EDA_ENZYMES_group9

December 6, 2020

1 Data Mining Programming Assignment

2 Task1 - Exploratory Data Analysis

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We assume that you have the generated Gram matrices and sparse vectors in the directories

kernels/node_labels

kernels/without_labels

And have the HiSC repository in: > ./HiSC

If not you can download them here. Repository: https://github.com/maxf-at/data_mining_group9.git

[2]:
```
# Load packages
import os
import numpy as np
from auxiliarymethods import datasets as dp
from auxiliarymethods.reader import tud_to_networkx
import pandas as pd
from sklearn.decomposition import KernelPCA, TruncatedSVD, PCA
from matplotlib import pyplot as plt
from nrkmeans import NrKmeans
from sklearn.cluster import SpectralClustering, KMeans, AgglomerativeClustering
from sklearn.metrics import normalized_mutual_info_score, pairwise_distances
import seaborn as sns
from scipy.sparse import load_npz
import auxiliarymethods.auxiliary_methods as aux
import networkx as nx
from sklearn.cluster import KMeans
from copy import deepcopy
from sklearn.manifold import TSNE
import umap
from sklearn.preprocessing import StandardScaler
from sklearn.manifold import TSNE
from sklearn.model_selection import train_test_split
from sklearn import preprocessing, svm, metrics
from scipy.sparse import csc_matrix
from sklearn.cluster import OPTICS, cluster_optics_dbscan
import matplotlib.gridspec as gridspec
import sys
sys.path.append(r'./HiSC/data_mining_group9/intermediate submission/') #may
from HiSC import process_csv, HiSC, reachability_plot, get_clusters
```

[4]:
```
# functions
def load_csv(path):
    return np.loadtxt(path, delimiter=";")

def load_sparse(path):
    return load_npz(path)

def select_from_list(l, indices):
    return [l[i] for i in indices]

def visualize(G, color=None, figsize=(5,5)):
    plt.figure(figsize=figsize)
    plt.xticks([])
    plt.yticks([])
    nx.draw_networkx(G,
                     pos=nx.spring_layout(G, seed=42),
                     with_labels=True,
                     node_color=color,
                     cmap="Set2")
    plt.show();

def plot_dr(reduced_dim, title, labels):
    targets = [1, 2, 3,4, 5, 6]
    colors = ['r', 'g', 'b', 'y', 'orange', "purple"]


    fig, ax = plt.subplots(figsize=(10,10))
    for color, target in zip(colors, targets):
        ind_to_keep = []
        for i in range(0, len(reduced_dim)):
            if labels[i] ==target:
                ind_to_keep.append(i)

        x = reduced_dim[ind_to_keep, 0]
        y = reduced_dim[ind_to_keep, 1]
        ax.scatter(x, y, c=color, label=target, alpha = 0.8)
    ax.legend()
    plt.title(title)
    plt.show();
```

```
[5]: #main named variables
base_path = os.path.join("kernels", "node_labels")
dataset = "ENZYMES"
classes = dp.get_dataset(dataset)
G = tud_to_networkx(dataset)
print(f"Number of graphs in data set is {len(G)}")
print(f"Number of classes {len(set(classes.tolist()))}")
```

```
Number of graphs in data set is 600
Number of classes 6
```

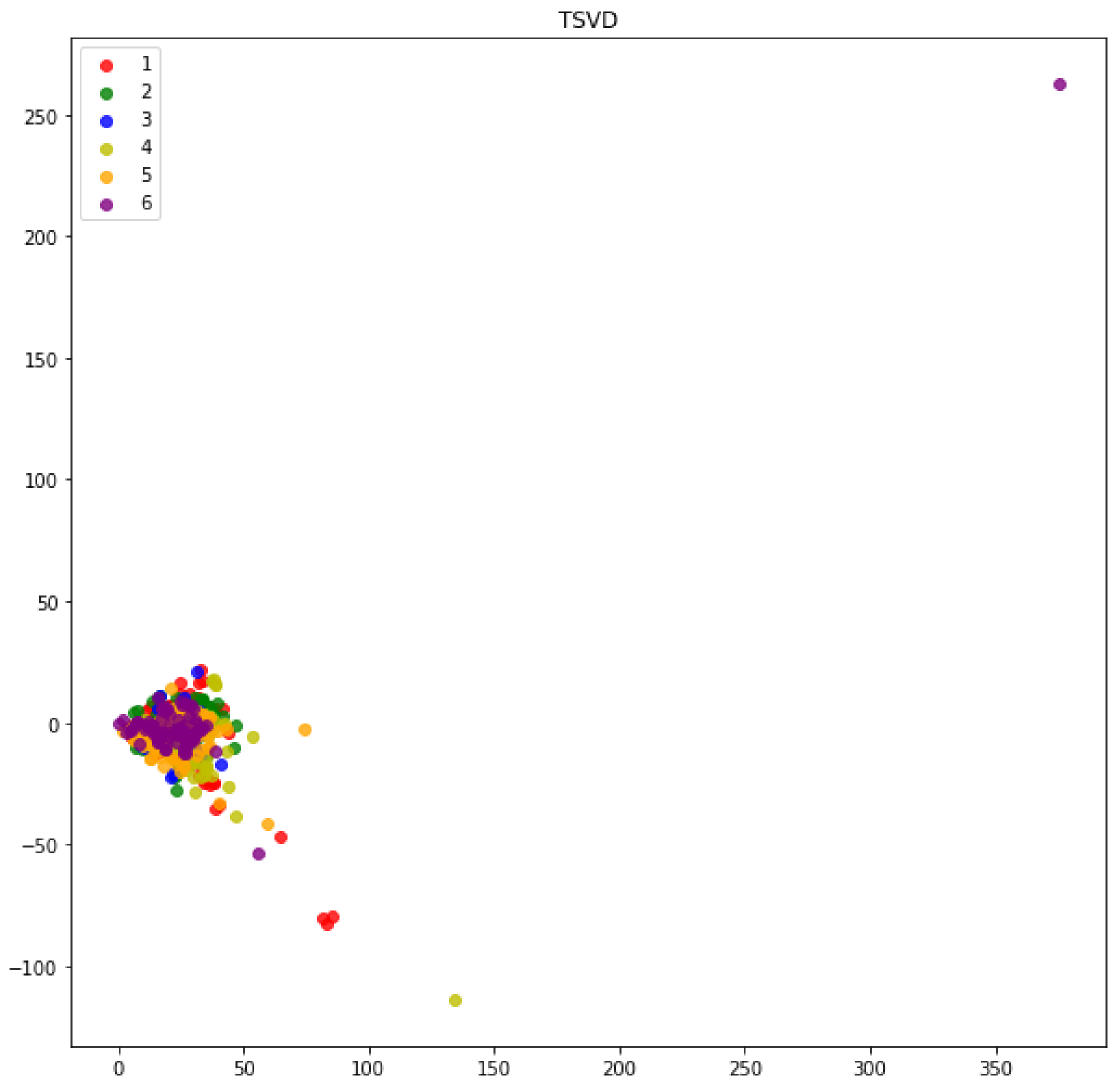
3 First look of the data: Dimensionality Reduction on raw data - WL kernel

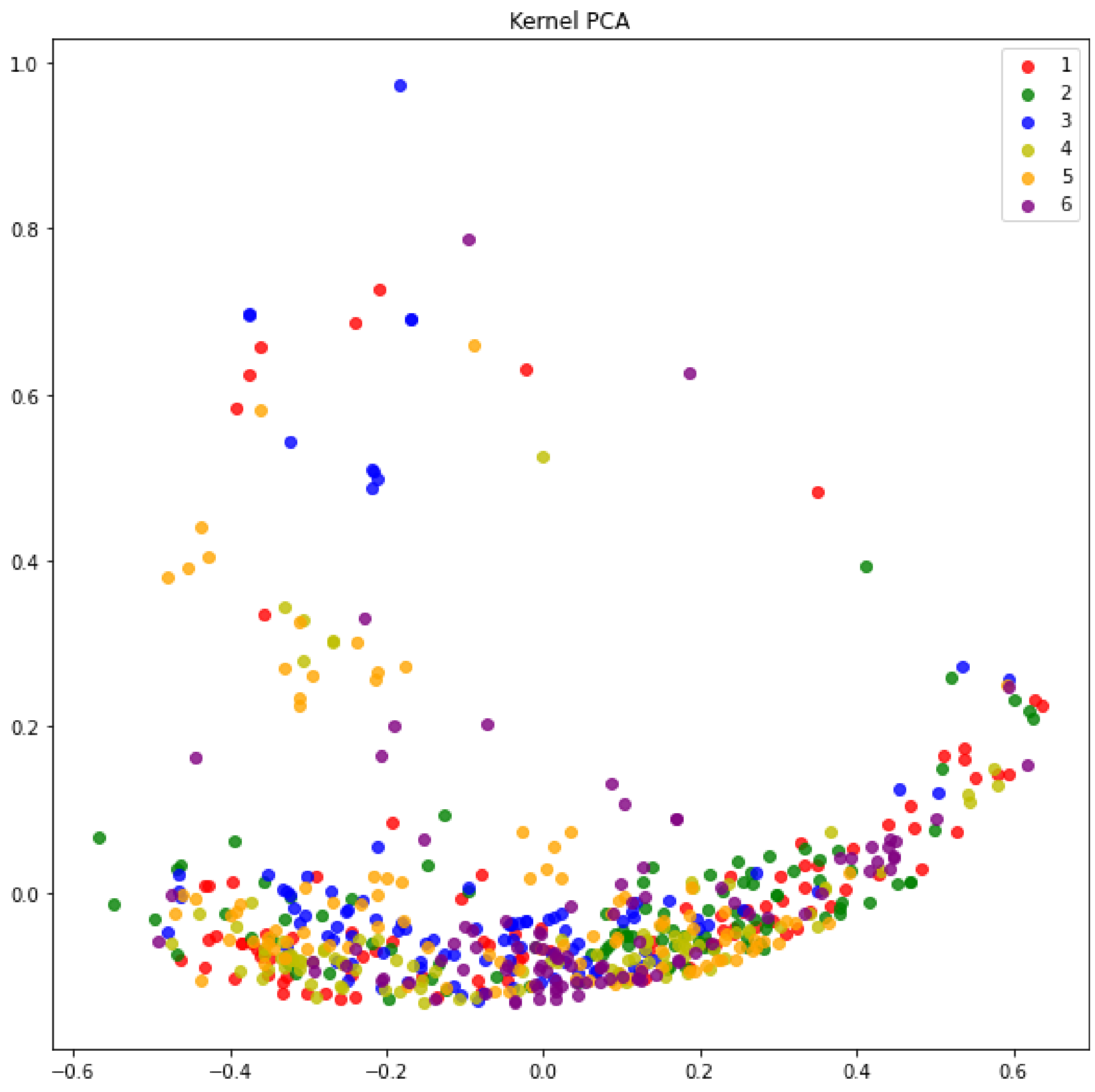
Let's see how our data looks like when unprocessed

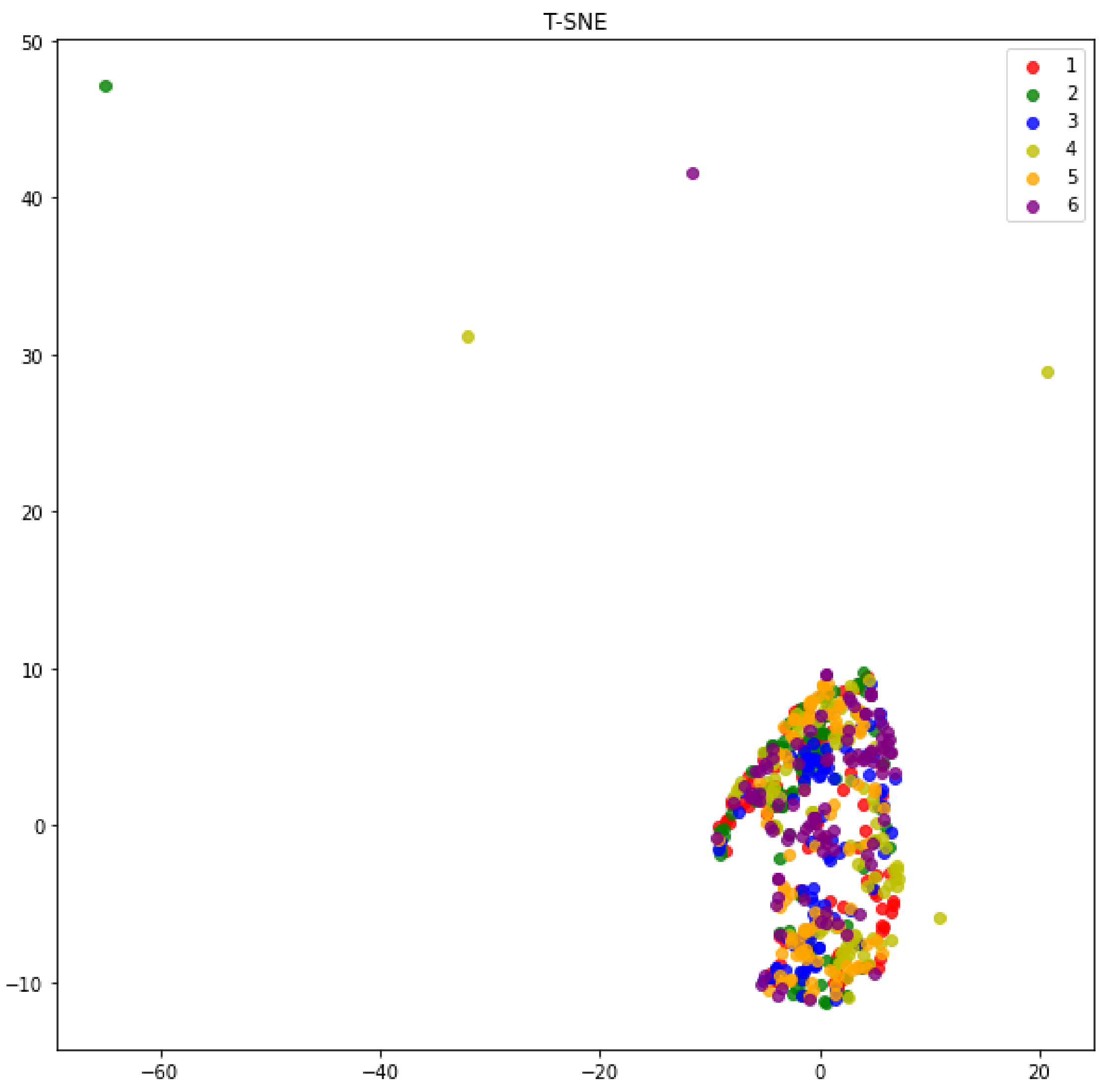
```
[6]: # triyng different iterations
dataset = "ENZYMES"
iterations = 5
base_path = os.path.join("kernels","node_labels")
#base_path = os.path.join("kernels","without_labels")

#---------------------------------------------
# Load graph representation from the kernel
#---------------------------------------------
#Gram Matrix for the Weisfeiler-Lehman subtree kernel
gram = load_csv(os.path.join(base_path,f"{dataset}_gram_matrix_wl{iterations}.
 ↪csv"))
gram = aux.normalize_gram_matrix(gram)

#Sparse Vectors for the Weisfeiler-Lehmann subtree kernel
vec = load_sparse(os.path.join(base_path,f"{dataset}_vectors_wl{iterations}.
 ↪npz"))
print(gram.shape, vec.shape)


# SVD
tsvd = TruncatedSVD(n_components=50)
reduced_tsvd = tsvd.fit_transform(vec)
plot_dr(reduced_tsvd, "TSVD", classes)

# Kernel PCA
kpca = KernelPCA(n_components=100, kernel="precomputed")
reduced_kpca= kpca.fit_transform(gram)
plot_dr(reduced_kpca, "Kernel PCA",classes)

# T-SNE
```

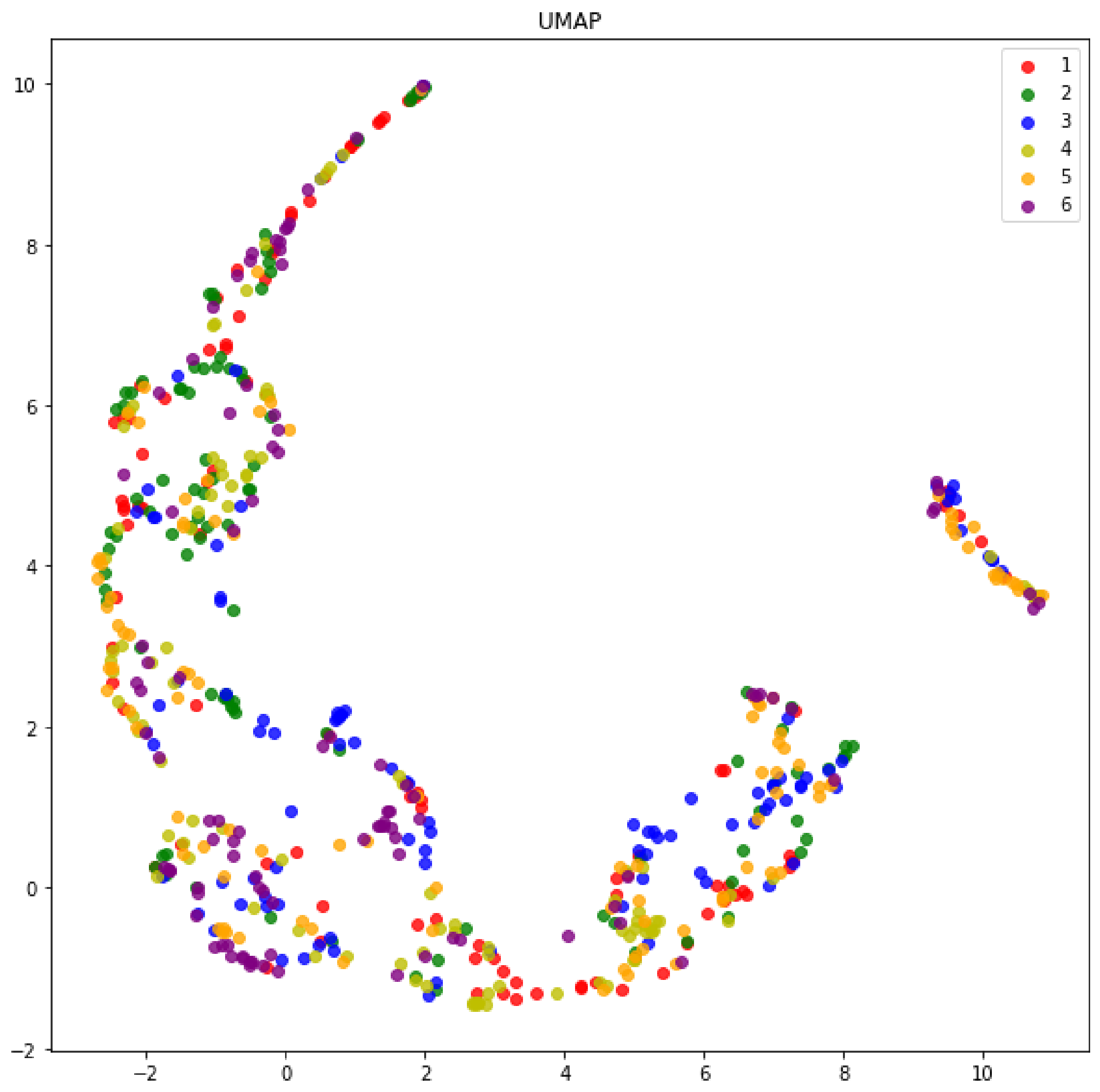
```
pca = TSNE(n_components=3)
reduced_tsne =  pca.fit_transform(gram)
plot_dr(reduced_tsne, "T-SNE",classes)

# UMAP
reducer = umap.UMAP()
scaled_gram = StandardScaler().fit_transform(gram)
embedding = reducer.fit_transform(scaled_gram)
plot_dr(embedding, "UMAP",classes)
```

```
(600, 600) (600, 76881)
```




Kernel PCA
1
2
3
4
5
6
1.0
0.8
0.6
0.4
0.2
0.0
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6


T-SNE
1
2
3
4
5
6
50
40
30
20
10
0
−10
−60
−40
−20
0
20



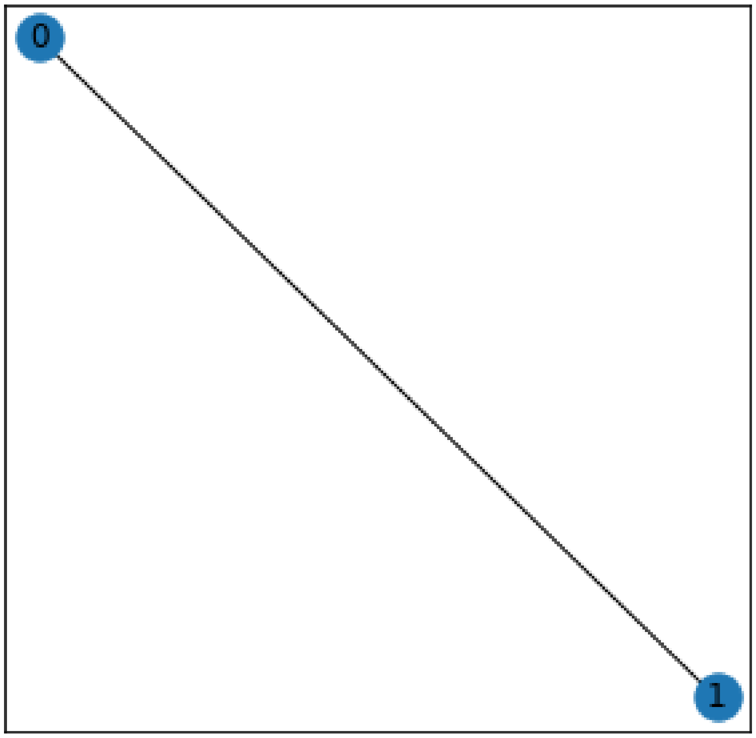
We can notice some outliers that occur in several vector representations, especially in kPCA. Let's visualize them to see if we can notice some patterns

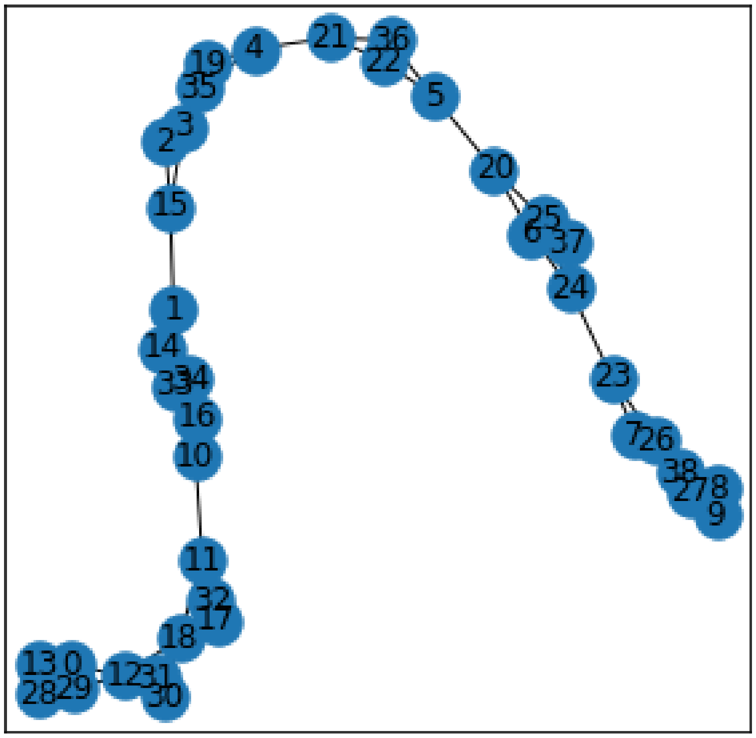
[7]:
```
# lets investiage the outliers in kPCA
reduced_kpca_2d = pd.DataFrame(data = reduced_kpca[:, 0:2], columns = ["PC1",␣
↪"PC2"])
index = reduced_kpca_2d.index
outliers = reduced_kpca_2d[(reduced_kpca_2d["PC2"] > 0.2) &␣
↪(reduced_kpca_2d["PC1"] < 0.5) ]

print("Num of outliers: ", len(outliers.index))
```

```
Num of outliers:  45
```

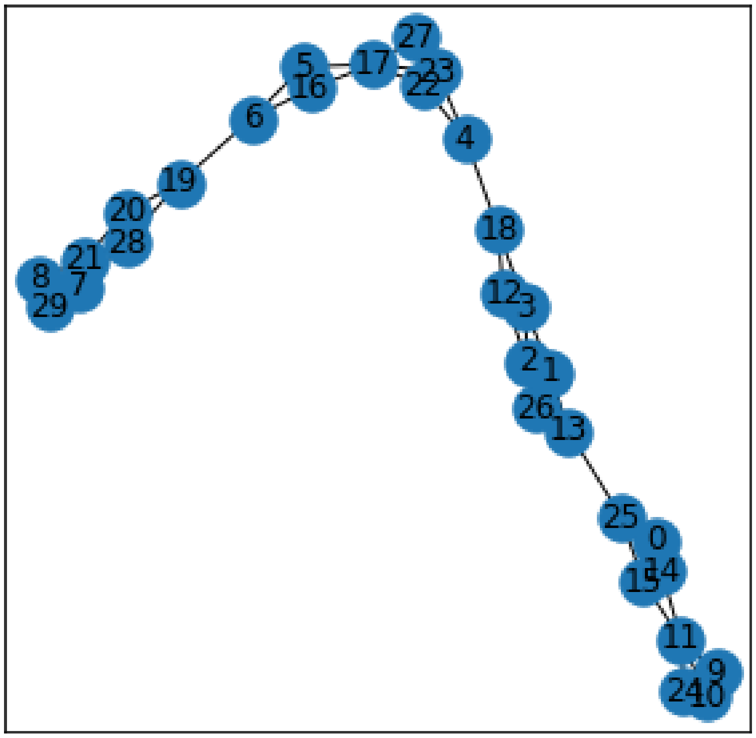
3.1 Visualizing the outliers

[48]:
```
for outlier in outliers.index[1:4]:
    visualize(G[outlier])
```





21
36
4
19
22
35
5
3
2
20
15
25
6
37
24
1
14
34
33
23
16
7
26
10
38
27
8
9
11
32
17
18
13
0
12
31
28
29
30



27
5
17
23
16
22
6
4
19
20
18
28
21
8
7
12
3
29
2
1
26
13
25
0
14
15
11
9
24
10

We can see that the outliers are associated with low/high number of nodes/edges.

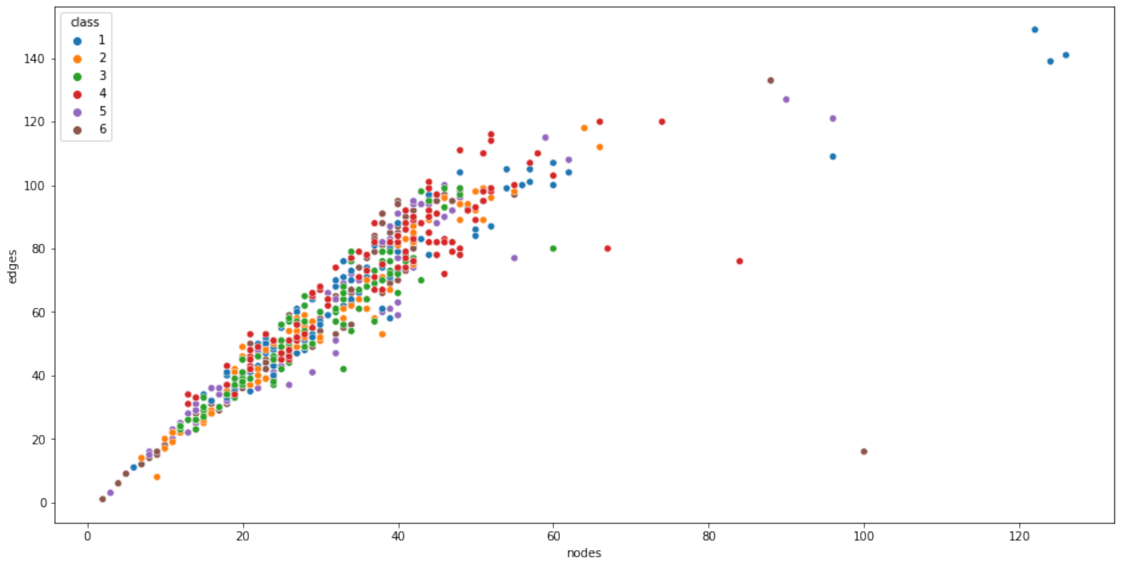
3.2 Exploring Dataset properties

3.2.1 Node - Edge correlation

[9]:
```
node_count = []
edge_count = []
for i in range(len(G)):
    node_count.append(len(G[i].nodes))
    edge_count.append(len(G[i].edges))
node_ser = pd.Series(node_count)
edge_ser = pd.Series(edge_count)
class_ser = pd.Series(classes)
df = pd.DataFrame({"class":class_ser,"nodes":node_ser,"edges":edge_ser})
```

[10]:
```
plt.subplots(figsize=(16,8))
sns.scatterplot(data=df, x="nodes", y="edges", hue="class", palette=("tab10"))
```

[10]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7fbf7f5c5b50>
```

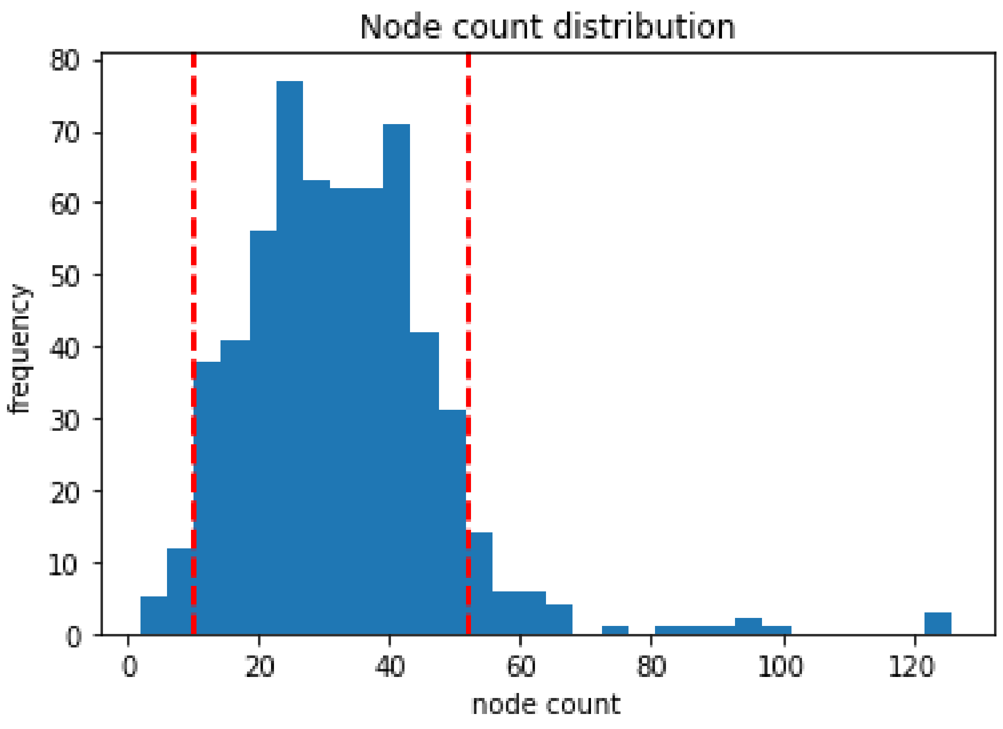


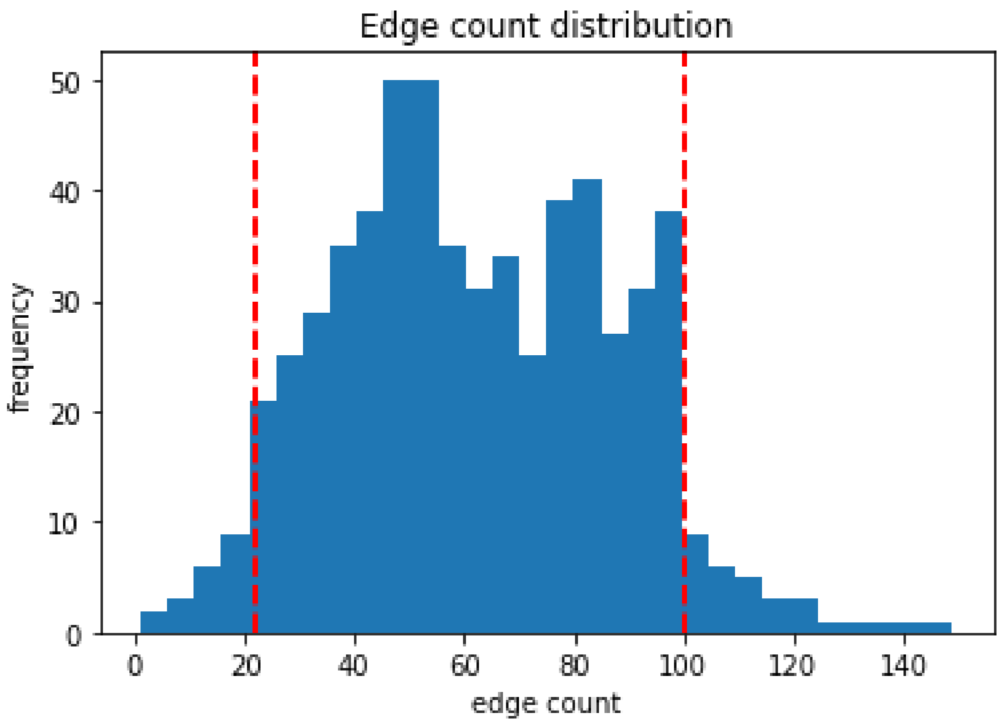
As expected, we can see that a strong linear correlation between the nodes and edges. Also we can notice that the in this vector representation the labels are more or less evently distributed. Which makes sense because the enzymes size, connectiveness is not a major factor that determines the EC of an enzyme.

Let's plot visualize the node and edge distribution of our dataset.

3.2.2 Node/edge count distributions

[11]:
```
# lets plot the node count distribution of the graphs
threshold_nodes= [10, 52]

node_lengths = [graph.number_of_nodes() for graph in G ]
plt.hist(node_lengths, bins =  30)
plt. axvline(x=threshold_nodes[0], color='r', linestyle='dashed', linewidth=2)
plt. axvline(x=threshold_nodes[1], color='r', linestyle='dashed', linewidth=2)
plt.xlabel("node count")
plt.ylabel("frequency")
plt.title("Node count distribution")
plt.show()

# lets plot the edge count distribution of the graphs
threshold_edges= [22, 100]

edge_lengths = [graph.number_of_edges() for graph in G ]
plt.hist(edge_lengths, bins =  30)
plt. axvline(x=threshold_edges[0], color='r', linestyle='dashed', linewidth=2)
plt. axvline(x=threshold_edges[1], color='r', linestyle='dashed', linewidth=2)
plt.xlabel("edge count")
plt.ylabel("frequency")
plt.title("Edge count distribution")
plt.show()
```





We can notice that there are quite some enzymes with extreme low/high node/edge counts.

For our preprocessing step we will apply edge and node count cutoffs, and remove the selected outliers because they are probably the source which make our dimensionality reduction less informative as they do not capture the esscence of data i.e. characteristics of ground truth labels.

3.3 Preprocessing

[12]:
```
# lets make some cutoffs to remove some extreme data points
G_filtered = []
indices_true = []
for graph, index in zip(G, range(0, len(G))):
    if threshold_nodes[0]  < graph.number_of_nodes() < threshold_nodes[1] \
        and threshold_edges[0]  < graph.number_of_edges() < threshold_edges[1] \
            and index not in outliers.index: #remove this line if you dont want␣
 ↪to filter out the outliers

            G_filtered.append(graph)
            indices_true.append(index)


indices_true = np.array(indices_true)
classes = dp.get_dataset(dataset)
classes = classes[indices_true] #subsetting the label list to remove OL
print("Size of filtered data: ",len(G_filtered))
```

```
Size of filtered data:  488
```

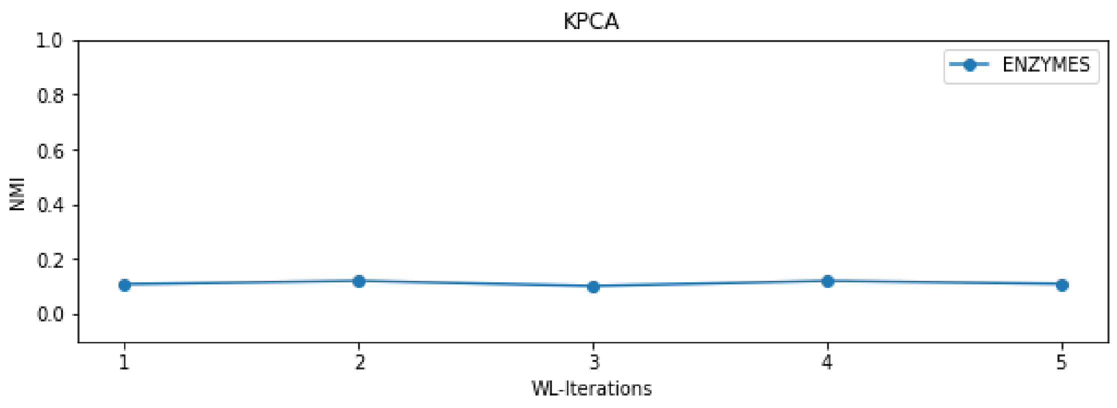
4 Dimensionality Reduction - WL

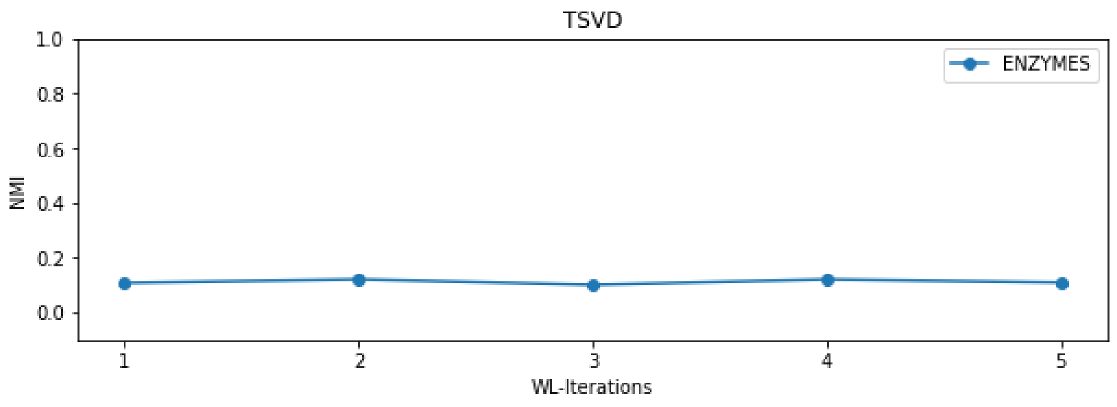
Here we want to try out clustering on different vector representations across different WL kernel iterations in order to see which WL iteration might capture the most amount of information. We also evaluate the clustering results with NMI metrics.

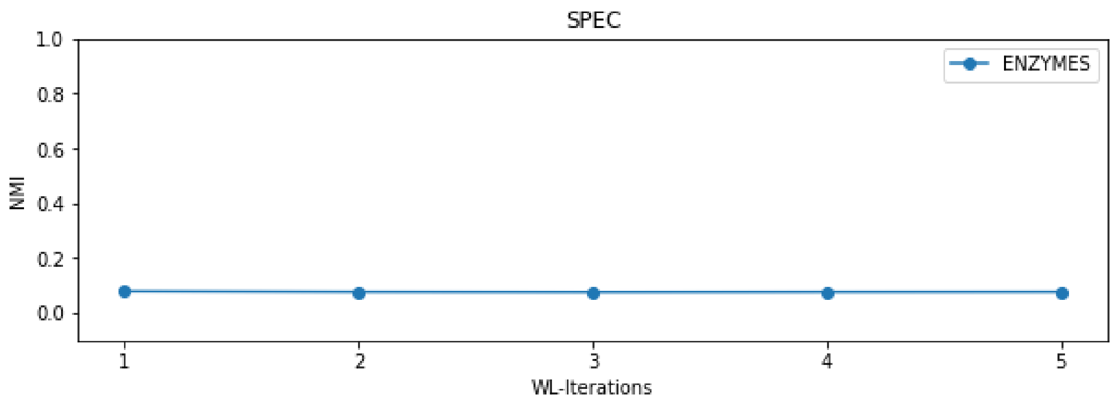
[ ]:
```
# Here we use the Wl kernel and for every WL iteration we apply DR and␣
 ↪Clustering and evaluate
# the clustering methods
# This is done on labeled and unlabeled dataset

for use_labels in [True, False]:
    if use_labels:
        base_path = os.path.join("kernels","node_labels")
        dataset = "ENZYMES"
    else:
        base_path = os.path.join("kernels","without_labels")
        dataset = "ENZYMES"

    print("##################################")
    print("Load from ", base_path)
    print("##################################")

    # dicts for storing nmi score
    nmis_kpca = {}
    nmis_tsvd = {}
    nmis_tsne = {}
    nmis_umap = {}
    nmis_spec = {}
    nmis_optics = {}


    nmis_kpca[dataset] = []
    nmis_tsvd[dataset] = []
    nmis_tsne[dataset] = []
    nmis_umap[dataset] = []
    nmis_spec[dataset] = []
    nmis_optics[dataset] = []

    # iterating over different Wl iterations
    for iterations in range(1,6):
        print("##################################")
        print("Dataset: ", dataset)
        print("Iteration: ", iterations)
        print("##################################")

        #---------------------------------------------
        # Load graph representation from the kernel
        #---------------------------------------------

        #Gram Matrix for the Weisfeiler-Lehman subtree kernel
        gram = load_csv(os.path.
↪join(base_path,f"{dataset}_gram_matrix_wl{iterations}.csv"))
        gram = aux.normalize_gram_matrix(gram) # normalizing for dr
        gram = gram[indices_true[:, None], indices_true] #removing outliers


        #Sparse Vectors for the Weisfeiler-Lehmann subtree kernel
        vec = load_sparse(os.path.
↪join(base_path,f"{dataset}_vectors_wl{iterations}.npz"))
        vec = vec[indices_true, :] #removing outliers
        vec = csc_matrix(vec, dtype=np.int8).toarray()
        #print(gram.shape, vec.shape)

        #---------------------------------------------
        # Dimensionality Reduction
        #---------------------------------------------

        # SVD
        tsvd = TruncatedSVD(n_components=100)
        reduced_tsvd = tsvd.fit_transform(vec)
        #plot_dr(reduced_tsvd, "TSVD", classes)

        # Kernel PCA
        kpca = KernelPCA(n_components=100, kernel="precomputed")
        reduced_kpca= kpca.fit_transform(gram)
        #plot_dr(reduced_kpca, "Kernel PCA",classes)

        # T-SNE
        pca = TSNE(n_components=3)
        reduced_tnse =  pca.fit_transform(gram)
        plot_dr(reduced_tnse, "T-SNE",classes)


        # UMAP
        reducer = umap.UMAP()
        #scaled_gram = StandardScaler().fit_transform(gram)
        #embedding = reducer.fit_transform(scaled_gram)
        embedding = reducer.fit_transform(gram)
        #plot_dr(embedding, "UMAP",classes)


        k = len(set(classes.tolist()))
        print("Number of labels: ", k)
        d = {0:"TSVD",1:"KPCA", 2:"T-SNE", 3:"UMAP",}
        n_d = {0:nmis_tsvd, 1:nmis_kpca, 2:nmis_tsne, 3:nmis_umap}

        for i, rep_i in enumerate([reduced_tsvd, reduced_kpca, reduced_tnse,␣
↪embedding]):

            # KMeans
            kmeans = KMeans(n_clusters=10 ,random_state=0).fit(reduced_kpca)
            plot_dr(rep_i, "KMeans in: {0}".format(d[i]),kmeans.labels_)
            km_nmi = normalized_mutual_info_score(kmeans.labels_ , classes)
            n_d[i][dataset].append(km_nmi)
            print(f"KMeans NMI:{km_nmi:.4f}")


        #Spectral Clustering
        spec = SpectralClustering(n_clusters=k, affinity="precomputed")
        spec.fit(gram)
        spec_nmi = normalized_mutual_info_score(spec.labels_,classes)
        plot_dr(reduced_kpca, "Spectral Clustering",spec.labels_)
        nmis_spec[dataset].append(spec_nmi)
        print("##################################")

        # OPTICS
        print("OPTICS")
        clust = OPTICS(min_samples=50, xi=.05, min_cluster_size=.01)
        clust.fit(gram)
        labels_050 = cluster_optics_dbscan(reachability=clust.reachability_,
                                           core_distances=clust.core_distances_,
                                           ordering=clust.ordering_, eps=0.5)

        space = np.arange(len(gram))
        reachability = clust.reachability_[clust.ordering_]
        labels = clust.labels_[clust.ordering_]
        optics_nmi = normalized_mutual_info_score(clust.labels_, classes)
        nmis_optics[dataset].append(optics_nmi)

        plt.figure(figsize=(10, 7))
        G = gridspec.GridSpec(2, 3)
        ax1 = plt.subplot(G[0, :])
        ax2 = plt.subplot(G[1, 0])

        # Reachability plot
        colors = ['g.', 'r.', 'b.', 'y.', 'c.']
        for klass, color in zip(range(0, 5), colors):
            Xk = space[labels == klass]
            Rk = reachability[labels == klass]
            ax1.plot(Xk, Rk, color, alpha=0.3)
        ax1.plot(space[labels == -1], reachability[labels == -1], 'k.', alpha=0.
↪3)
        ax1.plot(space, np.full_like(space, 2., dtype=float), 'k-', alpha=0.5)
        ax1.plot(space, np.full_like(space, 0.5, dtype=float), 'k-.', alpha=0.5)
        ax1.set_ylabel('Reachability (epsilon distance)')
        ax1.set_title('Reachability Plot')

        # OPTICS - clusters
        colors = ['g.', 'r.', 'b.', 'y.', 'c.']
        for klass, color in zip(range(0, 5), colors):
            Xk = gram[clust.labels_ == klass]
            ax2.plot(Xk[:, 0], Xk[:, 1], color, alpha=0.3)
        ax2.plot(gram[clust.labels_ == -1, 0], gram[clust.labels_ == -1, 1],␣
↪'k+', alpha=0.1)
        ax2.set_title('Automatic Clustering\nOPTICS')


    res = {"KPCA":nmis_kpca,"TSVD": nmis_tsvd, "SPEC": nmis_spec,
           "OPTICS":nmis_optics, "TSNE":nmis_tsne, "UMAP": nmis_umap, }
    for key, value in res.items():
        nmi_df = pd.DataFrame(res[key])
        nmi_df.to_csv(os.path.join(base_path, key + ".csv"))
```

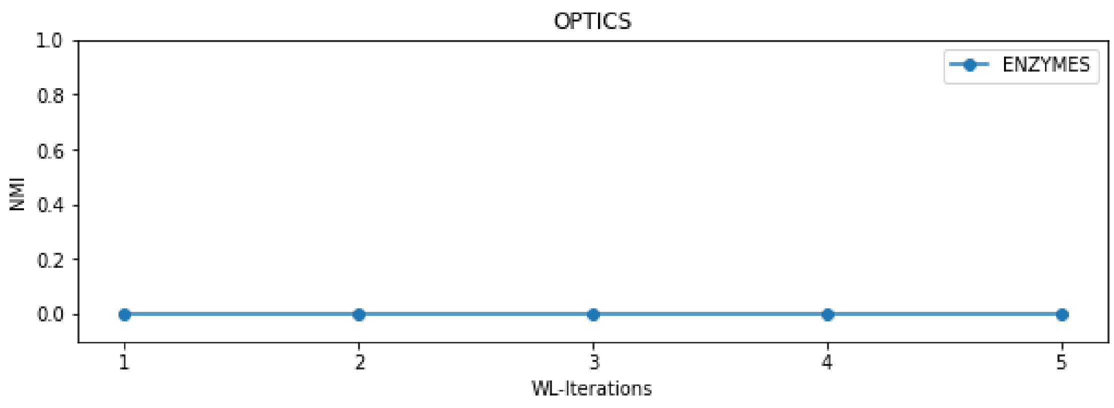
[16]:
```
result_names = ["KPCA", "TSVD", "SPEC", "OPTICS", "TSNE", "UMAP"]
for version in ["node_labels", "without_labels"]:
    print(f"#################{version}#################")
    for name_i in result_names:
        path_i = os.path.join("kernels", version, name_i+".csv")
        nmi_df = pd.read_csv(path_i, index_col=0)
        fig, ax = plt.subplots(figsize=(10,3))
        ax.set_ylabel("NMI")
        ax.set_xlabel("WL-Iterations")
        ax.set_ylim([-0.1,1])
        ax.set_xticks([0,1,2,3,4])
        ax.set_xticklabels([1,2,3,4,5])
        ax.set_title(name_i)
        nmi_df.plot(marker="o", ax=ax)
        plt.show();
```

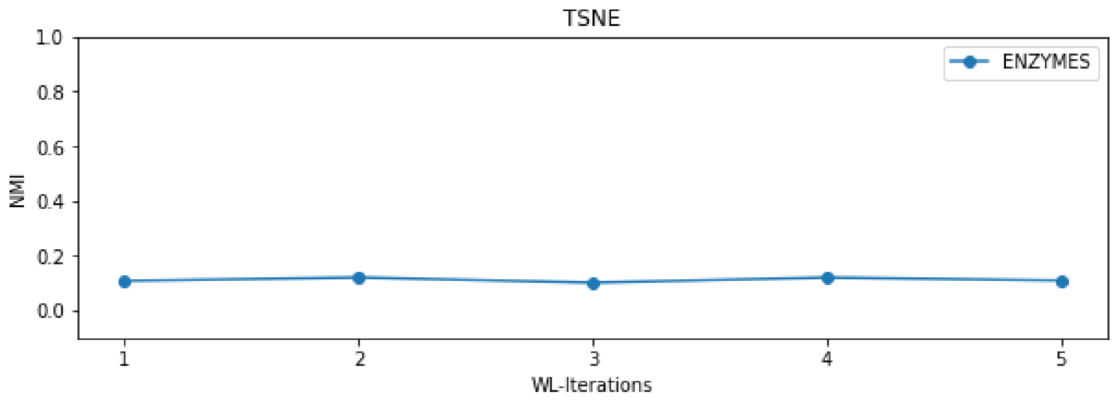
```
#################node_labels#################
```

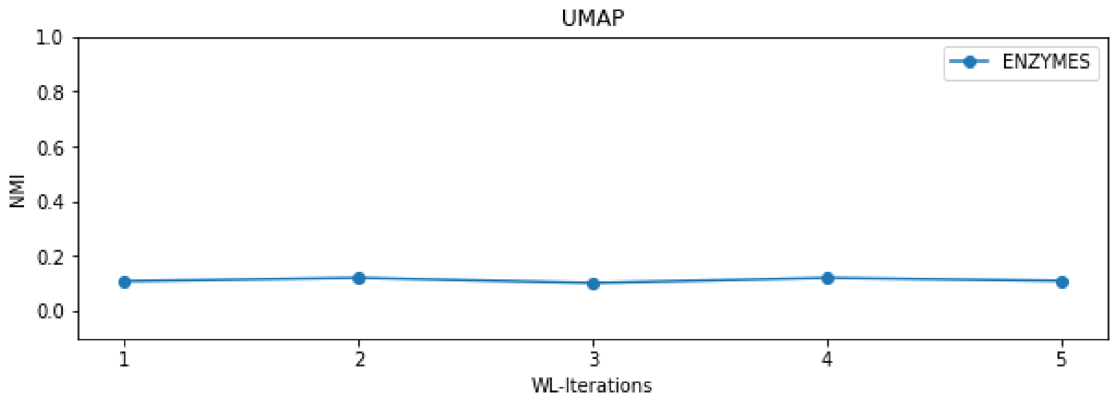

KPCA
ENZYMES
NMI
WL-Iterations
1.0
0.8
0.6
0.4
0.2
0.0
1
2
3
4
5


TSVD
ENZYMES
NMI
WL-Iterations
1.0
0.8
0.6
0.4
0.2
0.0
1
2
3
4
5

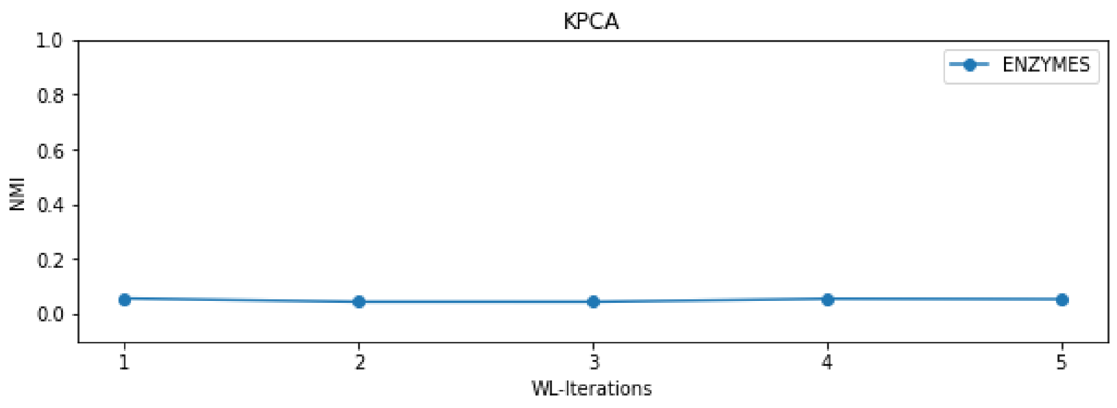

SPEC
ENZYMES
NMI
WL-Iterations
1.0
0.8
0.6
0.4
0.2
0.0
1
2
3
4
5

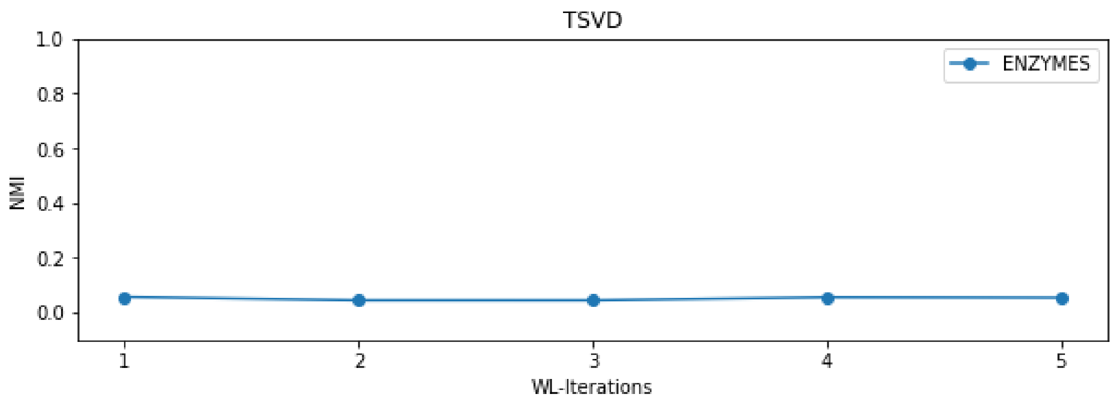


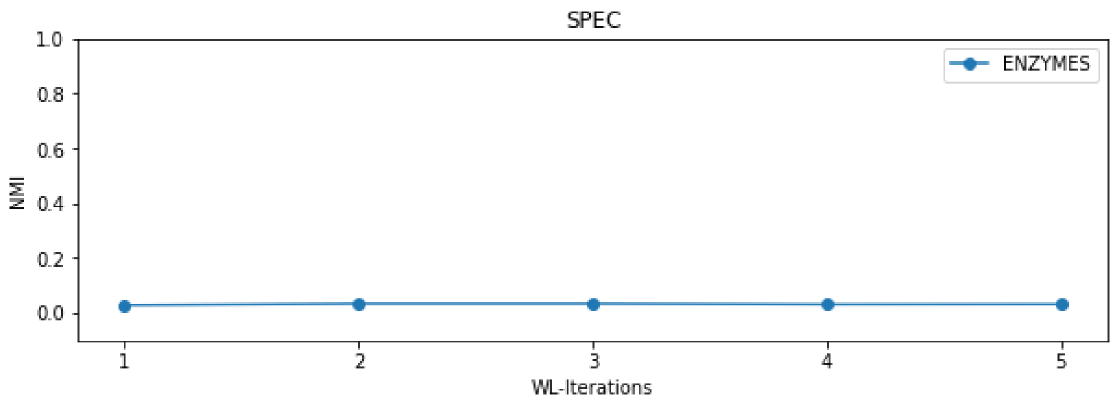


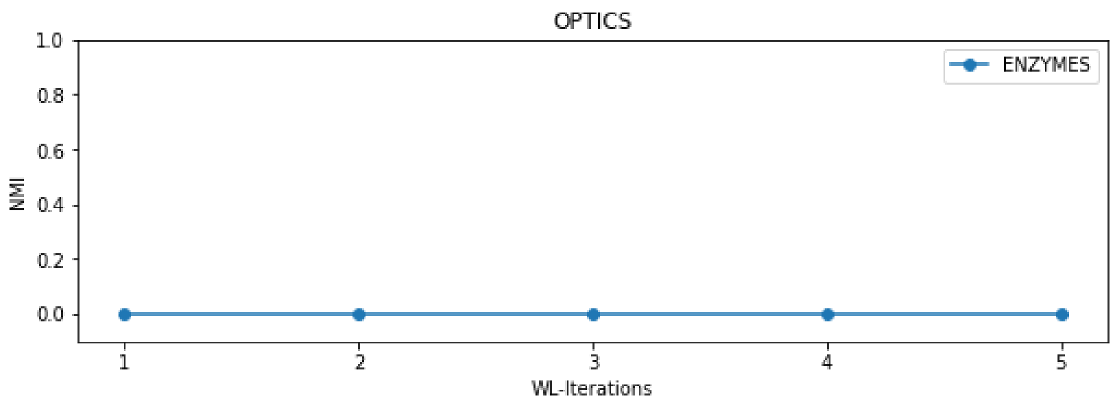


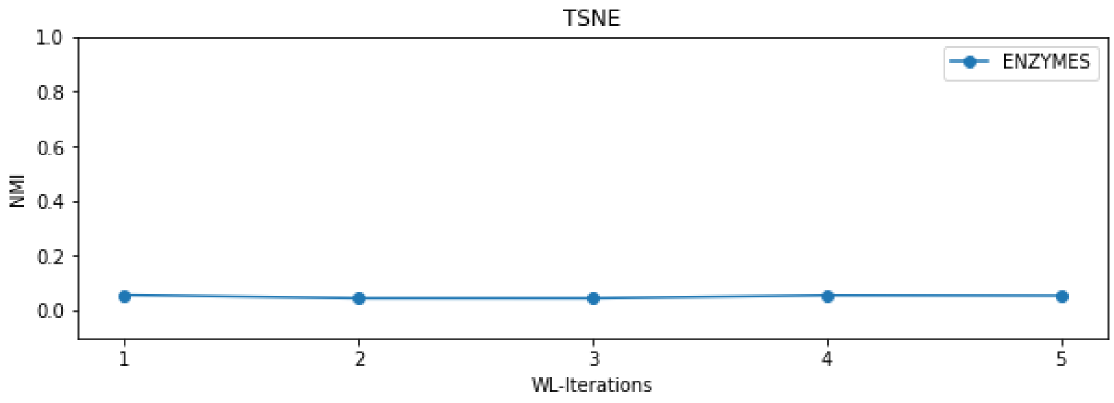
```
#################without_labels#################
```

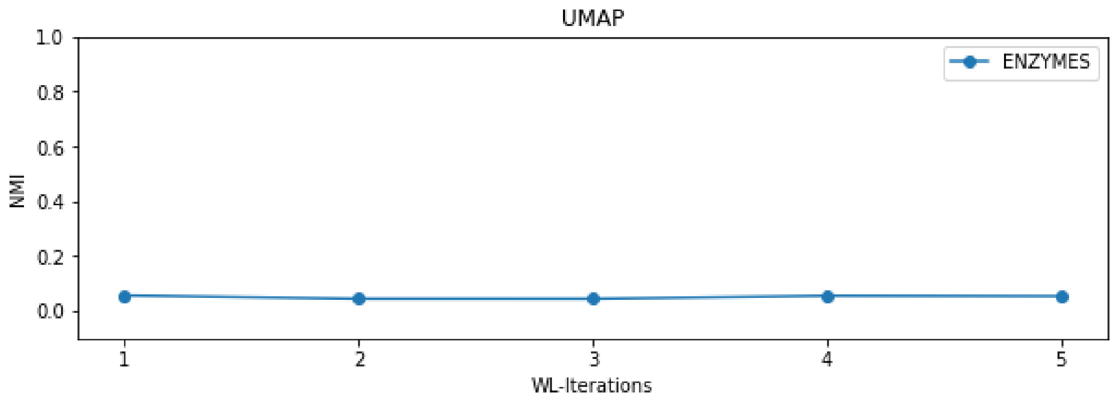

KPCA
1.0
0.8
0.6
0.4
0.2
0.0
NMI
ENZYMES
1
2
3
4
5
WL-Iterations


TSVD
1.0
0.8
0.6
0.4
0.2
0.0
NMI
ENZYMES
1
2
3
4
5
WL-Iterations


SPEC
1.0
0.8
0.6
0.4
0.2
0.0
NMI
ENZYMES
1
2
3
4
5
WL-Iterations







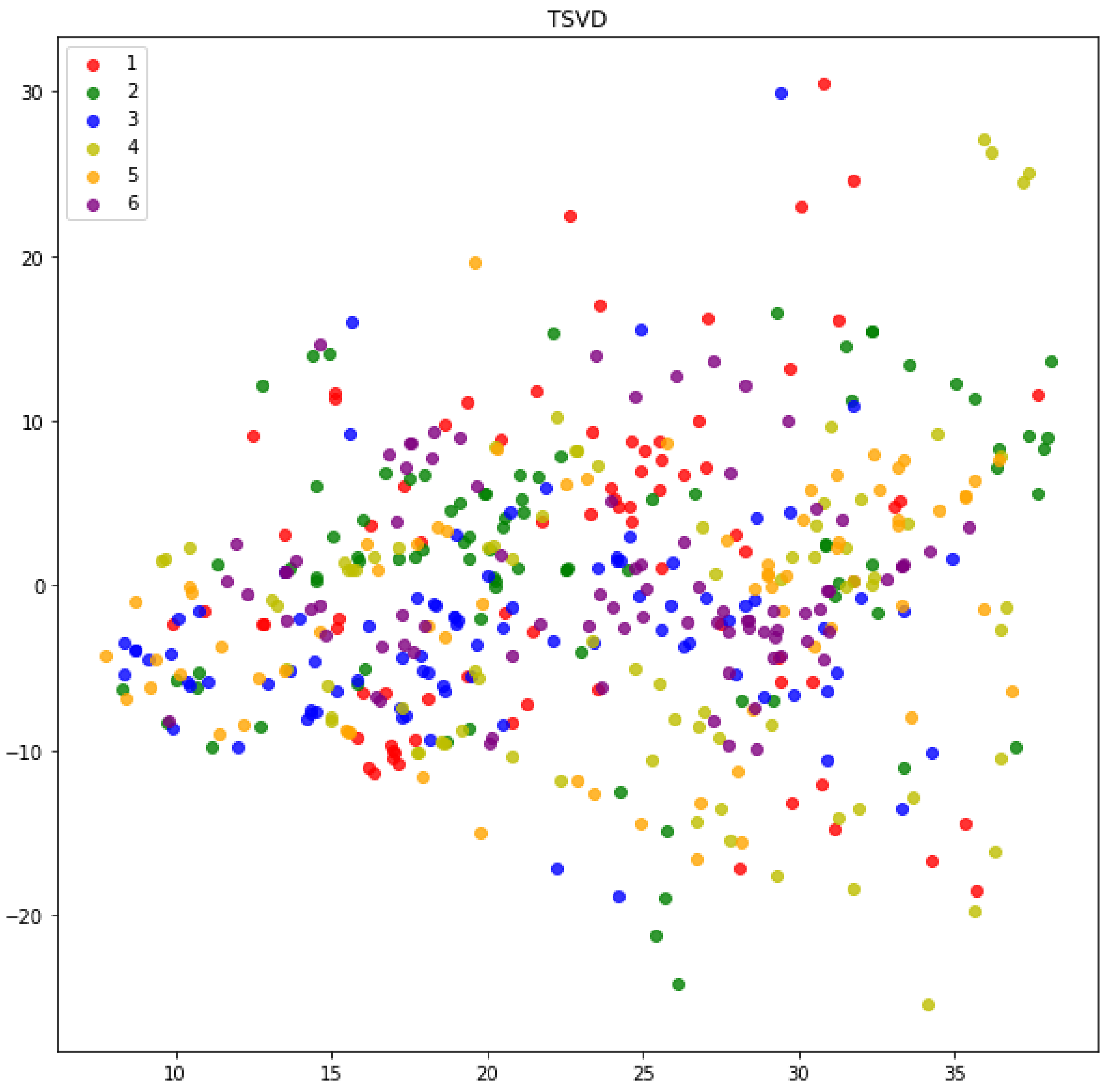
We can notice that the clustering results are a bit better in iteration 2 and 4 e.g. in kMeans clustering with UMAP, TSNE, kPCA. We will therefore use iteration 4 for our next part of the analysis.

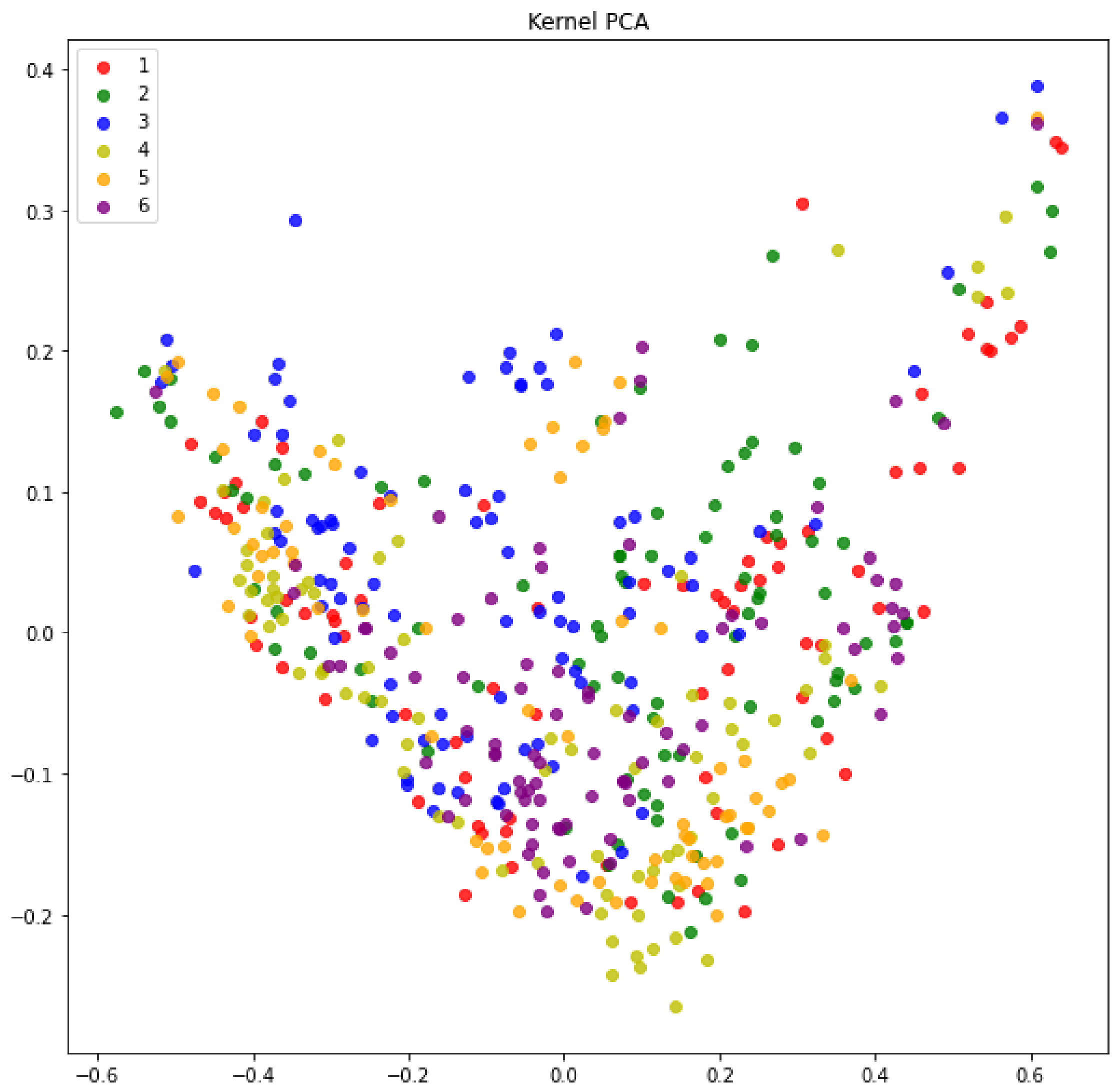
Lets visualize the WL4 DR representations.

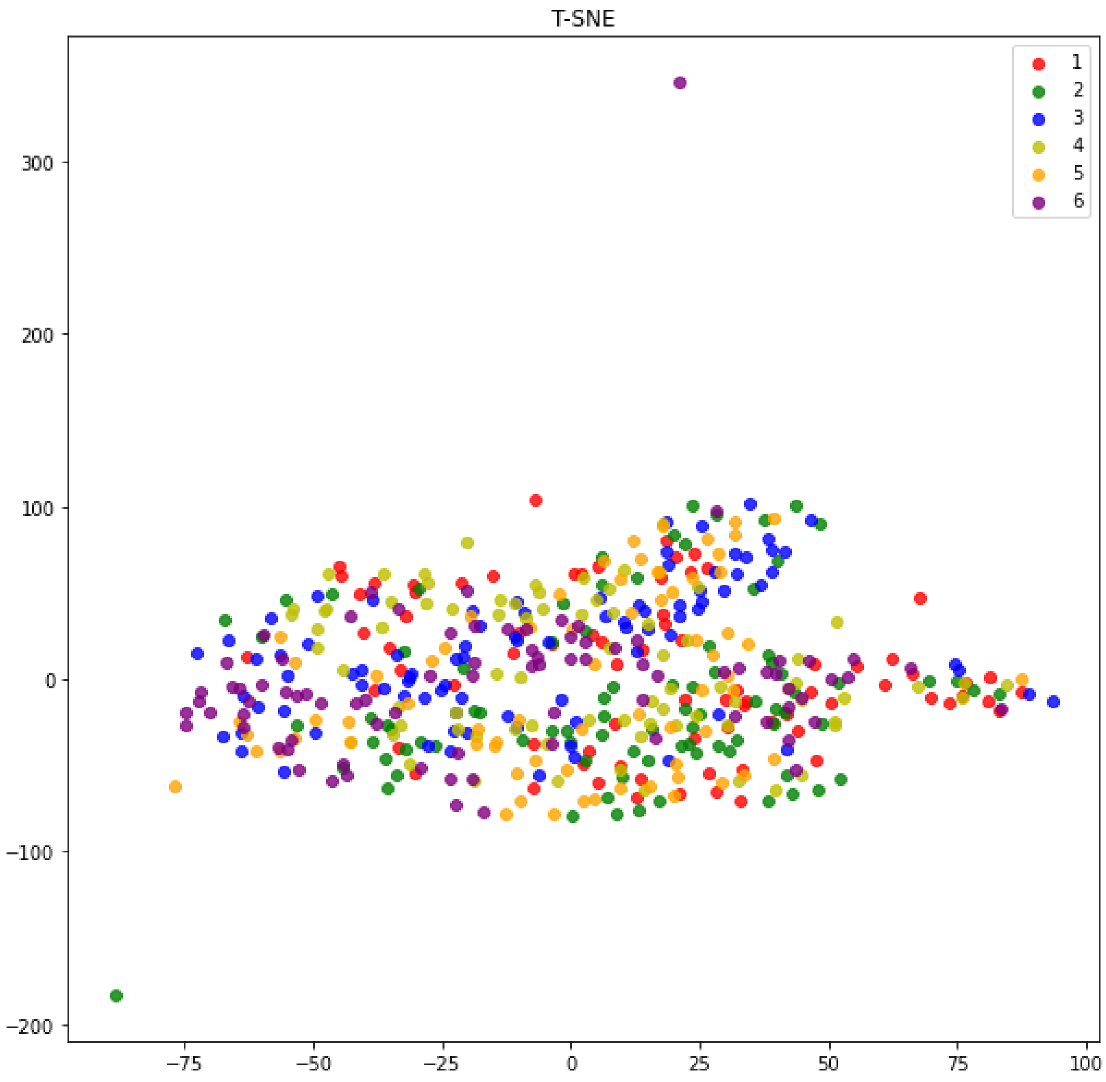
[17]:
```
# triyng different iterations
dataset = "ENZYMES"
iterations = 4
base_path = os.path.join("kernels","node_labels")
#base_path = os.path.join("kernels","without_labels")
classes = dp.get_dataset(dataset)
classes = classes[indices_true]
#--------------------------------------------
# Load graph representation from the kernel
#--------------------------------------------

#Gram Matrix for the Weisfeiler-Lehman subtree kernel
gram = load_csv(os.path.join(base_path,f"{dataset}_gram_matrix_wl{iterations}.
 ↪csv"))
gram = aux.normalize_gram_matrix(gram)
gram = gram[indices_true[:, None], indices_true] #removing outliers


#Sparse Vectors for the Weisfeiler-Lehmann subtree kernel
vec = load_sparse(os.path.join(base_path,f"{dataset}_vectors_wl{iterations}.
 ↪npz"))
vec = vec[indices_true, :] #removing outliers
vec = csc_matrix(vec, dtype=np.int8).toarray()
print(gram.shape, vec.shape)

# SVD
tsvd = TruncatedSVD(n_components=50)
reduced_tsvd = tsvd.fit_transform(vec)
plot_dr(reduced_tsvd, "TSVD", classes)

# Kernel PCA
kpca = KernelPCA(n_components=100, kernel="precomputed")
reduced_kpca= kpca.fit_transform(gram)
plot_dr(reduced_kpca, "Kernel PCA",classes)

# T-SNE

pca = TSNE(n_components=3)
reduced_tsne =  pca.fit_transform(gram)
plot_dr(reduced_tsne, "T-SNE",classes)

# UMAP
reducer = umap.UMAP()
scaled_gram = StandardScaler().fit_transform(gram)
embedding = reducer.fit_transform(scaled_gram)
```

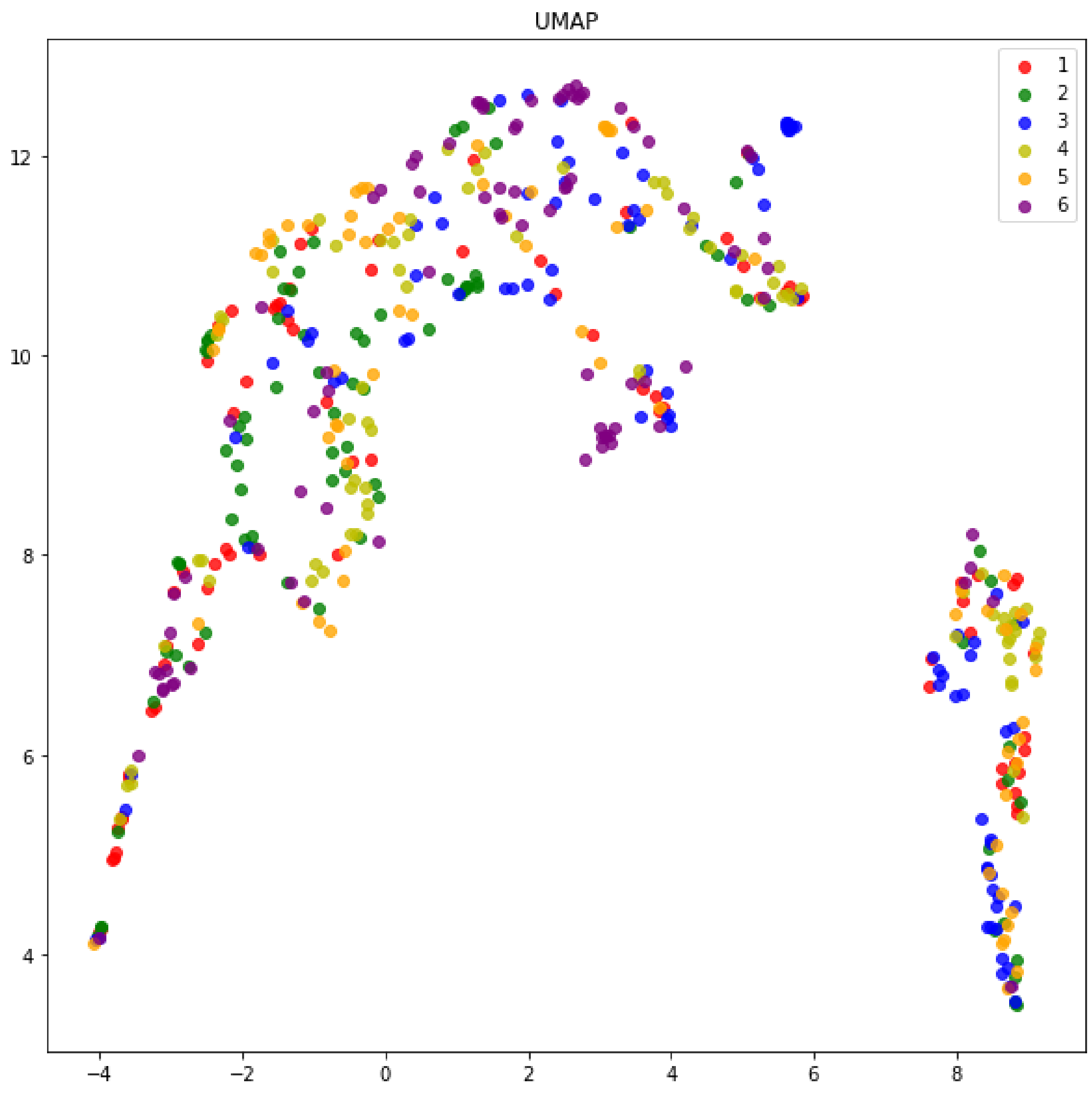
```
plot_dr(embedding, "UMAP",classes)
```

```
(488, 488) (488, 59599)
```




Kernel PCA
1
2
3
4
5
6
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6


T-SNE
1
2
3
4
5
6
300
200
100
0
−100
−200
−75
−50
−25
0
25
50
75
100



We can notice that there are some groupings of our truth labels in some places.

4.1 Clustering Evaluation

[18]:
```
dataset = "ENZYMES"
iterations = 4
base_path = os.path.join("kernels","node_labels")
#base_path = os.path.join("kernels","without_labels")
classes = dp.get_dataset(dataset)
classes = classes[indices_true]

# dicts for storing nmi score
nmis_kpca = {}
```

```
nmis_tsvd = {}
nmis_tsne = {}
nmis_umap = {}
nmis_spec = {}
nmis_optics = {}
nmis_hier = {}
nmis_hisc = {}


nmis_kpca[dataset] = []
nmis_tsvd[dataset] = []
nmis_tsne[dataset] = []
nmis_umap[dataset] = []
nmis_spec[dataset] = []
nmis_optics[dataset] = []
nmis_hier[dataset] = []
nmis_hisc[dataset] = []


iterations = 4
print("##################################")
print("Dataset: ", dataset)
print("Iteration: ", iterations)
print("##################################")

#--------------------------------------------
# Load graph representation from the kernel
#--------------------------------------------

#Gram Matrix for the Weisfeiler-Lehman subtree kernel
gram = load_csv(os.path.join(base_path,f"{dataset}_gram_matrix_wl{iterations}.
 ↪csv"))
gram = aux.normalize_gram_matrix(gram) # normalizing for dr
gram = gram[indices_true[:, None], indices_true] #removing outliers


#Sparse Vectors for the Weisfeiler-Lehmann subtree kernel
vec = load_sparse(os.path.join(base_path,f"{dataset}_vectors_wl{iterations}.
 ↪npz"))
vec = vec[indices_true, :] #removing outliers
vec = csc_matrix(vec, dtype=np.int8).toarray()
print(gram.shape, vec.shape)

#--------------------------------------------
# Dimensionality Reduction
#--------------------------------------------
```

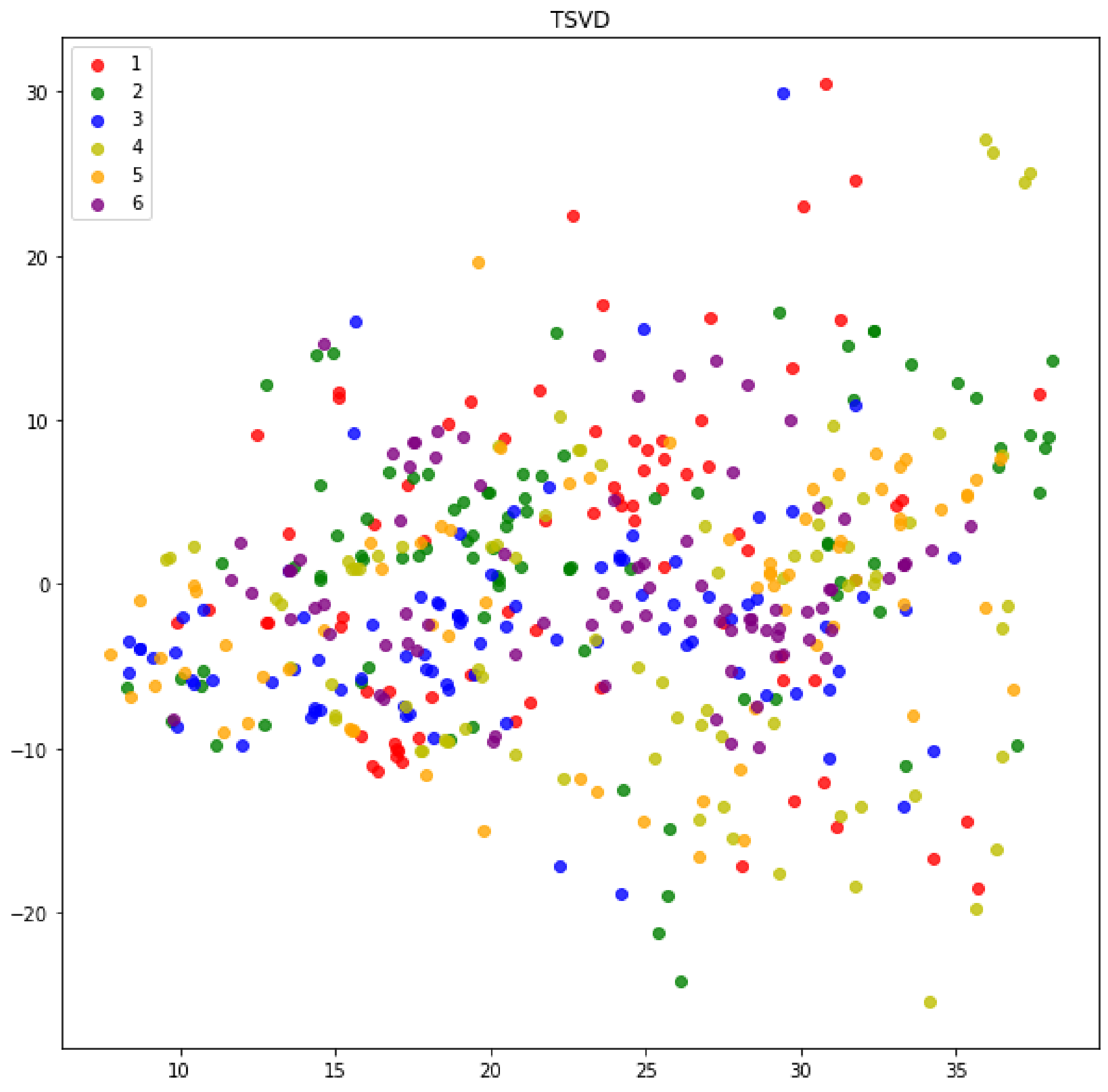
```
# SVD
tsvd = TruncatedSVD(n_components=100)
reduced_tsvd = tsvd.fit_transform(vec)
plot_dr(reduced_tsvd, "TSVD", classes)

# Kernel PCA
kpca = KernelPCA(n_components=100, kernel="precomputed")
reduced_kpca= kpca.fit_transform(gram)
plot_dr(reduced_kpca, "Kernel PCA",classes)

# T-SNE
pca = TSNE(n_components=3)
reduced_tnse =  pca.fit_transform(gram)
plot_dr(reduced_tnse, "T-SNE",classes)


# UMAP
reducer = umap.UMAP()
#scaled_gram = StandardScaler().fit_transform(gram)
#embedding = reducer.fit_transform(scaled_gram)
embedding = reducer.fit_transform(gram)
plot_dr(embedding, "UMAP",classes)


k = len(set(classes.tolist()))
print("Number of labels: ", k)
d = {0:"TSVD",1:"KPCA", 2:"T-SNE", 3:"UMAP",}
n_d = {0:nmis_tsvd, 1:nmis_kpca, 2:nmis_tsne, 3:nmis_umap}

for i, rep_i in enumerate([reduced_tsvd, reduced_kpca, reduced_tnse,␣
 ↪embedding]):
    print(d[i])


    # KMeans
    print("KMeans")
    kmeans = KMeans(n_clusters=10 ,random_state=0).fit(rep_i)
    plot_dr(reduced_kpca, "KMeans in: {0}".format(d[i]),kmeans.labels_)
    km_nmi = normalized_mutual_info_score(kmeans.labels_ , classes)
    n_d[i][dataset].append(km_nmi)
    print(f"KMeans NMI:{km_nmi:.4f}")



# Hierarchical clustering
clustering = AgglomerativeClustering(n_clusters=10, linkage="ward").fit(gram)
hc_nmi = normalized_mutual_info_score(clustering.labels_ , classes)
```

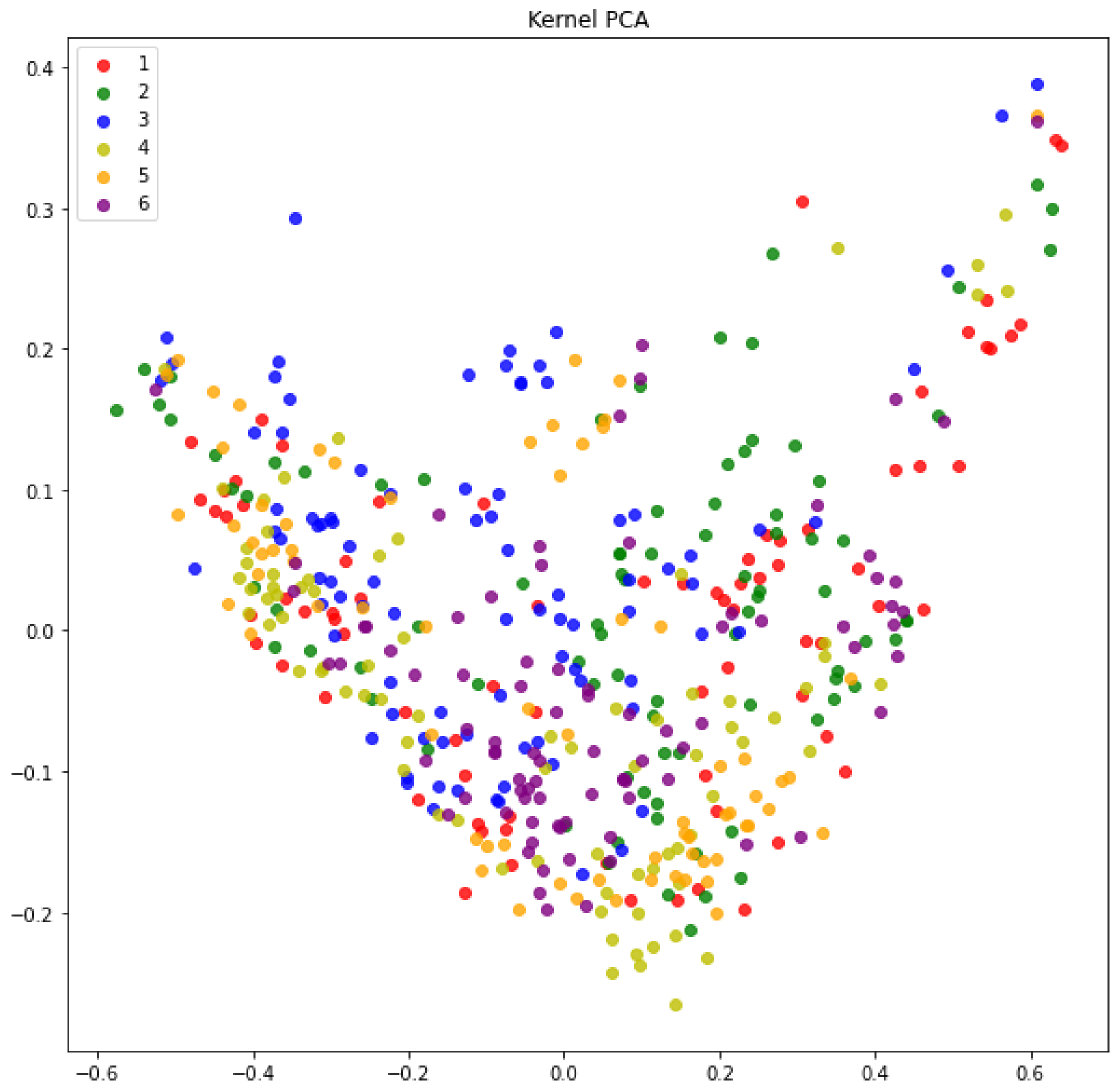
```python
nmis_hier[dataset].append(hc_nmi)
plot_dr(reduced_kpca, "hierarchical ward",clustering.labels_)
print(f"H clustering NMI:{hc_nmi:.4f}")



#Spectral Clustering
spec = SpectralClustering(n_clusters=k, affinity="precomputed")
spec.fit(gram)
spec_nmi = normalized_mutual_info_score(spec.labels_,classes)
plot_dr(reduced_kpca, "Spectral Clustering",clustering.labels_)
nmis_spec[dataset].append(spec_nmi)
print("###################################")

# OPTICS
print("OPTICS")
clust = OPTICS(min_samples=10, xi=.001, min_cluster_size=.01)
clust.fit(gram)
labels_050 = cluster_optics_dbscan(reachability=clust.reachability_,
                                   core_distances=clust.core_distances_,
                                   ordering=clust.ordering_, eps=0.5)

space = np.arange(len(gram))
reachability = clust.reachability_[clust.ordering_]
labels = clust.labels_[clust.ordering_]
optics_nmi = normalized_mutual_info_score(clust.labels_, classes)
print("optics nmi: ", optics_nmi)
nmis_optics[dataset].append(optics_nmi)

plt.figure(figsize=(10, 7))
G = gridspec.GridSpec(2, 3)
ax1 = plt.subplot(G[0, :])
ax2 = plt.subplot(G[1, 0])

# Reachability plot
colors = ['g.', 'r.', 'b.', 'y.', 'c.']
for klass, color in zip(range(0, 5), colors):
    Xk = space[labels == klass]
    Rk = reachability[labels == klass]
    ax1.plot(Xk, Rk, color, alpha=0.3)
ax1.plot(space[labels == -1], reachability[labels == -1], 'k.', alpha=0.3)
ax1.plot(space, np.full_like(space, 2., dtype=float), 'k-', alpha=0.5)
ax1.plot(space, np.full_like(space, 0.5, dtype=float), 'k-.', alpha=0.5)
ax1.set_ylabel('Reachability (epsilon distance)')
ax1.set_title('Reachability Plot')

# OPTICS - clusters
```

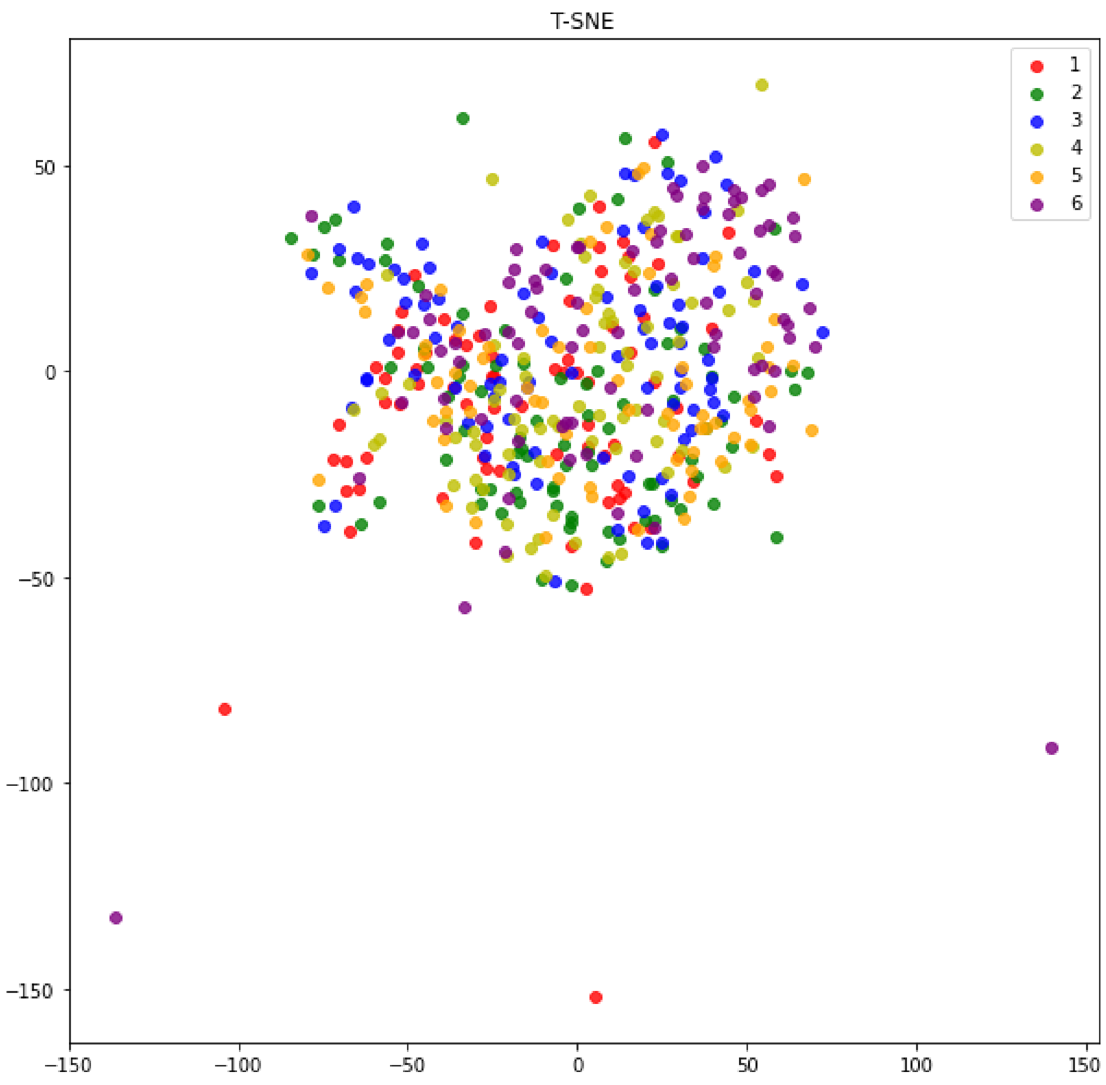
```
colors = ['g.', 'r.', 'b.', 'y.', 'c.']
for klass, color in zip(range(0, 5), colors):
    Xk = gram[clust.labels_ == klass]
    ax2.plot(Xk[:, 0], Xk[:, 1], color, alpha=0.3)
ax2.plot(gram[clust.labels_ == -1, 0], gram[clust.labels_ == -1, 1], 'k+',␣
 ↪alpha=0.1)
ax2.set_title('Automatic Clustering\nOPTICS')
plt.show()

# self-implemented HiSC
print("HISC")
gram = load_csv("./kernels/node_labels/ENZYMES_gram_matrix_wl4.csv")
gram = aux.normalize_gram_matrix(gram)
gram = gram[indices_true[:, None], indices_true]

label_file = load_csv("../tud_benchmark/datasets/ENZYMES/ENZYMES/raw/
 ↪ENZYMES_graph_labels.txt")[indices_true]
label_file = label_file.astype(int)
np.savetxt("./kernels/node_labels/ENZYMES_gram_matrix_wl4_filtered.csv", gram,␣
 ↪delimiter=";")
np.savetxt("../tud_benchmark/datasets/ENZYMES/ENZYMES/raw/
 ↪ENZYMES_graph_labels_filtered.txt", label_file,
           fmt="%d",newline="\n")
dataset_file = "./kernels/node_labels/ENZYMES_gram_matrix_wl4_filtered.csv"
label_file = "../tud_benchmark/datasets/ENZYMES/ENZYMES/raw/
 ↪ENZYMES_graph_labels_filtered.txt"

data, labels_true = process_csv(dataset_file, input_filename_labels=label_file,␣
 ↪sep=";")

alpha = 0.007
k = 4
clus_ord = HiSC(data, alpha, k, verbose=False, elki=True)
threshold=0.8
dimensions=[(0,9),(1,11)]

labels = get_clusters(clus_ord, threshold=threshold)

hisc_nmi = normalized_mutual_info_score(labels, classes)
print(hisc_nmi)
nmis_hisc[dataset].append(hisc_nmi)

reachability_plot(data, clus_ord, labels, dimensions=dimensions)
```

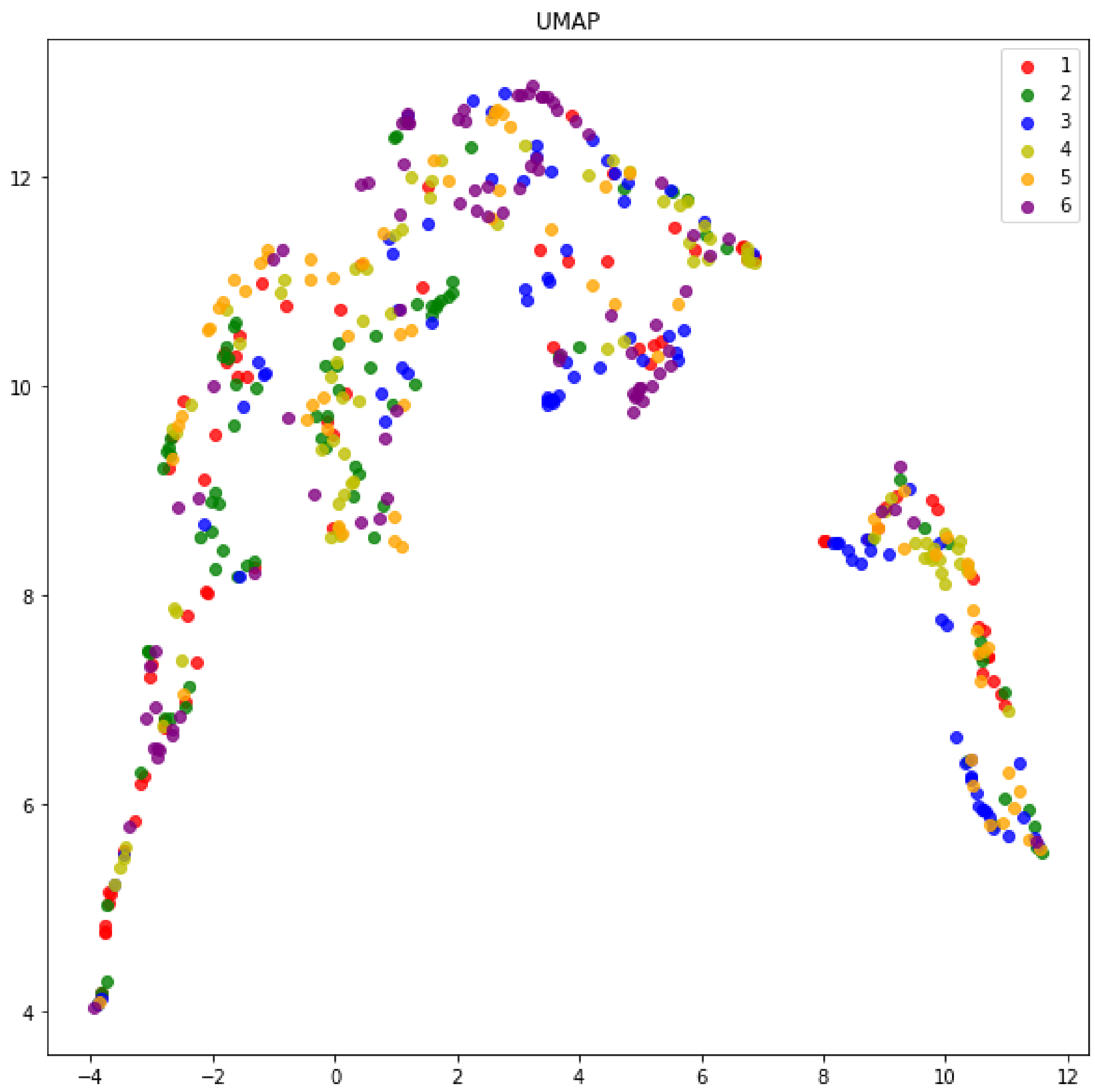
```
res = {"KPCA":nmis_kpca,"TSVD": nmis_tsvd, "SPEC": nmis_spec,
       "OPTICS":nmis_optics, "TSNE":nmis_tsne, "UMAP": nmis_umap, "HIER":␣
 ↪nmis_hier,
      "HISC": nmis_hisc}
for key, value in res.items():
    nmi_df = pd.DataFrame(res[key])
    nmi_df.to_csv(os.path.join(base_path, key + ".csv"))
```

```
##################################
Dataset:  ENZYMES
Iteration:  4
##################################
(488, 488) (488, 59599)
```

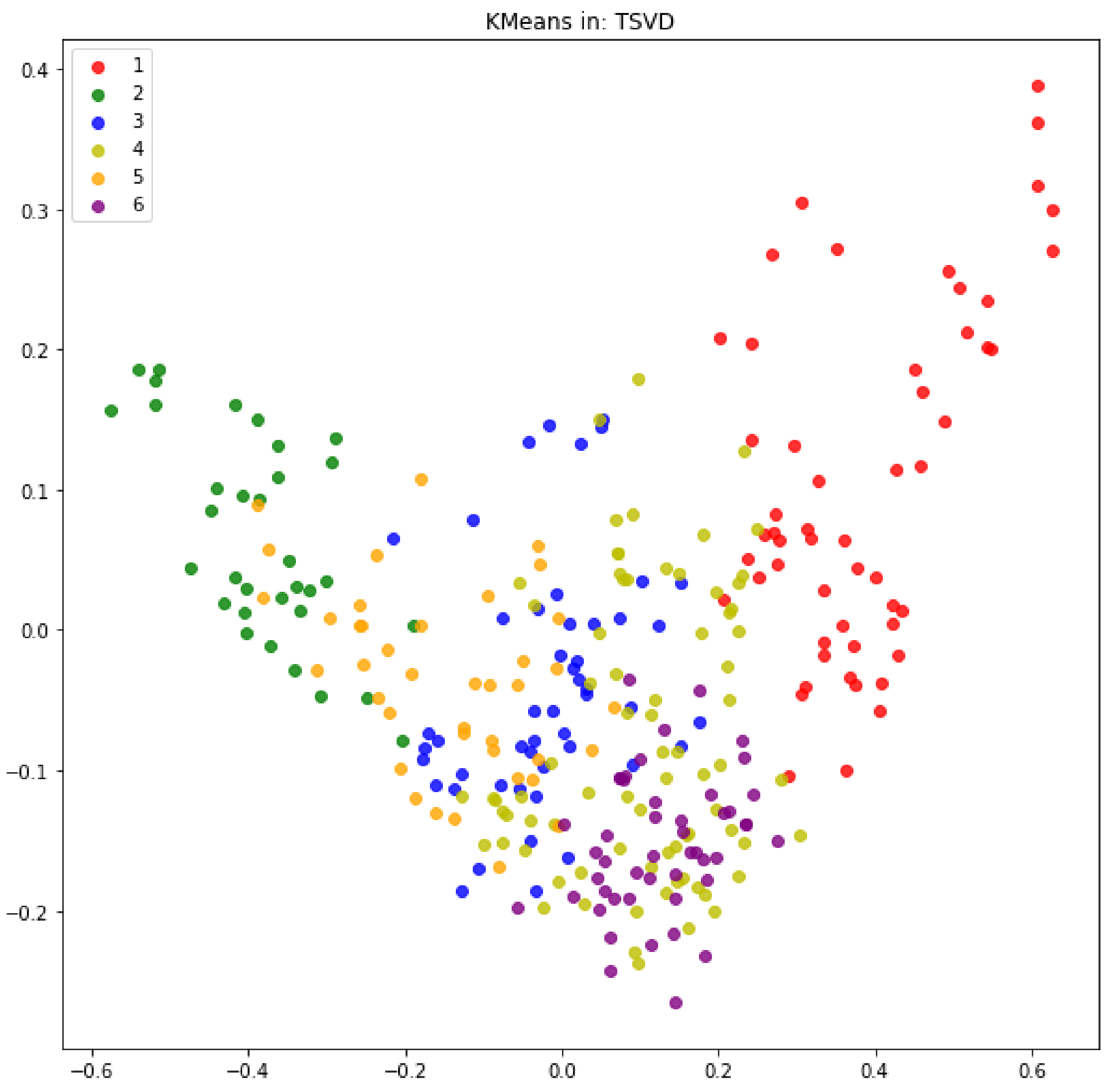



Kernel PCA
1
2
3
4
5
6
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6

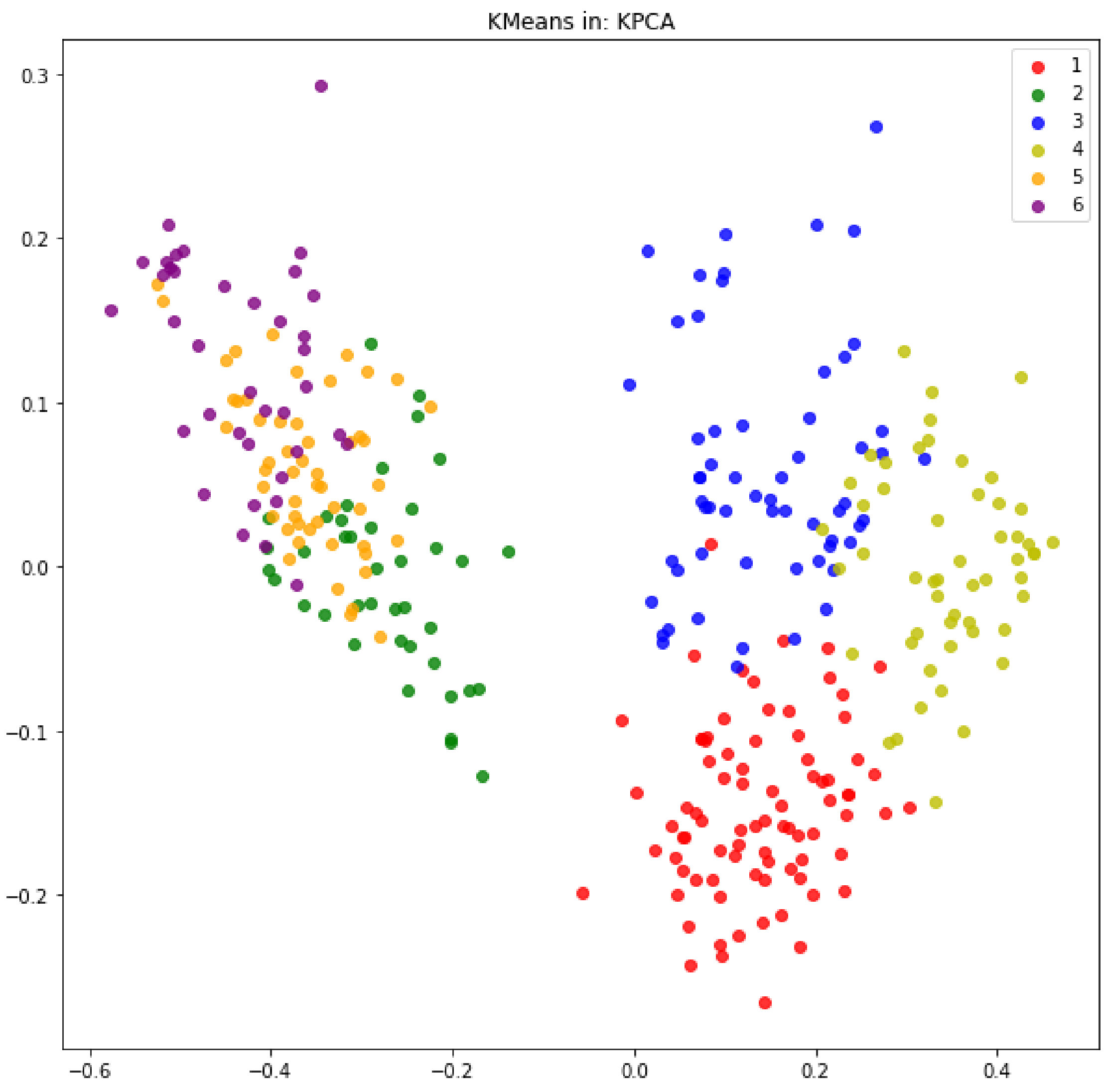

T-SNE
1
2
3
4
5
6
50
0
−50
−100
−150
−150
−100
−50
0
50
100
150



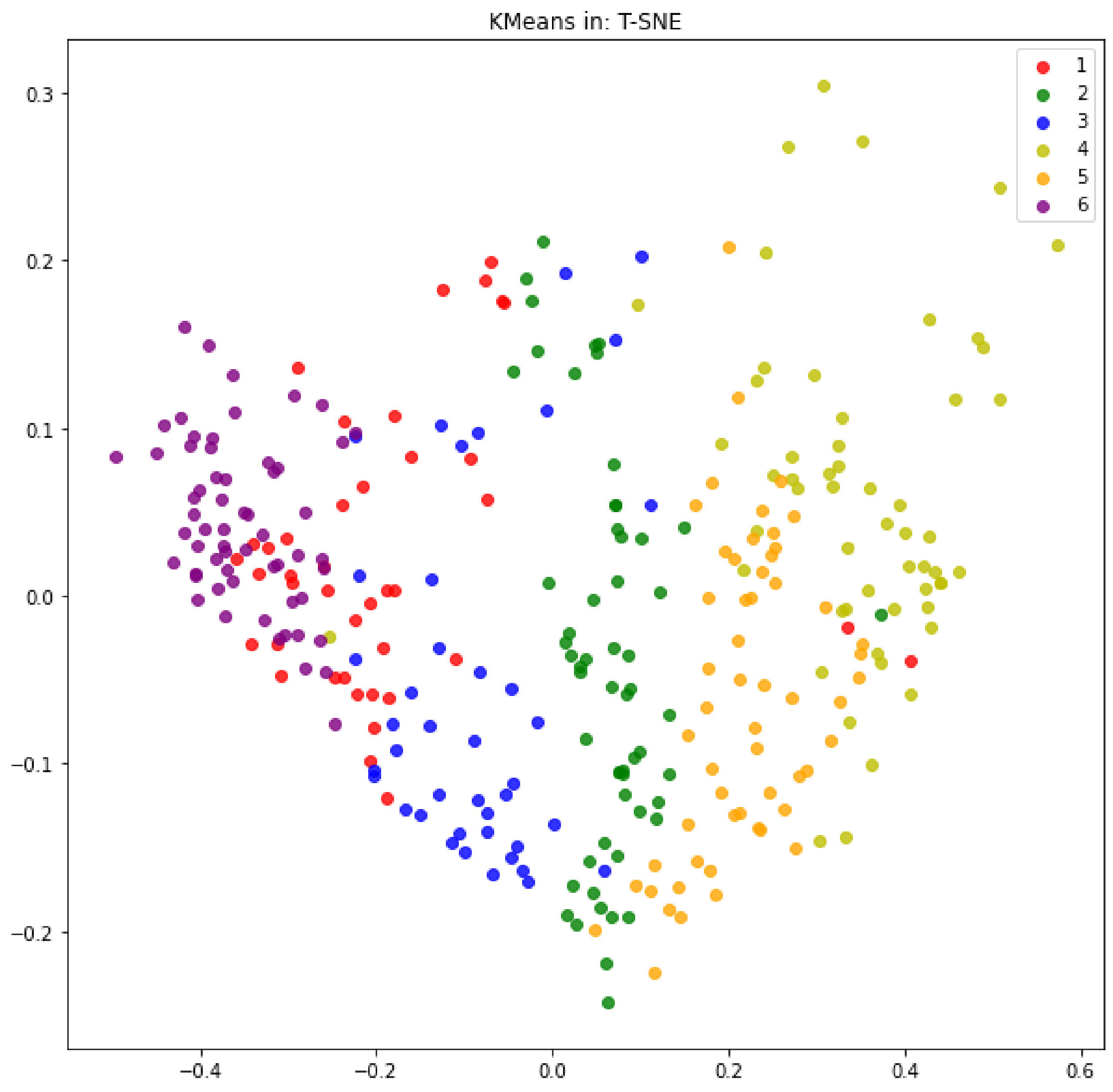
```
Number of labels:  6
TSVD
KMeans
```



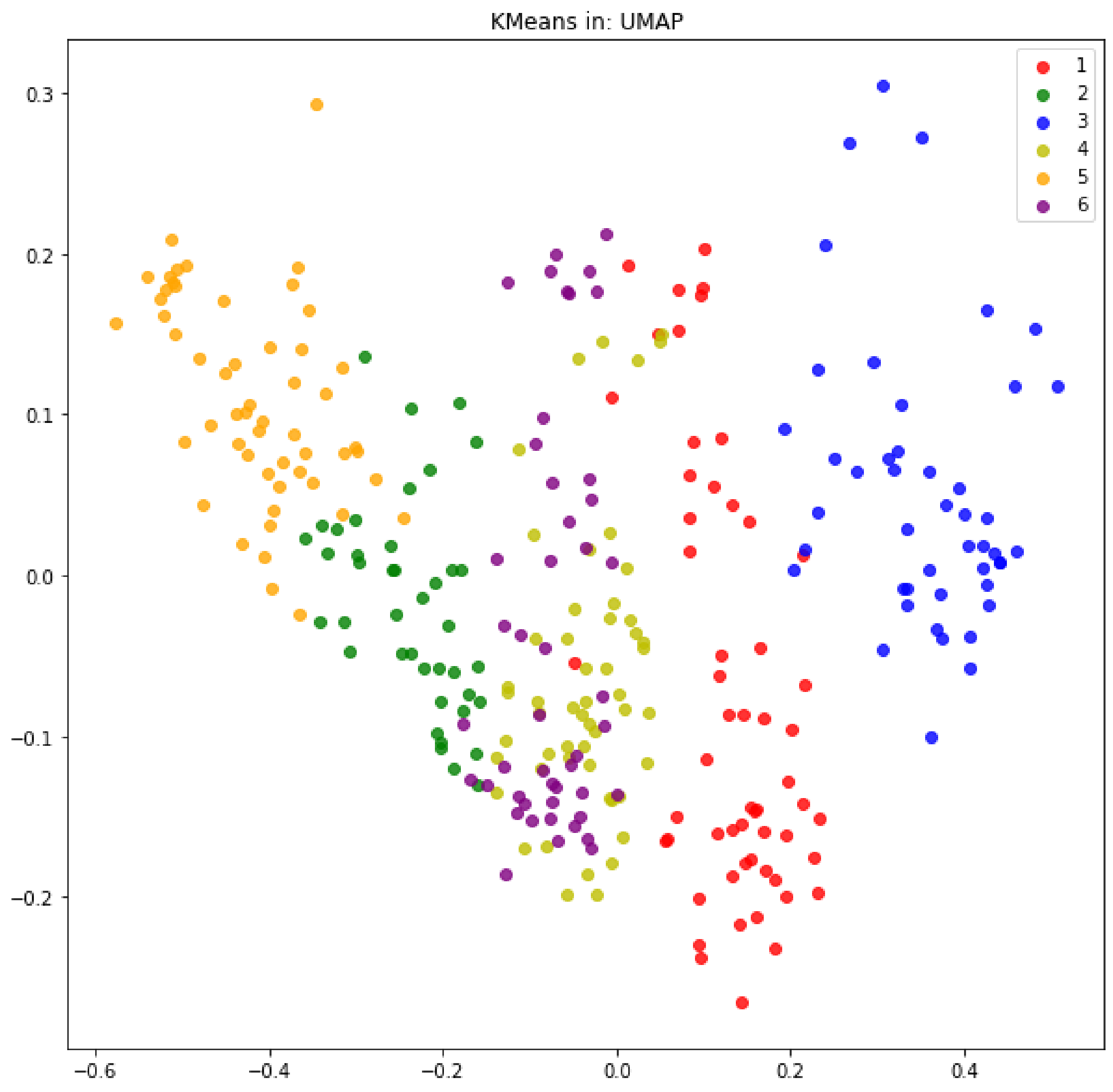
```
KMeans NMI:0.0923
KPCA
KMeans
```



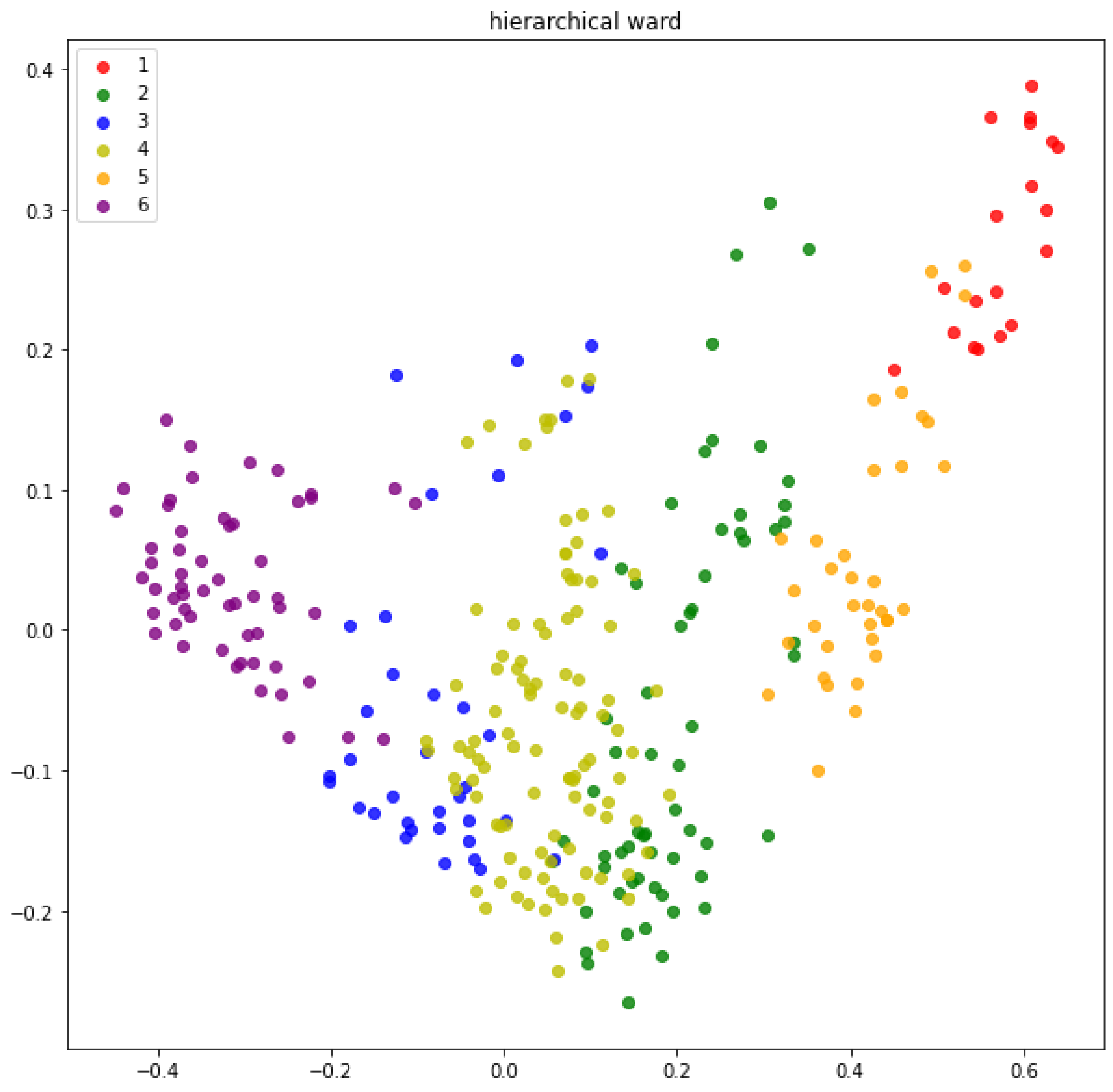
```
KMeans NMI:0.1205
T-SNE
KMeans
```



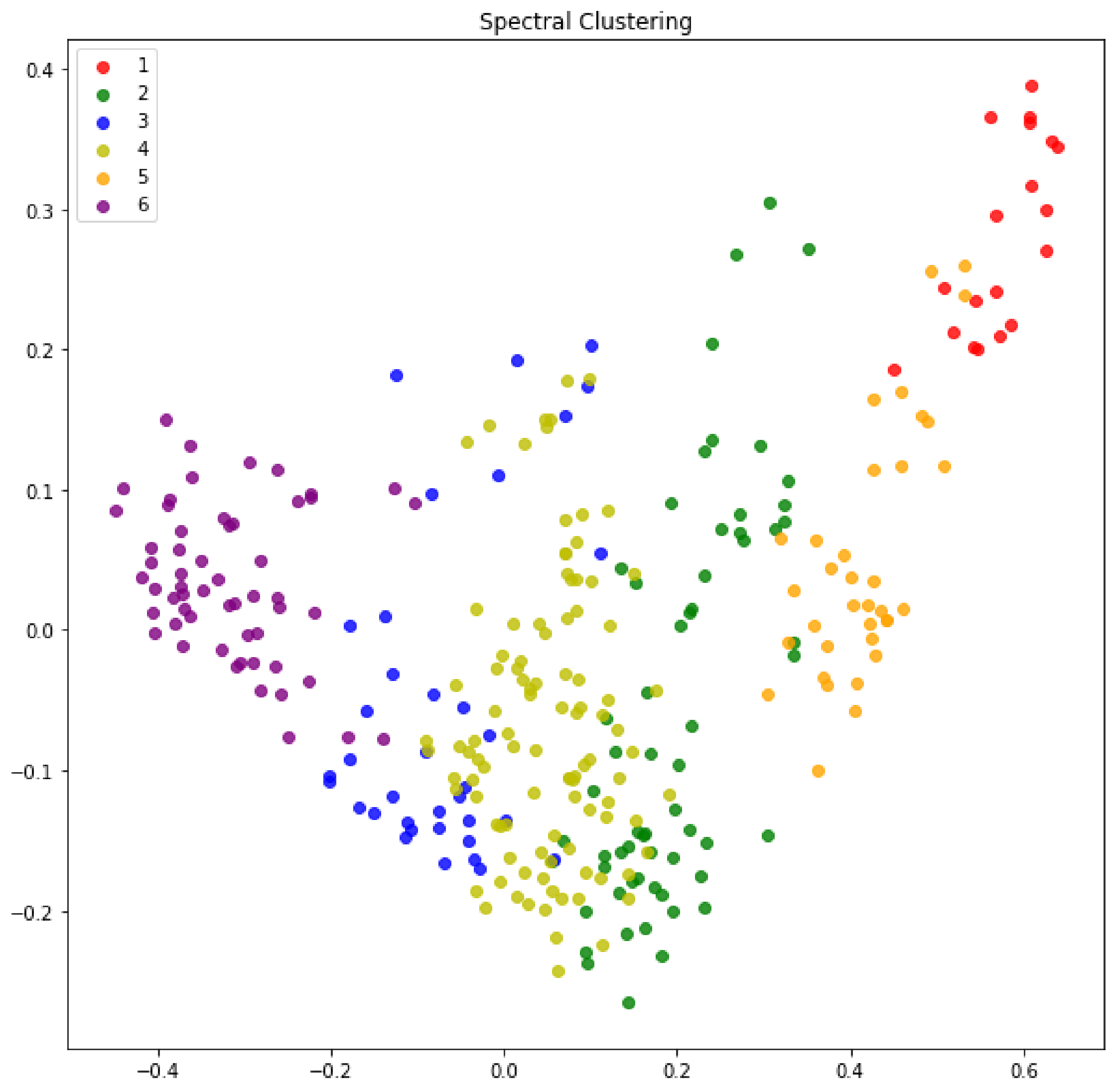
```
KMeans NMI:0.0979
UMAP
KMeans
```



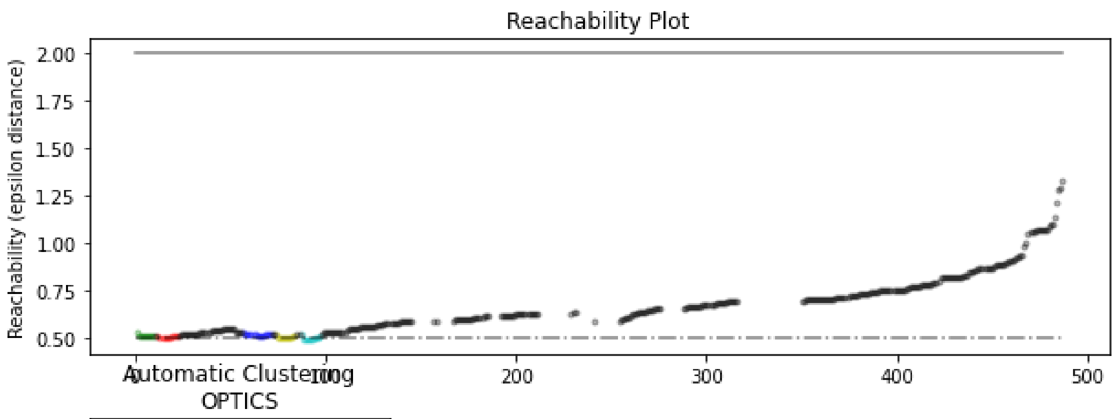
```
KMeans NMI:0.0968
```

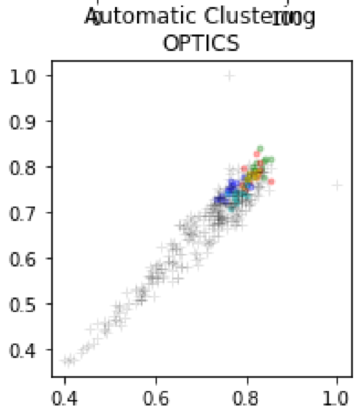


```
H clustering NMI:0.0956
```

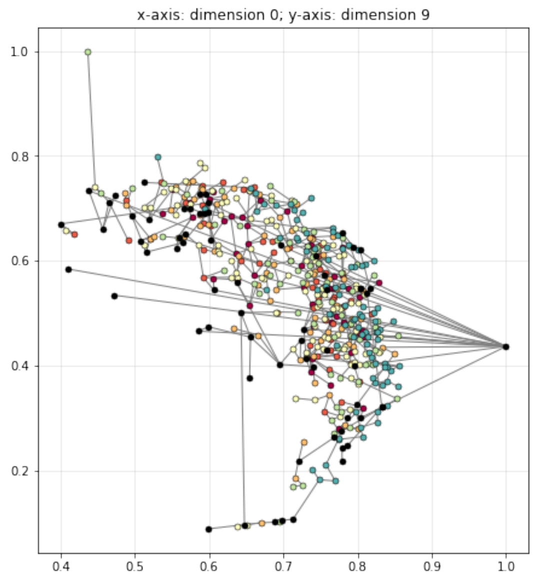


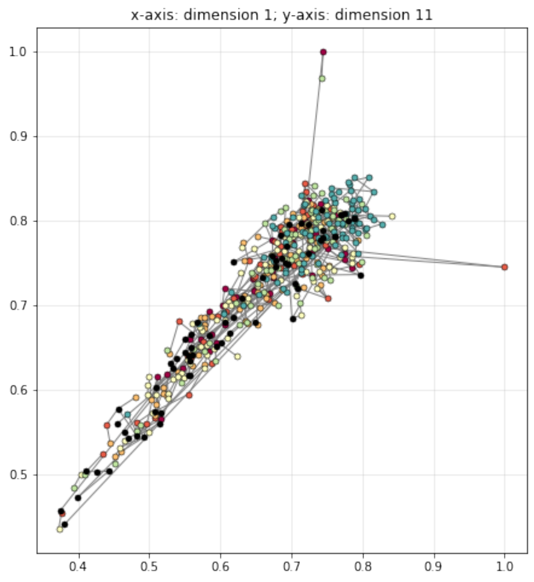
```
##################################
OPTICS
optics nmi:  0.13358307709649445
```

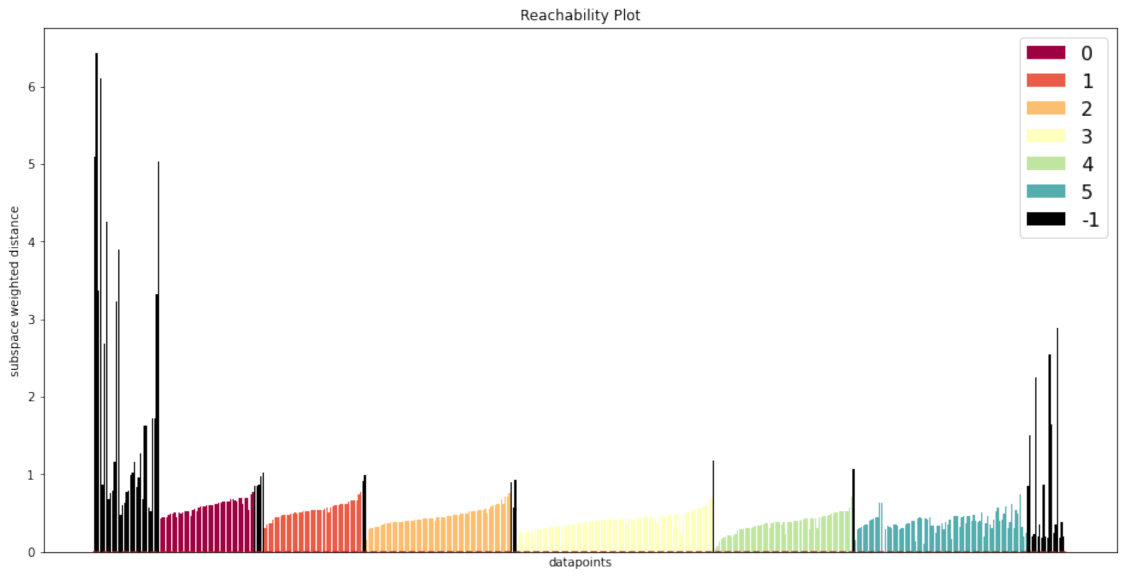




```
HISC
Running HiSC, input dataset has 488 entries with 488 dimensions
0.025576301418530626al structure |            | 100.0% complete
```

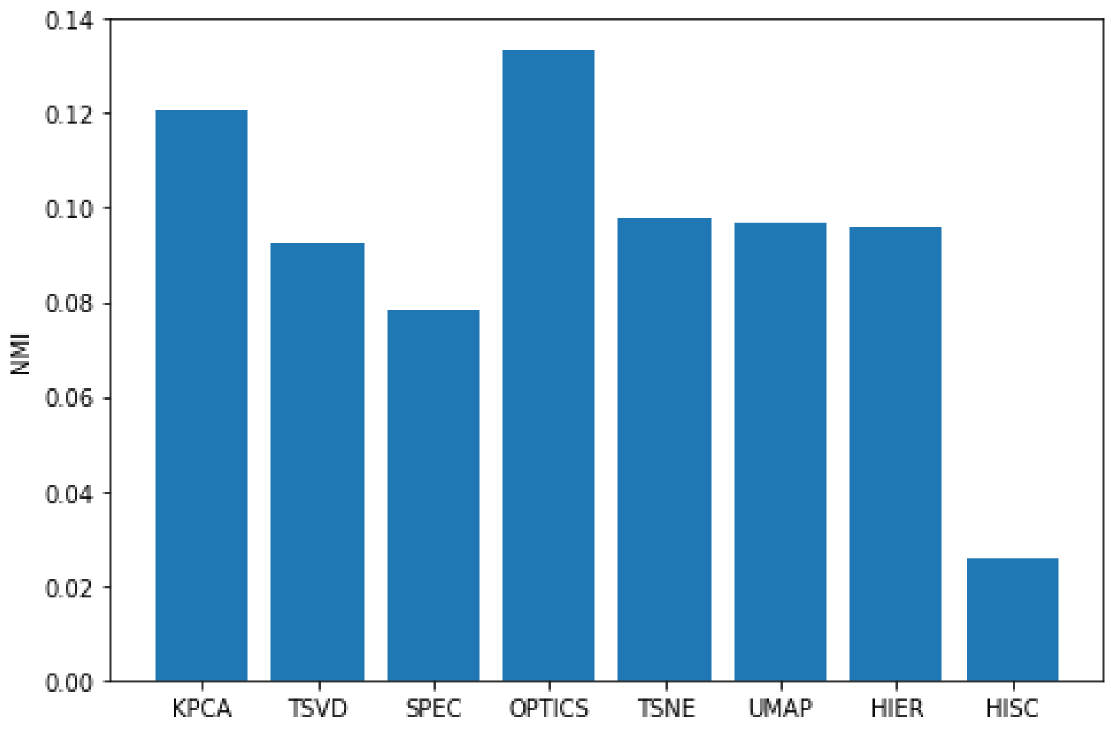






[19]:
```
result_names = ["KPCA", "TSVD", "SPEC", "OPTICS", "TSNE", "UMAP", "HIER",␣
 ↪"HISC"]
version = "node_labels"
#version = "without_labels"

nmis = []
print(f"#################{version}#################")
for name_i in result_names:
    path_i = os.path.join("kernels", version, name_i+".csv")

    nmi_df = pd.read_csv(path_i, index_col=0)
    nmis.append(float(nmi_df.values[0]))

fig = plt.figure()
ax = fig.add_axes([0,0,1,1])
ax.bar(result_names,nmis)
ax.set_ylabel('NMI')
plt.show()
```

```
#################node_labels#################
```

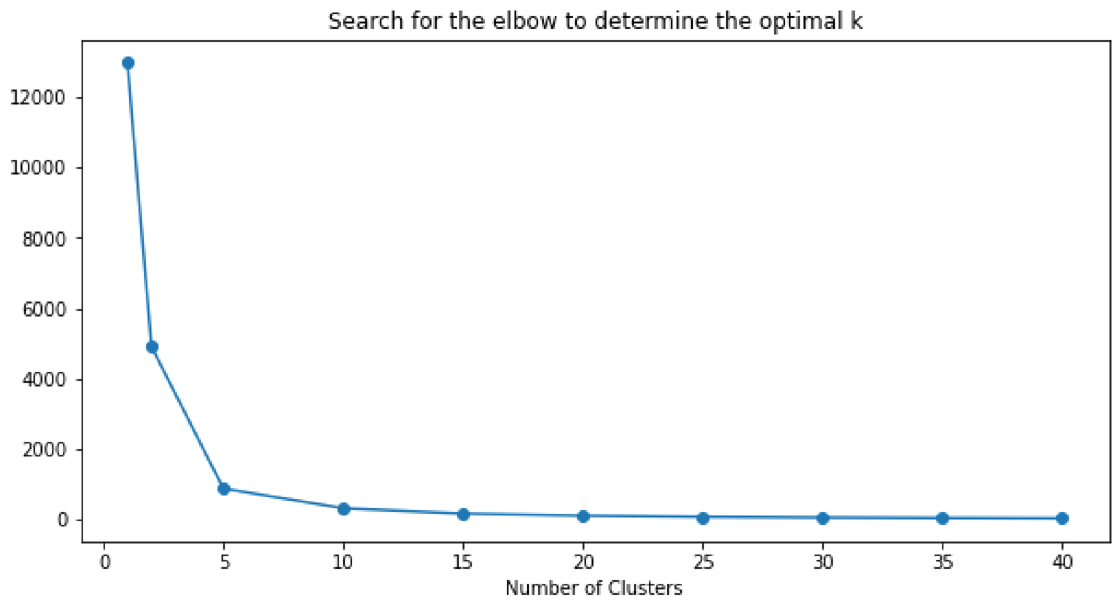


We notice that most of the clusters do not represent the ground truth labels with any clustering method. For the next part we will only use kmeans clustering as its NMI is descent. ALso HiSC clustering shows that it is not suitable for this kind of data.

4.2 Interpreting DR and Clusters found in UMAP

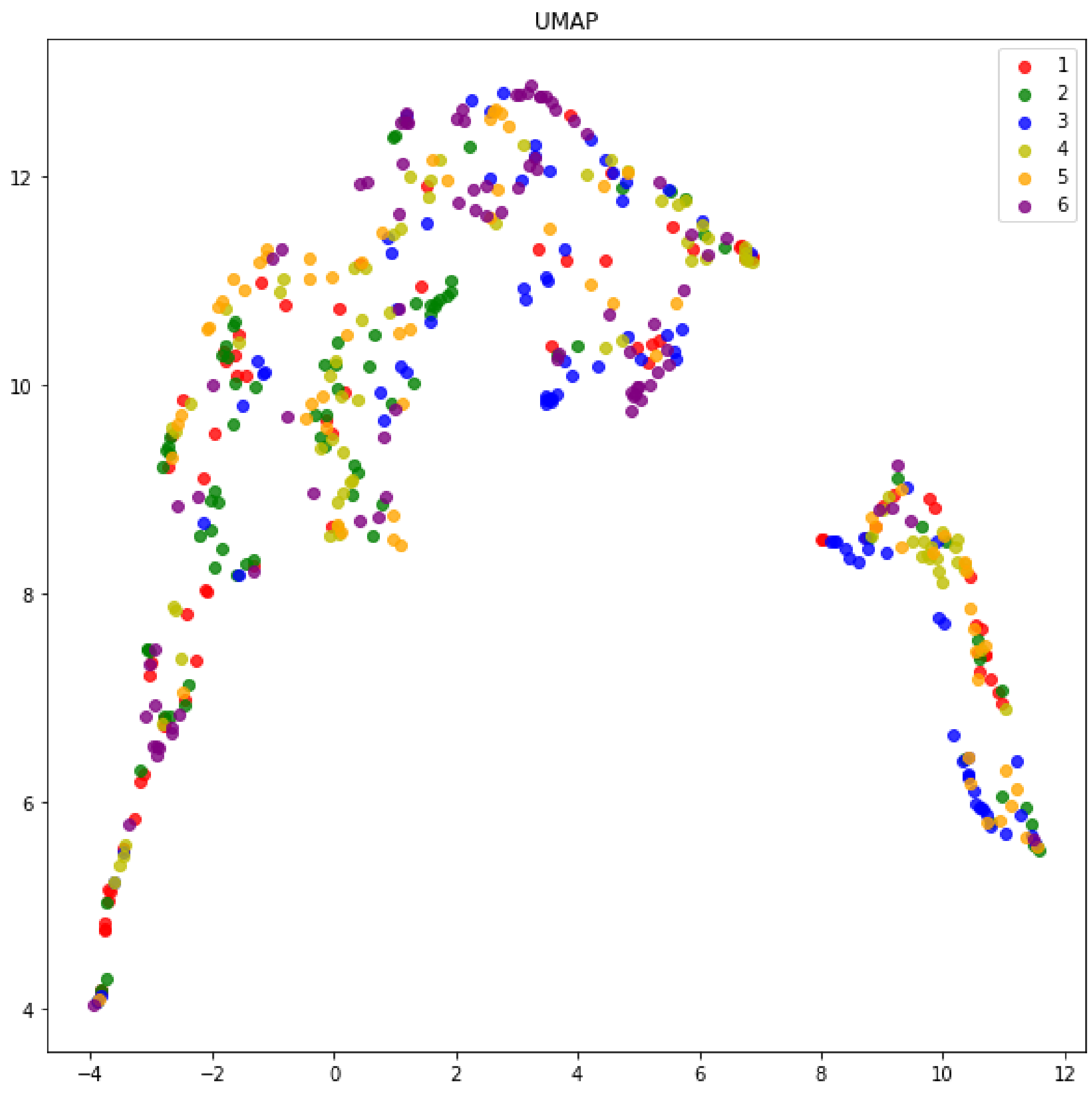
[20]:
```
costs = []
kmeans_runs = []
k_list = [1, 2, 5, 10, 15, 20, 25, 30, 35, 40]
for k in k_list:
    kmeans = KMeans(n_clusters=k)
    kmeans.fit(embedding)
    costs.append(kmeans.inertia_)
    kmeans_runs.append(deepcopy(kmeans))
```

[21]:
```
def scree_plot(k_list, costs):
    plt.figure(figsize=(10,5))
    plt.plot(k_list, costs, marker="o")
    plt.xlabel('Number of Clusters')
  #  plt.ylabel('KMeans loss')
    plt.title('Search for the elbow to determine the optimal k')
    plt.show();
scree_plot(k_list, costs)
```

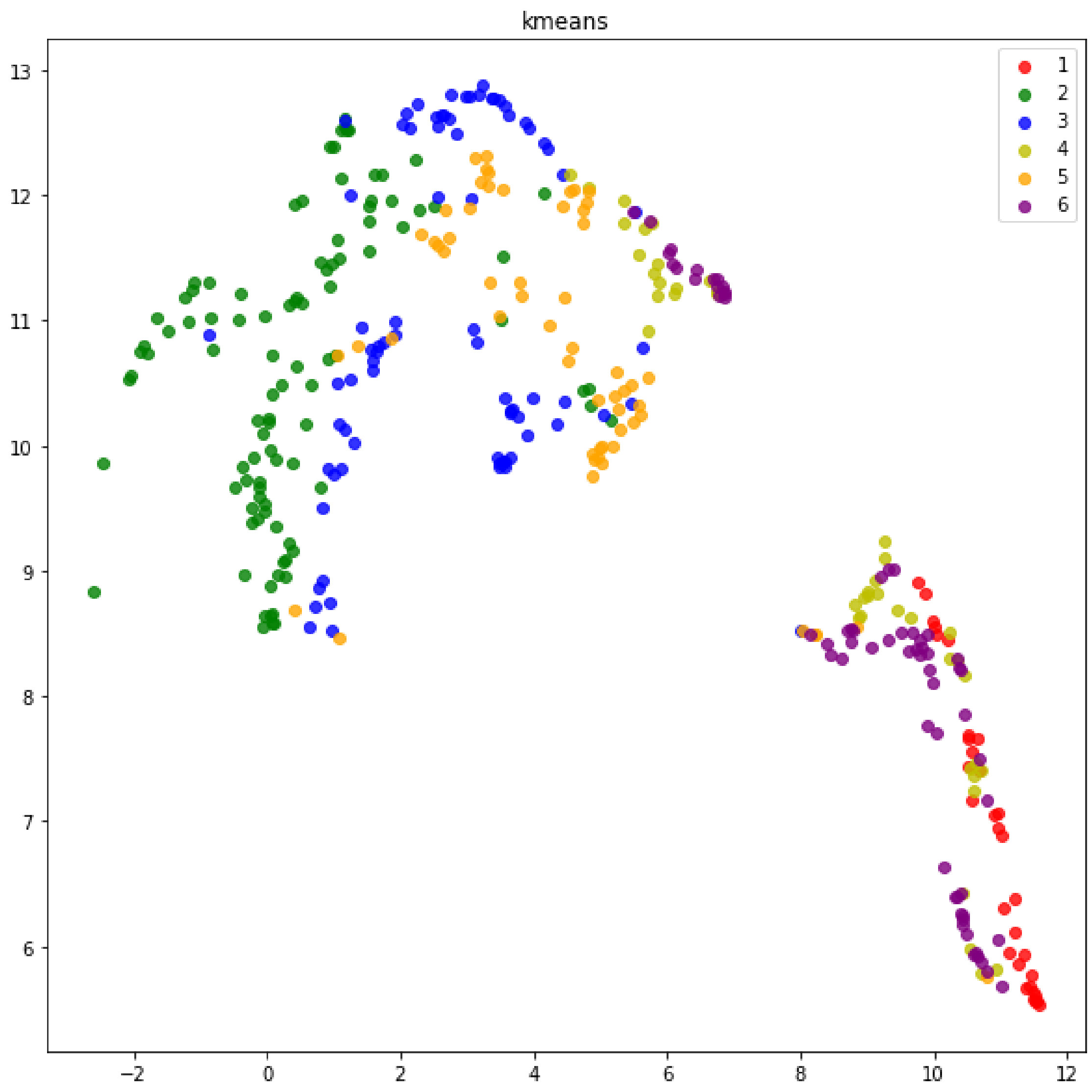


We use number of clusters between 5-10 as they are the most optimal

[22]:
```
plot_dr(embedding, "UMAP" ,classes)
plt.show();

# Instantiate the clustering model
kmeans = KMeans(n_clusters=8)
kmeans.fit(reduced_kpca)
print("KMeans")

plot_dr(embedding, "kmeans",kmeans.labels_)
```



KMeans



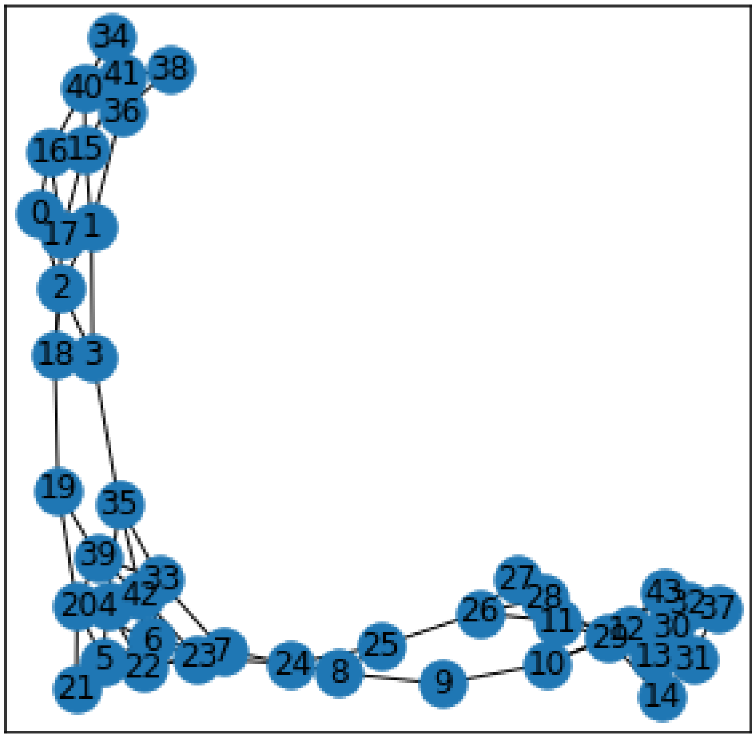
4.2.1 Visualizing data points in found clusters

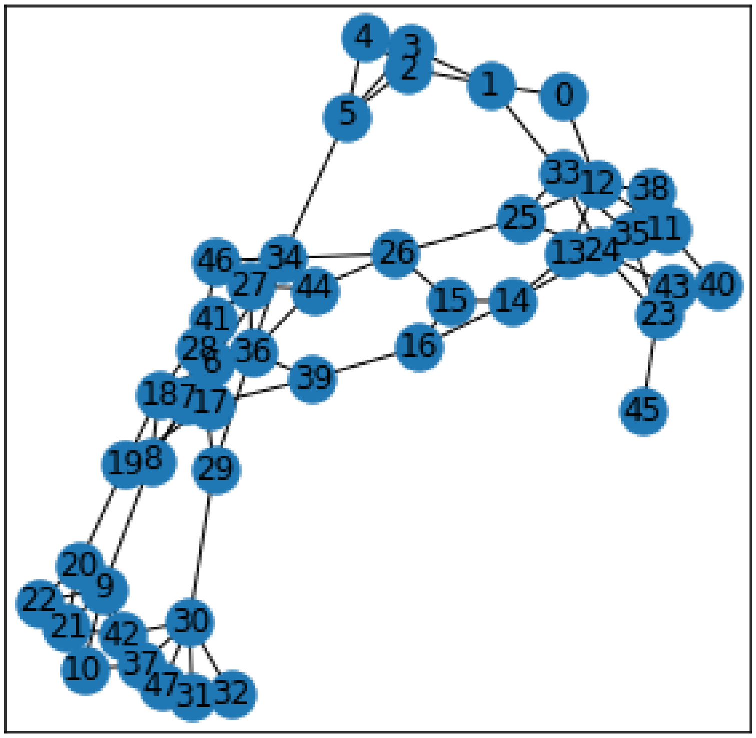
[23]:
```
# select first 2 nearest neighbours in for each cluster
nr_nearest = 2
nearest_indices = []
for cluster_i in set(kmeans.labels_):
    mask = (kmeans.labels_ == cluster_i)
    selection = reduced_kpca[mask]
    print(f"number of data points in cluster {cluster_i}: {selection.shape[0]}")
    center_i = kmeans.cluster_centers_[cluster_i].reshape(1,-1)
    distances_i = pairwise_distances(center_i, reduced_kpca)
    nearest_indices.append(np.argsort(distances_i, )[0][0:nr_nearest])
    print(f"Nearest data points in cluster {cluster_i}: {nearest_indices[-1]}")
```

```
number of data points in cluster 0: 84
Nearest data points in cluster 0: [233 240]
number of data points in cluster 1: 32
Nearest data points in cluster 1: [455 319]
number of data points in cluster 2: 100
Nearest data points in cluster 2: [276 133]
number of data points in cluster 3: 78
Nearest data points in cluster 3: [ 66 333]
number of data points in cluster 4: 42
Nearest data points in cluster 4: [475 409]
number of data points in cluster 5: 58
Nearest data points in cluster 5: [ 72 192]
number of data points in cluster 6: 64
Nearest data points in cluster 6: [485 481]
number of data points in cluster 7: 30
Nearest data points in cluster 7: [463 462]
```

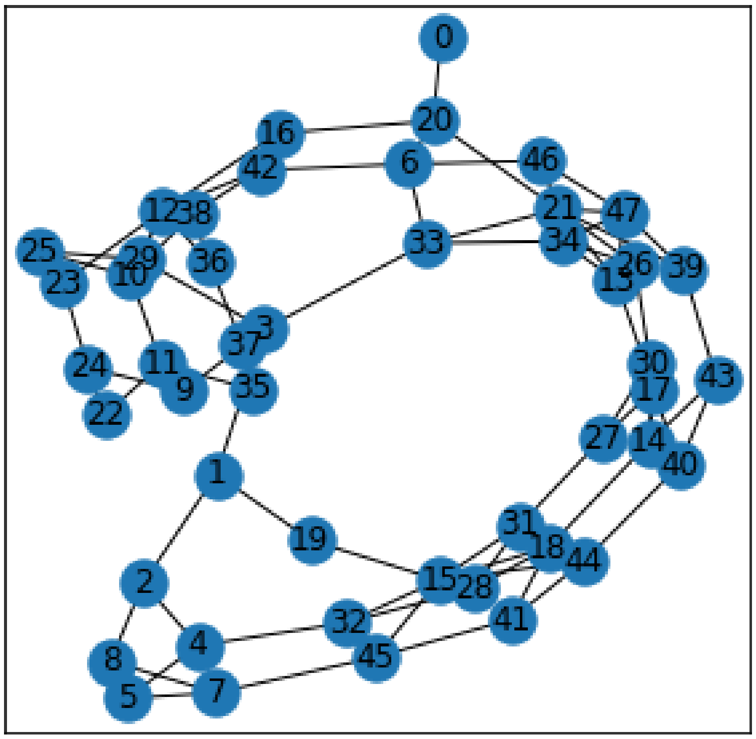
[24]:
```
for i, indices in enumerate(nearest_indices):
    print(f"Cluster {i}, Indices {indices}")
    G_selected = select_from_list(G_filtered, indices)
    for g_i in G_selected:
        print(g_i)
        visualize(g_i)
```

```
Cluster 0, Indices [233 240]
```





```
Cluster 1, Indices [455 319]
```


0
1
2
3
4
5
6
7
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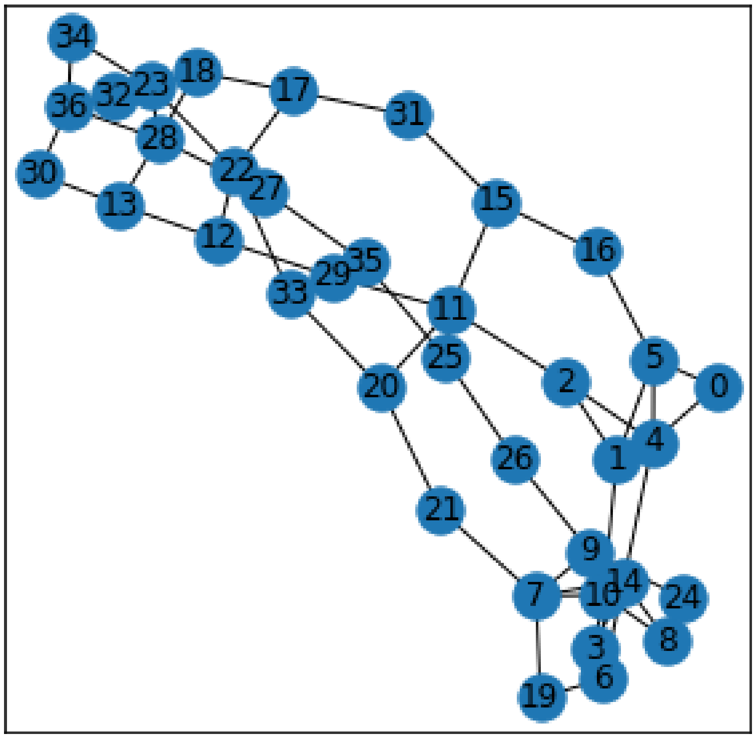
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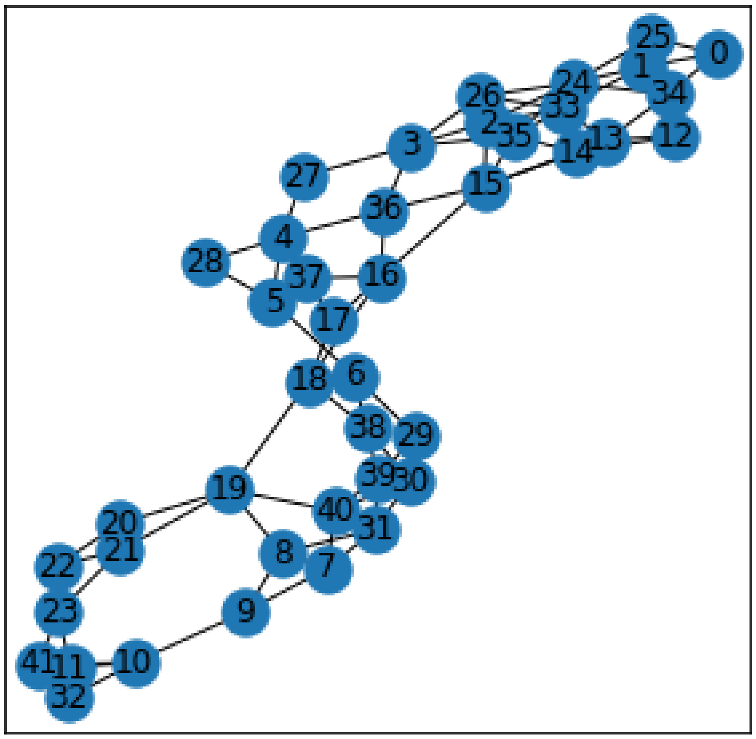
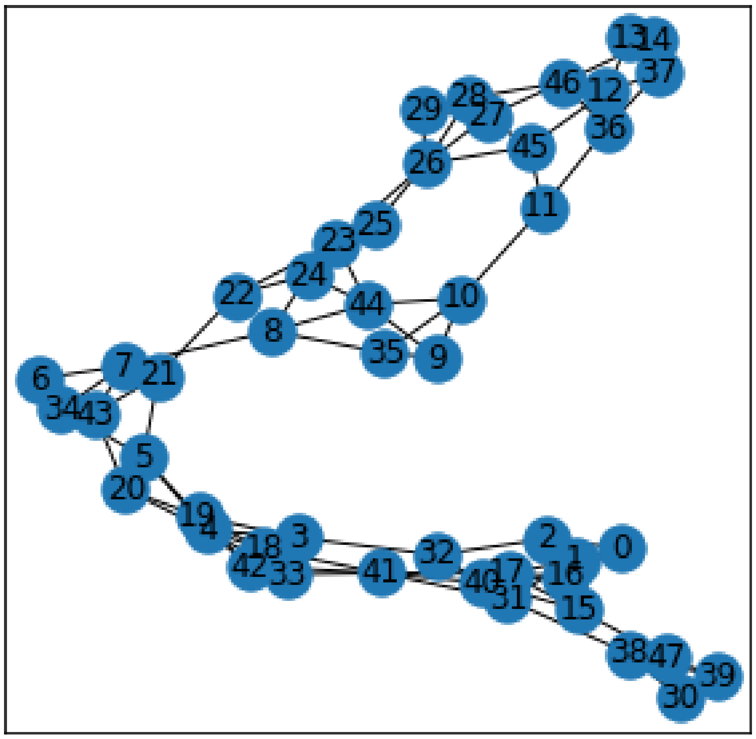
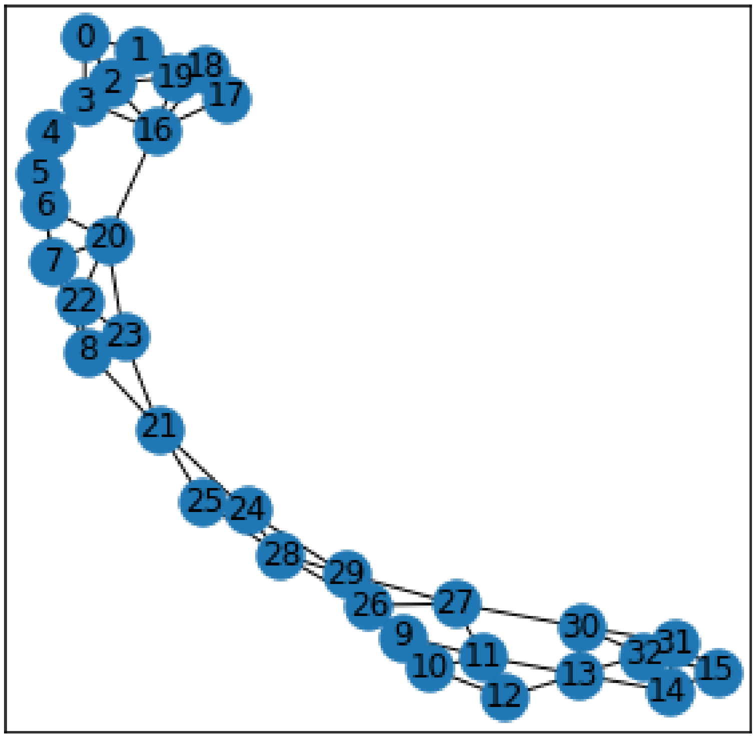
```
Cluster 2, Indices [276 133]
```





```
Cluster 3, Indices [ 66 333]
```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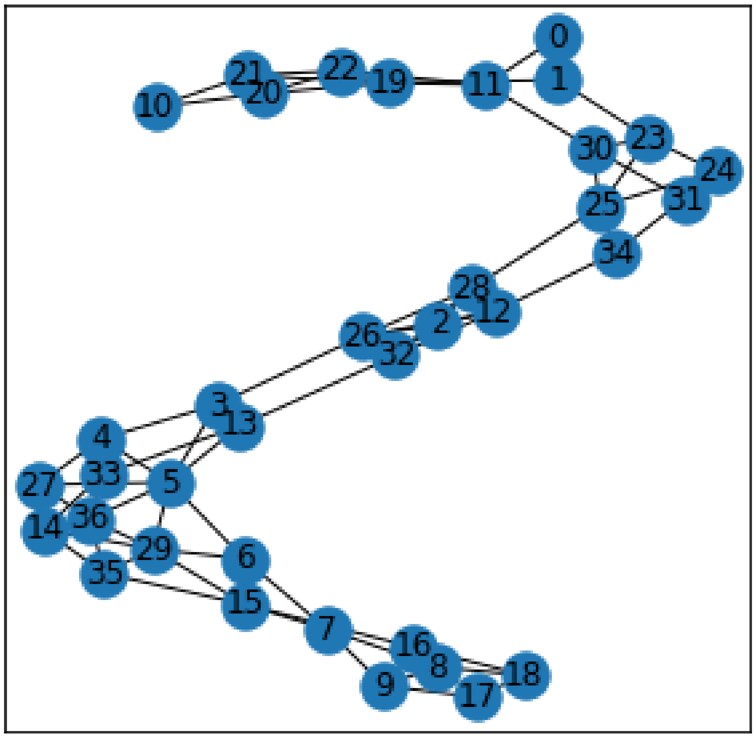
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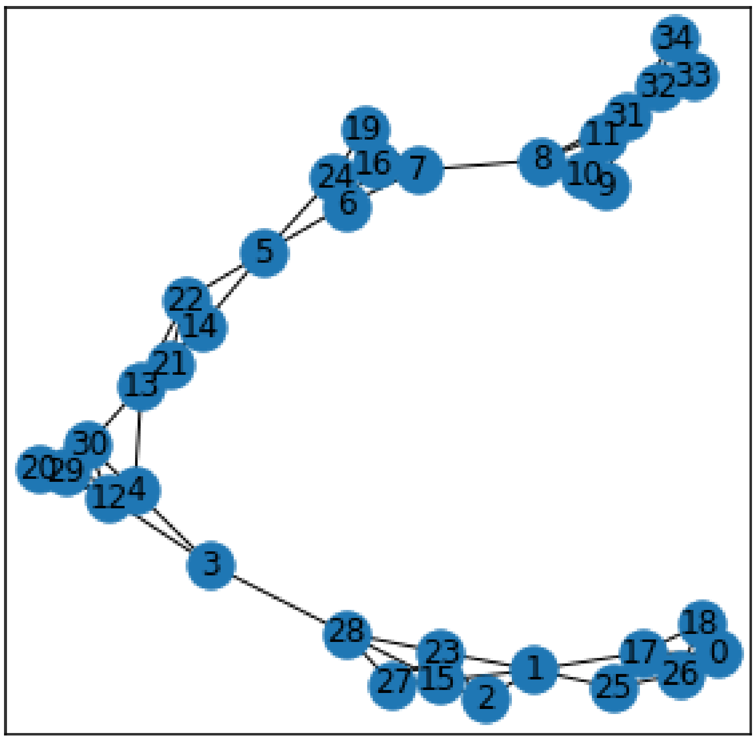
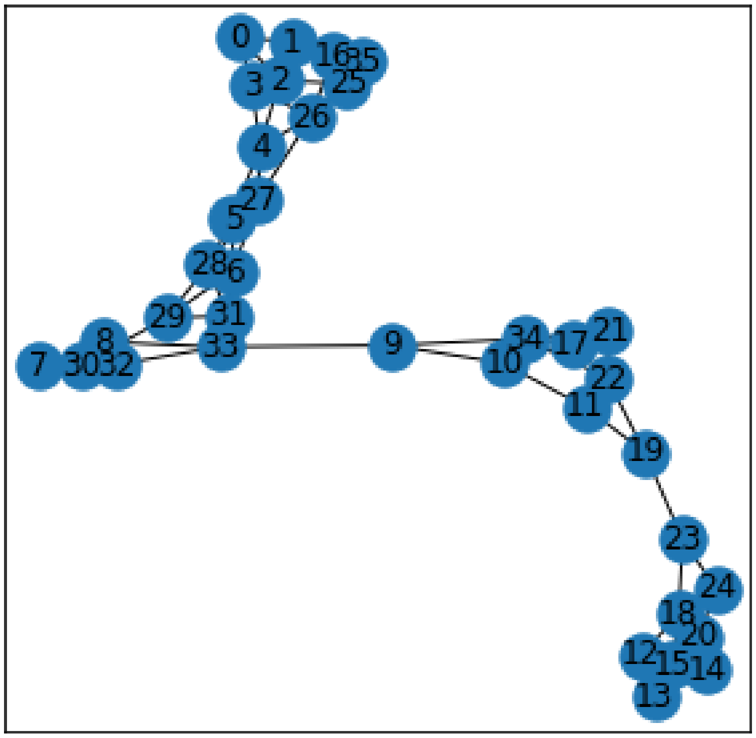
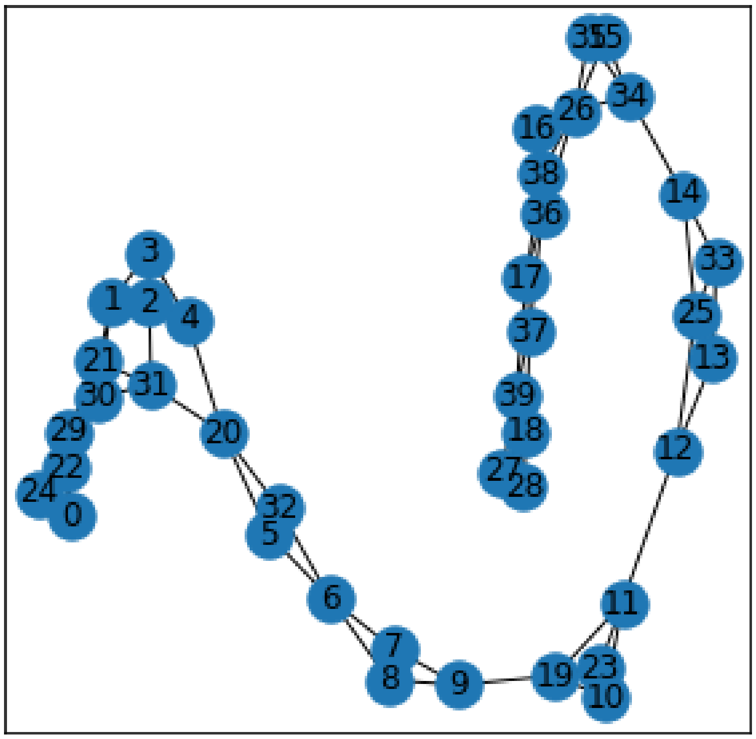
```
Cluster 4, Indices [475 409]
```





```
Cluster 5, Indices [ 72 192]
```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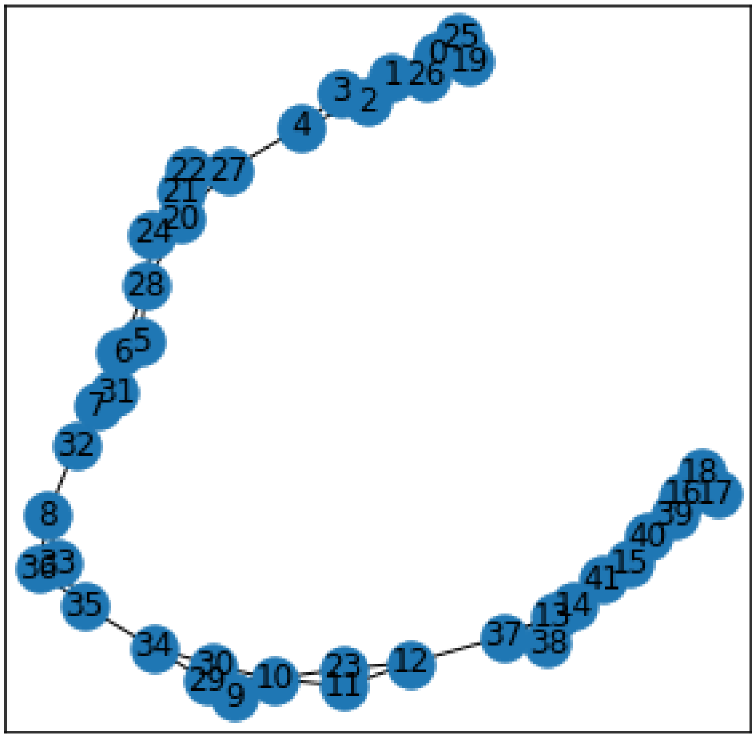
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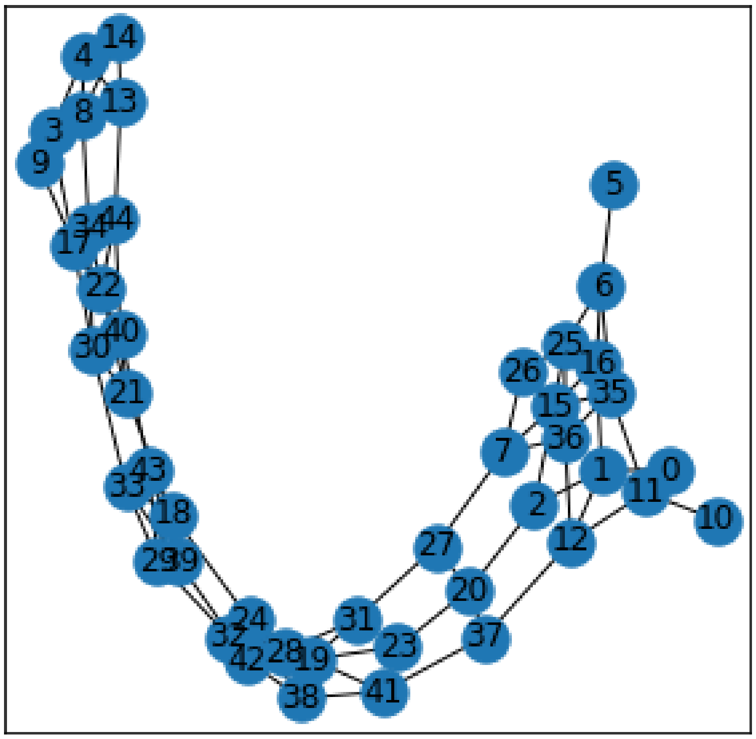
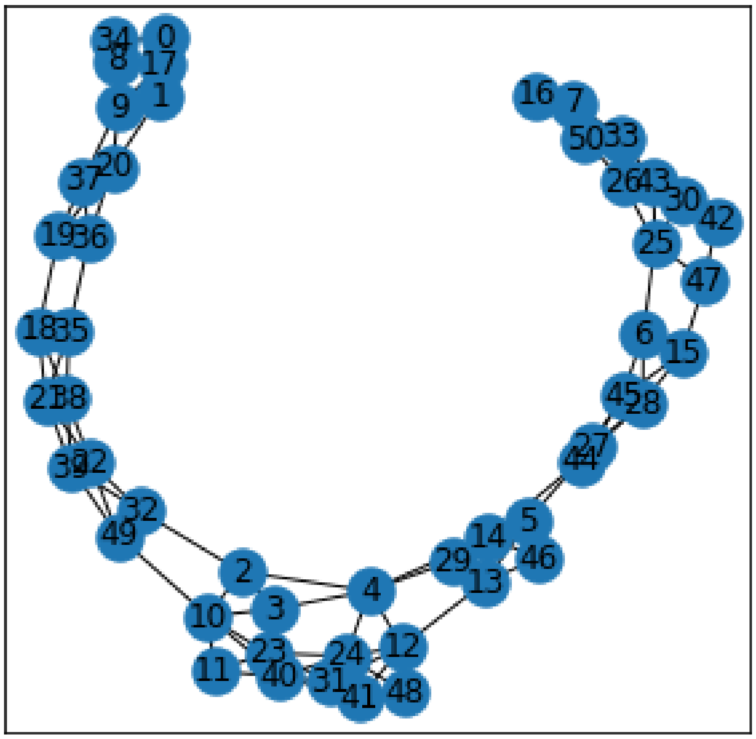
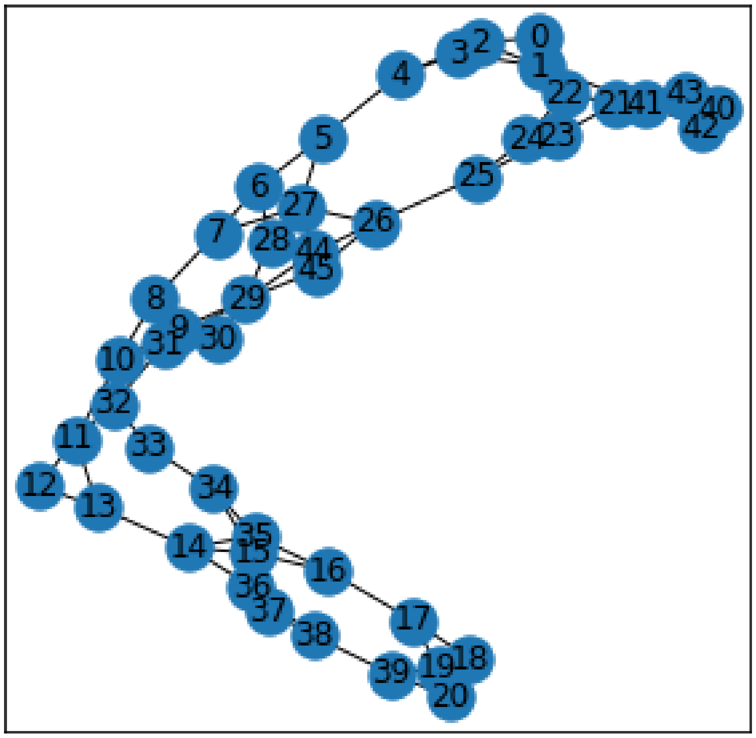
```
Cluster 6, Indices [485 481]
```





```
Cluster 7, Indices [463 462]
```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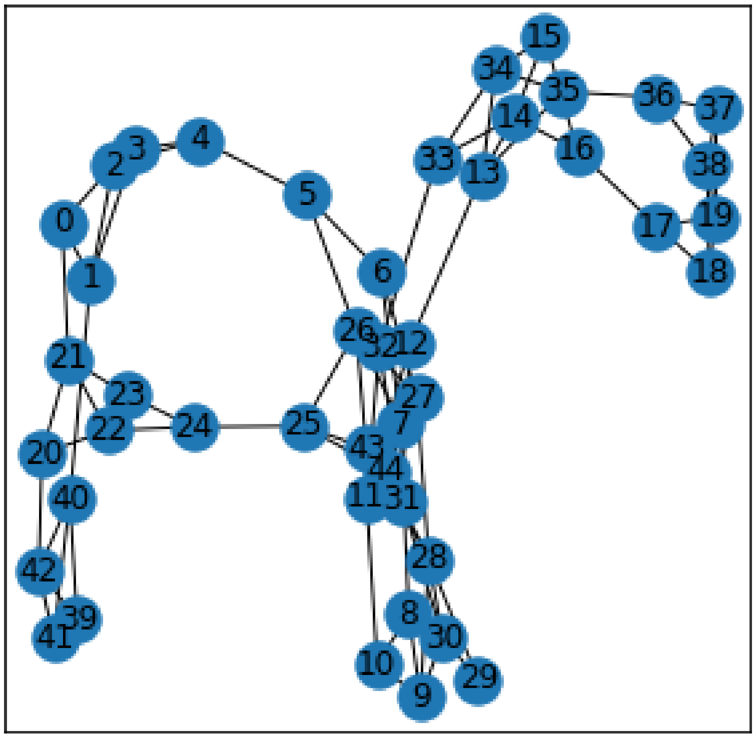
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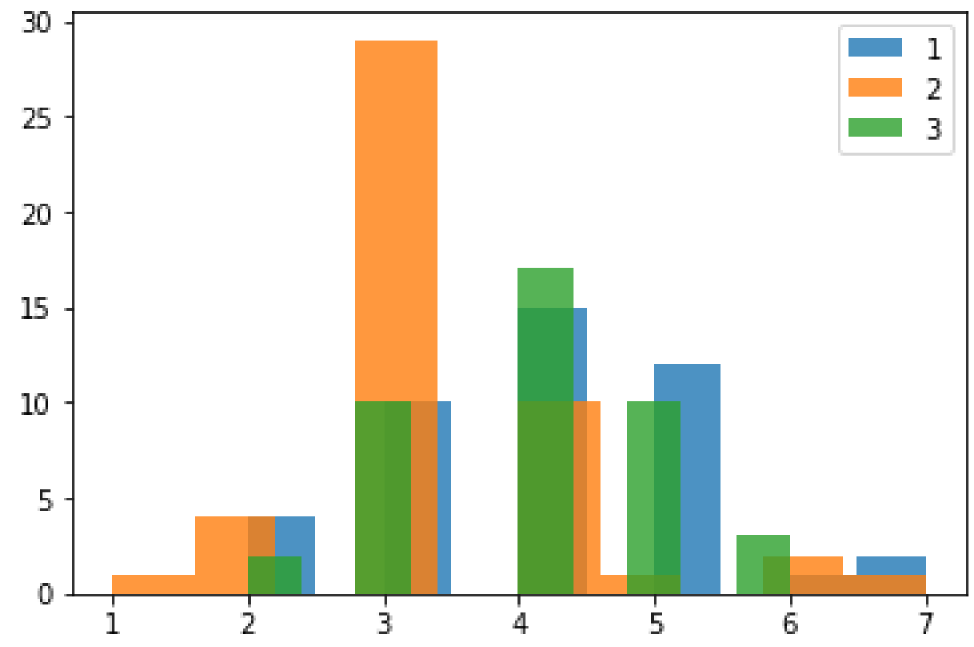
We can see that the clusters are strongly driven by the graph structure e.g. degree, node/edge counts.

[26]:
```python
def plot_degree_dist(G, labels):
    degrees= []
    for graph, label in zip(G, labels):
        degrees = [graph.degree(n) for n in graph.nodes()]
        plt.hist(degrees, alpha=0.8, label=label,bins= 10)
    plt.legend()
    plt.show()


graph_centers = []
for i, indices in enumerate(nearest_indices):
    G_selected = select_from_list(G_filtered, indices)
    graph_centers.append(G_selected[0])

plot_degree_dist(graph_centers[0:3], labels = ["1", "2", "3"])
plot_degree_dist(graph_centers[3:6], labels = ["4", "5", "6"])


avg_degree= []
for graph in G_filtered:
    degrees = [graph.degree(n) for n in graph.nodes()]
    avg= sum(degrees)/len(degrees)
    avg_degree.append(avg)


avg_centrality= []
for graph in G_filtered:
    degrees = nx.degree_centrality(graph)
    avg= sum(degrees.values())/len(degrees)
    avg_centrality.append(avg)


ax = sns.violinplot(x=classes, y=avg_degree)
plt.title("Average Degree in EC classes")
plt.show()

ax = sns.violinplot(x=classes, y=avg_centrality)
plt.title("Average Degree_centrality in EC classes")
plt.show()
```



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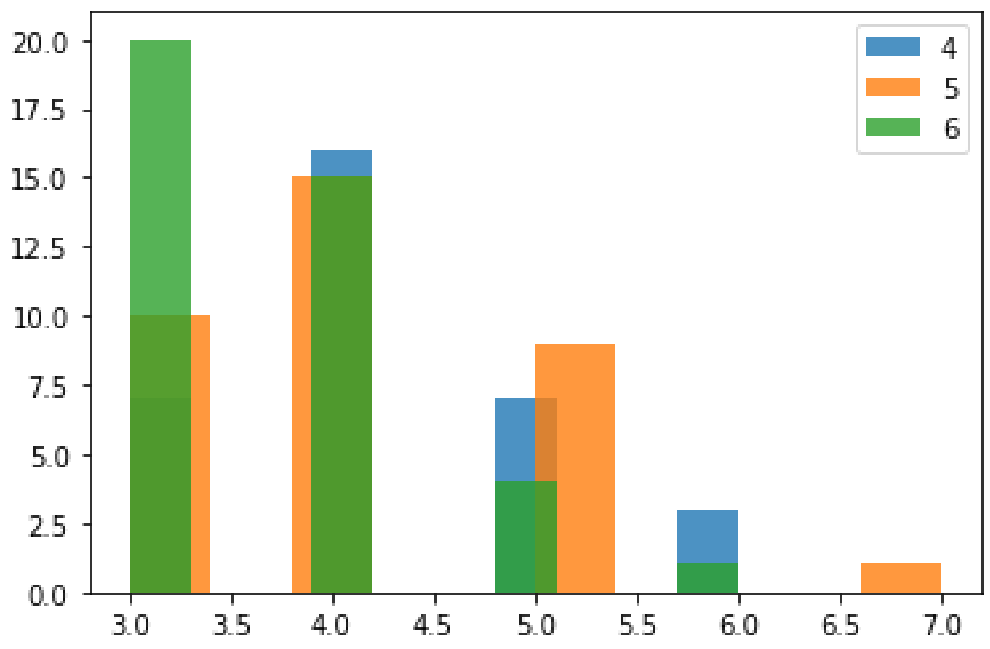

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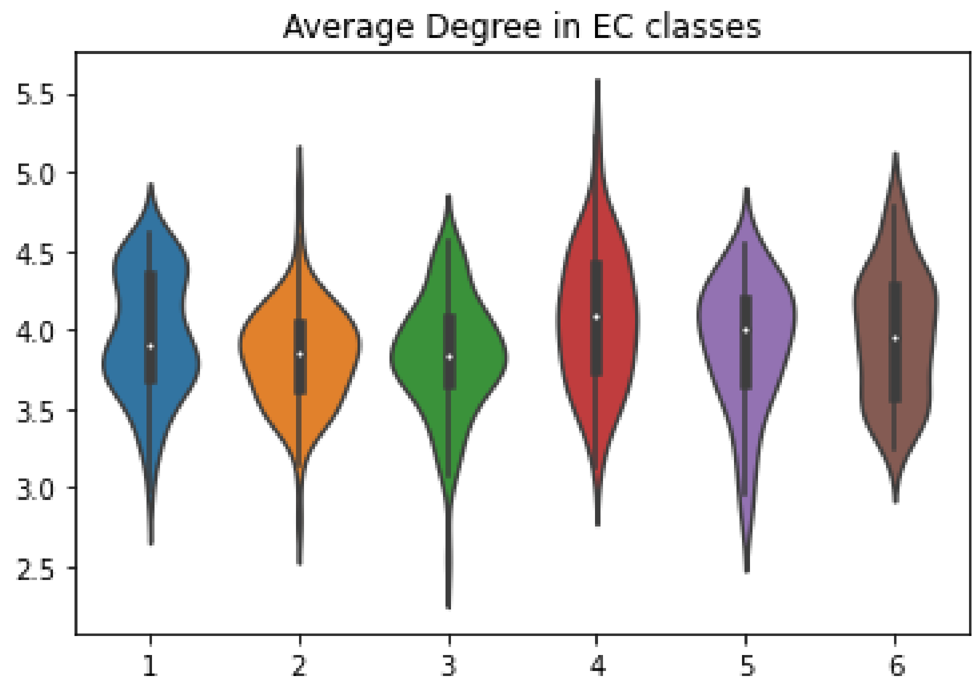
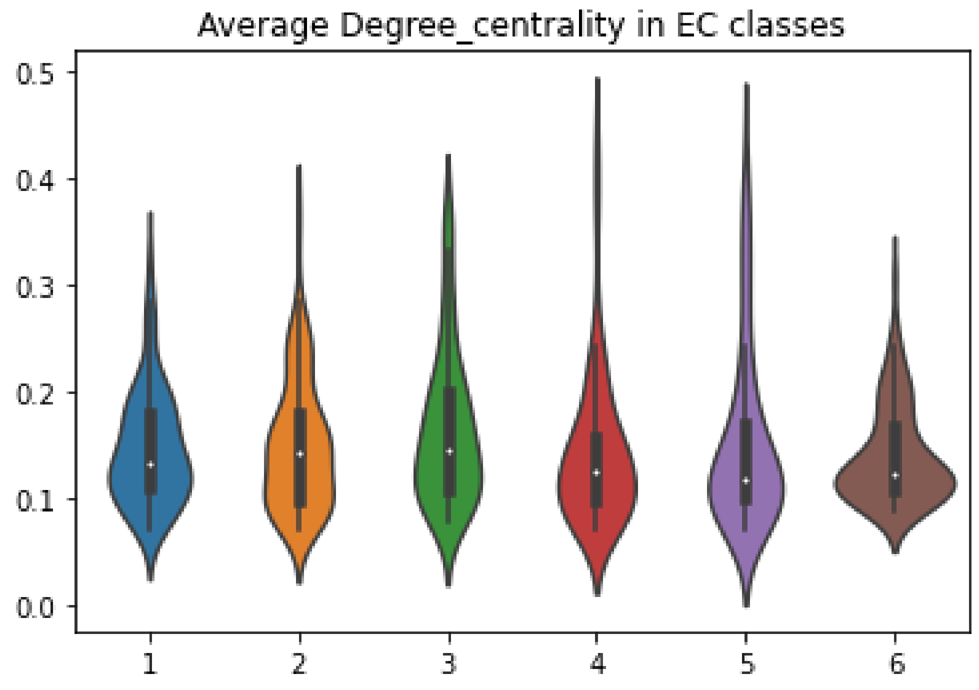




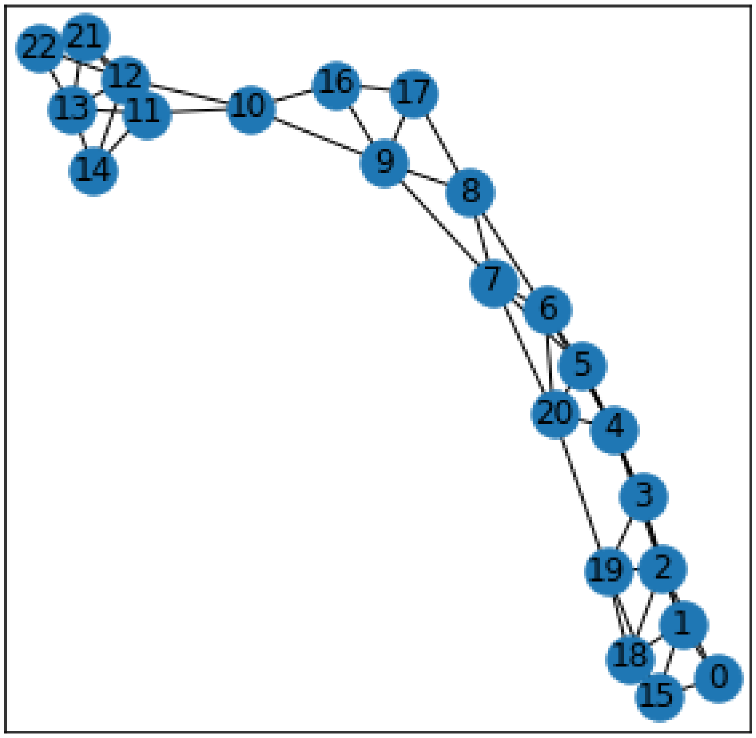
We can see that the EC classes have different degree distributions

4.3 Analyzing the labels

[27]:
```
G = tud_to_networkx(dataset)
class1_index = []
class2_index = []
class3_index = []
class4_index = []
class5_index = []
class6_index = []

for ind in classes:
    if ind == 1:
        class1_index.append(ind)

    if ind == 2:
        class2_index.append(ind)

    if ind == 3:
        class3_index.append(ind)

    if ind == 4:
        class4_index.append(ind)

    if ind == 5:
        class5_index.append(ind)

    if ind == 6:
        class6_index.append(ind)

ec_classes = [class1_index, class2_index, class3_index, class4_index,␣
 ↪class5_index, class6_index]
```

[28]:
```
labels = ["EC1", "EC2", "EC3", "EC4", "EC5", "EC6"]

for label, ec in zip(labels, ec_classes):
    print(label)

    visualize(G_filtered[ec[10]])
```

```
EC1
```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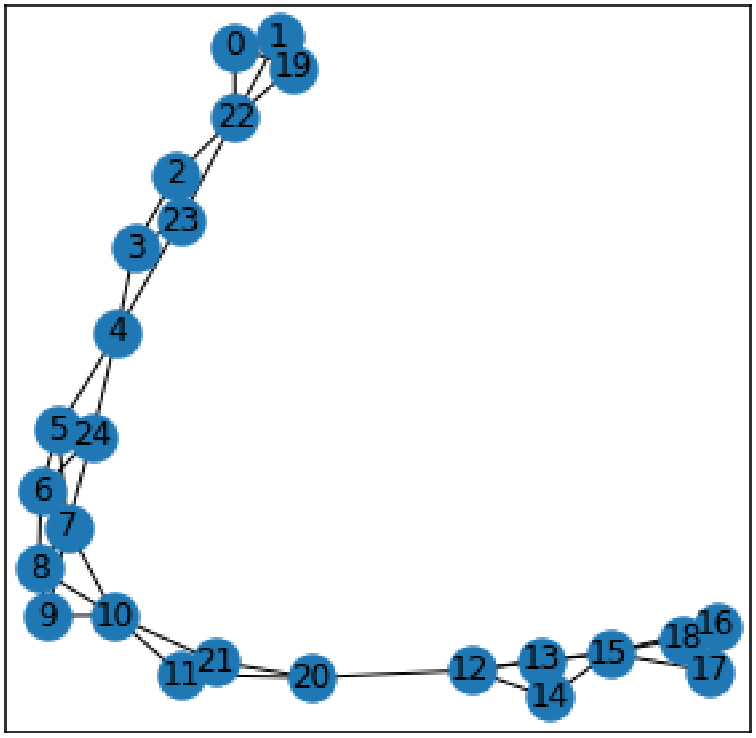
EC2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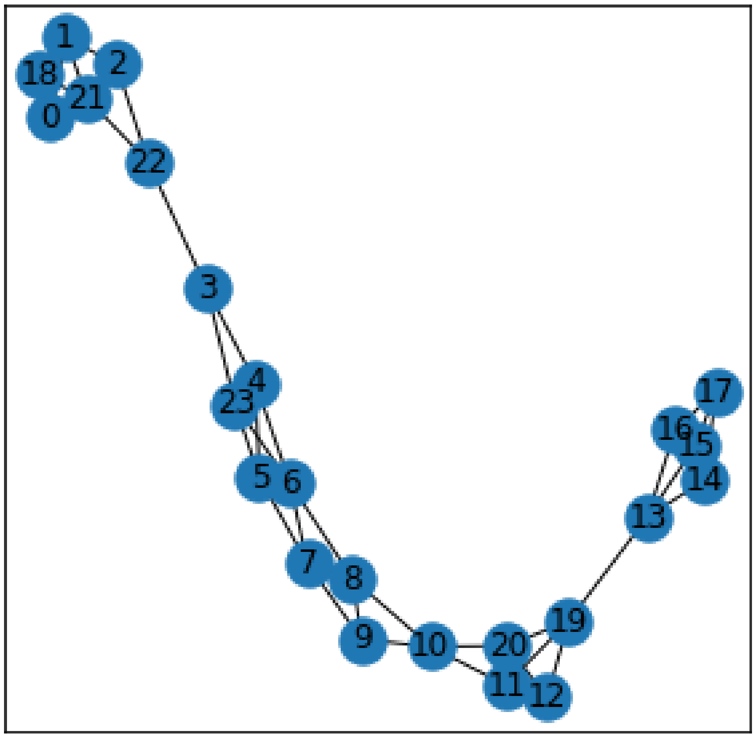
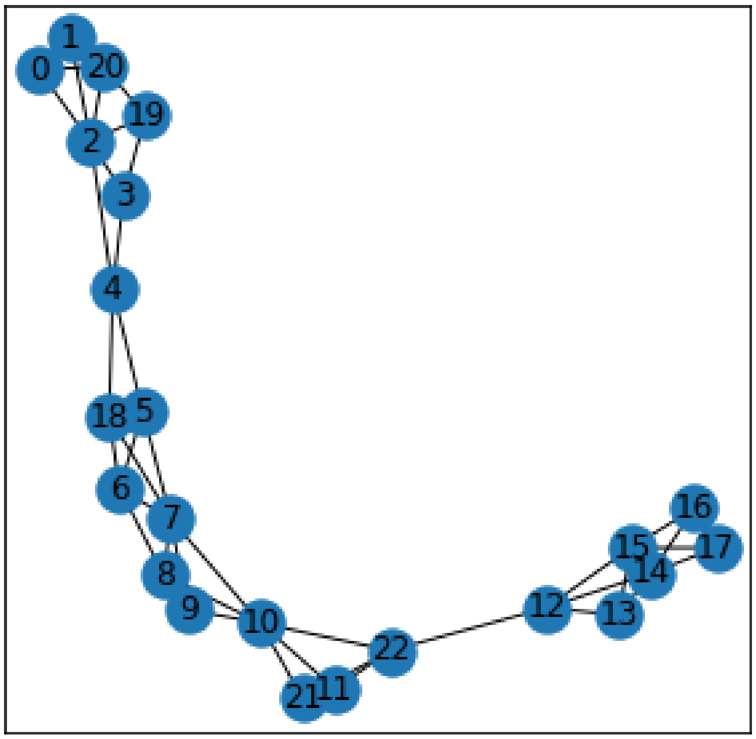
EC3



EC4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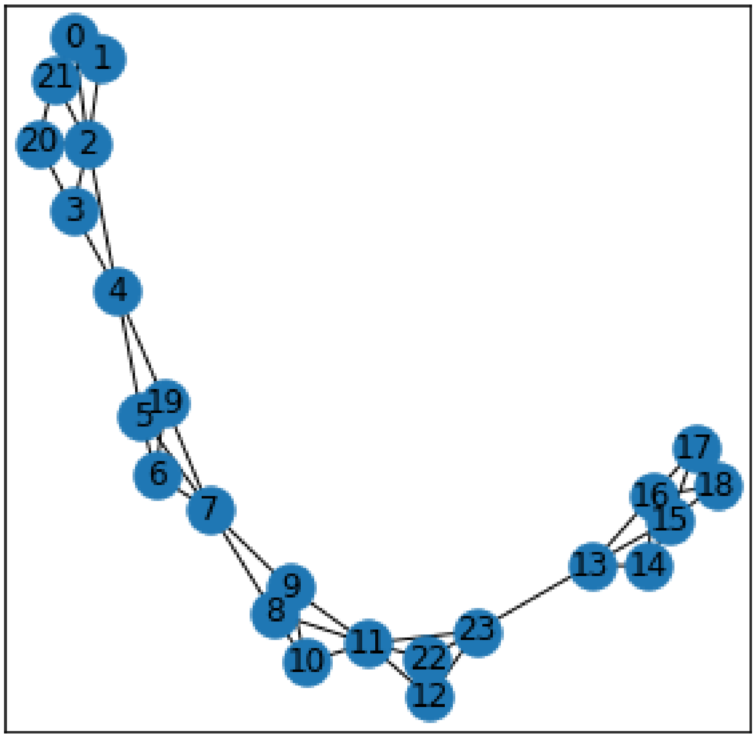
EC5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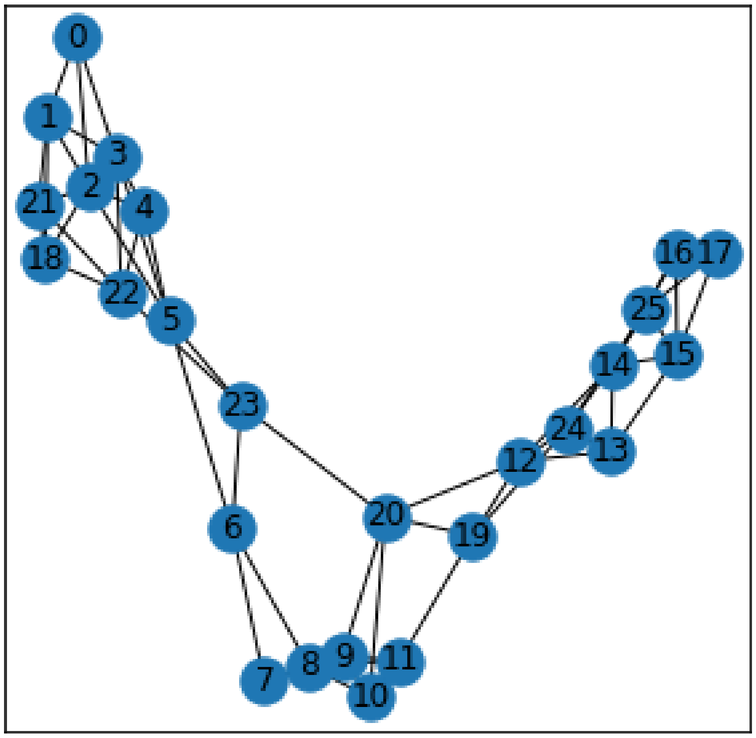
EC6



```
[29]: def get_label(G, attribute):
          data = []
          for graph in G:
              g_data = 0
              for node in range(0, len(graph)):
                  g_data += (graph.nodes.data()[node][attribute][0])

              data.append(g_data/len(graph))
          return(data)

      def get_property(G, attribute, index):
          data = []
          for gid, graph in enumerate(G):
              g_data = 0
              for node in range(0, len(graph)):
                  g_data += graph.nodes.data()[node][attribute][index]
              data.append(g_data/len(graph))

          return(data)
```

```
def get_EC(G):
    data  = []

    for i in range(0, len(classes)):
        data.append(classes[i])
    return data
```

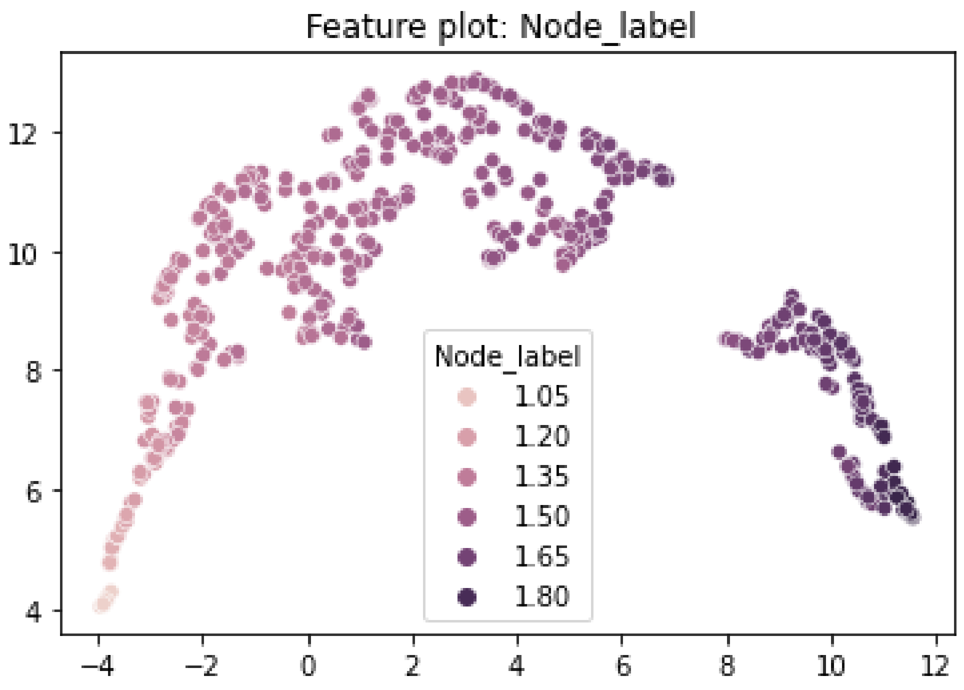
```
[43]: data = {'Node_label': get_label(G_filtered, "labels"),
          'Node_count': [graph.number_of_nodes() for graph in G_filtered ],
         'Edge_count': [graph.number_of_edges() for graph in G_filtered ],
         'AA_length': get_property(G_filtered, "attributes", 0),
          'low Waals': get_property(G_filtered, "attributes", 1),
          'med Waals': get_property(G_filtered, "attributes", 2),
          'high Waals': get_property(G_filtered, "attributes", 3),
          'low Hydro': get_property(G_filtered, "attributes", 4),
          'med Hydro': get_property(G_filtered, "attributes", 5),
          'high Hydro': get_property(G_filtered, "attributes", 6),
          'low Polarity': get_property(G_filtered, "attributes", 7),
          'med Polarity': get_property(G_filtered, "attributes", 8),
          'high Polarity': get_property(G_filtered, "attributes", 9),
          'low Polariz': get_property(G_filtered, "attributes", 10),
          'med Polariz': get_property(G_filtered, "attributes", 11),
          'high Polariz': get_property(G_filtered, "attributes", 12),
          '3d length': get_property(G_filtered, "attributes", 13),
          'Total Waals': get_property(G_filtered, "attributes", 14),
          'Total Hydro': get_property(G_filtered, "attributes", 15),
          'Total Polarity': get_property(G_filtered, "attributes", 16),
             'Total Polariz': get_property(G_filtered, "attributes", 17),
         'Avg_degree': avg_degree, 'Avg_degree_centrality': avg_centrality,

       }

df = pd.DataFrame(data)
df.head()
```

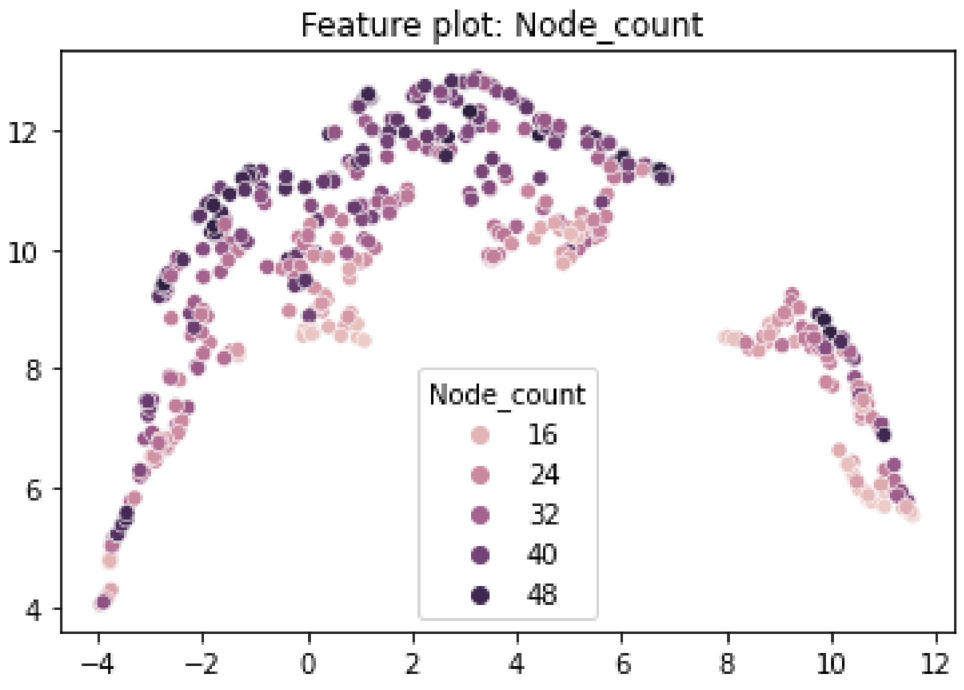
```
[43]:    Node_label  Node_count  Edge_count  AA_length  low Waals  med Waals  \
      0    1.351351          37          84   7.756757  12.753363  28.328919
      1    1.347826          23          51   9.434783  15.357012  35.580870
      2    1.240000          25          46   9.240000  14.165496  33.696000
      3    1.250000          24          45   8.875000  13.915350  32.902083
      4    1.217391          23          45   9.913043  15.458343  36.126957

         high Waals  low Hydro  med Hydro  high Hydro  …  low Polariz  \
      0    0.921081   1.299595  64.213514    2.189189  …     2.405405
```

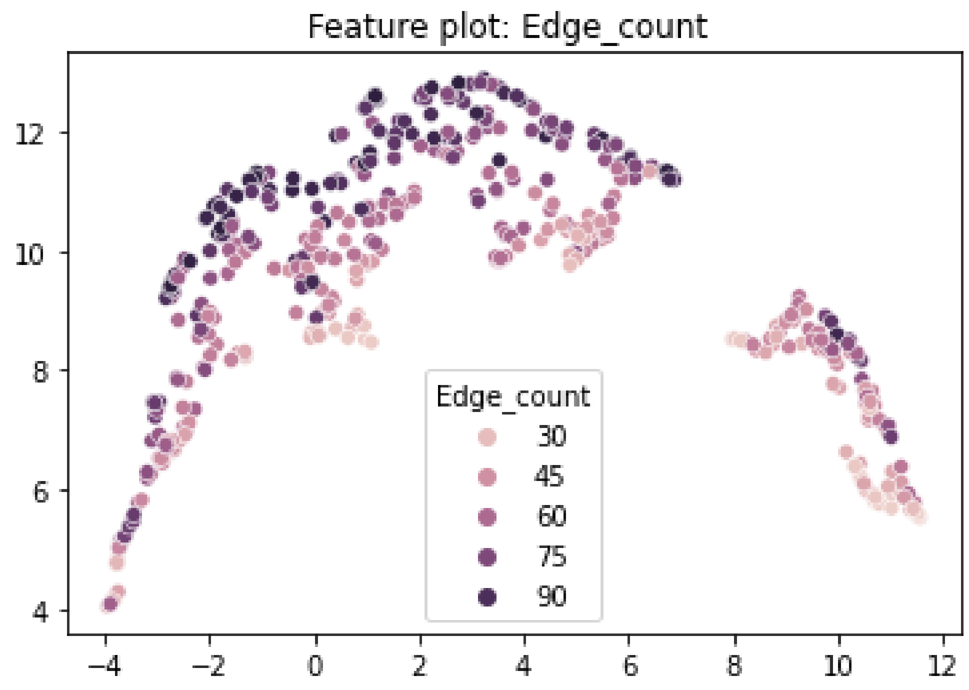
```
1    1.813913   1.626304  79.643478    2.217391  …     2.565217
2    0.684400   1.541600  78.580000    2.600000  …     2.800000
3    0.568750   1.501792  75.883333    2.416667  …     2.583333
4    0.715217   1.651348  84.521739    2.826087  …     3.000000

   med Polariz  high Polariz  3d length  Total Waals  Total Hydro  \
0     2.756757      3.027027   2.027027     2.702703     1.864865
1     3.391304      3.913043   1.739130     3.782609     1.913043
2     3.160000      3.560000   2.080000     3.600000     2.400000
3     3.000000      3.416667   1.875000     3.583333     2.250000
4     3.391304      3.826087   2.217391     3.869565     2.608696

   Total Polarity  Total Polariz  Avg_degree  Avg_degree_centrality
0        3.729730       2.162162    4.540541               0.126126
1        4.521739       3.000000    4.434783               0.201581
2        4.360000       2.480000    3.680000               0.153333
3        4.208333       2.416667    3.750000               0.163043
4        4.608696       2.695652    3.913043               0.177866

[5 rows x 23 columns]
```

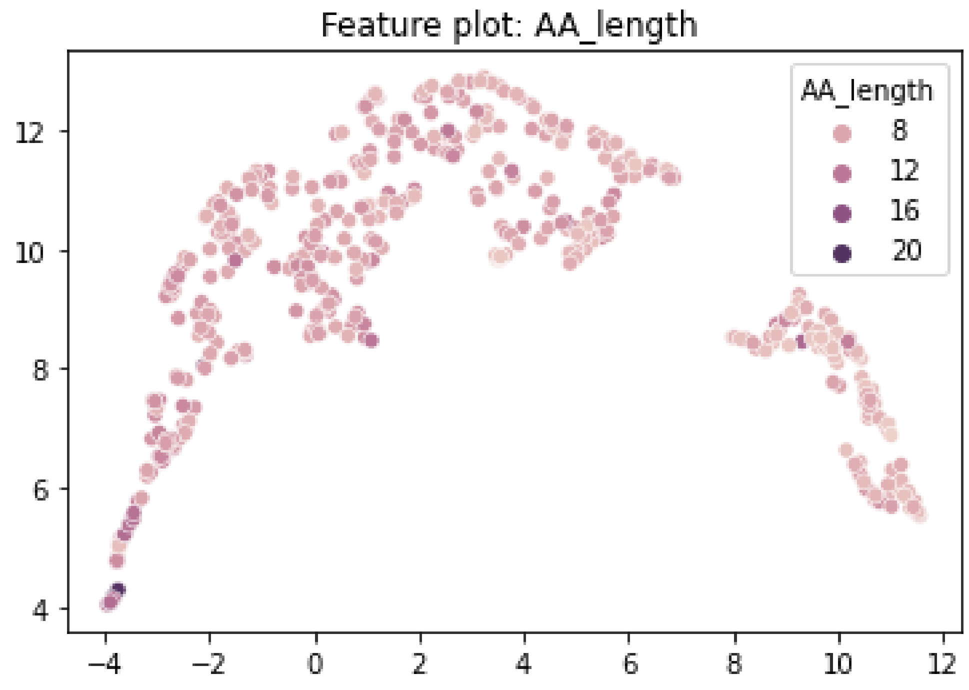
4.4 Interpreting UMAP with Featureplots of node attributes

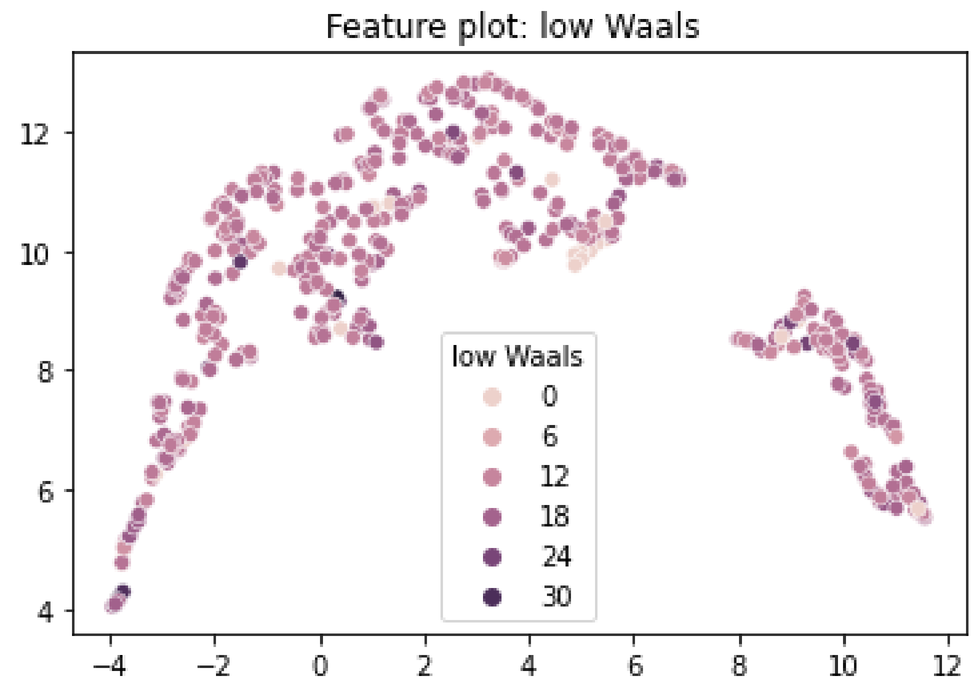
[44]:
```python
for feature in df.columns:
    sns.scatterplot(data=df, x=np.array(embedding[:,0]), y=np.array(embedding[:
 ↪,1]), hue=feature, )
    plt.title("Feature plot: {} ".format(feature))
    plt.show()
```

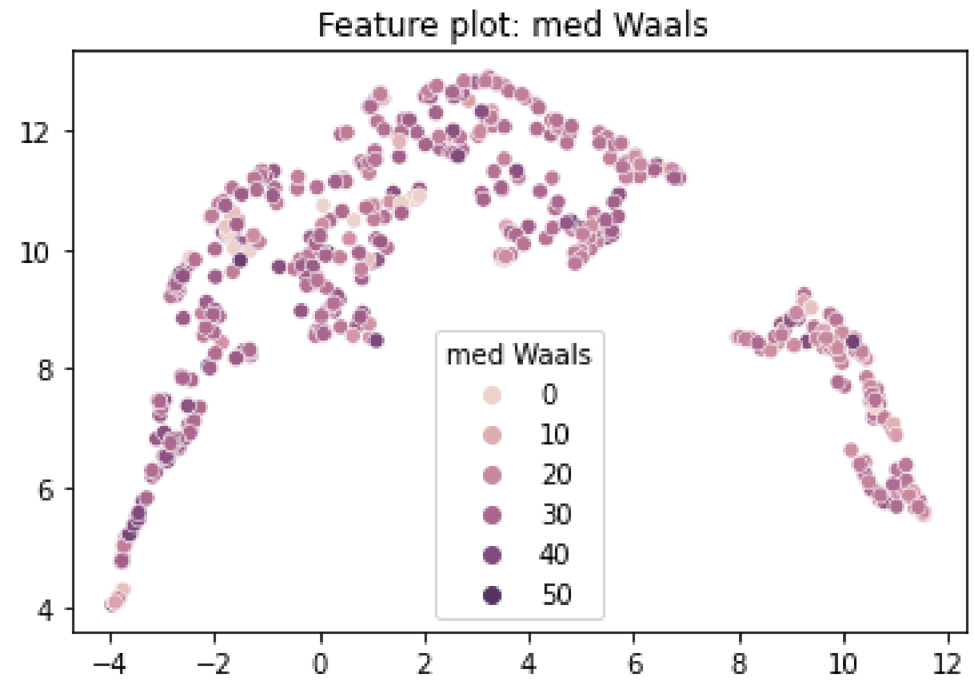

Feature plot: Node_label
Node_label
1.05
1.20
1.35
1.50
1.65
1.80
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

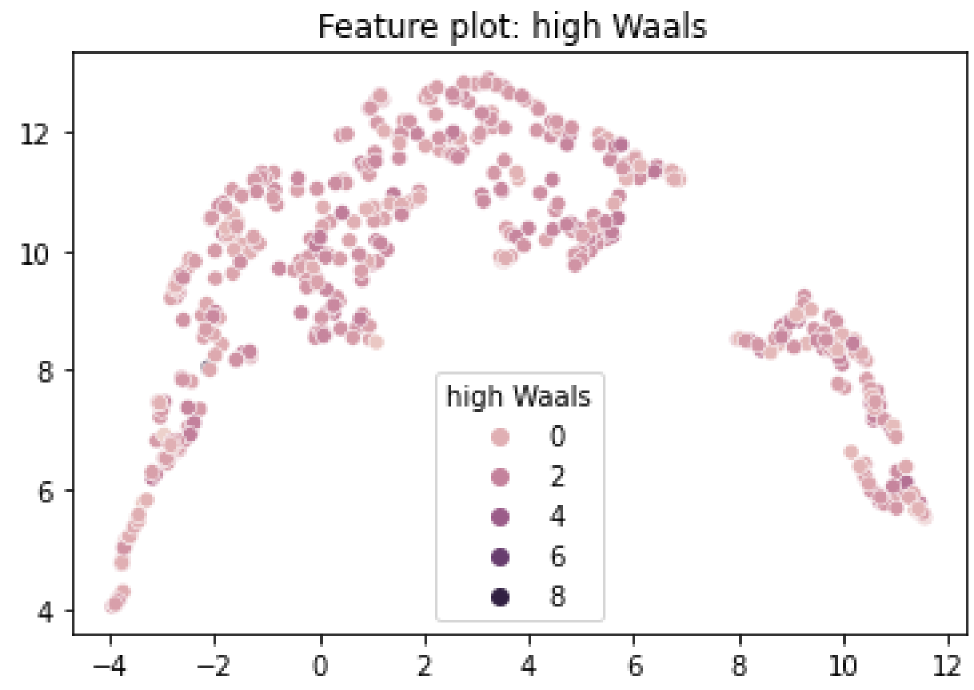

Feature plot: Node_count
Node_count
16
24
32
40
48
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

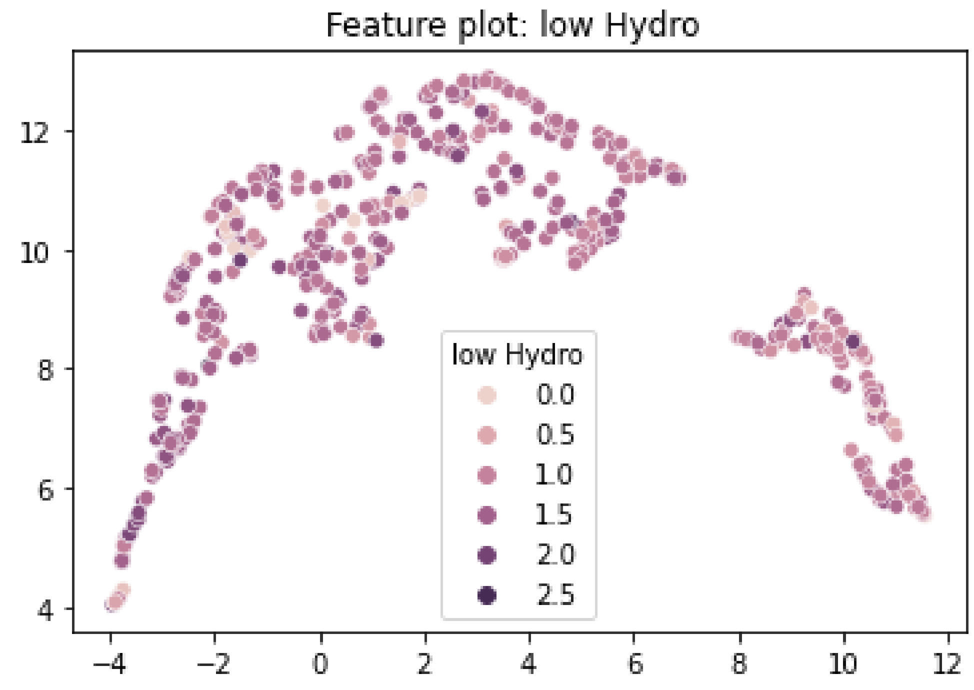

Feature plot: Edge_count
Edge_count
30
45
60
75
90
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

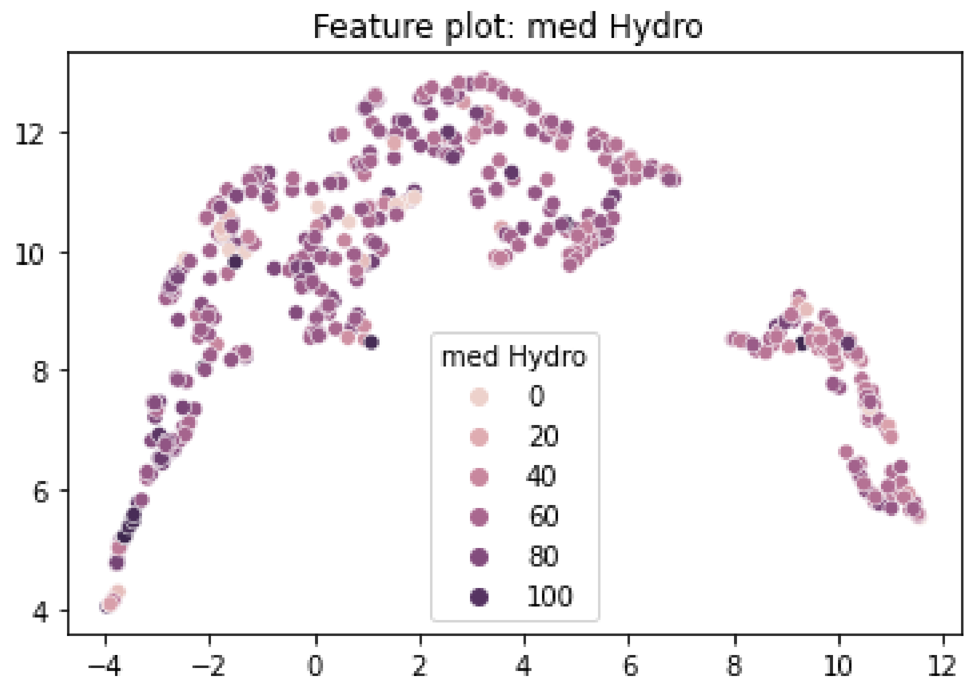

Feature plot: AA_length
AA_length
8
12
16
20
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

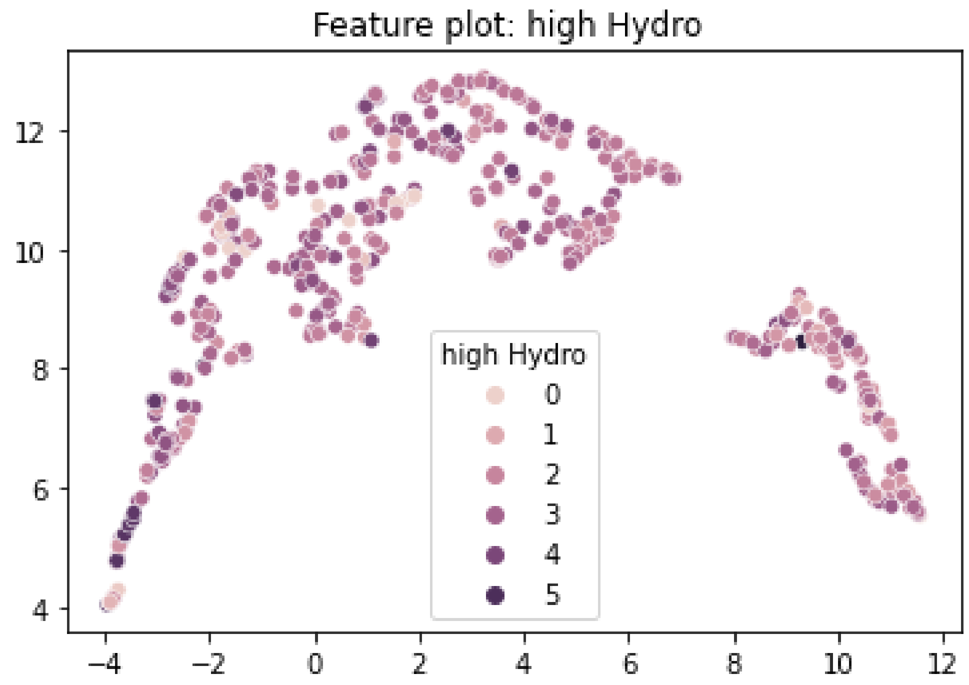

Feature plot: low Waals
low Waals
0
6
12
18
24
30
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

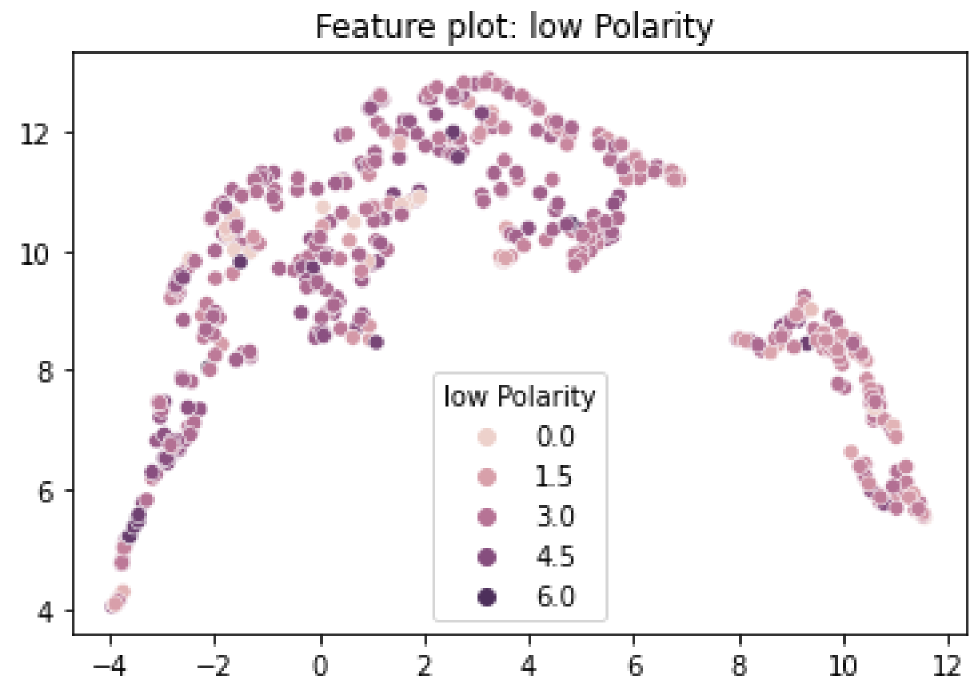

Feature plot: med Waals
med Waals
0
10
20
30
40
50
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

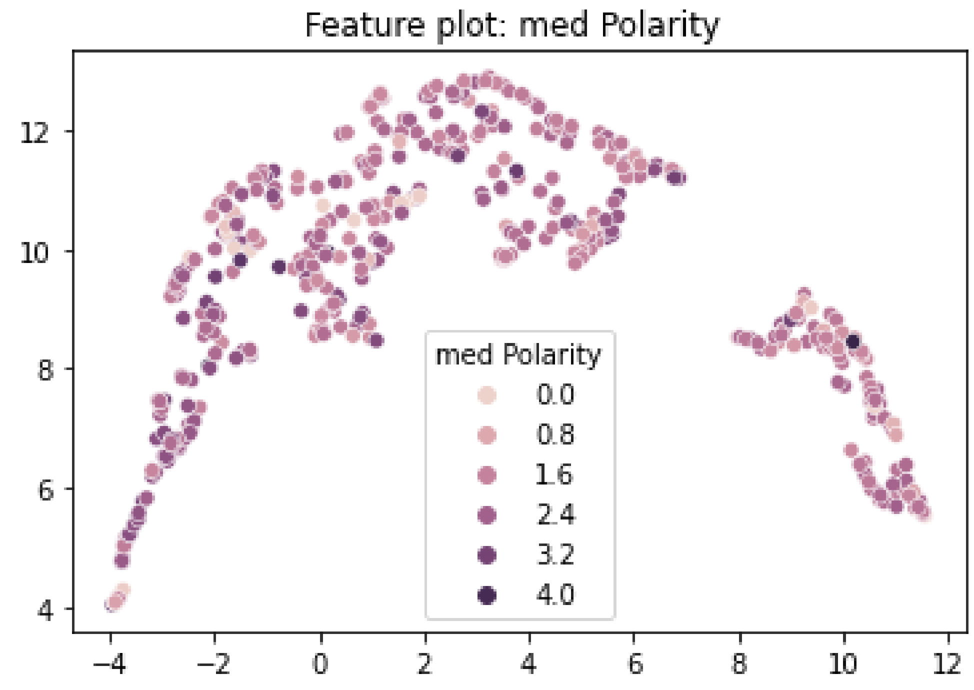

Feature plot: high Waals
high Waals
0
2
4
6
8

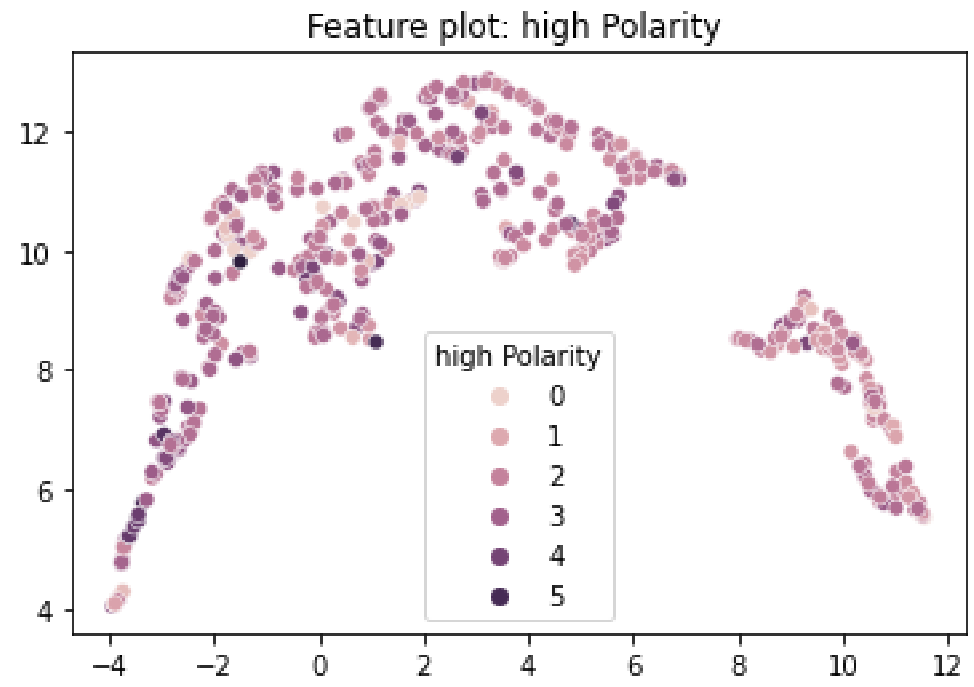

Feature plot: low Hydro
low Hydro
0.0
0.5
1.0
1.5
2.0
2.5

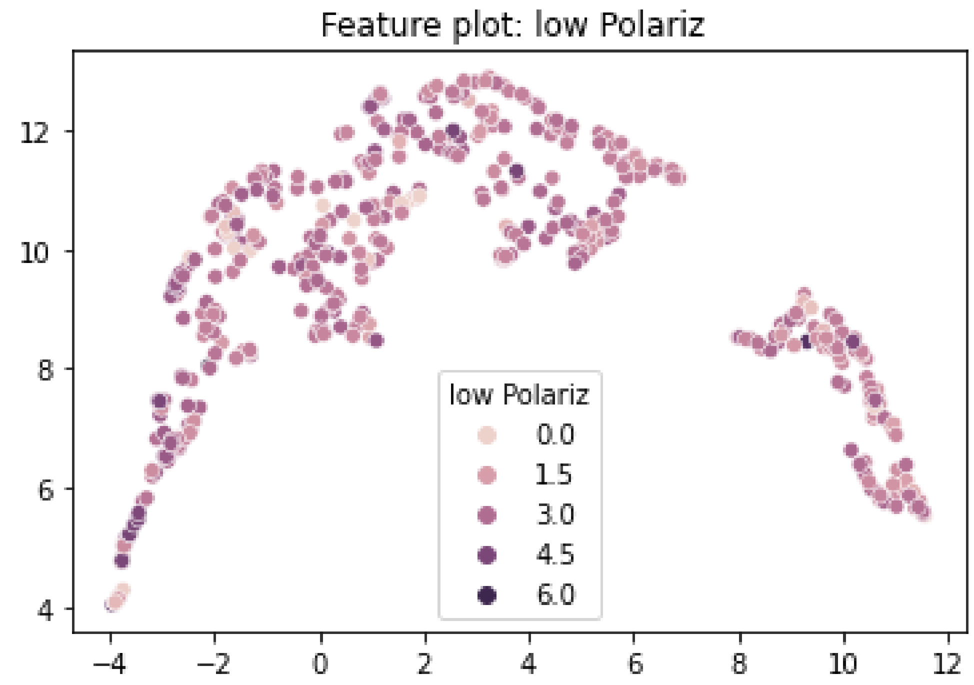

Feature plot: med Hydro
med Hydro
0
20
40
60
80
100
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

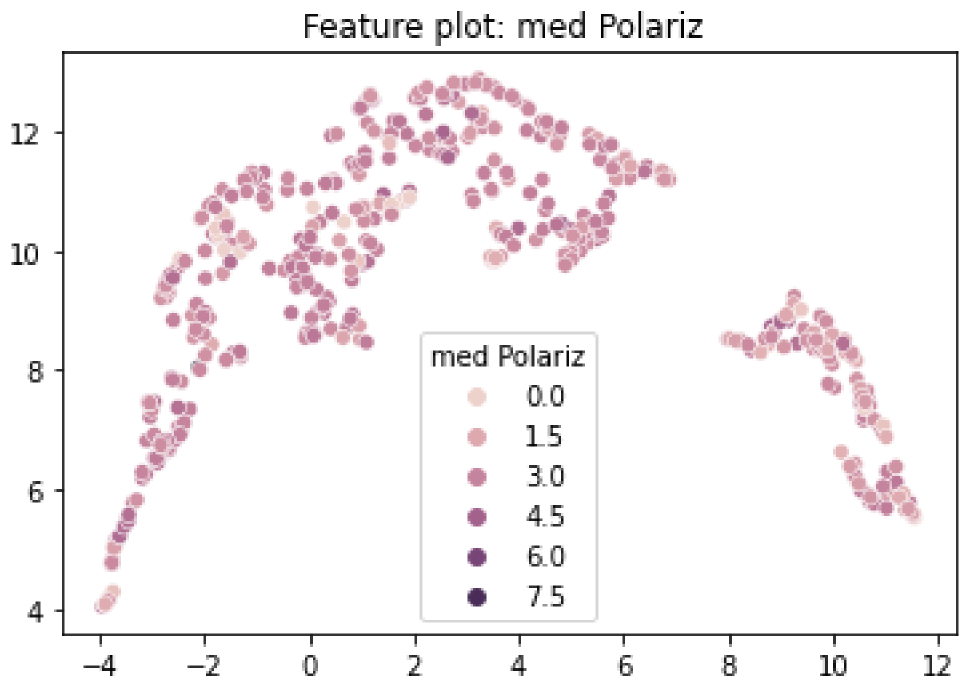

Feature plot: high Hydro
high Hydro
0
1
2
3
4
5
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

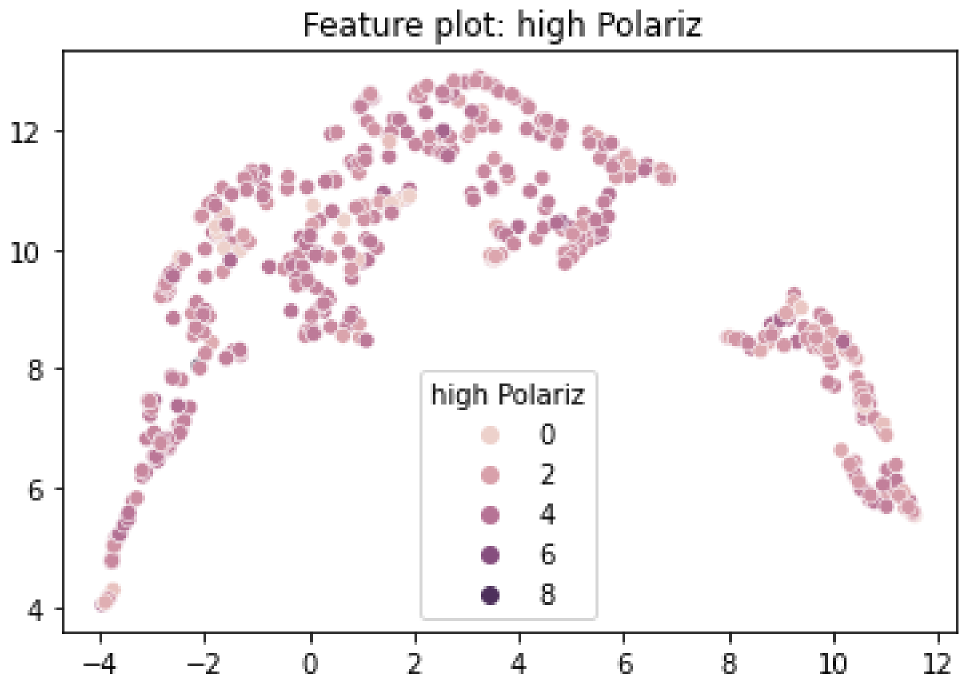

Feature plot: low Polarity
low Polarity
0.0
1.5
3.0
4.5
6.0
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

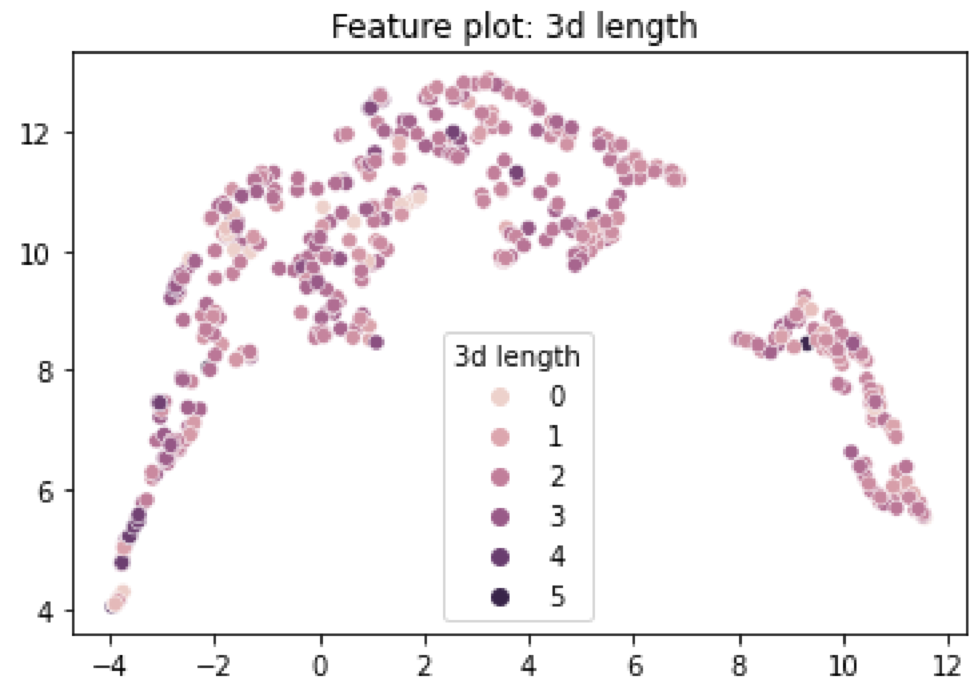

Feature plot: med Polarity
med Polarity
0.0
0.8
1.6
2.4
3.2
4.0
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

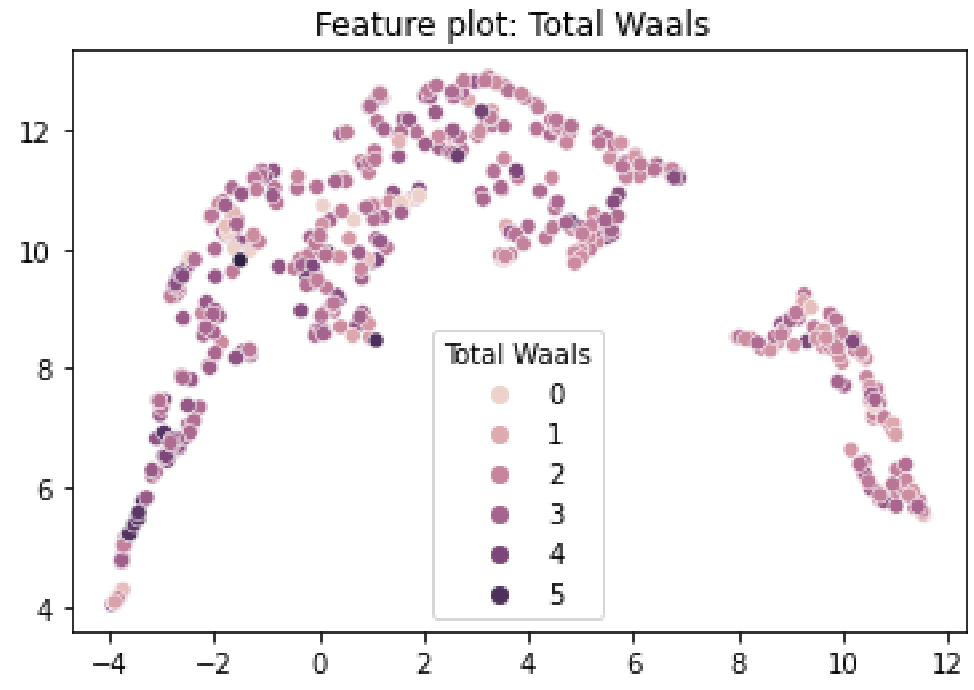

Feature plot: high Polarity
high Polarity
0
1
2
3
4
5
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

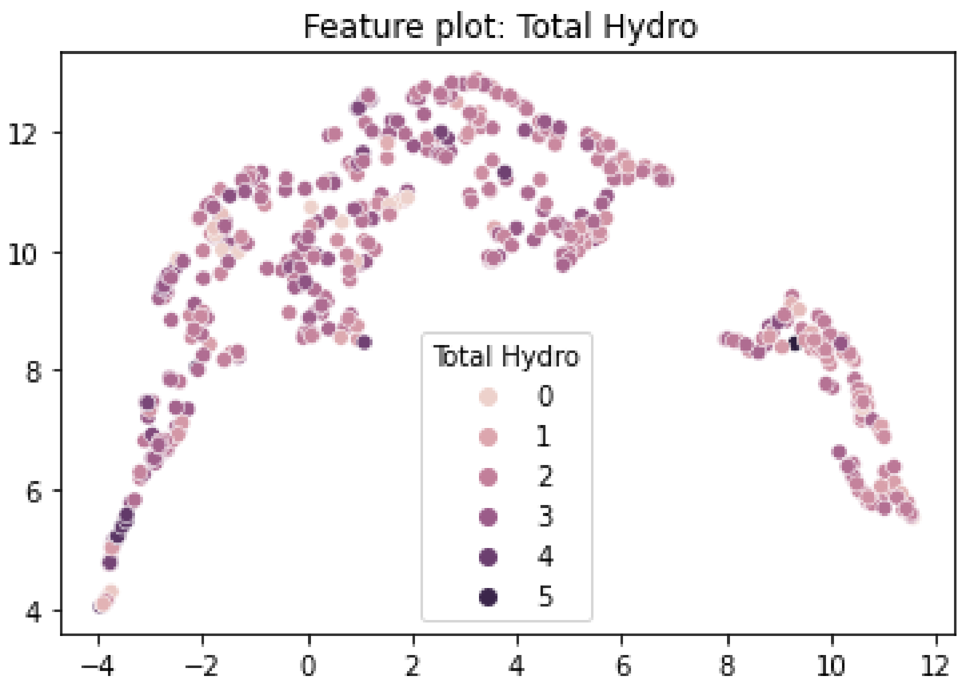

Feature plot: low Polariz
low Polariz
0.0
1.5
3.0
4.5
6.0
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12


Feature plot: med Polariz
med Polariz
0.0
1.5
3.0
4.5
6.0
7.5
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

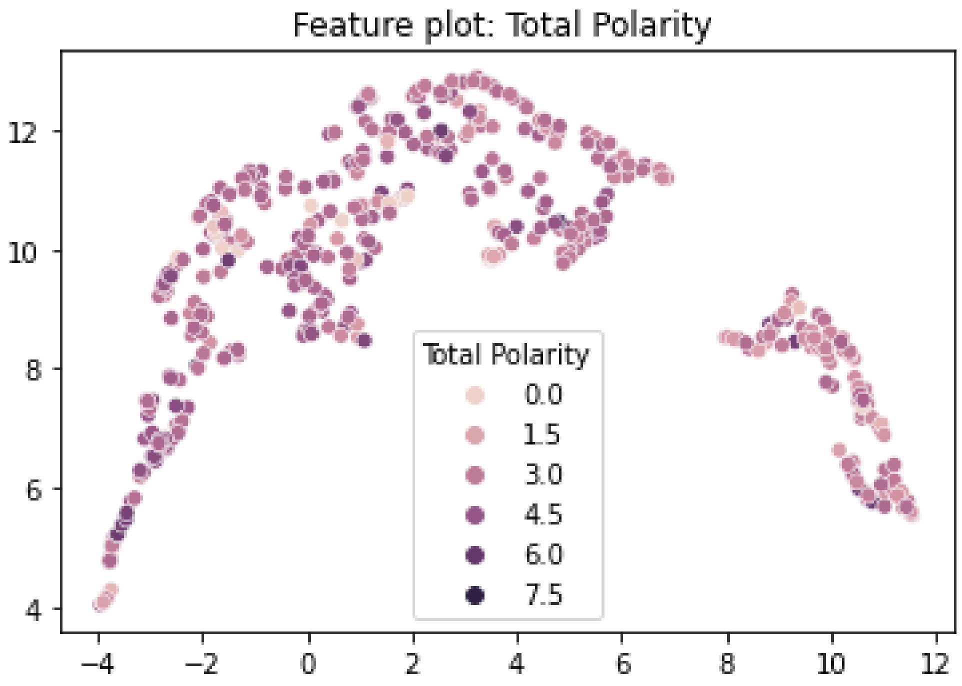

Feature plot: high Polariz
high Polariz
0
2
4
6
8
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12


Feature plot: 3d length
3d length
0
1
2
3
4
5
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

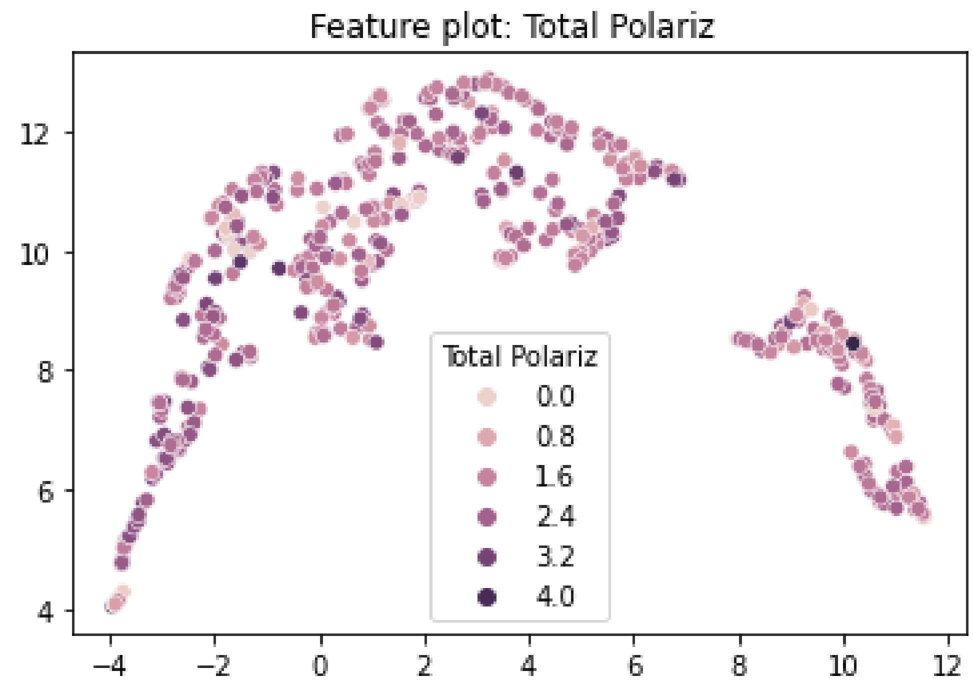

Feature plot: Total Waals
Total Waals
0
1
2
3
4
5
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12

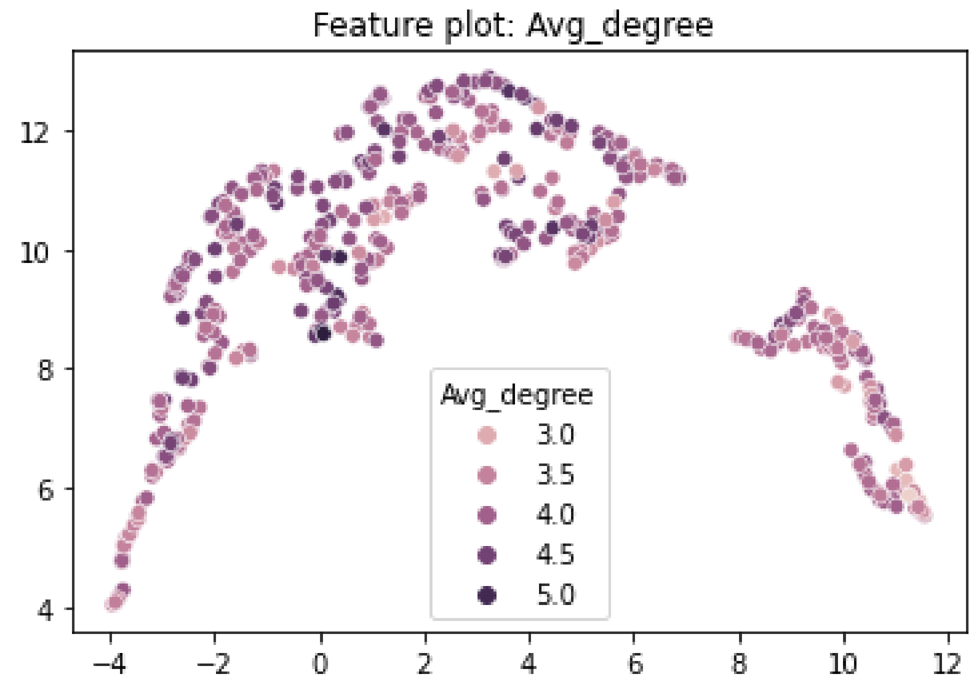


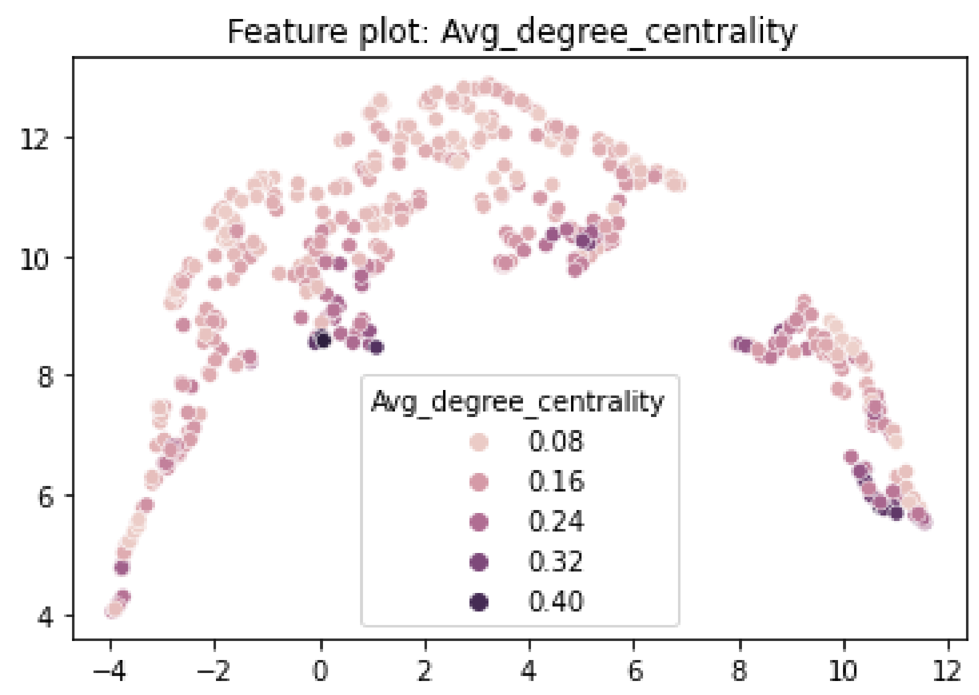
Feature plot: Total Hydro
Total Hydro
0
1
2
3
4
5



Feature plot: Total Polarity
Total Polarity
0.0
1.5
3.0
4.5
6.0
7.5


Feature plot: Total Polariz
Total Polariz
0.0
0.8
1.6
2.4
3.2
4.0
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12


Feature plot: Avg_degree
Avg_degree
3.0
3.5
4.0
4.5
5.0
12
10
8
6
4
−4
−2
0
2
4
6
8
10
12



We can notice that the Node_label has a strong effect on our UMAP1 vector. Also Node count and edge count have a strong effect on our UMAP2 vector.

```
[32]: x = df.values #returns a numpy array
      #df = preprocessing.normalize(x)
      min_max_scaler = preprocessing.MinMaxScaler()
      x_scaled = min_max_scaler.fit_transform(x)
      df = pd.DataFrame(x_scaled, columns= df.columns)

      data_norm= StandardScaler().fit_transform(x)

      df.head()
```

```
[32]:    Node_label  AA_length  low Waals  med Waals  high Waals  low Hydro  \
      0    0.392687   0.178778   0.373598   0.476537    0.246369   0.465153
      1    0.388747   0.270306   0.449869   0.598526    0.338841   0.582090
      2    0.268235   0.259682   0.414965   0.566819    0.221855   0.551772
      3    0.279412   0.239773   0.407637   0.553465    0.209877   0.537524
      4    0.242967   0.296393   0.452838   0.607712    0.225047   0.591053

         med Hydro  high Hydro  low Polarity  med Polarity  …  low Polariz  \
      0   0.535866    0.382577      0.493090      0.483840  …     0.373655
      1   0.664630    0.387505      0.610663      0.671329  …     0.398480
      2   0.655755    0.454369      0.602353      0.554965  …     0.434951
      3   0.633252    0.422330      0.585219      0.540793  …     0.401294
```

```
4   0.705340    0.493879     0.635845     0.603223  …     0.466019

   med Polariz  high Polariz  3d length  Total Waals  Total Hydro  \
0     0.325521      0.328355   0.386100     0.470035     0.349662
1     0.400449      0.424466   0.331263     0.657845     0.358696
2     0.373137      0.386169   0.396190     0.626087     0.450000
3     0.354244      0.370621   0.357143     0.623188     0.421875
4     0.400449      0.415033   0.422360     0.672968     0.489130

   Total Polarity  Total Polariz  Avg_degree  Avg_degree_centrality
0        0.491158       0.483840    0.742962               0.156686
1        0.595455       0.671329    0.703578               0.362102
2        0.574156       0.554965    0.422500               0.230754
3        0.554184       0.540793    0.448568               0.257189
4        0.606906       0.603223    0.509284               0.297540

[5 rows x 21 columns]
```

4.5 Investigating EC classes based on node features

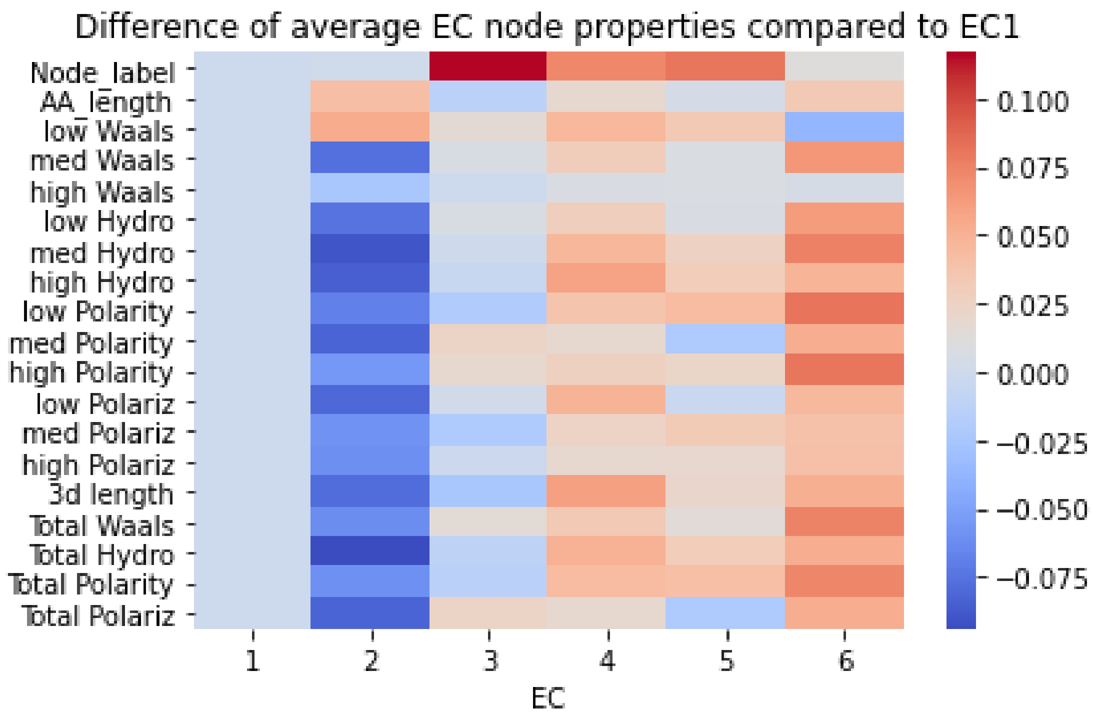
[45]:
```
# taking average values for each EC class
df.insert(1, "EC", get_EC(classes), True)
df = df.drop(columns=["Avg_degree", "Avg_degree_centrality", "Node_count",␣
 ↪"Edge_count"])
df_avg = df.groupby("EC").mean()
df_avg = df_avg.T
df_avg.head()
```

[45]:
```
EC                  1          2          3          4          5          6
Node_label   1.445366   1.446252   1.549962   1.510326   1.518212   1.457125
AA_length    7.720490   8.492352   7.485750   8.073502   7.801927   8.345070
low Waals   13.128959  14.967227  13.691902  14.707855  14.281851  11.869869
med Waals   25.073924  20.569776  25.489137  26.839942  25.592492  28.956227
high Waals   0.885641   0.662938   0.880228   0.961177   0.971233   0.936135
```

[34]:
```
df_diff = df_avg.sub(df_avg[1], axis= "rows")
```

[35]:
```
sns.heatmap(df_diff, cmap="coolwarm" )
plt.title("Difference of average EC node properties compared to EC1")
```

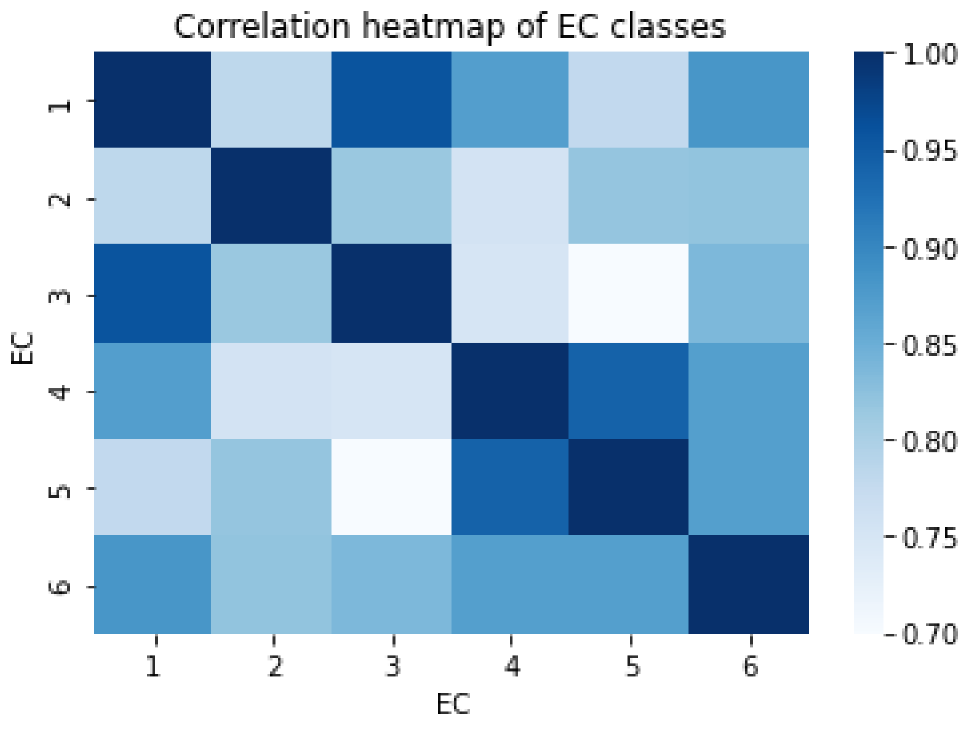
[35]:
```
Text(0.5, 1.0, 'Difference of average EC node properties compared to EC1')
```



We can see that node attributes play also an important role in EC classification.

```
[36]: sns.heatmap(df_avg.corr(method='spearman'), cmap="Blues")
      plt.title("Correlation heatmap of EC classes")
```

```
[36]: Text(0.5, 1.0, 'Correlation heatmap of EC classes')
```



We can see that EC 5,6 are highly correlatate thus they probably share some similarities Also EC 1,3 are highly correlated

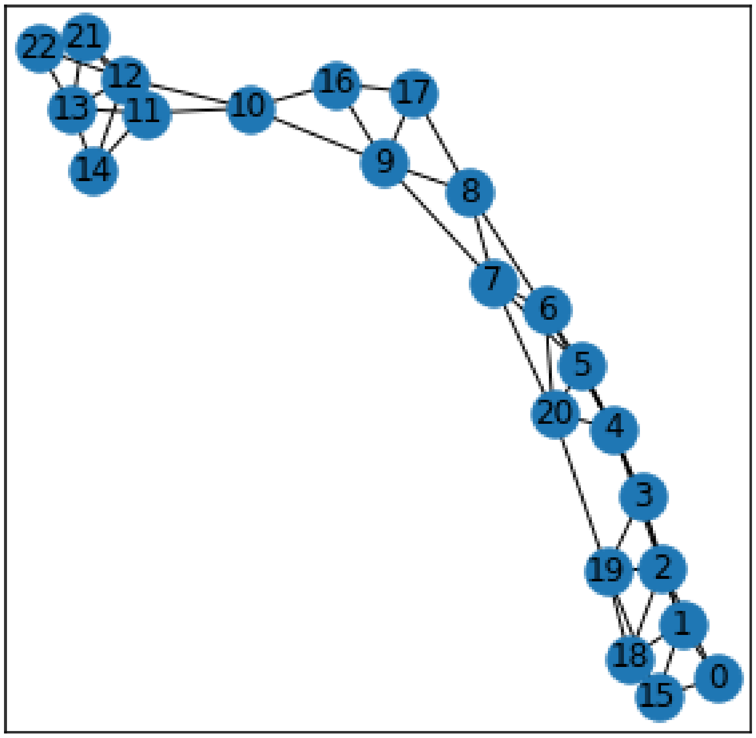
```
[37]: df = df.drop(columns=["EC"])
      df.head()
```

```
[37]:    Node_label  AA_length  low Waals  med Waals  high Waals  low Hydro  \
      0    0.392687   0.178778   0.373598   0.476537    0.246369   0.465153
      1    0.388747   0.270306   0.449869   0.598526    0.338841   0.582090
      2    0.268235   0.259682   0.414965   0.566819    0.221855   0.551772
      3    0.279412   0.239773   0.407637   0.553465    0.209877   0.537524
      4    0.242967   0.296393   0.452838   0.607712    0.225047   0.591053

         med Hydro  high Hydro  low Polarity  med Polarity  high Polarity  \
      0   0.535866    0.382577      0.493090      0.483840       0.465696
      1   0.664630    0.387505      0.610663      0.671329       0.624303
      2   0.655755    0.454369      0.602353      0.554965       0.588718
      3   0.633252    0.422330      0.585219      0.540793       0.590812
      4   0.705340    0.493879      0.635845      0.603223       0.632107

         low Polariz  med Polariz  high Polariz  3d length  Total Waals  \
      0     0.373655     0.325521      0.328355   0.386100     0.470035
      1     0.398480     0.400449      0.424466   0.331263     0.657845
      2     0.434951     0.373137      0.386169   0.396190     0.626087
```

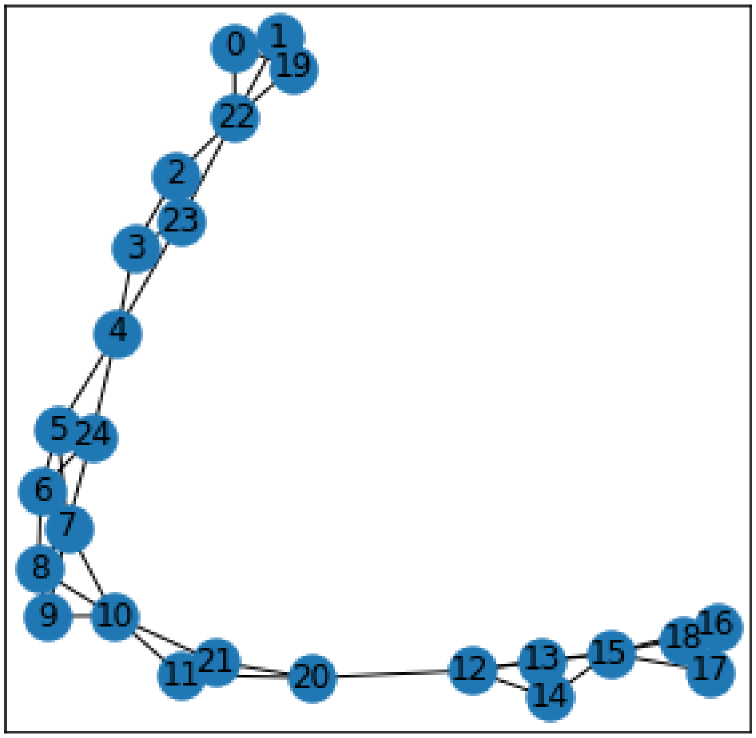
```
3     0.401294     0.354244     0.370621   0.357143     0.623188
4     0.466019     0.400449     0.415033   0.422360     0.672968

   Total Hydro  Total Polarity  Total Polariz
0     0.349662        0.491158       0.483840
1     0.358696        0.595455       0.671329
2     0.450000        0.574156       0.554965
3     0.421875        0.554184       0.540793
4     0.489130        0.606906       0.603223
```

[38]:
```
labels = ["EC1", "EC2", "EC3", "EC4", "EC5", "EC6"]

for label, ec in zip(labels, ec_classes):
    print(label)


    visualize(G_filtered[ec[10]])
```

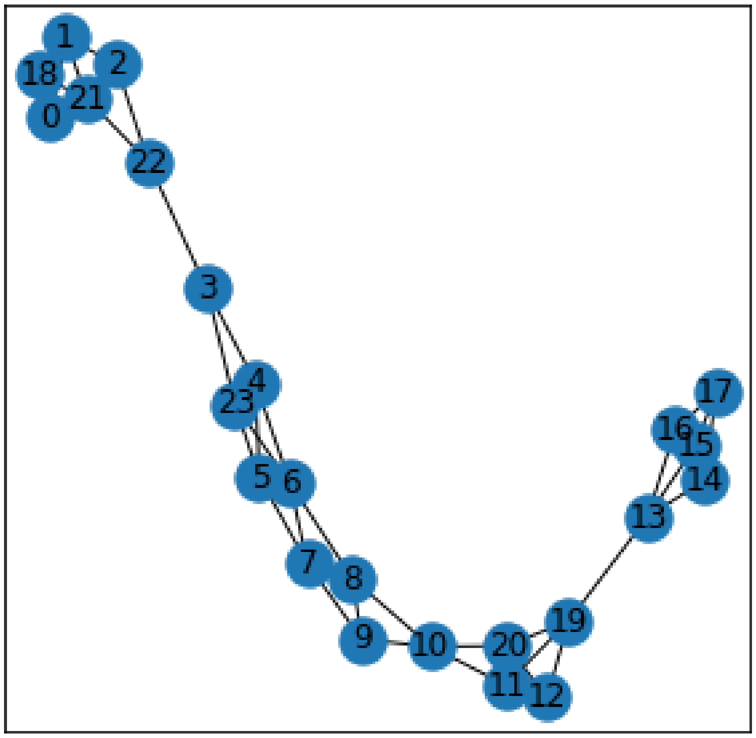
```
EC1
```



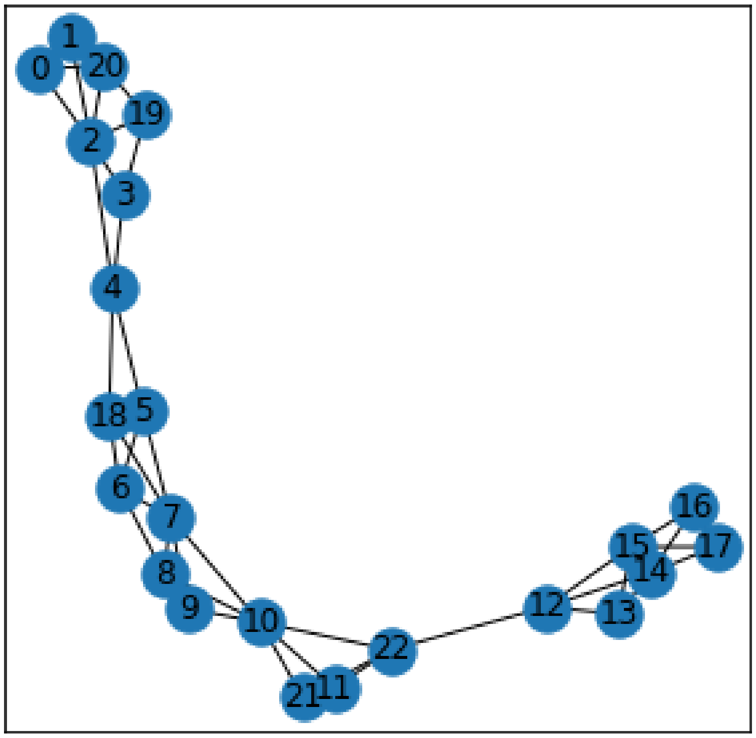
```
EC2
```


0
1
19
22
2
23
3
4
5
24
6
7
8
9
10
11
21
20
12
13
14
15
18
16
17

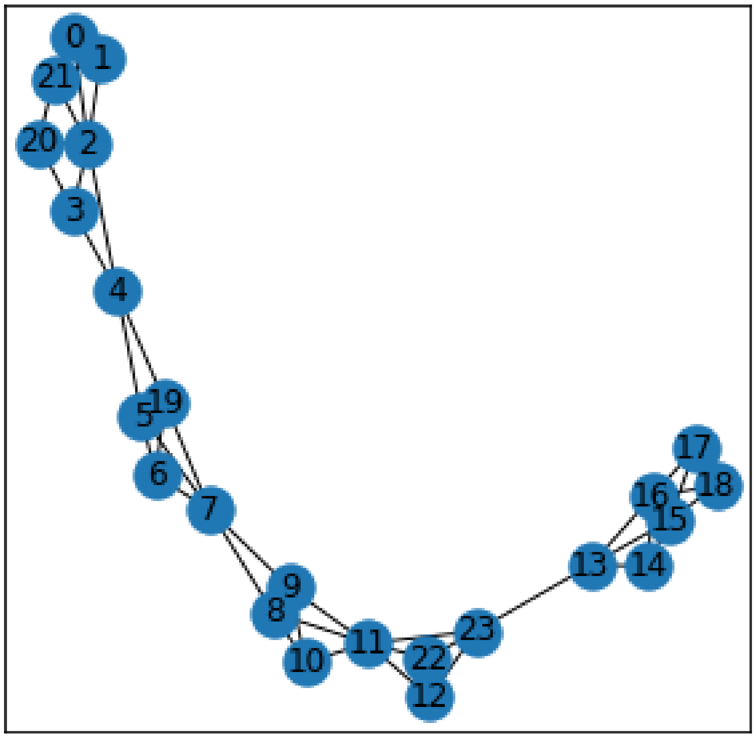
EC3


1
18
2
21
0
22
3
4
23
5
6
7
8
9
10
20
11
12
19
13
14
15
16
17

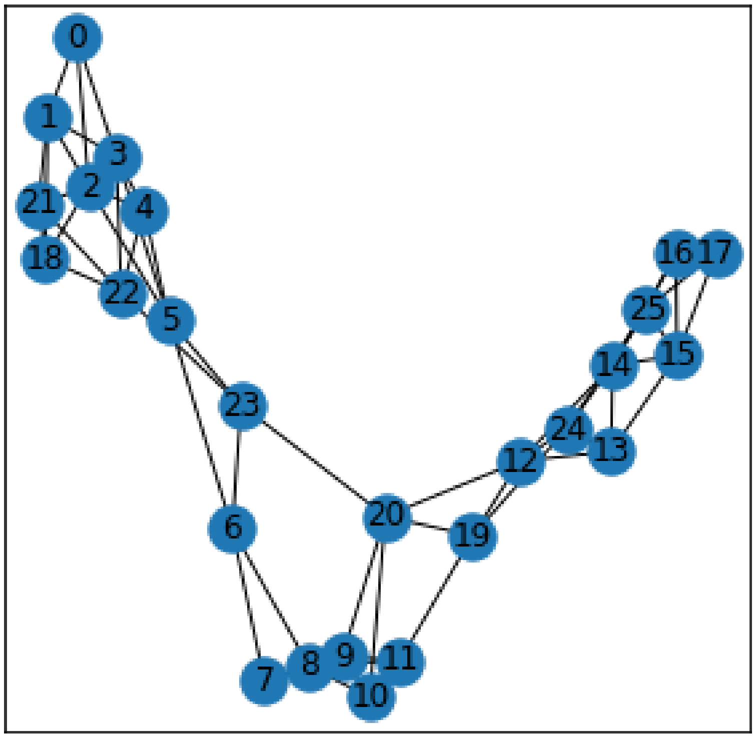
EC4



EC5


0
1
21
20
2
3
4
5
19
6
7
9
8
10
11
22
12
23
13
14
15
16
17
18

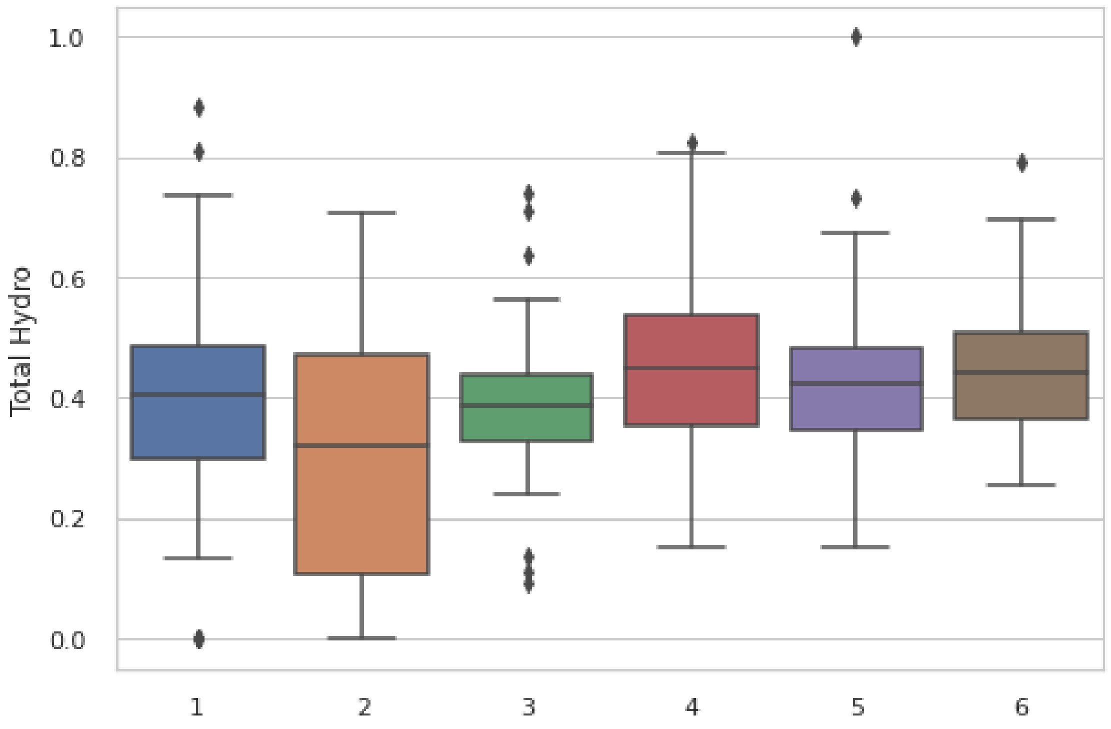
EC6


0
1
3
2
21
4
18
22
5
23
6
20
19
7
8
9
10
11
12
24
13
14
15
25
16
17

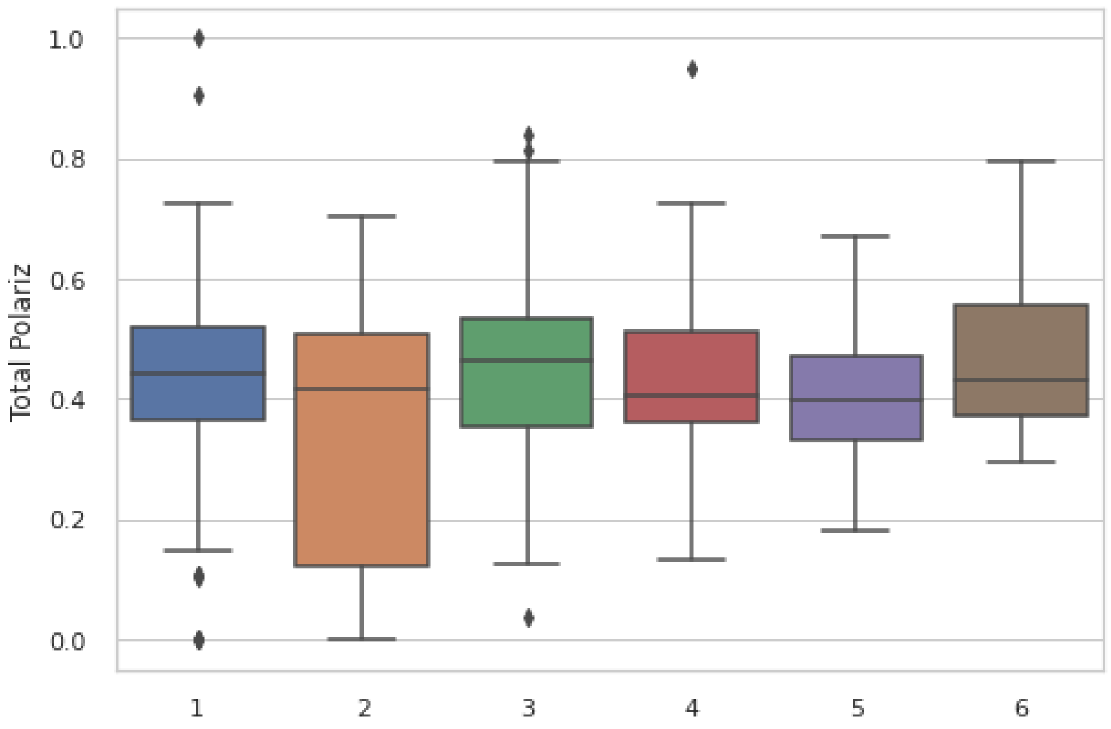
There is no clear structural difference between the EC classes

4.6 Additional: Quick analysis of Node attributes

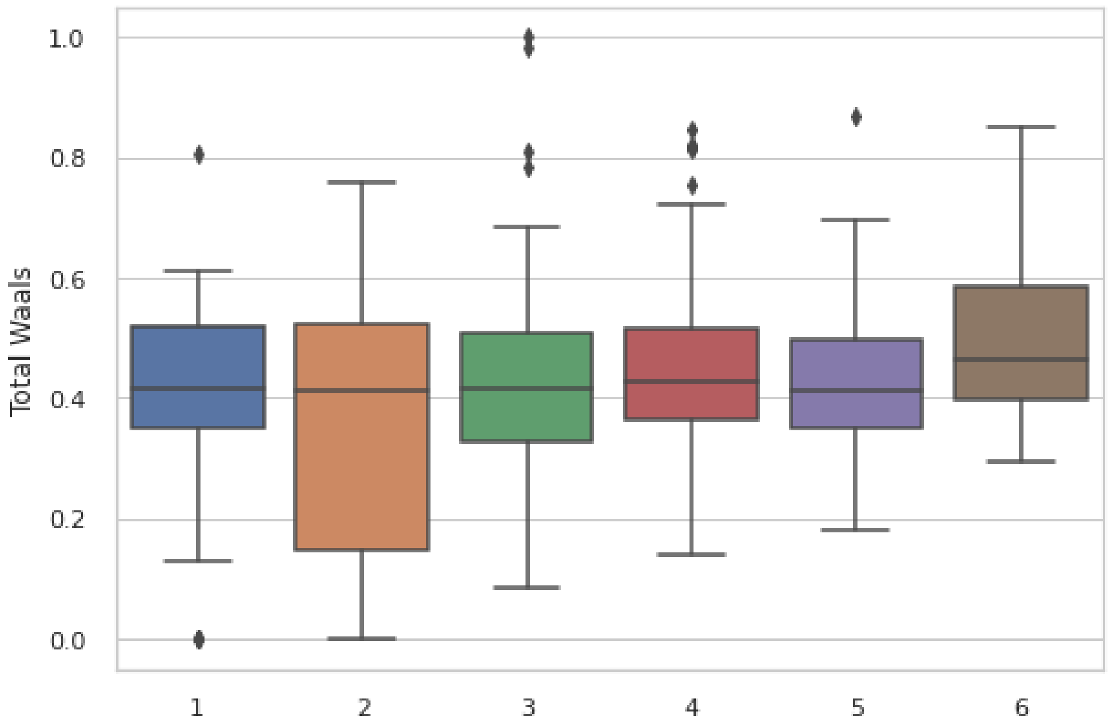
[81]:
```
sns.set_theme(style="whitegrid")
ax = sns.boxplot(x=classes, y="Total Hydro", data=df)
```



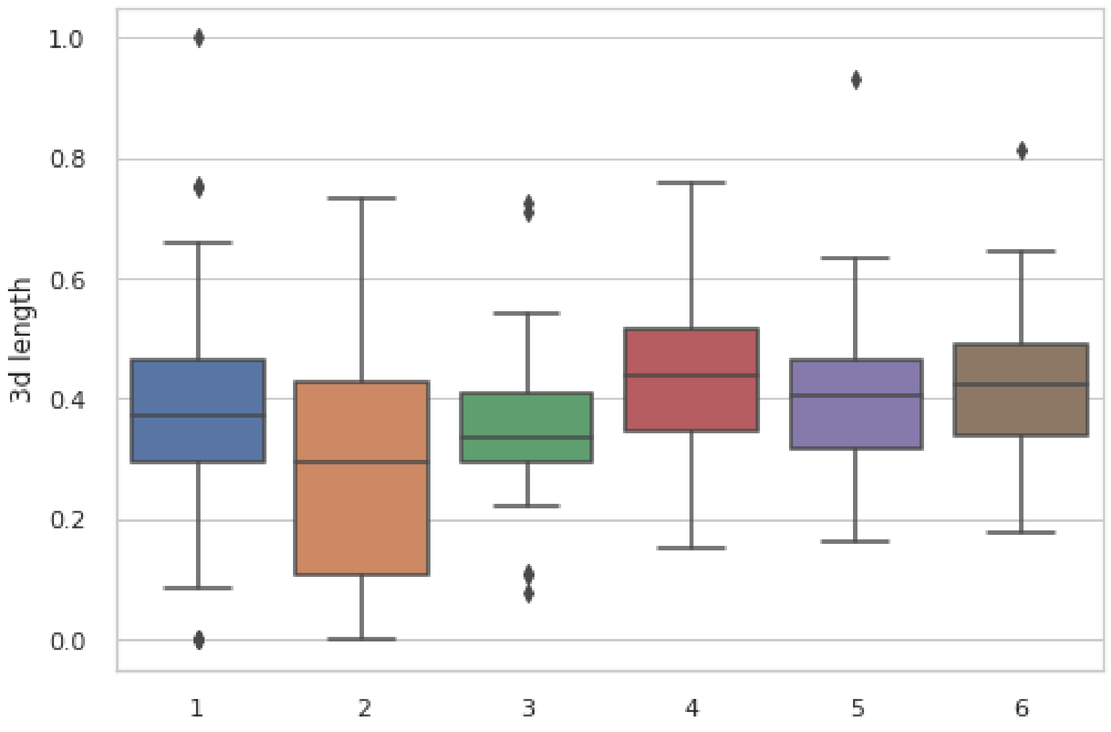
[82]:
```
sns.set_theme(style="whitegrid")
ax = sns.boxplot(x=classes, y="Total Polariz", data=df)
```



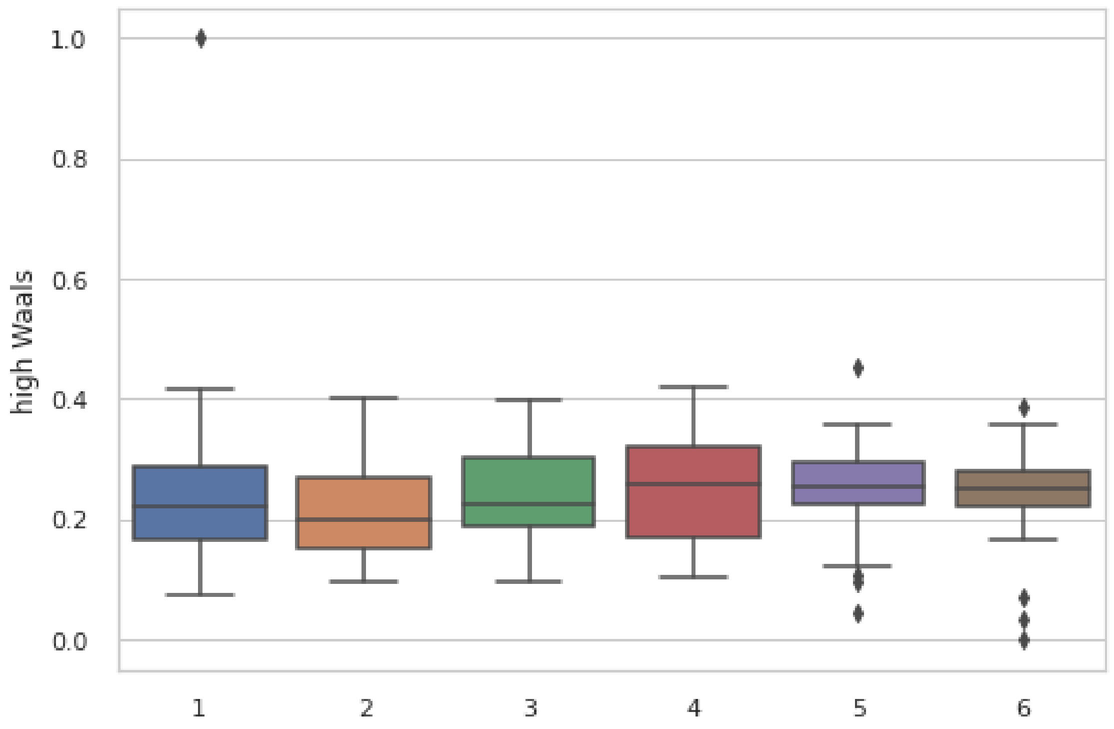
```
[83]: sns.set_theme(style="whitegrid")
      ax = sns.boxplot(x=classes, y="Total Waals", data=df)
```



[84]:
```
sns.set_theme(style="whitegrid")
ax = sns.boxplot(x=classes, y="3d length", data=df)
```

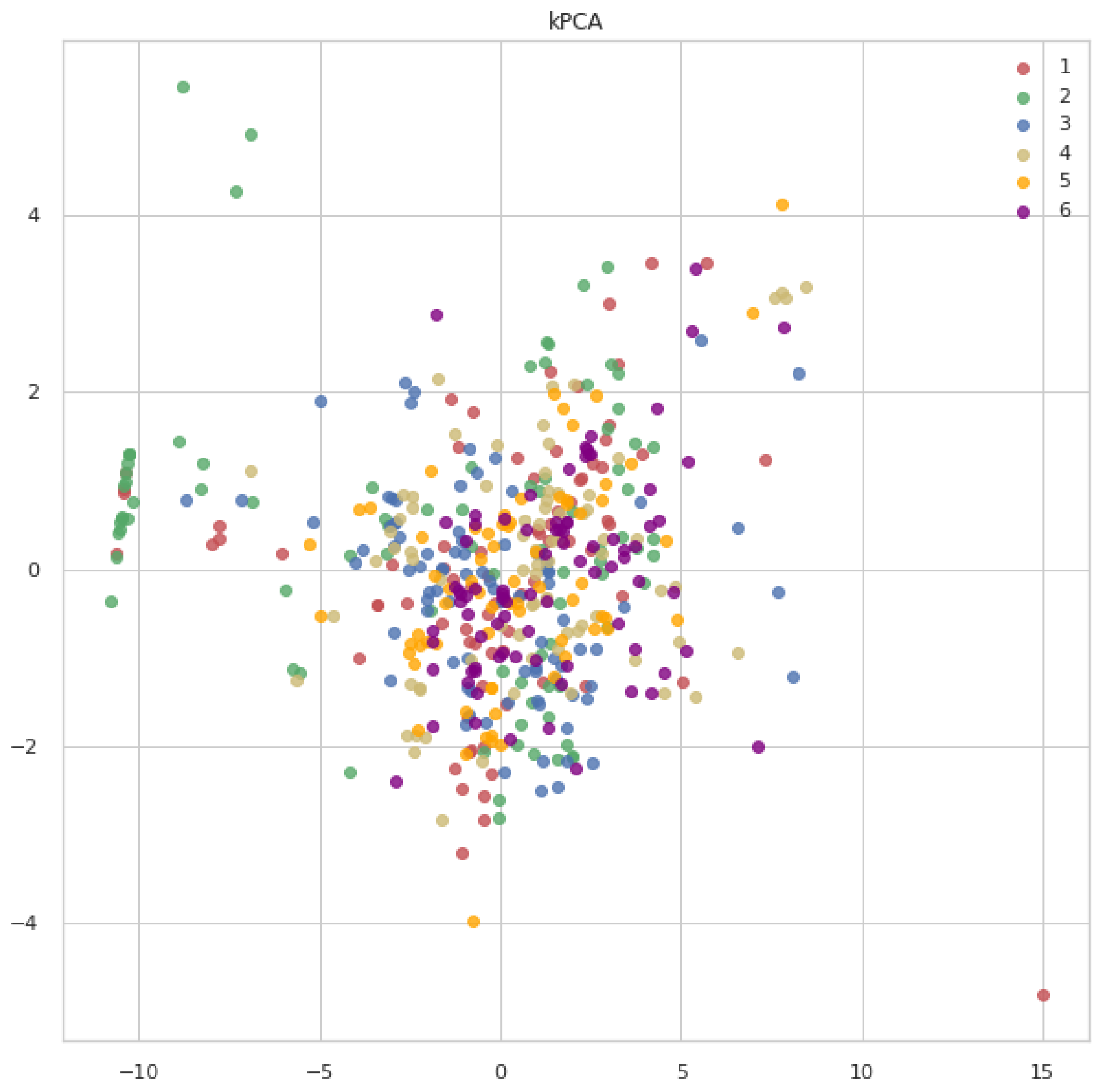


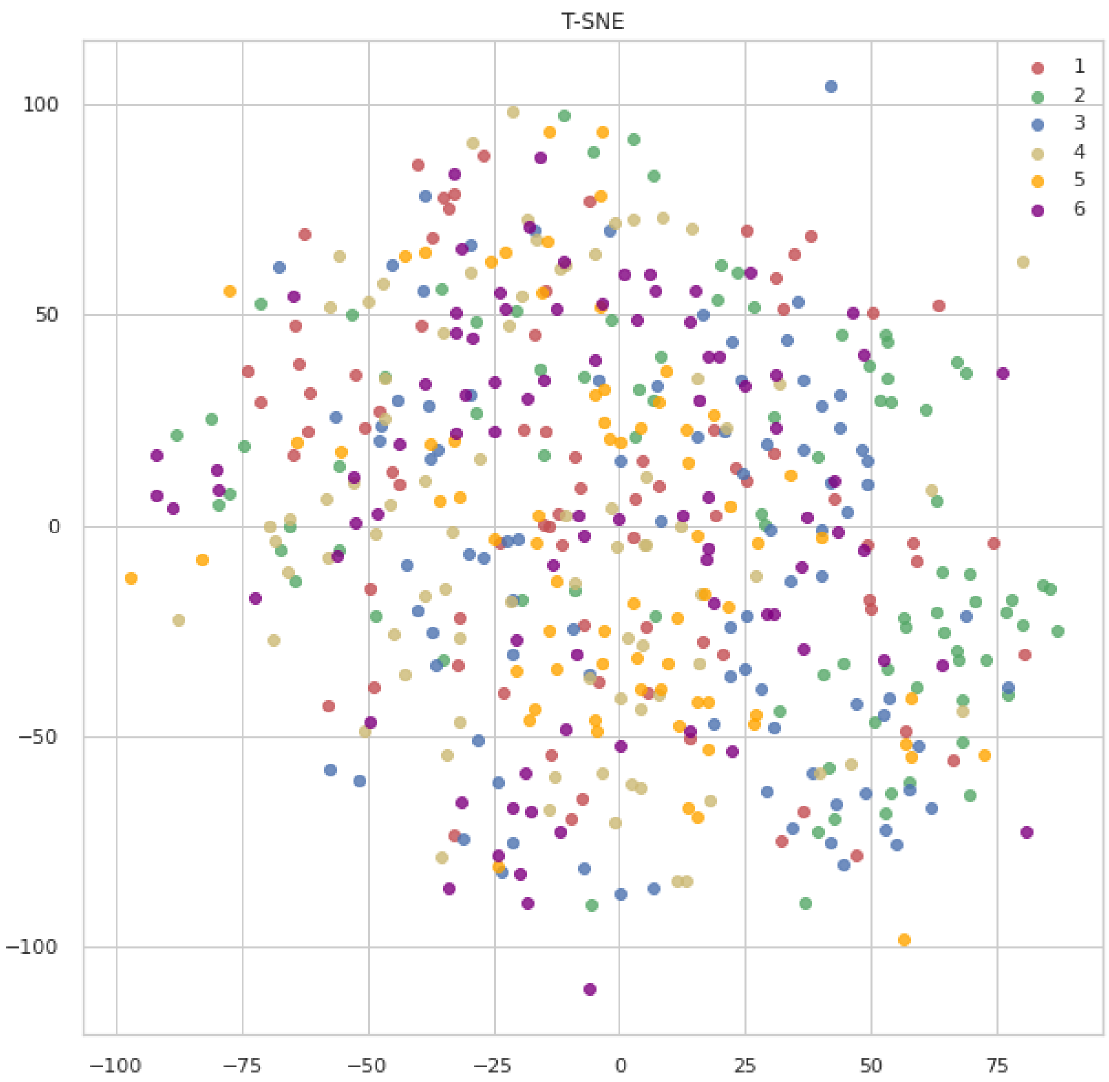
[85]:
```
sns.set_theme(style="whitegrid")
ax = sns.boxplot(x=classes, y="high Waals", data=df)
```

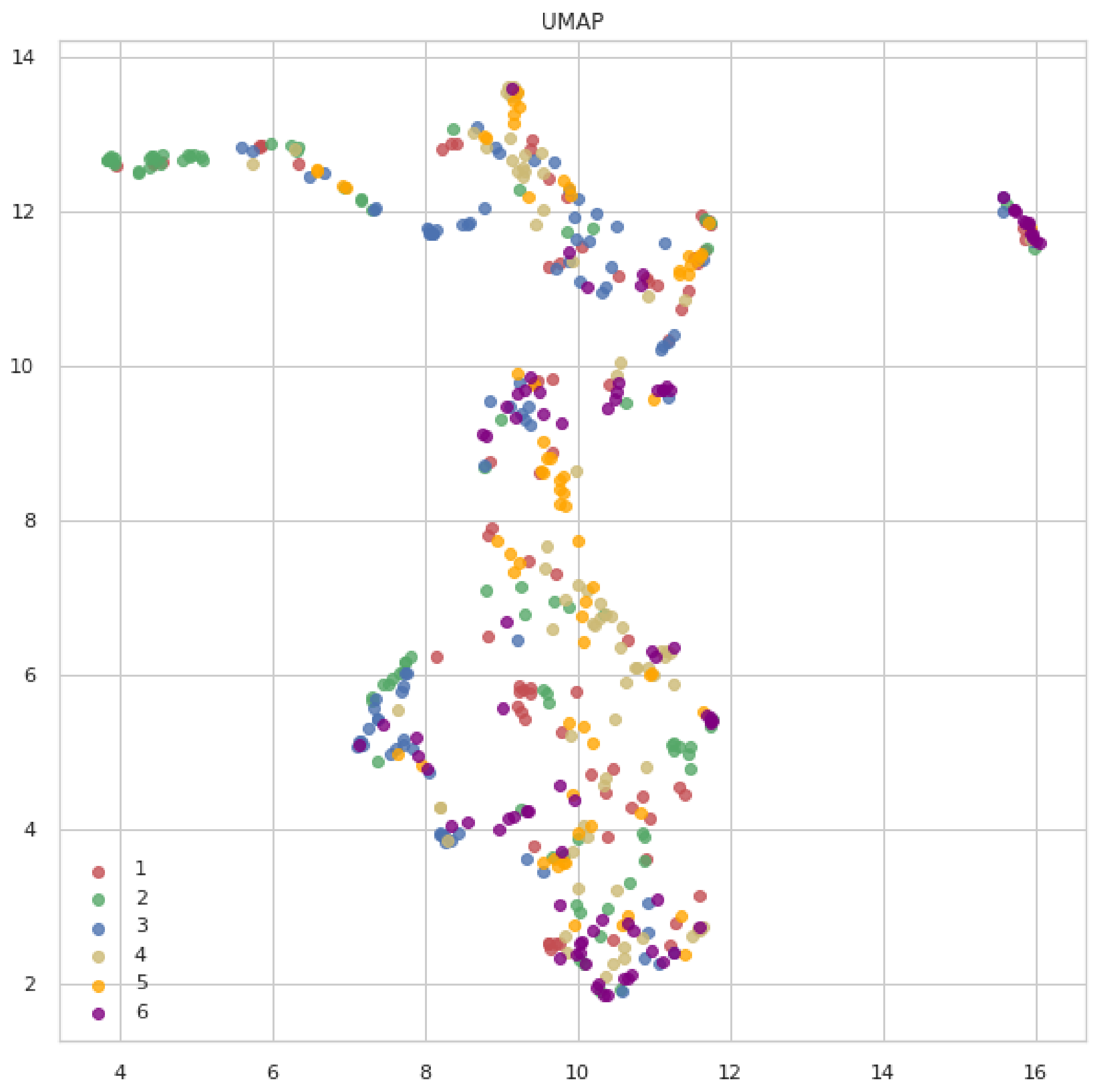


4.7 Dimensionality reduction based on Node attributes

[87]:
```
import umap
# Kernel PCA
kpca = PCA(n_components=18)
reduced_kpca= kpca.fit_transform(data_norm)
plot_dr(reduced_kpca, "kPCA",classes)

# T-SNE

pca = TSNE(n_components=3)
reduced_tsne =  pca.fit_transform(df.values)
plot_dr(reduced_tsne, "T-SNE",classes)

# UMAP
reducer = umap.UMAP()
embedding = reducer.fit_transform(df.values)
plot_dr(embedding, "UMAP",classes)
```


kPCA
1
2
3
4
5
6
4
2
0
−2
−4
−10
−5
0
5
10
15


T-SNE
1
2
3
4
5
6
100
50
0
−50
−100
−100
−75
−50
−25
0
25
50
75



Here we can see that node attributes also have big importance in the EC classification. E.g. EC2 and EC6 are nicely separated.

5 Support Vector machine prediction

[88]:
```
#sum on all iterations
for iterations in range(1,6,1):
    gram = load_csv(os.path.
 ↪join(base_path,f"{dataset}_gram_matrix_wl{iterations}.csv"))
    gram = aux.normalize_gram_matrix(gram)
    gram = gram[indices_true[:, None], indices_true]
    # Split dataset into training set and test set
    X_train, X_test, y_train, y_test = train_test_split(gram, classes,␣
↪test_size=0.2,random_state=109) # 70% training and 30% test
    clf = svm.SVC(kernel='poly') #Create a svm Classifier, 'poly' kernel is the␣
↪best by far!
    clf.fit(X_train, y_train) #Train the model using the training sets
    y_pred = clf.predict(X_test) #Predict the response for test dataset
    print(f"Iteration{iterations} accuracy:",metrics.accuracy_score(y_test,␣
↪y_pred)) # Model Accuracy: how often is the classifier correct?
```

```
Iteration1 accuracy: 0.4489795918367347
Iteration2 accuracy: 0.5612244897959183
Iteration3 accuracy: 0.5714285714285714
Iteration4 accuracy: 0.6224489795918368
Iteration5 accuracy: 0.6122448979591837
```

Best accuracy is reached on iterations 3-4, and significantly higher than what could result from randomness (~0.16).

[89]:
```
#svm on all iterations without "preprocessing"
classes_real = dp.get_dataset(dataset)
for iterations in range(1,6,1):
    gram = load_csv(os.path.
↪join(base_path,f"{dataset}_gram_matrix_wl{iterations}.csv"))
    gram = aux.normalize_gram_matrix(gram)

    # Split dataset into training set and test set
    X_train, X_test, y_train, y_test = train_test_split(gram, classes_real,␣
↪test_size=0.2,random_state=109) # 70% training and 30% test
    clf = svm.SVC(kernel='poly') #Create a svm Classifier, 'poly' kernel is the␣
↪best by far!
    clf.fit(X_train, y_train) #Train the model using the training sets
    y_pred = clf.predict(X_test) #Predict the response for test dataset
    print(f"Iteration{iterations} accuracy:",metrics.accuracy_score(y_test,␣
↪y_pred)) # Model Accuracy: how often is the classifier correct?
```

```
Iteration1 accuracy: 0.4583333333333333
Iteration2 accuracy: 0.575
Iteration3 accuracy: 0.625
Iteration4 accuracy: 0.625
Iteration5 accuracy: 0.6083333333333333
```

The svm works a bit better on the unprocessed kernel for most iterations, except for iteration5, but the difference is small.

6 Trying different kernels out

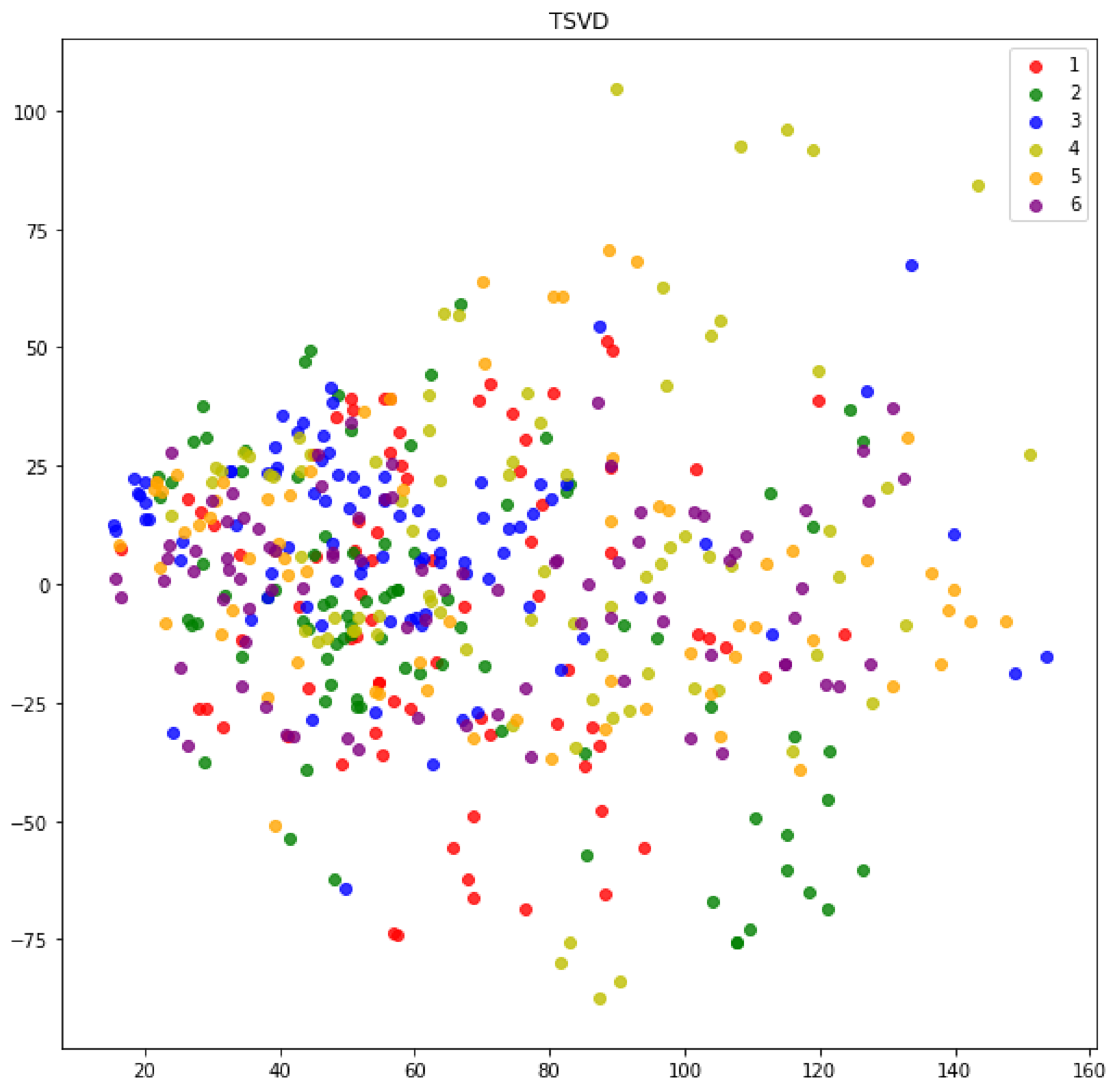
6.1 Graphlet kernel

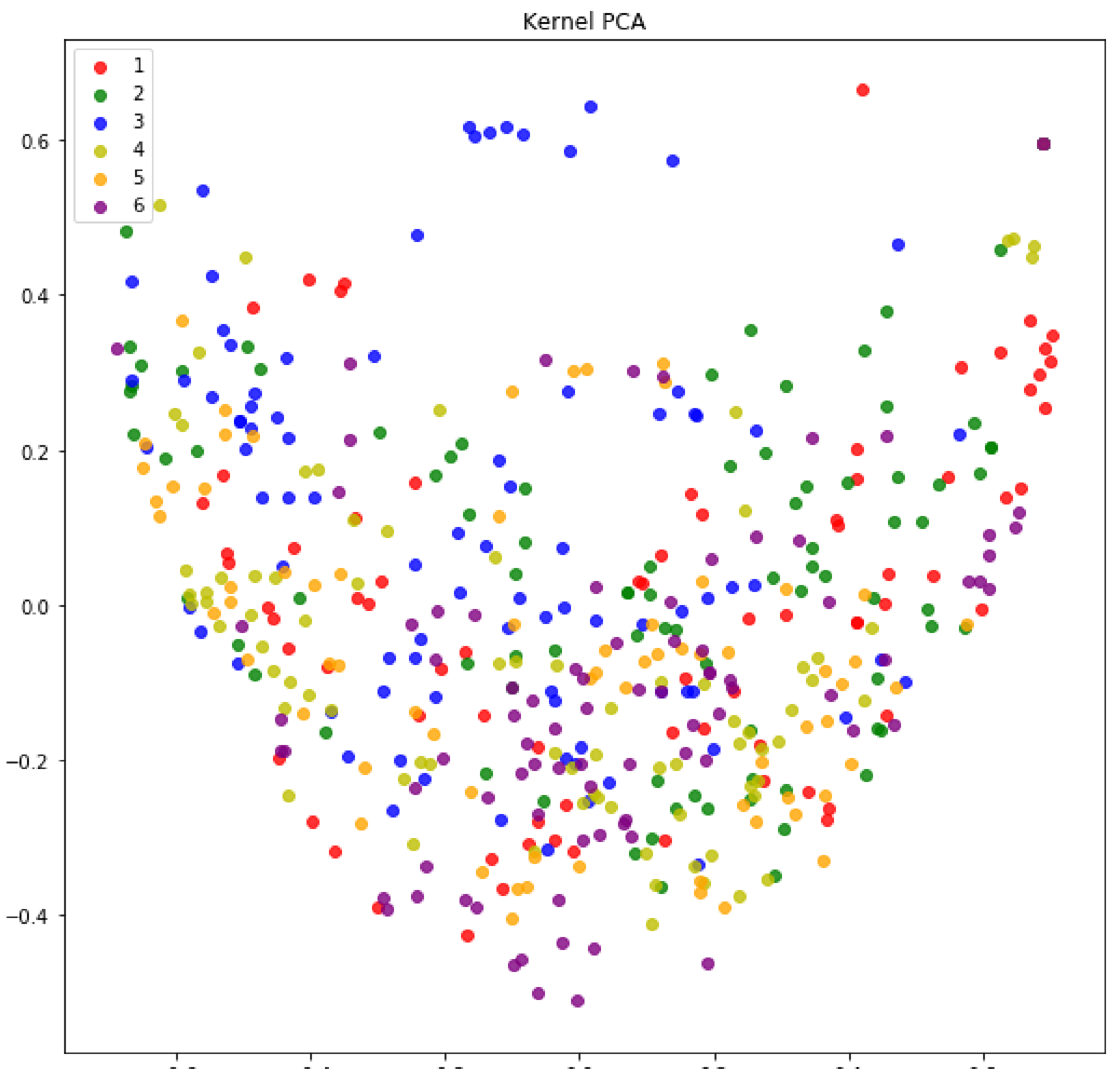
6.1.1 Dim red

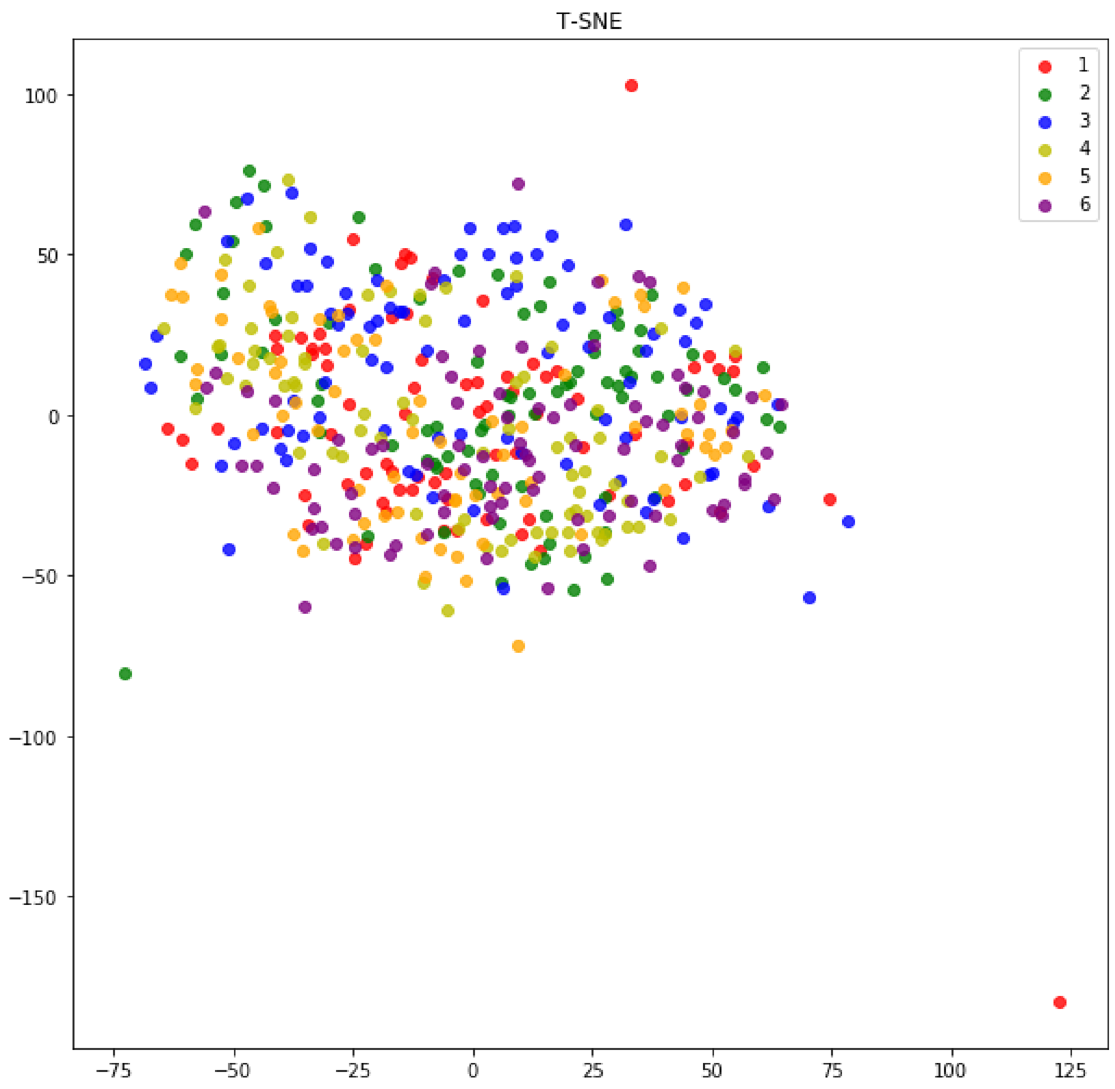
[37]:
```python
use_edge_labels = False
for use_labels in [True]:
    if use_labels:
        base_path = os.path.join("kernels","node_labels")
        datasets = ["ENZYMES"]
    else:
        base_path = os.path.join("kernels","without_labels")
        datasets = ["ENZYMES"]
    print("Load from ", base_path)
    nmis_kpca = {}
    nmis_tsvd = {}
    nmis_tsne = {}
    nmis_spec = {}
    dataset= datasets[0]

    nmis_kpca[dataset] = []
    nmis_tsvd[dataset] = []
    nmis_tsne[dataset] = []
    nmis_spec[dataset] = []

    print("###################################")
    print("Dataset ", dataset)
    #print("Iteration ", iterations)
    print("###################################")

    #--------------------------------------------
    # Load graph representation from the kernel
    #--------------------------------------------
    #Gram Matrix for the Weisfeiler-Lehman subtree kernel
    gram = load_csv(os.path.join(base_path,f"{dataset}_gram_matrix_graphlet.
↪csv"))
    #gram = load_csv(os.path.
↪join(base_path,f"{dataset}_gram_matrix_shortestpath.csv"))
    gram = aux.normalize_gram_matrix(gram)
    gram = gram[indices_true[:, None], indices_true]

    #Sparse Vectors for the Weisfeiler-Lehmann subtree kernel
    vec = load_sparse(os.path.join(base_path,f"{dataset}_vectors_graphlet.npz"))
    vec = vec[indices_true, :]
    #vec = load_sparse(os.path.join(base_path,f"{dataset}_vectors_shortestpath.
↪npz"))
    print(gram.shape, vec.shape)
```

```
#---------------------------------------------
# Dimensionality Reduction
#---------------------------------------------

# SVD
tsvd = TruncatedSVD(n_components=50)
reduced_tsvd = tsvd.fit_transform(vec)
plot_dr(reduced_tsvd, "TSVD", classes)

# Kernel PCA
kpca = KernelPCA(n_components=50, kernel="precomputed")
reduced_kpca= kpca.fit_transform(gram)
plot_dr(reduced_kpca, "Kernel PCA",classes)

# T-SNE
pca = TSNE(n_components=3)
reduced_tnse =  pca.fit_transform(gram)
plot_dr(reduced_tnse, "T-SNE",classes)

k = len(set(classes.tolist()))
print("n_clusters: ", k)
d = {0:"TSVD",1:"KPCA", 2:"T-SNE"}
n_d = {0:nmis_tsvd, 1:nmis_kpca, 2:nmis_tsne}
```

```
Load from  kernels\node_labels
##################################
Dataset  ENZYMES
##################################
(488, 488) (488, 3455)
```


TSVD
1
2
3
4
5
6
100
75
50
25
0
−25
−50
−75
20
40
60
80
100
120
140
160


Kernel PCA
1
2
3
4
5
6
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6



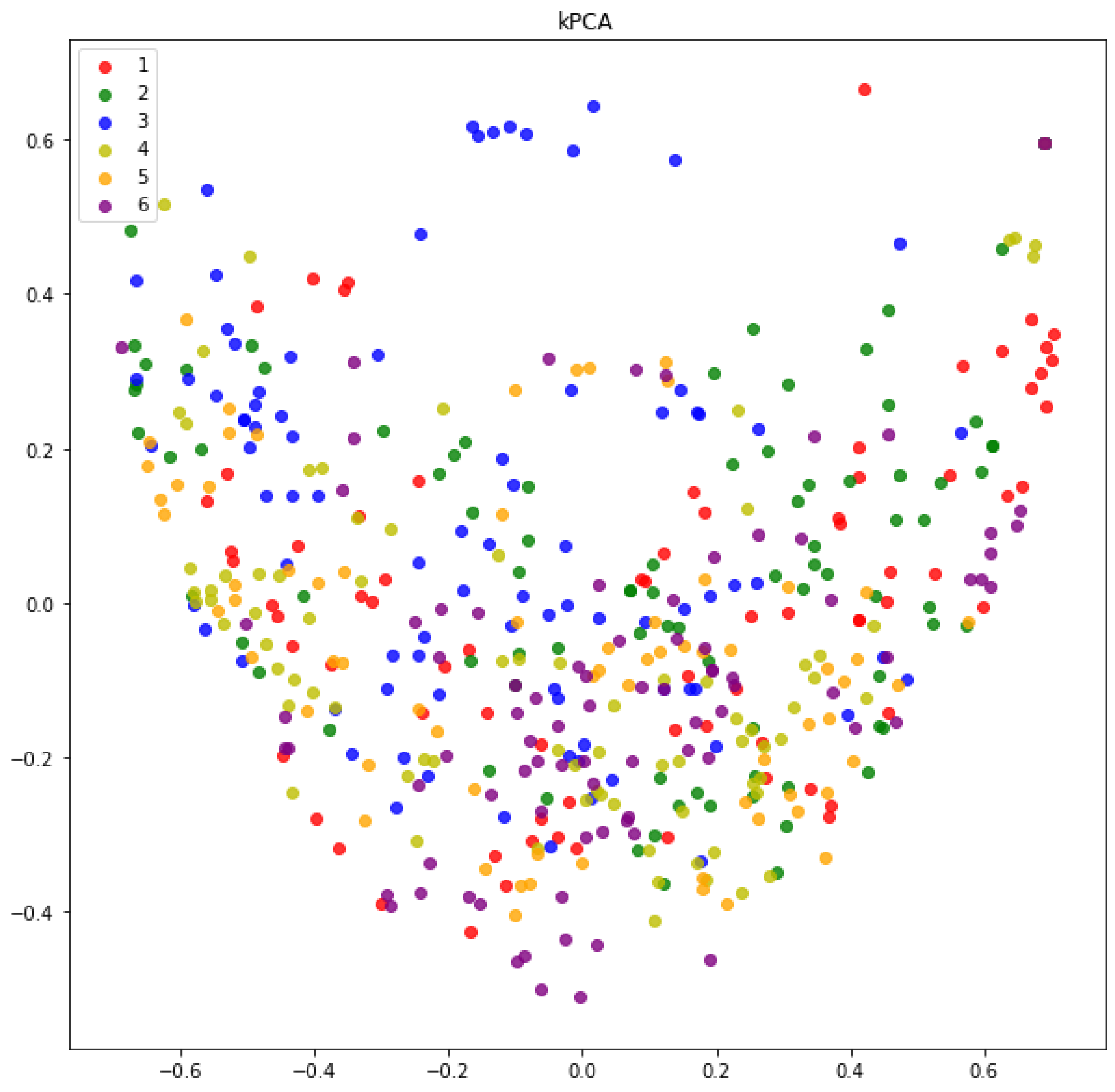
```
n_clusters:  6
```

6.1.2 Clustering

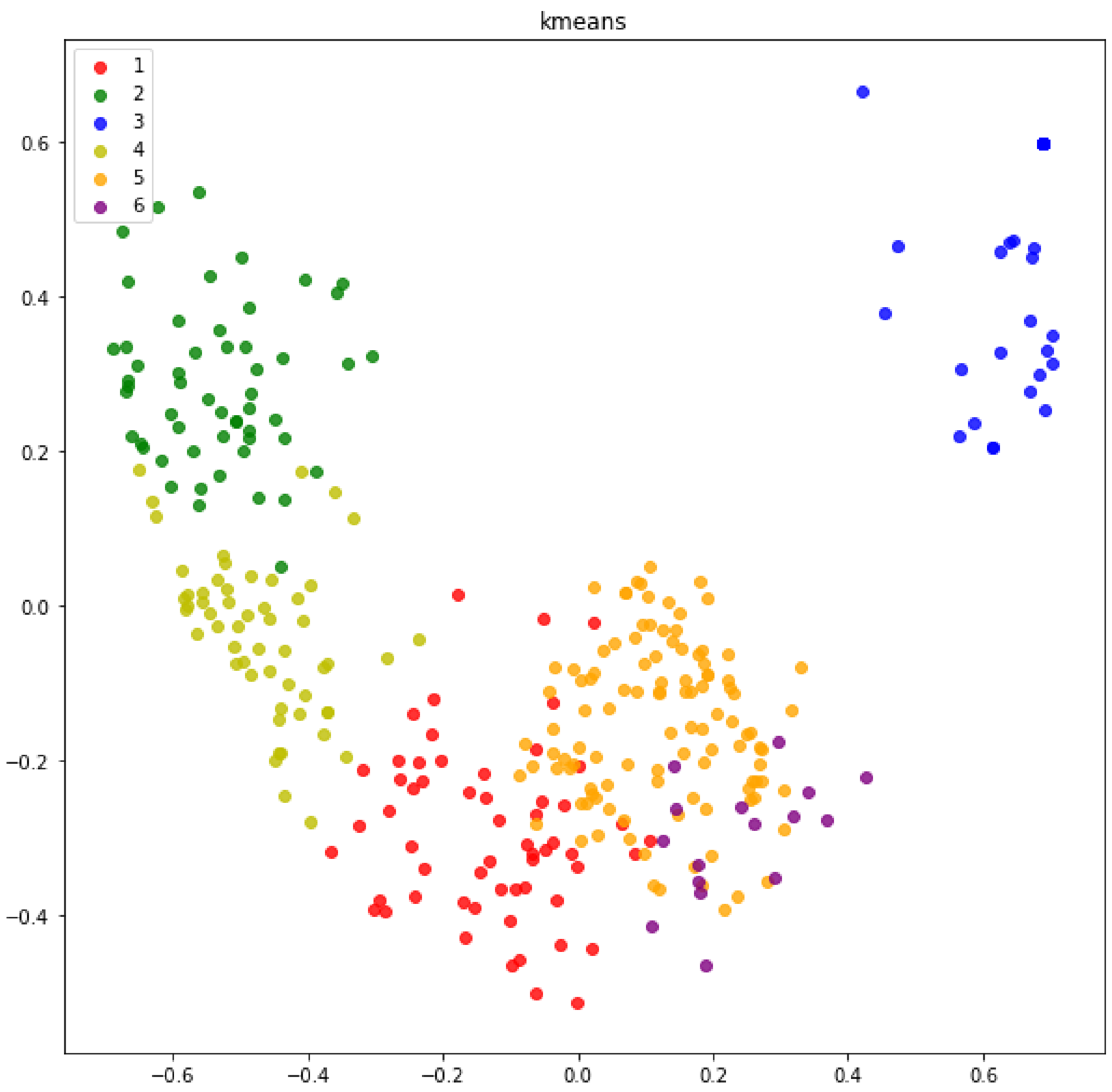
[38]:
```
print("Dimensionality reduction: kPCA")
plot_dr(reduced_kpca, "kPCA",classes)
plt.show();

# KMeans
print("KMeans")
kmeans = KMeans(n_clusters=10 ,random_state=0).fit(reduced_kpca)
km_nmi = normalized_mutual_info_score(kmeans.labels_ , classes)
print(len(kmeans.labels_))
print(len(classes))
```

```
plot_dr(reduced_kpca, "kmeans",kmeans.labels_)
print(f"KMeans NMI:{km_nmi:.4f}")

# Hierarchical clustering
clustering = AgglomerativeClustering(n_clusters=30, linkage="ward").
 ↪fit(reduced_kpca)
hc_nmi = normalized_mutual_info_score(clustering.labels_ , classes)
plot_dr(reduced_kpca, "hierarchical ward",clustering.labels_)
print(f"H clustering NMI:{hc_nmi:.4f}")

clustering = AgglomerativeClustering(n_clusters=30, linkage="complete").
 ↪fit(reduced_kpca)
hc_nmi = normalized_mutual_info_score(clustering.labels_ , classes)
plot_dr(reduced_kpca, "hierarchical complete",clustering.labels_)
print(f"H clustering NMI:{hc_nmi:.4f}")

clustering = AgglomerativeClustering(n_clusters=10, linkage="average").
 ↪fit(reduced_kpca)
hc_nmi = normalized_mutual_info_score(clustering.labels_ , classes)
plot_dr(reduced_kpca, "hierarchical average",clustering.labels_)
print(f"H clustering NMI:{hc_nmi:.4f}")

clustering = AgglomerativeClustering(n_clusters=10, linkage="single").
 ↪fit(reduced_kpca)
hc_nmi = normalized_mutual_info_score(clustering.labels_ , classes)
plot_dr(reduced_kpca, "hierarchical single",clustering.labels_)
print(f"H clustering NMI:{hc_nmi:.4f}")

# Apply Subkmeans
k = len(set(classes.tolist()))
print("SubKMeans")
nrkm = NrKmeans(n_clusters=[k,1])#, allow_larger_noise_space=False)
nrkm.fit(reduced_kpca, best_of_n_rounds=10, verbose=False)
print("Found Cluster Subspaces: ", nrkm.m)
subkm_nmi = normalized_mutual_info_score(nrkm.labels[0], classes)
print(f"Subkmeans NMI:{subkm_nmi:.4f}")
#n_d[i][dataset].append(subkm_nmi)
# Plot rotated space
V = nrkm.V
rotated = np.dot(reduced_kpca,V)
reduced_df = pd.DataFrame(rotated[:,0:2])
reduced_df["labels"] = nrkm.labels[0] #classes[true_nodes]
sns.pairplot(reduced_df, hue="labels", diag_kind="hist", palette=("tab10"))
plt.show();
```

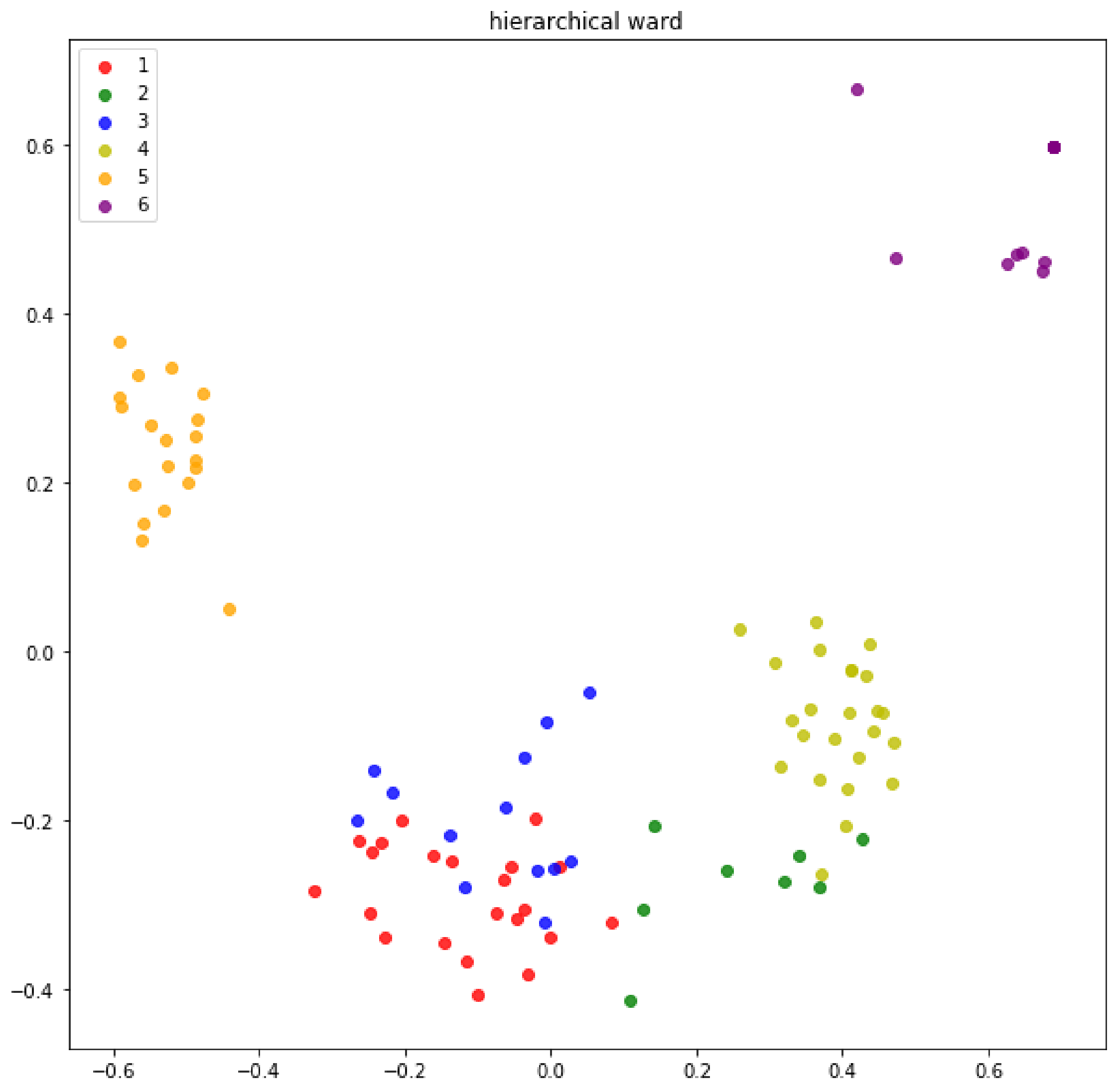
```
Dimensionality reduction: kPCA
```



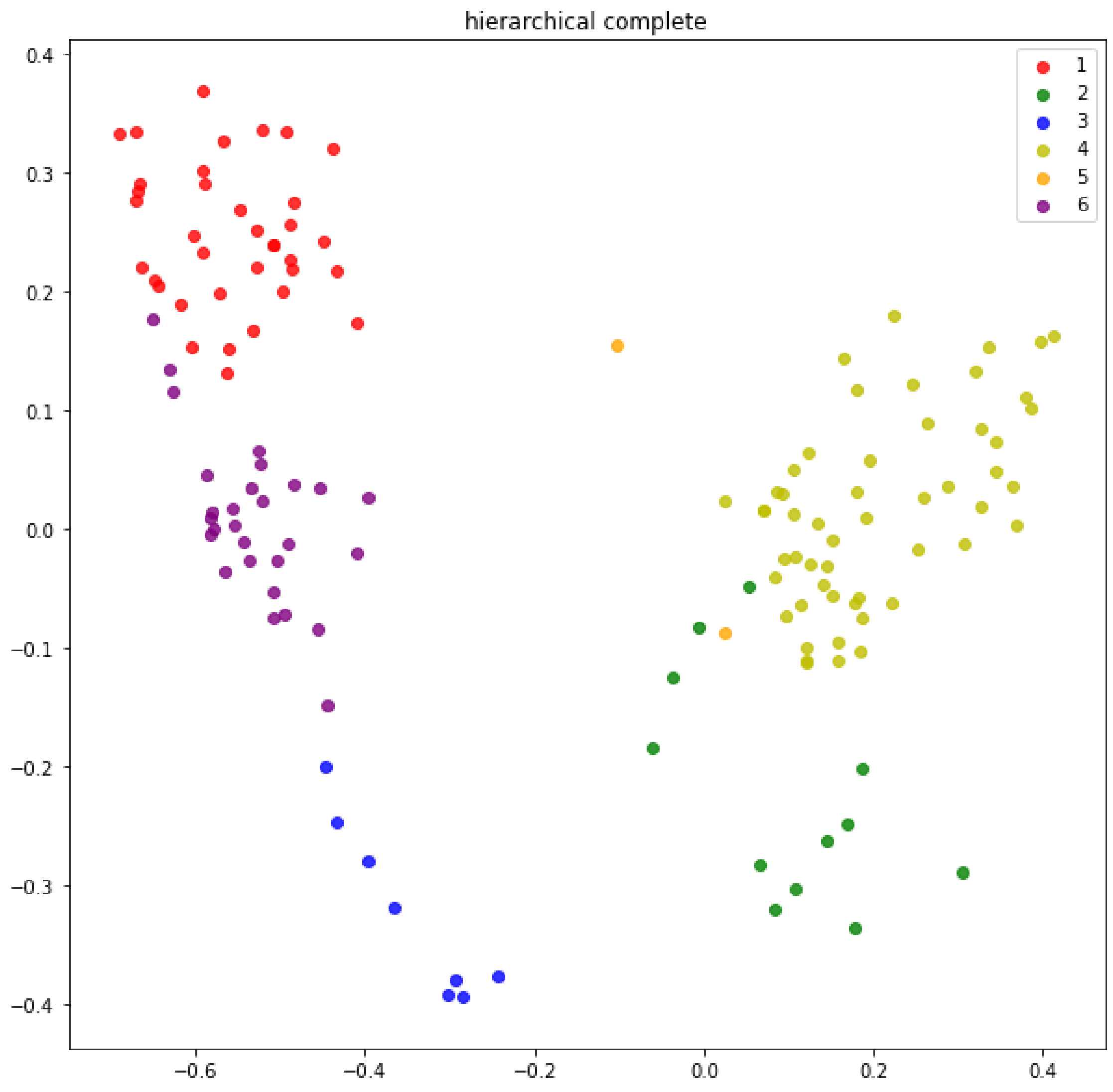
```
KMeans
488
488
```



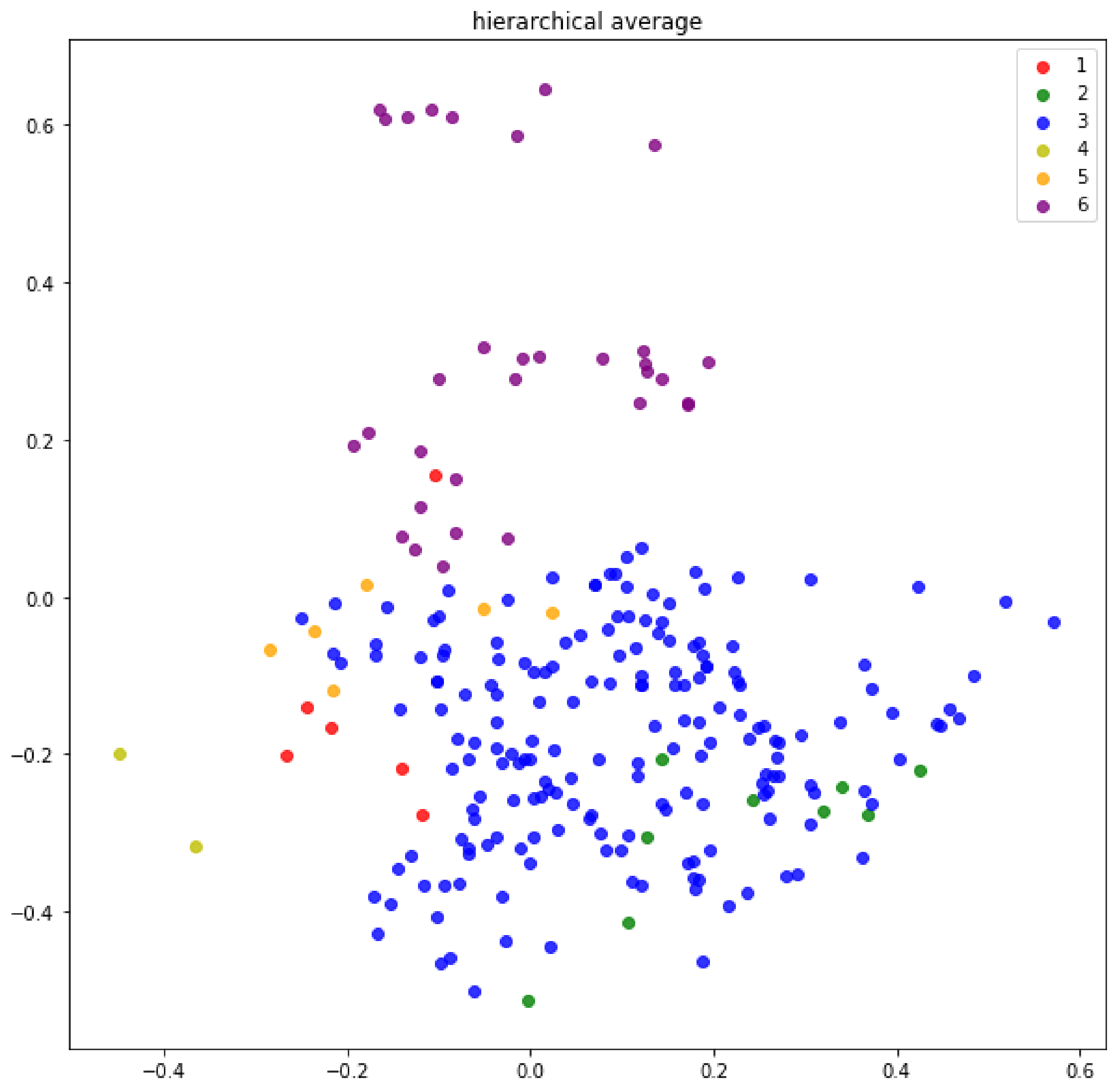
```
KMeans NMI:0.0828
```



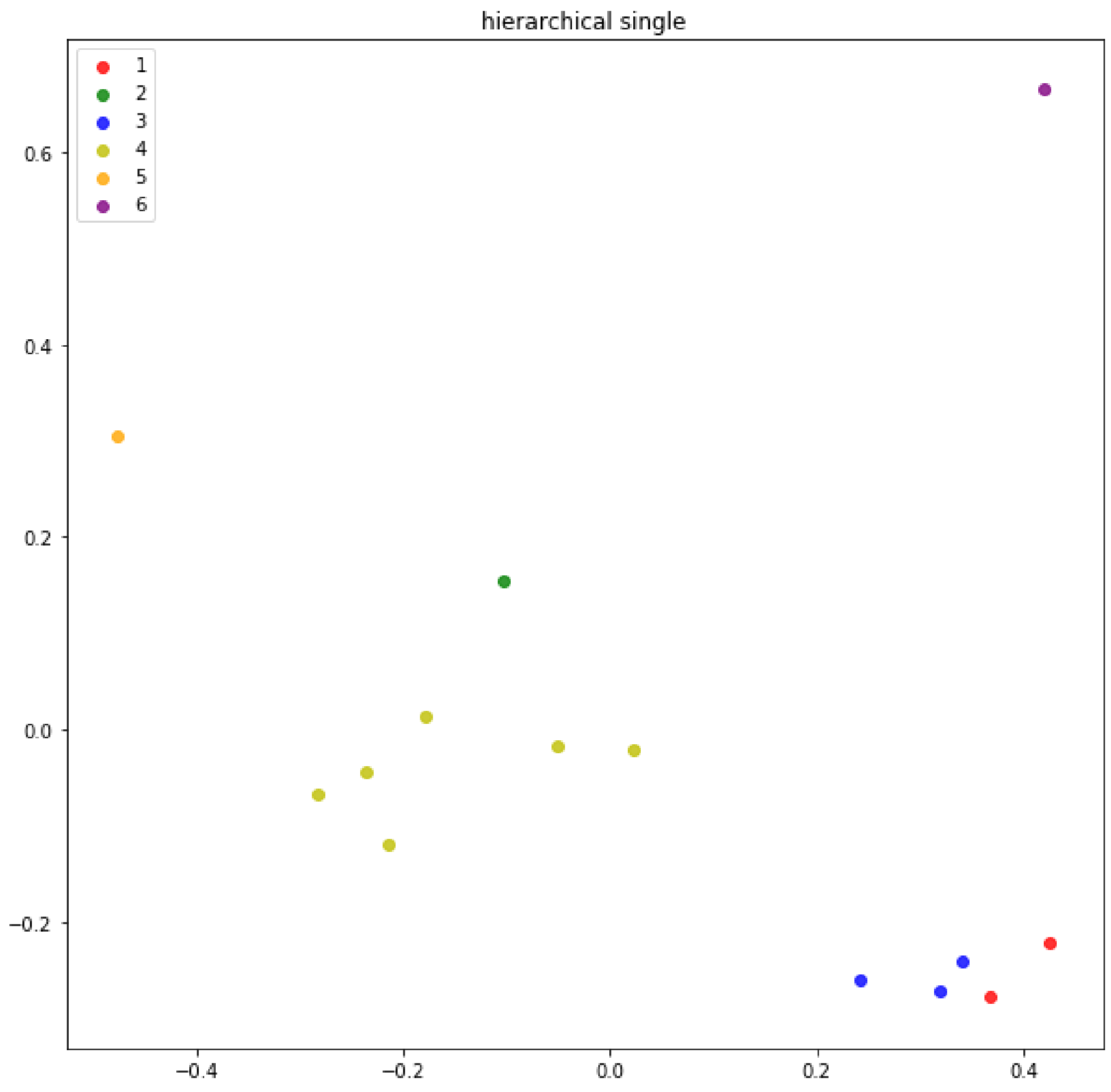
```
H clustering NMI:0.1710
```



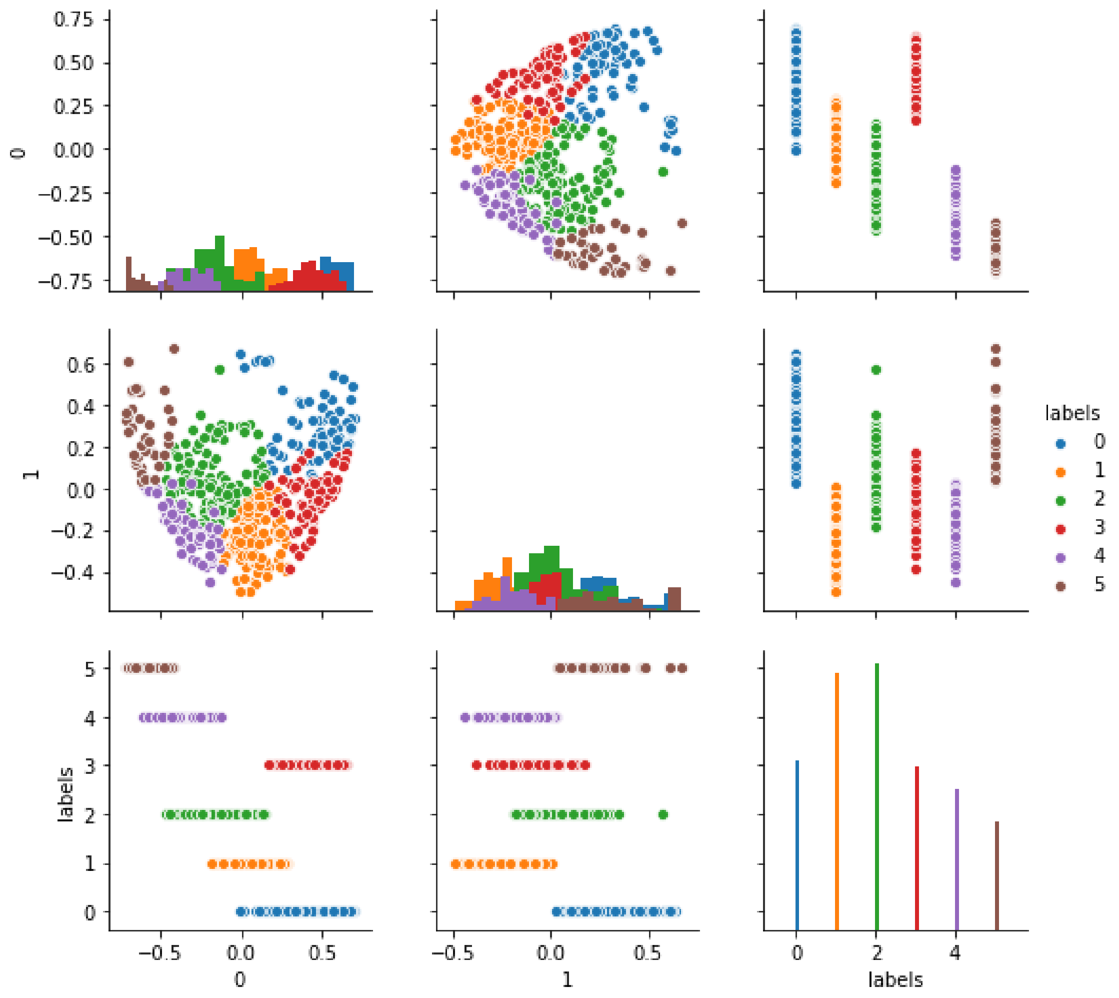
```
H clustering NMI:0.1576
```



```
H clustering NMI:0.0887
```



```
H clustering NMI:0.0551
SubKMeans
Found Cluster Subspaces:  [5, 45]
Subkmeans NMI:0.0717
```



6.1.3 SVM

[39]:
```
    # Split dataset into training set and test set
X_train, X_test, y_train, y_test = train_test_split(gram, classes, test_size=0.
↪2,random_state=109) # 70% training and 30% test
clf = svm.SVC(kernel='poly') #Create a svm Classifier, 'poly' kernel is the␣
↪best by far!
clf.fit(X_train, y_train) #Train the model using the training sets
y_pred = clf.predict(X_test) #Predict the response for test dataset
print("Graphlet accuracy:",metrics.accuracy_score(y_test, y_pred)) # Model␣
↪Accuracy: how often is the classifier correct?
```

```
Graphlet accuracy: 0.32653061224489793
```

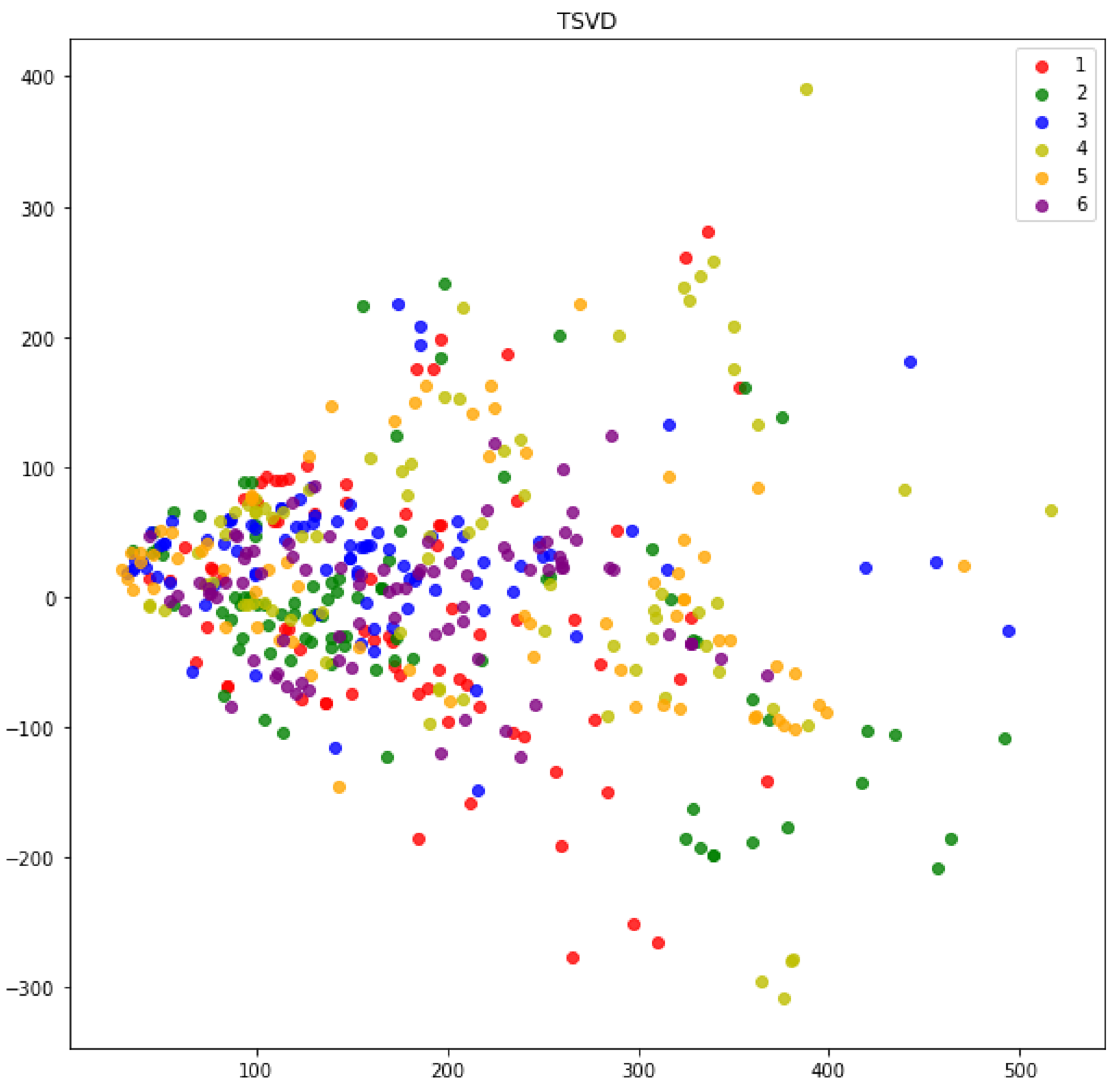
6.2 Shortest path kernel

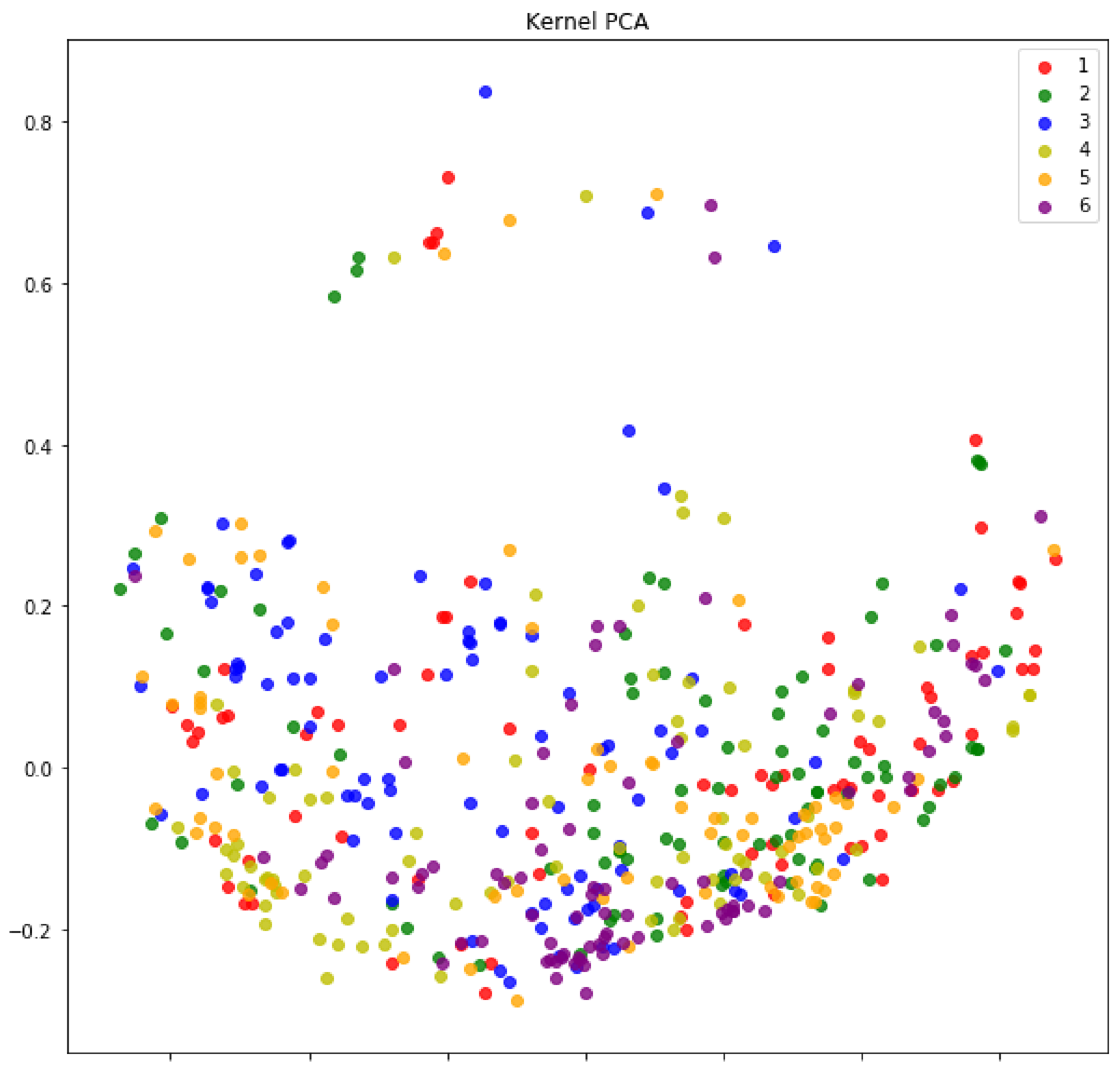
6.2.1 Dim red

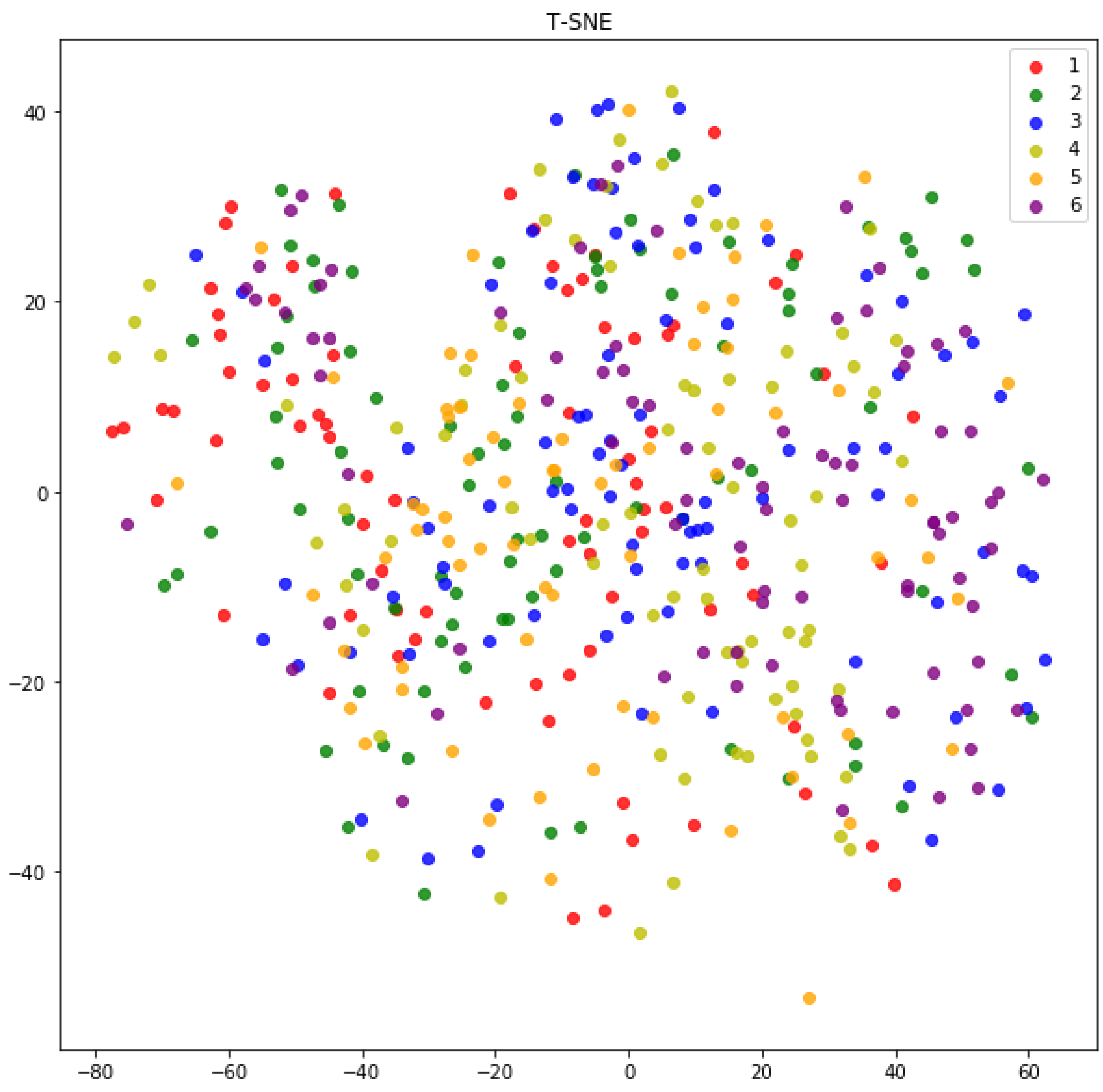
[40]:
```
use_edge_labels = False
for use_labels in [True]:
    if use_labels:
        base_path = os.path.join("kernels","node_labels")
        datasets = ["ENZYMES"]
    else:
        base_path = os.path.join("kernels","without_labels")
        datasets = ["ENZYMES"]
    print("Load from ", base_path)
    nmis_kpca = {}
    nmis_tsvd = {}
    nmis_tsne = {}
    nmis_spec = {}
    dataset= datasets[0]

    nmis_kpca[dataset] = []
    nmis_tsvd[dataset] = []
    nmis_tsne[dataset] = []
    nmis_spec[dataset] = []

    print("##################################")
    print("Dataset ", dataset)
    #print("Iteration ", iterations)
    print("##################################")

    #---------------------------------------------
    # Load graph representation from the kernel
    #---------------------------------------------
    #Gram Matrix for the Weisfeiler-Lehman subtree kernel
    gram = load_csv(os.path.join(base_path,f"{dataset}_gram_matrix_shortestpath.
 ↪csv"))
    #gram = load_csv(os.path.
 ↪join(base_path,f"{dataset}_gram_matrix_shortestpath.csv"))
    gram = aux.normalize_gram_matrix(gram)
    gram = gram[indices_true[:, None], indices_true]

    #Sparse Vectors for the Weisfeiler-Lehmann subtree kernel
    vec = load_sparse(os.path.join(base_path,f"{dataset}_vectors_shortestpath.
 ↪npz"))
    #vec = load_sparse(os.path.join(base_path,f"{dataset}_vectors_shortestpath.
 ↪npz"))
    vec = vec[indices_true, :]
    print(gram.shape, vec.shape)
```

```python
    #---------------------------------------------
    # Dimensionality Reduction
    #---------------------------------------------

    # SVD
    tsvd = TruncatedSVD(n_components=50)
    reduced_tsvd = tsvd.fit_transform(vec)
    plot_dr(reduced_tsvd, "TSVD", classes)

    # Kernel PCA
    kpca = KernelPCA(n_components=50, kernel="precomputed")
    reduced_kpca= kpca.fit_transform(gram)
    plot_dr(reduced_kpca, "Kernel PCA",classes)

    # T-SNE
    pca = TSNE(n_components=3)
    reduced_tnse =  pca.fit_transform(gram)
    plot_dr(reduced_tnse, "T-SNE",classes)

    k = len(set(classes.tolist()))
    print("n_clusters: ", k)
    d = {0:"TSVD",1:"KPCA", 2:"T-SNE"}
    n_d = {0:nmis_tsvd, 1:nmis_kpca, 2:nmis_tsne}
```

```
Load from  kernels\node_labels
##################################
Dataset  ENZYMES
##################################
(488, 488) (488, 25460)
```


TSVD
1
2
3
4
5
6
400
300
200
100
0
−100
−200
−300
100
200
300
400
500


Kernel PCA
1
2
3
4
5
6
0.8
0.6
0.4
0.2
0.0
−0.2
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6



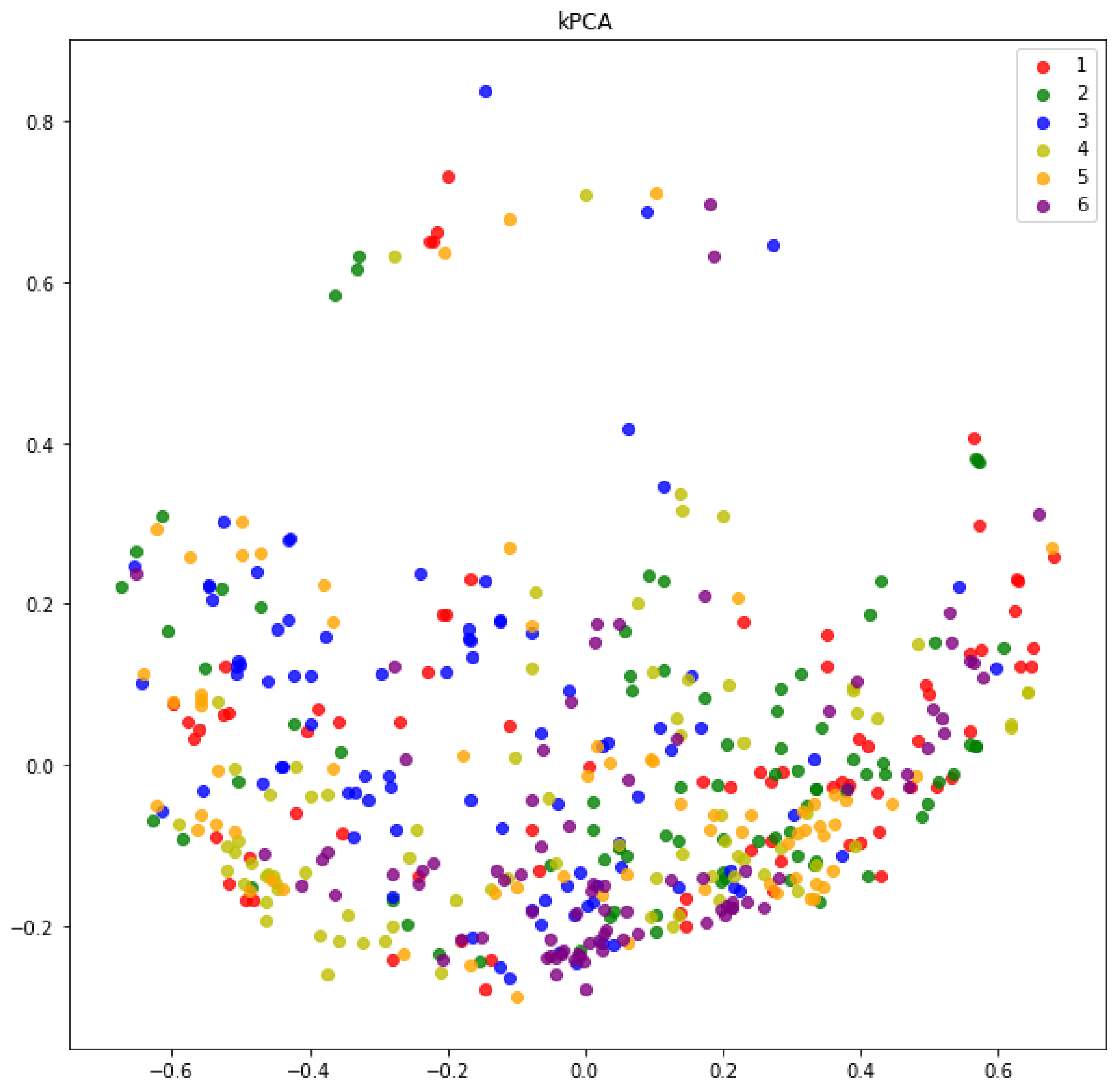
```
n_clusters:  6
```

6.2.2 Clustering

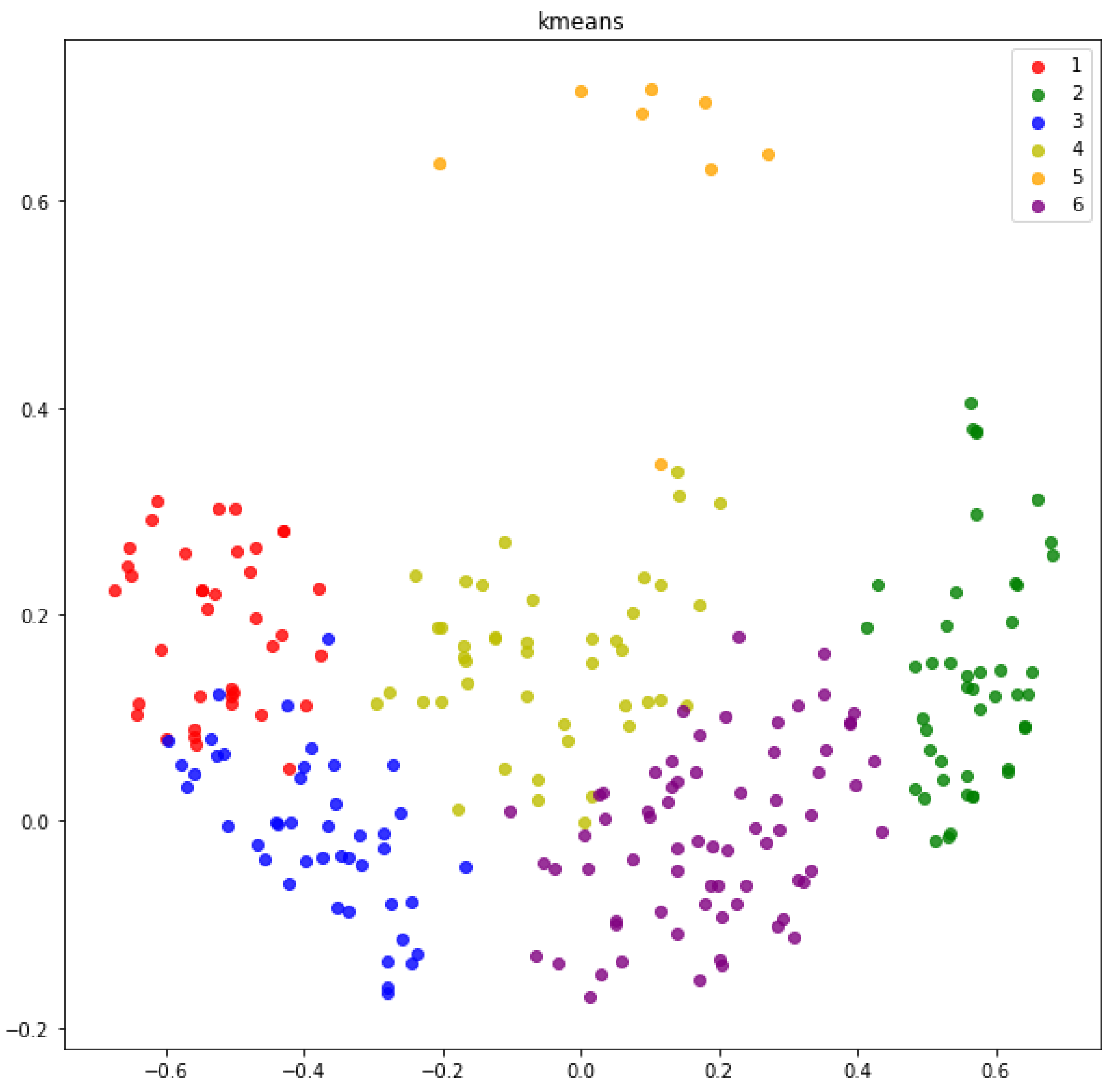
```
[41]: print("Dimensionality reduction: kPCA")
      plot_dr(reduced_kpca, "kPCA",classes)
      plt.show();

      # KMeans
      print("KMeans")
      kmeans = KMeans(n_clusters=10 ,random_state=0).fit(reduced_kpca)
      km_nmi = normalized_mutual_info_score(kmeans.labels_ , classes)
      print(len(kmeans.labels_))
      print(len(classes))
```

```
plot_dr(reduced_kpca, "kmeans",kmeans.labels_)
print(f"KMeans NMI:{km_nmi:.4f}")

# Hierarchical clustering
clustering = AgglomerativeClustering(n_clusters=30, linkage="ward").
 ↪fit(reduced_kpca)
hc_nmi = normalized_mutual_info_score(clustering.labels_ , classes)
plot_dr(reduced_kpca, "hierarchical ward",clustering.labels_)
print(f"H clustering NMI:{hc_nmi:.4f}")

clustering = AgglomerativeClustering(n_clusters=30, linkage="complete").
 ↪fit(reduced_kpca)
hc_nmi = normalized_mutual_info_score(clustering.labels_ , classes)
plot_dr(reduced_kpca, "hierarchical complete",clustering.labels_)
print(f"H clustering NMI:{hc_nmi:.4f}")

clustering = AgglomerativeClustering(n_clusters=10, linkage="average").
 ↪fit(reduced_kpca)
hc_nmi = normalized_mutual_info_score(clustering.labels_ , classes)
plot_dr(reduced_kpca, "hierarchical average",clustering.labels_)
print(f"H clustering NMI:{hc_nmi:.4f}")

clustering = AgglomerativeClustering(n_clusters=10, linkage="single").
 ↪fit(reduced_kpca)
hc_nmi = normalized_mutual_info_score(clustering.labels_ , classes)
plot_dr(reduced_kpca, "hierarchical single",clustering.labels_)
print(f"H clustering NMI:{hc_nmi:.4f}")

# Apply Subkmeans
k = len(set(classes.tolist()))
print("SubKMeans")
nrkm = NrKmeans(n_clusters=[k,1])#, allow_larger_noise_space=False)
nrkm.fit(reduced_kpca, best_of_n_rounds=10, verbose=False)
print("Found Cluster Subspaces: ", nrkm.m)
subkm_nmi = normalized_mutual_info_score(nrkm.labels[0], classes)
print(f"Subkmeans NMI:{subkm_nmi:.4f}")
#n_d[i][dataset].append(subkm_nmi)
# Plot rotated space
V = nrkm.V
rotated = np.dot(reduced_kpca,V)
reduced_df = pd.DataFrame(rotated[:,0:2])
reduced_df["labels"] = nrkm.labels[0] #classes[true_nodes]
sns.pairplot(reduced_df, hue="labels", diag_kind="hist", palette=("tab10"))
plt.show();
```

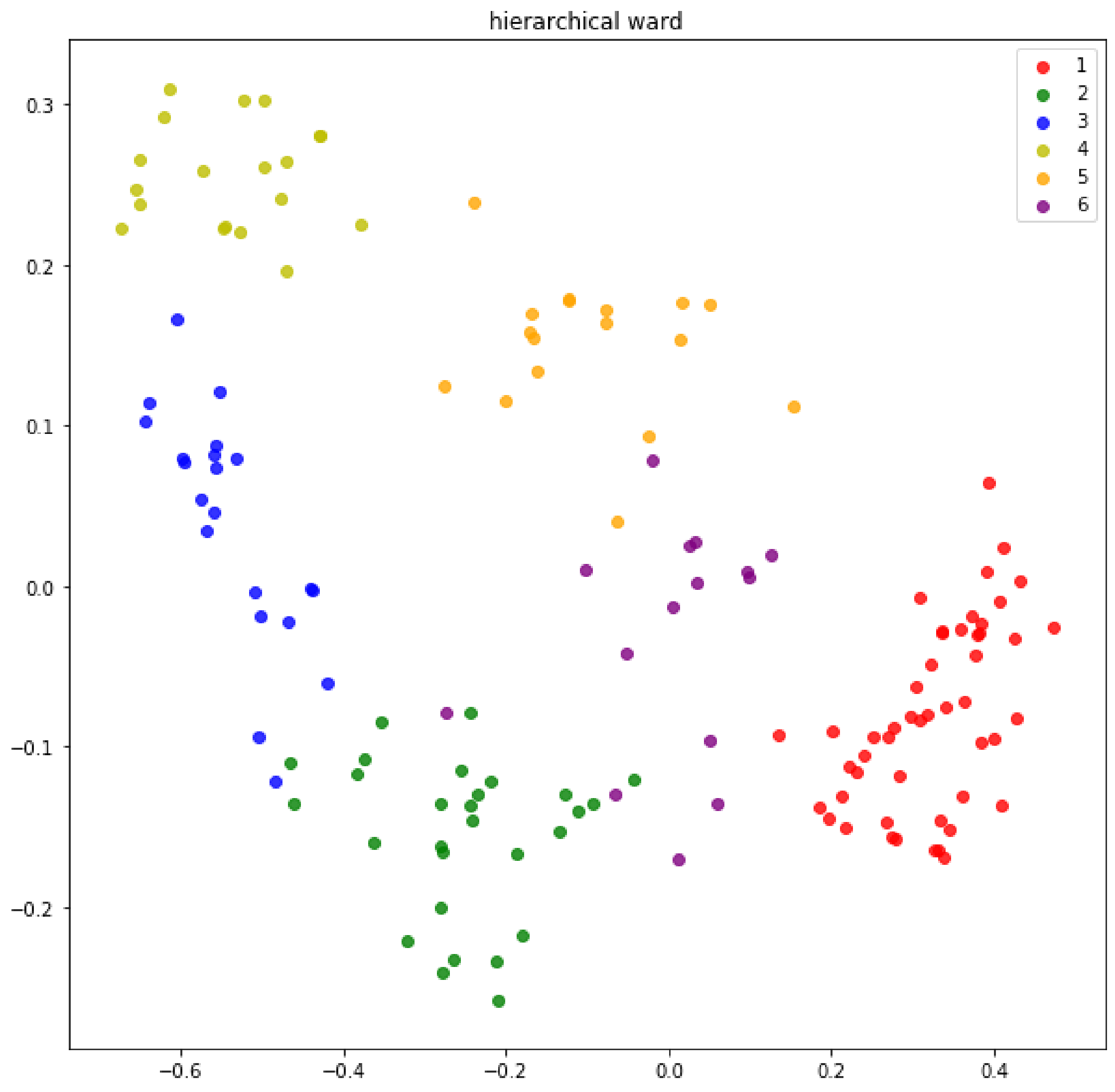
```
Dimensionality reduction: kPCA
```



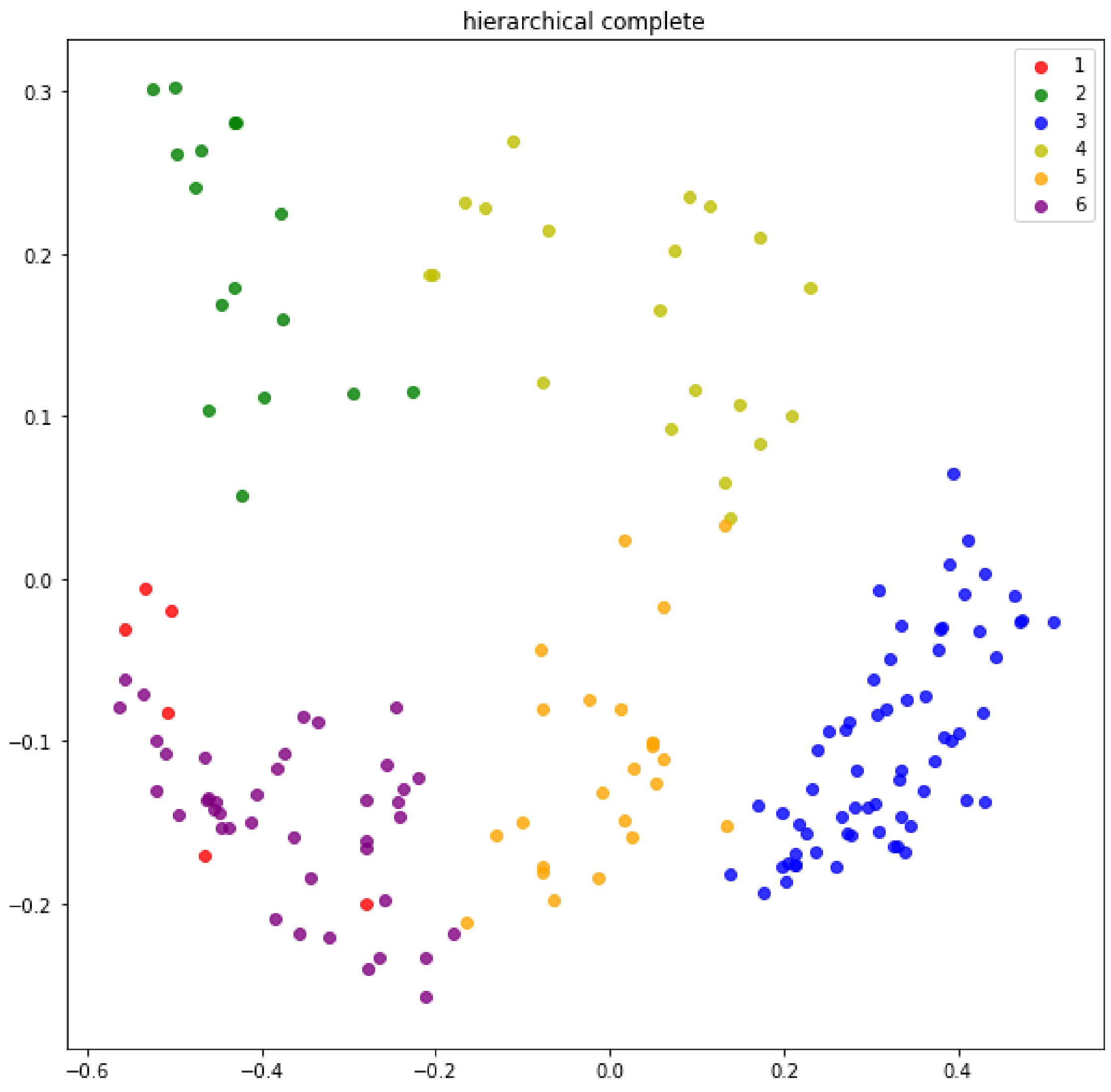
```
KMeans
488
488
```



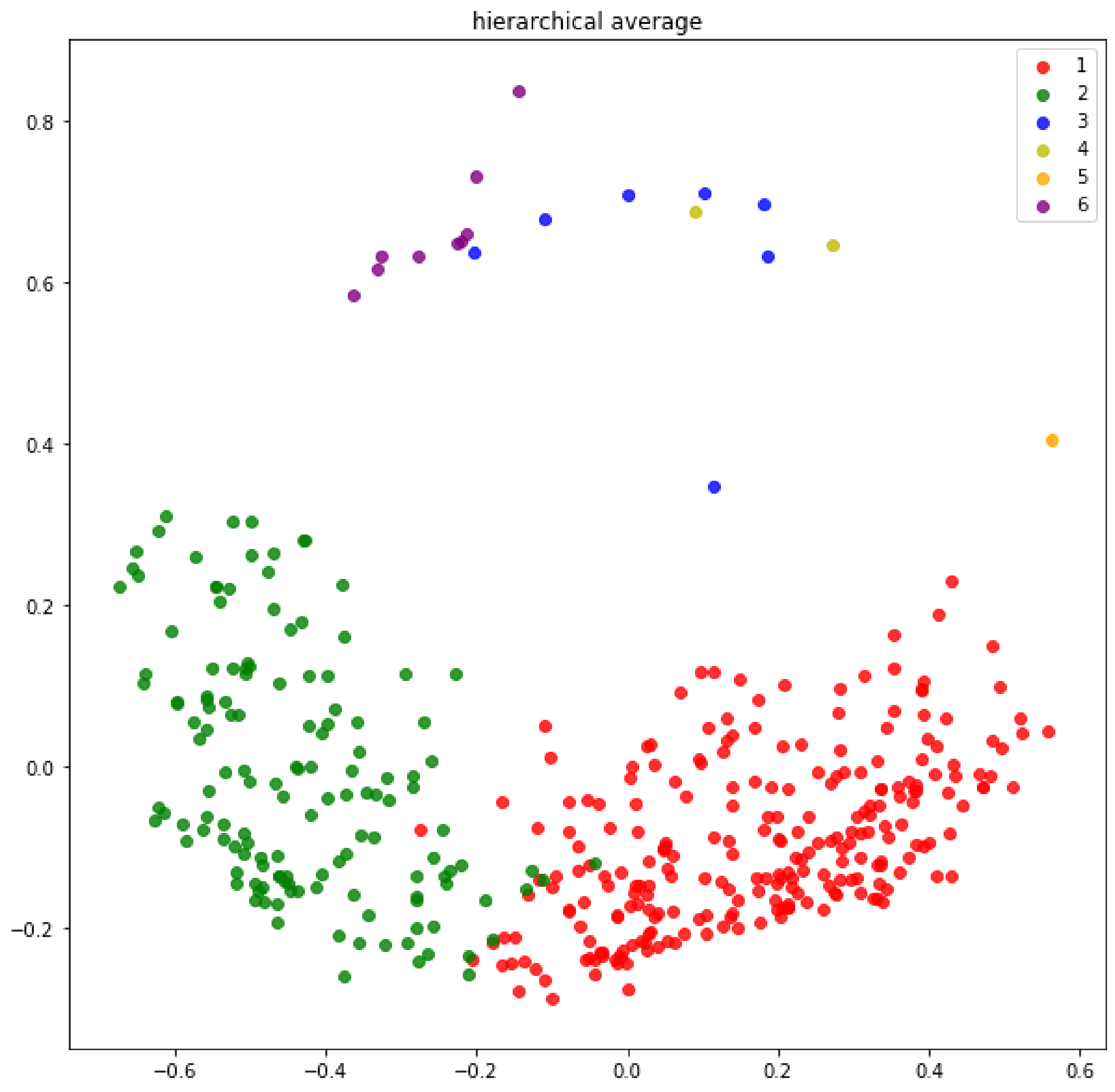
```
KMeans NMI:0.1091
```



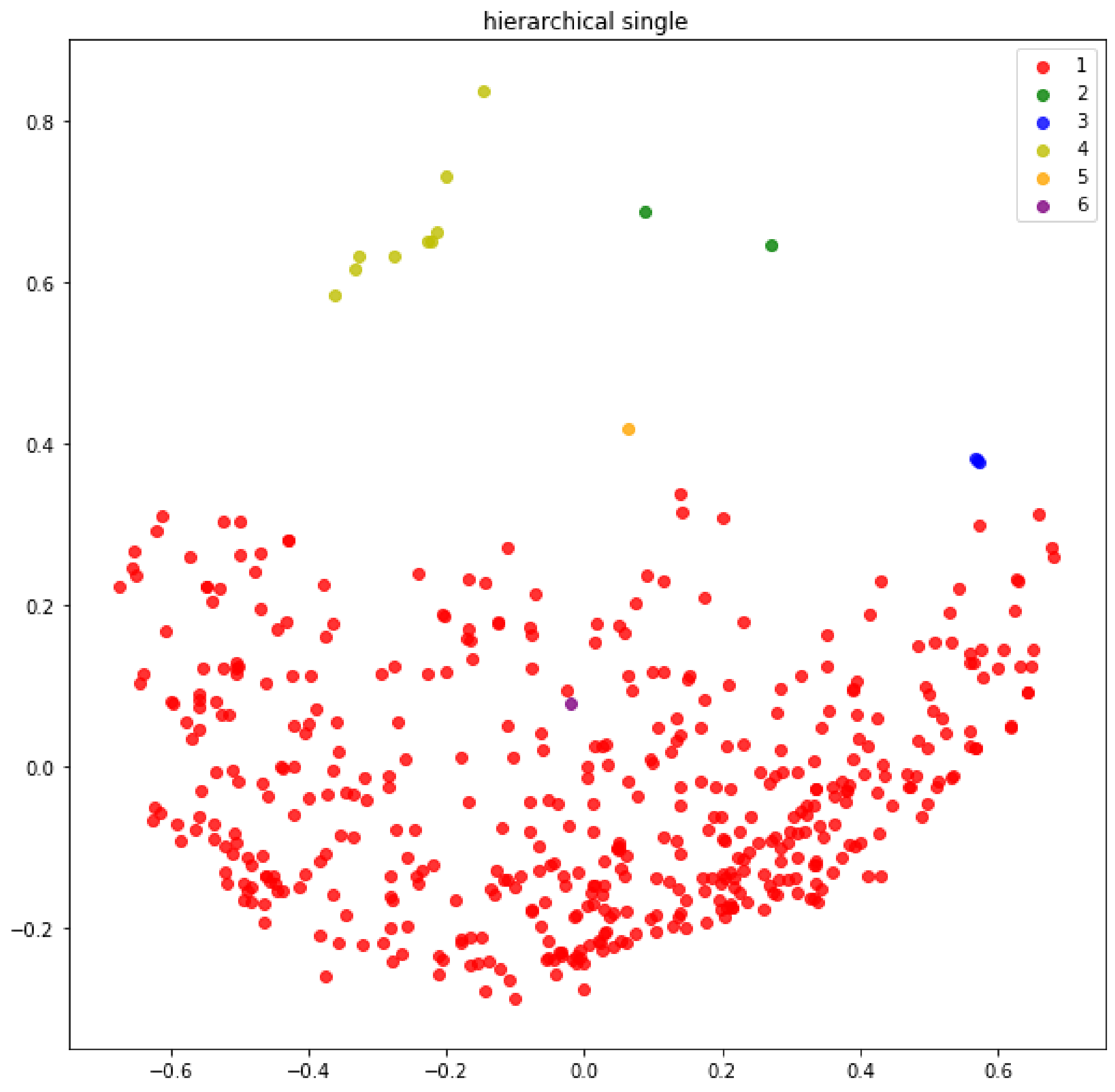
```
H clustering NMI:0.1866
```



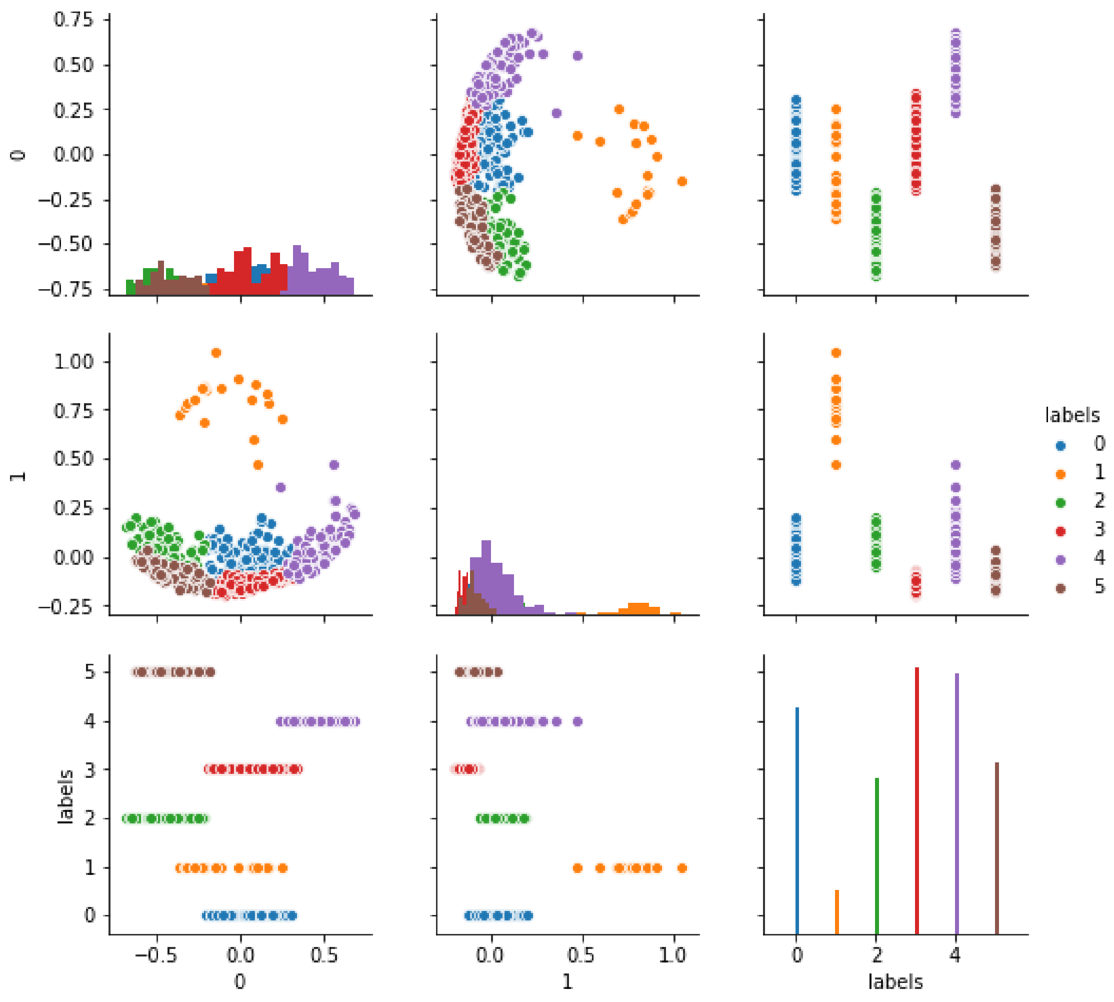
```
H clustering NMI:0.1601
```



```
H clustering NMI:0.0602
```



```
H clustering NMI:0.0508
SubKMeans
Found Cluster Subspaces:  [5, 45]
Subkmeans NMI:0.0754
```



6.2.3 SVM

```
[42]: # Split dataset into training set and test set
      X_train, X_test, y_train, y_test = train_test_split(gram, classes, test_size=0.
       ↪2,random_state=109) # 70% training and 30% test
      clf = svm.SVC(kernel='poly') #Create a svm Classifier, 'poly' kernel is the␣
       ↪best by far!
      clf.fit(X_train, y_train) #Train the model using the training sets
      y_pred = clf.predict(X_test) #Predict the response for test dataset
      print("Shortest path accuracy:",metrics.accuracy_score(y_test, y_pred)) # Model␣
       ↪Accuracy: how often is the classifier correct?
```

```
Shortest path accuracy: 0.4897959183673469
```

7 Conclusion

- UMAP vector representation is strongly driven by node labels (SSE elements), edge/node count
- Clusters do not represent the ground truth labels
- Clusters are formed based on different SSE composition, and structural differences e.g. degree distribution
- Node attributes play also an important role in EC classification which could be used for building better kernels