the collection of ego and all nodes to whom ego has a connection at some path length. In social network analysis, the "neighborhood" is almost always one-step; that is, it includes only ego and actors that are directly adjacent. The neighborhood also includes all of the ties among all of the actors to whom ego has a direct connection. The boundaries of ego networks are defined in terms of neighborhoods.

```
# Create an empty dictionary to store ego networks
ego networks = {}
# Iterate through each node in the graph
for node in filtered G.nodes():
   \# Create the ego network for the current node with 1-hop neighbors
   ego_network = nx.ego_graph(filtered_G, node)
    # Store the ego network in the dictionary with the node as the key
    ego networks[node] = ego network
# Basic data exploration of ego_graph
for node in range(2):
   print(f"Ego Network for Node {node}:")
   print("Nodes:", ego_networks[node].nodes())
   print("Edges:", ego_networks[node].edges())
   print()
   # Visualization of ego graph
   pos = nx.spring_layout(ego_networks[node], seed=42) # Layout for visualization
   nx.draw(ego_networks[node], pos, with_labels=True, node_size=100, font_size=8)
   plt.title(f'Ego Graph')
   plt.show()
```

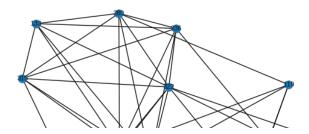
```
Ego Network for Node 0:
Nodes: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 3]
Edges: [(0, 1), (0, 2), (0, 3), (0, 4), (0, 5), (0, 6), (0, 7), (0, 8), (0, 9), (0, 10)
```

Ego Graph



```
Ego Network for Node 1:
Nodes: [0, 1, 194, 280, 322, 133, 73, 299, 236, 48, 53, 54, 119, 88, 346, 315, 92,
Edges: [(0, 1), (0, 48), (0, 53), (0, 54), (0, 73), (0, 88), (0, 92), (0, 119), (0
```

Ego Graph



Feature Engineering

Define and extract local node features such as degree, centrality measures, clustering coefficients etc from the ego graph Create a feature matrix that includes these features for each node. Normalize or scale the feature matrix if required.

Feature Defination -

Degree: The number of edges connected to the node, indicating its local connectivity.

Centrality Measures:

- Betweenness Centrality: Measures the extent to which a node lies on the shortest paths between other nodes in the ego graph.
- Closeness Centrality: Measures how close a node is to all other nodes in the ego graph in terms of geodesic distance.

Local Clustering Coefficient: The clustering coefficient of the node itself. Local Clustering Coefficient of a node in a Graph is the fraction of pairs of the node's neighbours that are adjacent to each other.

Eigenvector Centrality: Measures a node's importance based on its connections to other highly central nodes in the ego graph.

Average Neighbor Degree: The average degree of a node's neighbors.

ego_sizes Size of ego network is the number of nodes that one-step out neighbors of ego, plus ego itself.

num_directed_ties Number of directed ties is the number of connections among all the nodes in the ego network.

num_ordered_pairs Number of ordered pairs is the number of possible directed ties in each ego network.

densities Density is the number of ties divided by the number of pairs. That is, what percentage of all possible ties in each ego network are actually present?

avg_geodesic_distances Average geodesic distance is the mean of the shortest path lengths among all connected pairs in the ego network.

diameters Diameter of an ego network is the length of the longest path between connected actors (just as it is for any network).

pairs_not_directly_connecteds Brokerage (number of pairs not directly connected). The idea of brokerage (more on this, below) is that ego is the "go-between" for pairs of other actors. In an ego network, ego is connected to every other actor (by definition). If these others are not connected directly to one another, ego may be a "broker" ego falls on a the paths between the others. One item of interest is simply how much potential for brokerage there is for each actor (how many times pairs of neighbors in ego's network are not directly connected).

normalized_brokerages Normalized brokerage (brokerage divided by number of pairs) assesses the extent to which ego's role is that of broker.

ego_betweennesses Betweenness is an aspect of the larger concept of "centrality."

normalized_ego_betweennesses Normalized Betweenness compares the actual betweenness of ego to the maximum possible betweenness in neighborhood of the size and connectivity of ego's. The "maximum" value for betweenness would be achieved where ego is the center of a "star" network; that is, no neighbors communicate directly with one another, and all directed communications between pairs of neighbors go through ego.

dyadic_redundancies The dyadic redundancy measure calculates, for each actor in ego's neighborhood, how many of the other actors in the neighborhood are also tied to the other.

```
# Create empty lists to store features
nodes = []
degrees = []
betweenness_centralities = []
closeness_centralities = []
eigenvector_centralities = []
avg_neighbor_degrees = []
ego_sizes = []
num_directed_ties = []
num ordered pairs = []
densities = []
avg_geodesic_distances = []
diameters = []
pairs_not_directly_connecteds = []
normalized_brokerages = []
ego betweennesses = []
normalized ego betweennesses = []
clustering_coefficients = []
dyadic_redundancies = []
# Iterate through the dictionary of nodes and ego graphs
for node, ego_graph in ego_networks.items():
    # Calculate the specified features for each node and append to the respective lists
   nodes.append(node)
    degrees.append(ego_graph.degree(node))
   betweenness_centralities.append(nx.betweenness_centrality(ego_graph)[node])
    closeness_centralities.append(nx.closeness_centrality(ego_graph)[node])
    eigenvector_centralities.append(nx.eigenvector_centrality(ego_graph)[node])
    avg_neighbor_degrees.append(nx.average_neighbor_degree(ego_graph)[node])
    ego sizes.append(len(ego graph))
    num directed ties.append(len(list(ego graph.neighbors(node))))
    num_ordered_pairs.append(len(list(ego_graph.edges(node))))
    densities.append(nx.density(ego_graph))
    avg_geodesic_distances.append(nx.average_shortest_path_length(ego_graph))
    diameters.append(nx.diameter(ego_graph))
    # Calculate brokerage (number of pairs not directly connected)
    pairs not directly connected = 0
    for node1 in ego_graph.nodes():
        for node2 in ego_graph.nodes():
            if node1 != node2 and not ego_graph.has_edge(node1, node2):
                pairs_not_directly_connected += 1
```

```
pairs_not_directly_connecteds.append(pairs_not_directly_connected)
    # Calculate normalized brokerage
    num possible pairs = (len(ego graph) * (len(ego graph) - 1)) / 2
    normalized brokerage = pairs not directly connected / num possible pairs
    normalized_brokerages.append(normalized_brokerage)
    # Calculate ego betweenness
    ego betweenness = nx.betweenness_centrality(ego_graph)[node]
    ego betweennesses.append(ego betweenness)
    # Calculate normalized ego betweenness
    normalized ego betweenness = ego betweenness / (len(ego graph) - 1)
    normalized_ego_betweennesses.append(normalized_ego_betweenness)
    # Calculate clustering coefficient
    clustering coefficient = nx.clustering(ego graph, node)
    clustering coefficients.append(clustering coefficient)
    # Calculate dyadic redundancy
    dyadic_redundancy = nx.density(nx.ego_graph(ego_graph, node))
    dyadic_redundancies.append(dyadic_redundancy)
# Create a DataFrame from the lists of features
features df = pd.DataFrame({
    'Node': nodes,
    'Degree': degrees,
    'Betweenness Centrality': betweenness_centralities,
    'Closeness Centrality': closeness_centralities,
    'Eigenvector Centrality': eigenvector_centralities,
    'Average Neighbor Degree': avg_neighbor_degrees,
    'Ego Size': ego sizes,
    'Number of Directed Ties': num_directed_ties,
    'Number of Ordered Pairs': num_ordered_pairs,
    'Density': densities,
    'Average Geodesic Distance': avg_geodesic_distances,
    'Diameter': diameters,
    'Pairs Not Directly Connected': pairs not directly connecteds,
    'Normalized Brokerage': normalized brokerages,
    'Ego Betweenness': ego_betweennesses,
    'Normalized Ego Betweenness': normalized_ego_betweennesses,
    'Clustering Coefficient': clustering_coefficients,
    'Dyadic Redundancy': dyadic_redundancies
})
features df.shape
    (4039, 18)
features df.info()
    <class 'pandas.core.frame.DataFrame'>
    RangeIndex: 4039 entries, 0 to 4038
    Data columns (total 18 columns):
        Column
                                       Non-Null Count Dtype
        Node
                                       4039 non-null
     1
         Degree
                                       4039 non-null int64
         Betweenness Centrality
                                       4039 non-null
                                                       float64
                                       4039 non-null float64
         Closeness Centrality
        Eigenvector Centrality
                                      4039 non-null float64
         Average Neighbor Degree
                                       4039 non-null float64
     6
         Ego Size
                                       4039 non-null
                                                       int64
         Number of Directed Ties
                                       4039 non-null
                                                       int64
         Number of Ordered Pairs
                                       4039 non-null int64
         Density
                                       4039 non-null float64
     10 Average Geodesic Distance
                                       4039 non-null
                                                       float64
                                       4039 non-null
                                                       int64
     11
         Diameter
     12 Pairs Not Directly Connected 4039 non-null
                                                       int.64
     13 Normalized Brokerage
                                       4039 non-null
                                                       float64
                                       4039 non-null
     14 Ego Betweenness
                                                       float.64
```

15 Normalized Ego Betweenness 4039 non-null float64 16 Clustering Coefficient 4039 non-null float64 17 Dyadic Redundancy 4039 non-null float64 dtypes: float64(11), int64(7)

features_df

memory usage: 568.1 KB

Node	Degree	Betweenness Centrality	Closeness Centrality	Eigenvector Centrality	Average Neighbor Degree	Ego Size	Number of Directed Ties	О
0	347	0.823842	1.0	0.289796	15.518732	348	347	
1	17	0.204902	1.0	0.392721	7.705882	18	17	
2	10	0.018333	1.0	0.322646	9.000000	11	10	
3	17	0.113320	1.0	0.294592	11.117647	18	17	
4	10	0.033333	1.0	0.321293	8.800000	11	10	
4034	2	0.000000	1.0	0.577350	2.000000	3	2	
4035	1	0.000000	1.0	0.707107	1.000000	2	1	
4036	2	0.000000	1.0	0.577350	2.000000	3	2	
4037	4	0.166667	1.0	0.510036	3.000000	5	4	
4038	9	0.164352	1.0	0.416579	5.444444	10	9	
	0 1 2 3 4 4034 4035 4036 4037	0 347 1 17 2 10 3 17 4 10 4034 2 4035 1 4036 2 4037 4	Node Degree Centrality 0 347 0.823842 1 17 0.204902 2 10 0.018333 3 17 0.113320 4 10 0.033333 4034 2 0.000000 4035 1 0.000000 4036 2 0.000000 4037 4 0.166667	Node Degree Centrality Centrality 0 347 0.823842 1.0 1 17 0.204902 1.0 2 10 0.018333 1.0 3 17 0.113320 1.0 4 10 0.033333 1.0 4034 2 0.000000 1.0 4035 1 0.000000 1.0 4036 2 0.000000 1.0 4037 4 0.166667 1.0	Node Degree Centrality Centrality Centrality 0 347 0.823842 1.0 0.289796 1 17 0.204902 1.0 0.392721 2 10 0.018333 1.0 0.322646 3 17 0.113320 1.0 0.294592 4 10 0.0333333 1.0 0.321293 4034 2 0.000000 1.0 0.577350 4035 1 0.000000 1.0 0.577350 4037 4 0.166667 1.0 0.510036	Node Degree Betweenness Centrality Closeness Centrality Eigenvector Degree 0 347 0.823842 1.0 0.289796 15.518732 1 17 0.204902 1.0 0.392721 7.705882 2 10 0.018333 1.0 0.322646 9.000000 3 17 0.113320 1.0 0.294592 11.117647 4 10 0.033333 1.0 0.321293 8.800000 4034 2 0.000000 1.0 0.577350 2.000000 4035 1 0.000000 1.0 0.577350 2.000000 4036 2 0.000000 1.0 0.577350 2.000000 4037 4 0.166667 1.0 0.510036 3.000000	Node Degree Betweenness Centrality Closeness Centrality Eigenvector Centrality Neighbor Degree Egg Size 0 347 0.823842 1.0 0.289796 15.518732 348 1 17 0.204902 1.0 0.392721 7.705882 18 2 10 0.018333 1.0 0.322646 9.000000 11 3 17 0.113320 1.0 0.294592 11.117647 18 4 10 0.0333333 1.0 0.321293 8.800000 11 4034 2 0.000000 1.0 0.577350 2.000000 2 4035 1 0.000000 1.0 0.577350 2.000000 2 4036 2 0.000000 1.0 0.577350 2.000000 3 4037 4 0.166667 1.0 0.510036 3.000000 5	Node Degree Betweenness Centrality Closeness Centrality Eigenvector Centrality Average Neighbor Degree Ego Size of Size Directed Ties 0 347 0.823842 1.0 0.289796 15.518732 348 347 1 17 0.204902 1.0 0.392721 7.705882 18 17 2 10 0.018333 1.0 0.322646 9.000000 11 10 3 17 0.113320 1.0 0.294592 11.117647 18 17 4 10 0.033333 1.0 0.321293 8.800000 11 10 4034 2 0.000000 1.0 0.577350 2.000000 2 1 4035 1 0.000000 1.0 0.577350 2.000000 3 2 4036 2 0.000000 1.0 0.577350 2.000000 3

4039 rows × 18 columns

```
features_df['Closeness Centrality'].unique()
    array([1.])

features_df['Diameter'].unique()
    array([2, 1])
```

Removing "Closeness Centrality" feature as it has only one unique value features_df.drop('Closeness Centrality', axis=1, inplace=True)

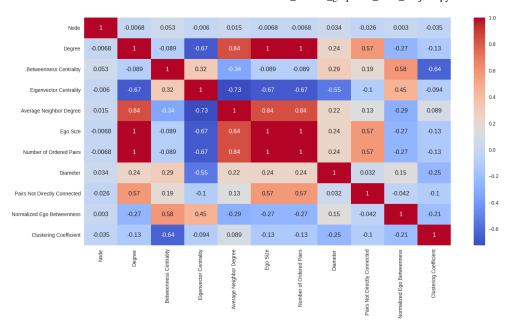
Feature Removal using Correlation Matrix

```
# Assuming 'features_df' is your feature data in a DataFrame
correlation_matrix = features_df.corr()

plt.figure(figsize=(16, 8))
sns.heatmap(correlation_matrix, annot=True, cmap='coolwarm')
plt.show()
```

plt.show()

```
Node 1 -0.0068 0.053 -0.006 0.015 -0.0068-0.0068-0.0068 -0.051 0.051 0.034 -0.026 0.051 0.053 0.003 -0.035 -0.051
                 Degree -0.0068 1 -0.089 -0.67 0.84 1 1 1 -0.29 0.29 0.24 0.57 0.29 -0.089 -0.27 -0.13 -0.29
                                                                                                         0.75
                               1 0.32 -0.34 -0.089 -0.089 -0.089
                                                          -0.67 0.67 0.29 0.19
          Eigenvector Centrality -0.006 -0.6
                               0.32
                                                          0.29 -0.29
                                                                       .0.1 .0.29 0.32 0.45 .0.094 0.29
                                                                                                         0.50
        Average Neighbor Degree 0.015
                               -0.34
                                                          -0.058 0.058 0.22 0.13 0.058 -0.34 -0.29 0.089 -0.058
                Ego Size -0.0068
                               -0.089
                                                          -0.29 0.29 0.24
                                                                            0.29 -0.089 -0.27 -0.13
                               -0.089
                                                          -0.29 0.29 0.24
                                                                                                         0.25
        Number of Ordered Pairs -0.0068
                               -0.089
                                                          -0.29
                                                                            0.29 -0.089 -0.27 -0.13
                                                               0.29 0.24
                                   0.29 -0.058 -0.29 -0.29 -0.29
                                                                                   -0.11
                 Density -0.051 -0.29
                                                                       -0.14
                                                                                                         0.00
       Average Geodesic Distance 0.051 0.29 0.67
                                   -0.29 0.058 0.29 0.29 0.29
                                                                       0.14
                                                                                    0.11
               Diameter 0.034 0.24 0.29 -0.55 0.22 0.24 0.24 0.24
       Pairs Not Directly Connected -0.026 0.57 0.19 -0.1 0.13
                                                          Normalized Brokerage 0.051 0.29 0.67 -0.29 0.058 0.29 0.29 0.29
                                                                       0.14
                                                                                                          -0.50
           Ego Betweenness 0.053 -0.089 1 0.32 -0.34 -0.089 -0.089 -0.089
                                                          -0.67 0.67 0.29 0.19
      Normalized Ego Betweenness 0.003 -0.27
                                   0.45 -0.29 -0.27 -0.27 -0.27 -0.11 0.11 0.15 -0.042 0.11
          Clustering Coefficient -0.035 -0.13
                                   -0.094 0.089 -0.13 -0.13 -0.13
                                                                   -0.25
                                                                       -0.1
           Dyadic Redundancy -0.051 -0.29
                                   0.29 -0.058 -0.29 -0.29 -0.29
                                                                       -0.14
# Identify Highly Correlated Features
threshold = 0.7
highly_correlated_pairs = []
for i in range(len(correlation_matrix.columns)):
     for j in range(i):
          if abs(correlation matrix.iloc[i, j]) > threshold:
               pair = (correlation_matrix.columns[i], correlation_matrix.columns[j])
               highly correlated pairs.append(pair)
print("Highly Correlated Feature Pairs:")
print(highly_correlated_pairs)
     Highly Correlated Feature Pairs:
      [('Average Neighbor Degree', 'Degree'), ('Average Neighbor Degree', 'Eigenvector Centrality'), ('Ego Size', 'Degree
print(features_df.columns)
     Index(['Node', 'Degree', 'Betweenness Centrality', 'Eigenvector Centrality',
               'Average Neighbor Degree', 'Ego Size', 'Number of Directed Ties', 'Number of Ordered Pairs', 'Density', 'Average Geodesic Distance',
               'Diameter', 'Pairs Not Directly Connected', 'Normalized Brokerage',
               'Ego Betweenness', 'Normalized Ego Betweenness',
               'Clustering Coefficient', 'Dyadic Redundancy'],
             dtype='object')
# Based on heat map analysis and importance of features
highly_correlated_pairs =['Average Geodesic Distance','Number of Directed Ties', 'Density','Dyadic Redundancy', 'Normali:
# Remove one of the features from each highly correlated pair
for feature1 in highly correlated pairs:
     features df.drop(feature1, axis=1, inplace=True) # Remove feature1
# features_df now contains the remaining non-correlated features
#for feature1, feature2 in highly_correlated_pairs:
     # Decide which feature to keep, e.g., based on importance or domain knowledge
     # Remove one of the features
     #features df.drop(feature1, axis=1, inplace=True) # Remove feature1
correlation_matrix = features_df.corr()
plt.figure(figsize=(16, 8))
sns.heatmap(correlation_matrix, annot=True, cmap='coolwarm')
```



```
features_df.drop('Ego Size', axis=1, inplace=True)

features_df.drop('Number of Ordered Pairs', axis=1, inplace=True)

features_df.drop('Average Neighbor Degree', axis=1, inplace=True)

correlation_matrix = features_df.corr()

plt.figure(figsize=(16, 8))
sns.heatmap(correlation_matrix, annot=True, cmap='coolwarm')
plt.show()
```



Perform standardization and normalization

```
# Perform standardization and normalization
scaler = StandardScaler()
normalized_df = scaler.fit_transform(features_df.drop(columns=['Node']))
minmax_scaler = MinMaxScaler()
normalized_df = minmax_scaler.fit_transform(normalized_df)
```

▼ Perform PCA

```
# Perform PCA
pca = PCA(n_components=0.95)
pca_result = pca.fit_transform(normalized_df)

# Create a DataFrame for PCA results
pca_df = pd.DataFrame(data=pca_result, columns=[f'PCA_{i+1}' for i in range(pca_result.shape[1])])
```

Finding the optimal number of clusters is a crucial step in clustering analysis.

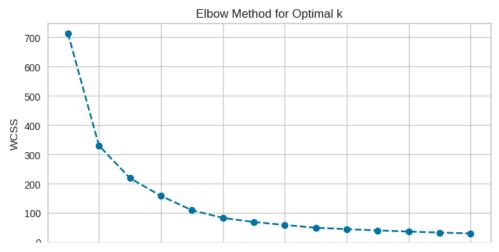
We will use below 2 methods to determine the optimal number of clusters

1. Elbow Method:

The elbow method involves plotting the within-cluster sum of squares (WCSS) against the number of clusters and looking for the "elbow" point where the rate of decrease in WCSS starts to slow down. Use scikit-learn's KMeans and calculate WCSS for different values of k. Then, plot the WCSS values and look for the elbow point.

```
wcss = []
for k in range(1, 15):
    kmeans = KMeans(n_clusters=k, init='k-means++', max_iter=300, n_init=10, random_state=0)
    kmeans.fit(pca_df)
    wcss.append(kmeans.inertia_)

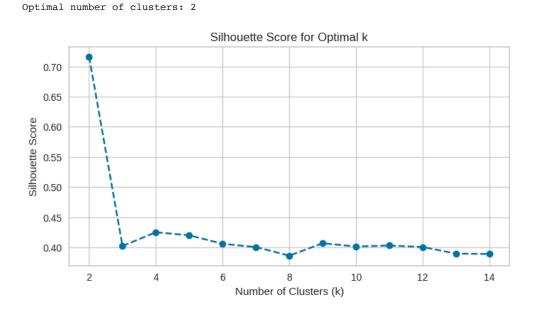
# Plot the WCSS values
plt.figure(figsize=(8, 4))
plt.plot(range(1, 15), wcss, marker='o', linestyle='--')
plt.xlabel('Number of Clusters (k)')
plt.ylabel('WCSS')
plt.title('Elbow Method for Optimal k')
plt.show()
```



2. Silhouette Score:

The silhouette score measures how similar each data point is to its own cluster compared to other clusters. Higher silhouette scores indicate better cluster separation. Calculate the silhouette score for different values of k and choose the k that maximizes the silhouette score.

```
# Calculate Silhouette Score for different k values
silhouette_scores = []
for i in range(2, 15):
    kmeans = KMeans(n_clusters=i, init='k-means++', max_iter=300, n_init=10, random_state=0)
    kmeans.fit(pca_df)
    silhouette_scores.append(silhouette_score(pca_df, kmeans.labels_))
# Find the number of clusters with the highest Silhouette Score
optimal_num_clusters = silhouette_scores.index(max(silhouette_scores)) + 2 # Add 2 due to starting from 2 clusters
print("Optimal number of clusters:", optimal_num_clusters)
print()
# Plot the silhouette scores
plt.figure(figsize=(8, 4))
plt.plot(range(2, 15), silhouette_scores, marker='o', linestyle='--')
plt.xlabel('Number of Clusters (k)')
plt.ylabel('Silhouette Score')
plt.title('Silhouette Score for Optimal k')
plt.show()
```



▼ Perform Clustering Analysis

- · Apply various clustering algorithms (e.g., k-means, hierarchical clustering, DBSCAN) to the feature-engineered data.
- Experiment with different parameter settings for each clustering algorithm.
- Evaluate the quality of clusters using appropriate metrics.

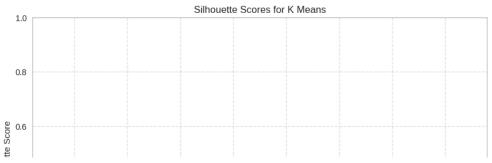
```
# Perform k-means clustering with different values of 'k'
k \text{ values} = [3, 4, 5, 8, 10]
kmeans results = []
for k in k_values:
    kmeans = KMeans(n_clusters=k, random_state=42)
    kmeans_labels = kmeans.fit_predict(pca_df)
    # Evaluate k-means clustering using Silhouette Score
    silhouette avg = silhouette score(pca df, kmeans labels)
    ch score = calinski harabasz score(pca df, kmeans labels)
    db_score = davies_bouldin_score(pca_df, kmeans_labels)
    kmeans_results.append({
        'k': k,
        'labels': kmeans labels,
        'silhouette score': silhouette avg,
        'calinski harabasz score': ch score,
        'davies_bouldin_score': db_score
    })
# Perform hierarchical clustering with different linkage methods
linkage methods = ['ward', 'complete', 'average', 'single']
hierarchical results = []
for linkage in linkage_methods:
    hierarchical = AgglomerativeClustering(n_clusters=3, linkage=linkage)
    hierarchical_labels = hierarchical.fit_predict(pca_df)
    # Evaluate hierarchical clustering using Silhouette Score
    silhouette avg = silhouette score(pca df, hierarchical labels)
    ch score = calinski harabasz score(pca df, hierarchical labels)
   db_score = davies_bouldin_score(pca_df, hierarchical_labels)
   hierarchical_results.append({
        'linkage': linkage,
        'labels': hierarchical labels,
        'silhouette score': silhouette avg,
        'calinski harabasz score': ch score,
        'davies_bouldin_score': db_score
    })
# Perform DBSCAN clustering with different parameters
eps values = [0.1, 0.2, 0.3]
min_samples_values = [5, 10, 20]
dbscan_results = []
for eps in eps_values:
    for min_samples in min_samples_values:
        dbscan = DBSCAN(eps=eps, min samples=min samples)
        dbscan labels = dbscan.fit predict(pca df)
        # Evaluate DBSCAN clustering using Silhouette Score
        if len(np.unique(dbscan_labels)) > 1:
            silhouette_avg = silhouette_score(pca_df, dbscan_labels)
            db_score = davies_bouldin_score(pca_df, dbscan_labels)
        else:
            silhouette avg = -1 # DBSCAN may result in a single cluster
            db_score = -1
        dbscan_results.append({
            'eps': eps,
            'min samples': min samples,
            'labels': dbscan labels,
```

```
'silhouette_score': silhouette_avg,
            'davies_bouldin_score': db_score
        })
# Print and analyze the clustering results
print("K-Means Clustering Results:")
kmeans_df = pd.DataFrame(kmeans_results)
print(kmeans df)
print("\nHierarchical Clustering Results:")
hierarchical df = pd.DataFrame(hierarchical results)
print(hierarchical df)
print("\nDBSCAN Clustering Results:")
dbscan_df = pd.DataFrame(dbscan_results)
print(dbscan_df)
    K-Means Clustering Results:
                                                      labels silhouette score
          [2, 2, 0, 0, 0, 2, 0, 2, 2, 2, 0, 1, 1, 0, 0, ...
                                                                      0.402197
        4 [0, 0, 2, 2, 2, 0, 2, 0, 0, 0, 2, 3, 3, 2, 2, ...
    1
                                                                      0.424260
           [2, 2, 4, 4, 4, 2, 4, 2, 4, 0, 4, 3, 3, 0, 4, ...
                                                                      0.419997
       8 [0, 0, 3, 6, 3, 0, 3, 5, 6, 5, 3, 4, 4, 7, 3, ...
                                                                      0.387652
      10 [8, 8, 4, 0, 4, 8, 4, 6, 5, 6, 4, 2, 2, 0, 7, ...
                                                                      0.401961
       calinski harabasz score davies bouldin score
                   4539.921230
                                            0.866599
                   4694.149920
                                            0.627045
    1
    2
                   5533.225626
                                            0.615727
                   6272.916611
                                            0.710755
    3
                   6591,660442
                                            0.714848
    Hierarchical Clustering Results:
        linkage
           ward [2, 2, 1, 1, 1, 2, 1, 2, 1, 2, 1, 0, 0, 1, 1, ...
    1 complete [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, ...
        average [2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 0, 0, 2, 2, ...
         single [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, ...
       silhouette score calinski harabasz score davies bouldin score
               0.387328
                                     4367.152165
                                                              0.869414
               0.689910
                                     2355.479069
                                                              0.445870
    1
    2
               0.689910
                                     2355.479069
                                                              0.445870
               0.724309
                                                              0.266044
    3
                                     3313.092339
    DBSCAN Clustering Results:
       eps min_samples
                         [-1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, \dots]
       0.1
                     5
      0.1
                     10 [-1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0,...
    2 0.1
                     20 [-1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0,...
       0.2
                     5 [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, ...
      0.2
                     10
                         [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, ...
      0.2
                     20 [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, ...
    6 0.3
                     5 [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, ...
    7
       0.3
                     10 [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, ...
    8
      0.3
                     20 [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, ...
       silhouette_score davies_bouldin_score
    0
               0.583294
                                     0.497956
    1
               0.553122
                                     0.485767
    2
                                     0.505796
               0.549505
    3
               0.650925
                                     0.756948
               0.650925
    4
                                     0.756948
    5
               0.650925
                                     0.756948
               0.702717
                                     0.248047
    6
                                     0.248047
               0.702717
                                     0.248047
               0.702717
# Define a list of parameter combinations to try
eps_values = [0.1, 0.2, 0.3] # Adjust these values as needed
min_samples_values = [5, 10, 20] # Adjust these values as needed
best dbscan = None
```

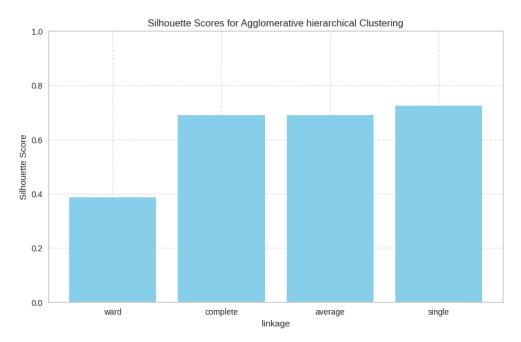
```
best_labels = None
best_silhouette_score = -1 # Initialize with a low value
for eps in eps values:
    for min samples in min samples values:
        dbscan = DBSCAN(eps=eps, min_samples=min_samples)
        labels = dbscan.fit_predict(pca_df)
        # Exclude noise points (-1) from the silhouette score calculation
        if len(np.unique(labels)) > 1:
            silhouette avg = silhouette score(pca df, labels)
            silhouette avg = -1
        if silhouette_avg > best_silhouette_score:
            best_silhouette_score = silhouette_avg
            best dbscan = dbscan
            best labels = labels
# Print the best DBSCAN parameters and silhouette score
print("Best DBSCAN Parameters:")
print("Eps:", best_dbscan.eps)
print("Min Samples:", best_dbscan.min_samples)
print("Silhouette Score:", best silhouette score)
    Best DBSCAN Parameters:
    Eps: 0.3
    Min Samples: 5
    Silhouette Score: 0.7027174022770256
```

▼ Evaluate Clustering Performance

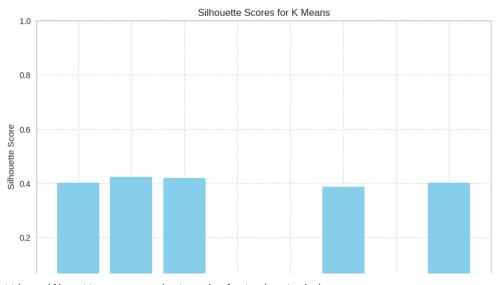
Calculate Silhouette Score to evaluate the quality of clusters.



```
# Create a bar plot for Silhouette Scores for Agglomerative hierarchical Clustering using different linkage
plt.figure(figsize=(10, 6))
plt.bar(hierarchical_df['linkage'], hierarchical_df['silhouette_score'], color='skyblue')
plt.xlabel('linkage')
plt.ylabel('Silhouette Score')
plt.title('Silhouette Scores for Agglomerative hierarchical Clustering')
plt.ylim(0, 1) # Set y-axis limits (0 to 1)
plt.grid( linestyle='--', alpha=0.6)
plt.show()
```



```
plt.figure(figsize=(10, 6))
plt.bar(kmeans_df['k'], kmeans_df['silhouette_score'], color='skyblue')
plt.xlabel('Number of Clusterring')
plt.ylabel('Silhouette Score')
plt.title('Silhouette Scores for K Means')
plt.ylim(0, 1) # Set y-axis limits (0 to 1)
plt.grid( linestyle='--', alpha=0.6)
plt.show()
```



Plotting silhouette_score against each clustering technique

```
data = {
    'clustering_technique': ['K Means', 'Agglomerative', 'DBScan'],
    'silhouette_score': [max(kmeans_df['silhouette_score']), max(hierarchical_df['silhouette_score']), max(dbscan_df['silhouette_score'])
}
# Create the DataFrame
df = pd.DataFrame(data)
plt.figure(figsize=(10, 6))
plt.bar(df['clustering_technique'], df['silhouette_score'], color='skyblue',)
# Add labels to the bars
for i, v in enumerate(df['silhouette_score']):
   plt.annotate(str(v), (i, v), ha='center', va='bottom')
plt.xlabel('Clustering Technique')
plt.ylabel('Silhouette Score')
plt.title('Comparaing Silhouette Scores for different Clustering Technique')
plt.ylim(0, 1) # Set y-axis limits (0 to 1)
plt.grid( linestyle='--', alpha=0.6,)
plt.show()
```

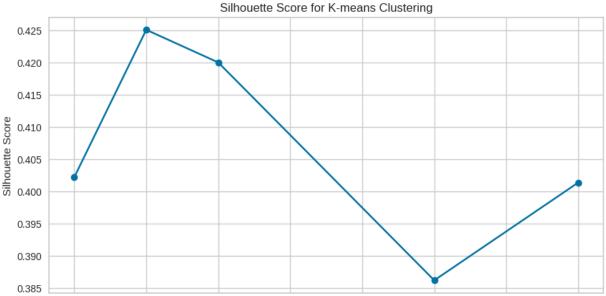
```
Comparaing Silhouette Scores for different Clustering Technique
Double-click (or enter) to edit
# Print and analyze the K Means clustering results
max_silhouette_score_row = kmeans_df[ kmeans_df['silhouette_score'] == kmeans_df['silhouette_score'].max() ]
cluster_no_silhouette_score = max_silhouette_score_row['k'].values[0]
max_silhouette_score = max_silhouette_score_row['silhouette_score'].values[0]
print("K Means clustering results")
print()
print(f"Based on Maximum Silhouette Score: {max_silhouette_score}, Optimal number of clusters (k) : {cluster_no_silhouette
max ch score row = kmeans df[ kmeans df[ 'calinski harabasz score'] == kmeans df[ 'calinski harabasz score'].max() ]
cluster_no_ch_score = max_ch_score_row['k'].values[0]
max_sch_score = max_ch_score_row['calinski_harabasz_score'].values[0]
print(f"Based on Maximum calinski harabasz score: {max sch score}, Optimal number of clusters (k) : {cluster no ch score
min db score row = kmeans df[ kmeans df['davies bouldin score'] == kmeans df['davies bouldin score'].min() ]
cluster_no_db_score = min_db_score_row['k'].values[0]
max_db_score = min_db_score_row['davies_bouldin_score'].values[0]
print(f"Based on Maximum davies bouldin score: {max_db_score}, Optimal number of clusters (k) : {cluster_no_db_score} ")
       K Means clustering results
       Based on Maximum Silhouette Score: 0.42425986444227004, Optimal number of clusters (k): 4
       Based on Maximum calinski harabasz score: 6591.660441794133, Optimal number of clusters (k): 10
       Based on Maximum davies bouldin score: 0.6157272403290853, Optimal number of clusters (k): 5
# Print and analyze the Agglomerative hierarchical Clustering results
max_silhouette_score_row = hierarchical_df[ hierarchical_df['silhouette_score'] == hierarchical_df['silhouette_score'].max_silhouette_score'].max_silhouette_score_row = hierarchical_df['silhouette_score'].max_silhouette_score'].max_silhouette_score_row = hierarchical_df['silhouette_score'].max_silhouette_score'].max_silhouette_score_row = hierarchical_df['silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silhouette_score'].max_silh
best linkage = max silhouette score row['linkage'].values[0]
max_silhouette_score = max_silhouette_score_row['silhouette_score'].values[0]
print("Agglomerative hierarchical Clustering results")
print()
print(f"Based on Maximum Silhouette Score: {max silhouette score}, Best linkage method : {best linkage} ")
max_ch_score_row = hierarchical_df[ hierarchical_df['calinski_harabasz_score'] == hierarchical_df['calinski_harabasz_score']
best_linkage_ch = max_ch_score_row['linkage'].values[0]
max_sch_score = max_ch_score_row['calinski_harabasz_score'].values[0]
print(f"Based on Maximum calinski harabasz score: {max sch score}, Best linkage method : {best linkage ch} ")
min_db_score_row = hierarchical_df[ hierarchical_df['davies_bouldin_score'] == hierarchical_df['davies_bouldin_score'].m:
best_linkage_db = min_db_score_row['linkage'].values[0]
max_db_score = min_db_score_row['davies_bouldin_score'].values[0]
print(f"Based on Maximum davies bouldin score: {max db score}, Best linkage method : {best linkage db} ")
       Agglomerative hierarchical Clustering results
       Based on Maximum Silhouette Score: 0.7243092232756921, Best linkage method : single
```

9/27/23, 11:27 PM Bhaskar_Boruah_graphML_Mini_Project.ipynb - Colaboratory Based on Maximum calinski harabasz score: 4367.1521653584105, Best linkage method : ward Based on Maximum davies bouldin score: 0.2660437294743572, Best linkage method : single # Print and analyze the DB Scan Clustering results max silhouette score row = dbscan df[dbscan df['silhouette score'] == dbscan df['silhouette score'].max()] best_eps = max_silhouette_score_row['eps'].values[0] best_min_samples = max_silhouette_score_row['min_samples'].values[0] max silhouette score = max silhouette score row['silhouette score'].values[0] print("DB Scan Clustering results") print() print(f"Based on Maximum Silhouette Score: {max_silhouette_score}, Optimal parameters: epsilon = {best_eps}, min_samples min db score row = dbscan df[dbscan df['davies bouldin score'] == dbscan df['davies bouldin score'].min()] best eps db = min db score row['eps'].values[0] best_min_samples_db = min_db_score_row['min_samples'].values[0] min_db_score = min_db_score_row['silhouette_score'].values[0] print(f"Based on Minimum davies bouldin Score: {min_db_score}, Optimal parameters: epsilon = {best_eps_db}, min_samples : DB Scan Clustering results Based on Maximum Silhouette Score: 0.7027174022770256, Optimal parameters: epsilon = 0.3, min_samples = 5 Based on Minimum davies bouldin Score: 0.7027174022770256, Optimal parameters: epsilon = 0.3, min_samples = 5 pca_df.info PCA_2 <bound method DataFrame.info of</pre> PCA 1 PCA 3 -0.266123 0.678498 0.194019 -0.042757 0.267334 -0.0747451 0.015212 -0.229019 -0.204234 -0.067590 -0.011802 -0.061474 0.008447 -0.207056 -0.194363 4034 1.083664 -0.175628 -0.027383 4035 0.973585 0.736624 0.330775 4036 1.083664 -0.175628 -0.027383 4037 0.103814 0.148554 -0.323705 4038 0.007791 0.162999 -0.164085 [4039 rows x 3 columns]> # Extract the features for clustering X = pca_df[['PCA_1', 'PCA_2', 'PCA_3']] # Perform K-means clustering with different numbers of clusters (adjust k_values) $k_{values} = [3, 4, 5, 8, 10] # You can adjust these values$ silhouette_scores_kmeans = [] for k in k_values: kmeans = KMeans(n_clusters=k, random_state=0) labels = kmeans.fit_predict(X) silhouette_score_kmeans = silhouette_score(X, labels) silhouette_scores_kmeans.append(silhouette_score_kmeans) # Plot the silhouette scores for K-means plt.figure(figsize=(10, 5)) plt.plot(k_values, silhouette_scores_kmeans, marker='o', linestyle='-') plt.title('Silhouette Score for K-means Clustering')

plt.xlabel('Number of Clusters (k)') plt.ylabel('Silhouette Score')

plt.grid(True) plt.show()

plt.grid(True)
plt.show()



```
# Perform Hierarchical Clustering with different linkage methods (adjust linkage_methods)
linkage_methods = ['ward', 'complete', 'average', 'single'] # You can adjust these values
silhouette_scores_hierarchy = []

for linkage in linkage_methods:
    hierarchical = AgglomerativeClustering(n_clusters=3, linkage=linkage)
    labels = hierarchical.fit_predict(X)
    silhouette_score_hierarchy = silhouette_score(X, labels)
    silhouette_scores_hierarchy.append(silhouette_score_hierarchy)

# Plot the silhouette scores for Hierarchical Clustering
plt.figure(figsize=(10, 5))
plt.bar(linkage_methods, silhouette_scores_hierarchy)
plt.title('Silhouette Score for Hierarchical Clustering')
plt.xlabel('Linkage Method')
plt.ylabel('Silhouette Score')
```



Model Evaluation using Pycaret

Initialize the PyCaret environment
exp_clu = setup(data=pca_df, normalize=True, session_id=123)

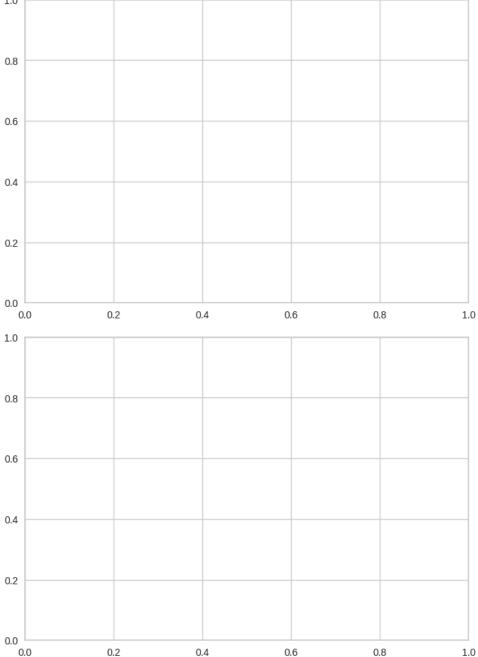
	Description	Value
0	Session id	123
1	Original data shape	(4039, 3)
2	Transformed data shape	(4039, 3)
3	Numeric features	3
4	Preprocess	True
5	Imputation type	simple
6	Numeric imputation	mean
7	Categorical imputation	mode
8	Normalize	True
9	Normalize method	zscore
10	CPU Jobs	-1
11	Use GPU	False
12	Log Experiment	False
13	Experiment Name	cluster-default-name
14	USI	d3a6

```
# Import necessary functions from pycaret.clustering module
from pycaret.clustering import create_model, evaluate_model
```

```
# Create and evaluate KMeans clustering model
kmeans = create_model('kmeans')
evaluate_model(kmeans)
```

- # Create and evaluate Hierarchical clustering model
 hierarchical = create_model('hclust')
 evaluate_model(hierarchical)
- # Create and evaluate DBScan clustering model
 dbscan = create_model('dbscan')
 evaluate_model(dbscan)
- # Create and evaluate BIRCH clustering model birch = create_model('birch') evaluate_model(birch)

<Figure size 800x550 with 0 Axes>
1.0



<Figure size 800x550 with 0 Axes>
<Figure size 800x550 with 0 Axes>

```
# Visualize KMeans clusters
plot_model(kmeans, plot='cluster')
# Visualize Hierarchical clusters
plot_model(hierarchical, plot='cluster')
# Visualize DBScan clusters
plot_model(dbscan, plot='cluster')
# Visualize BIRCH clusters
plot_model(birch, plot='cluster')
```