Cluster_metrics_graphs

May 16, 2021

[1]:
```
import numpy as np
import pandas as pd
from tdc.multi_pred import DTI
from rdkit import Chem
import torch
from sklearn.cluster import AgglomerativeClustering
from sklearn.cluster import KMeans
from sklearn.cluster import SpectralClustering
from sklearn.metrics import silhouette_samples, silhouette_score
import matplotlib.pyplot as plt
import matplotlib.cm as cm
from sklearn import metrics
import sklearn as sk
```

```
RDKit WARNING: [23:56:10] Enabling RDKit 2019.09.3 jupyter extensions
```

[2]:
```
# ============================================================================
# torch_data Loading
# ============================================================================
data = DTI(name = 'BindingDB_Kd')
bindingDB_data = data.get_data()[['Drug_ID','Drug']]

bindingDB_data = bindingDB_data.drop_duplicates().reset_index(drop=True)


bindingDB_data['Drug_vector'] = ''

for ind, drug in enumerate(bindingDB_data['Drug']):
    mol = Chem.MolFromSmiles(drug)
    fp = Chem.RDKFingerprint(mol)
    intmap = map(int, fp.ToBitString())
    bindingDB_data['Drug_vector'][ind] = np.array(list(intmap))

torch_data = torch.tensor(list(bindingDB_data['Drug_vector']))
```

```
Found local copy...
Loading...
Done!
```

[13]:
```
# ================================================================================
# Agglomerative
# ================================================================================

clusters={}
silhouette_avg={}
cluster_num_list = [i*10 for i in range(1,16)]

for n_cluster in cluster_num_list:
    clustering = AgglomerativeClustering(linkage='average',␣
 ↪n_clusters=n_cluster)
    clustering.fit(torch_data)
    clusters[n_cluster] = clustering.labels_
    silhouette_avg[n_cluster] = silhouette_score(torch_data, clustering.labels_)
```

[25]:
```
# ================================================================================
# Kmeans
# ================================================================================

clusters_kmeans={}
silhouette_avg_kmeans={}
cluster_num_list = [i*10 for i in range(1,16)]

for n_cluster in cluster_num_list:
    model = KMeans(n_clusters=n_cluster)
    model.fit(torch_data)
    clusters_kmeans[n_cluster] = model.labels_
    silhouette_avg_kmeans[n_cluster] = silhouette_score(torch_data, model.
 ↪labels_)
```

[26]:
```
# ================================================================================
# spectral
# ================================================================================

clusters_spectral={}
silhouette_avg_spectral={}
cluster_num_list = [i*10 for i in range(1,16)]
spectral_Data = torch_data
spectral_Data = sk.metrics.pairwise.pairwise_distances(spectral_Data,␣
 ↪metric='euclidean')    # converts the distance matrix in above step to a␣
 ↪similarity matrix
beta = 1.0
spectral_Data = np.exp(-beta * spectral_Data / spectral_Data.std())
```

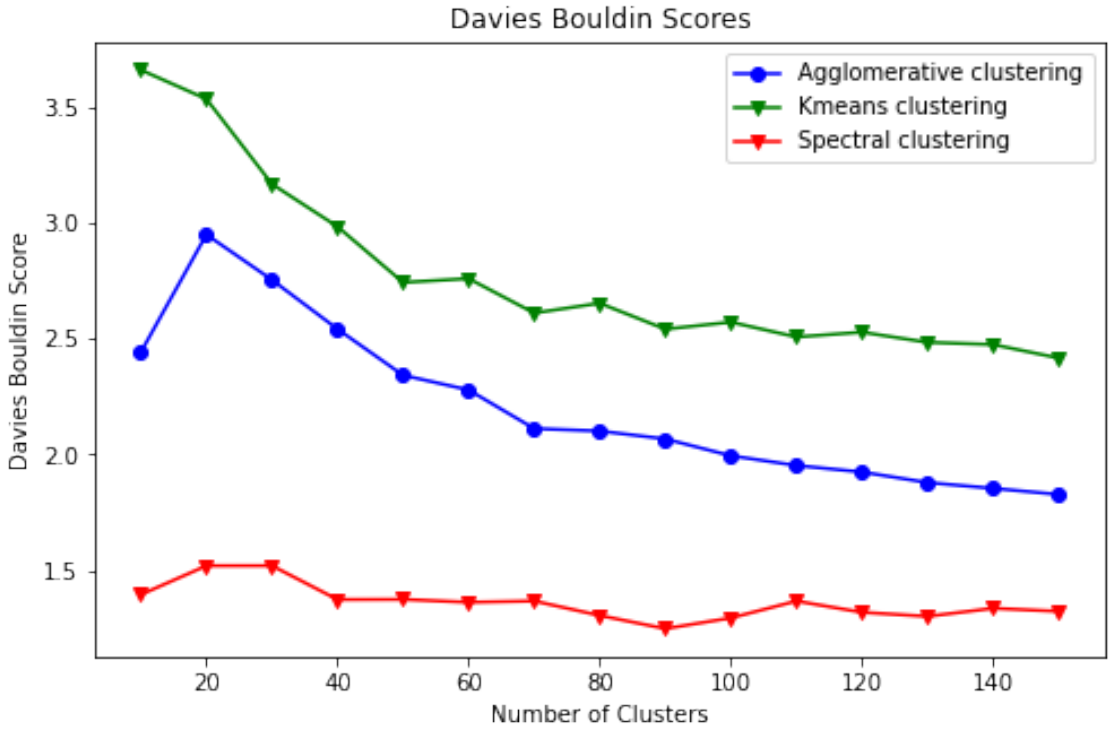
[27]:
```
for n_cluster in cluster_num_list:

    model = SpectralClustering(n_clusters=n_cluster, n_init=1, n_neighbors=5,␣
 ↪eigen_tol=0.000001,
                                                                              ␣
 ↪n_jobs=-1,random_state=46,eigen_solver='amg',affinity='precomputed')
    model.fit(spectral_Data)
    clusters_spectral[n_cluster] = model.labels_
    silhouette_avg_spectral[n_cluster] = silhouette_score(spectral_Data, model.
 ↪labels_)
```

[28]:
```
# ============================================================================
# Plots
# ============================================================================

n_clusters = 50

X = torch_data
y = clusters[n_clusters]
```

1 Davies Bouldin

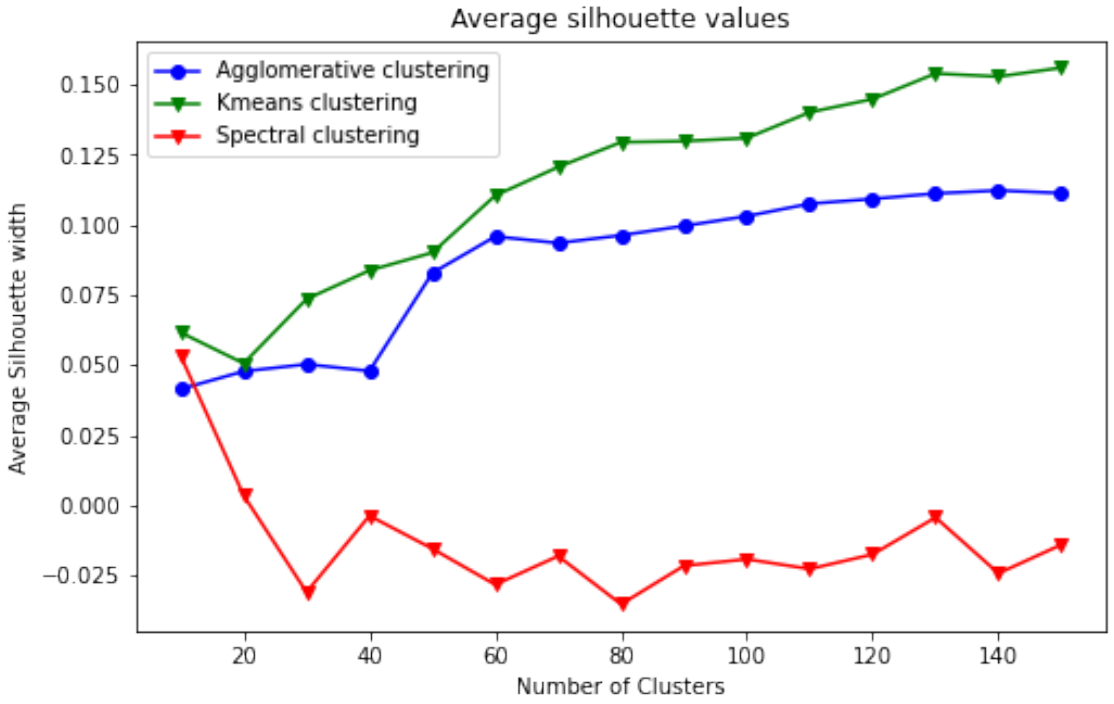
[37]:
```
# ============================================================================
# Davies Bouldin
# ============================================================================

from sklearn.metrics import davies_bouldin_score

davies_bouldin_mapping_agg={}
davies_bouldin_mapping_kmeans={}
davies_bouldin_mapping_spectral={}

for n_cluster in cluster_num_list:
    davies_bouldin_mapping_spectral[n_cluster] = davies_bouldin_score(X,␣
 ↪clusters_spectral[n_cluster])

for n_cluster in cluster_num_list:
    davies_bouldin_mapping_agg[n_cluster] = davies_bouldin_score(X,␣
 ↪clusters[n_cluster])

for n_cluster in cluster_num_list:
    davies_bouldin_mapping_kmeans[n_cluster] = davies_bouldin_score(X,␣
 ↪clusters_kmeans[n_cluster])

plt.figure(figsize=(8,5))
plt.xlabel('Number of Clusters')
```

```
plt.ylabel('Davies Bouldin Score')
plt.title('Davies Bouldin Scores')
plt.plot(cluster_num_list, list(davies_bouldin_mapping_agg.
 ↪values()),'bo-',label="Agglomerative clustering" )
plt.plot(cluster_num_list, list(davies_bouldin_mapping_kmeans.
 ↪values()),'gv-',label="Kmeans clustering")
plt.plot(cluster_num_list, list(davies_bouldin_mapping_spectral.
 ↪values()),'rv-',label='Spectral clustering')
plt.legend(loc="upper right")
plt.show()
```



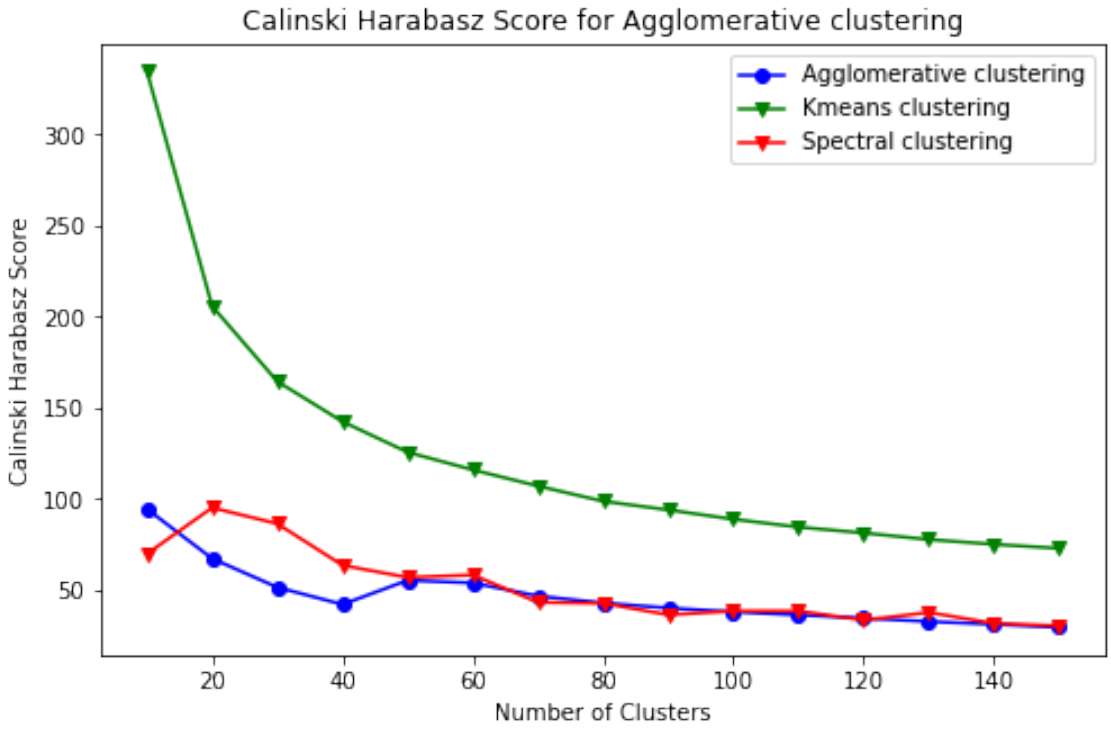
[39]:
```
# ============================================================================
# silhouette
# ============================================================================

plt.figure(figsize=(8,5))
plt.xlabel('Number of Clusters')
plt.ylabel('Average Silhouette width')
plt.title('Average silhouette values')
plt.plot(cluster_num_list, list(silhouette_avg.
 ↪values()),'bo-',label="Agglomerative clustering")
```

```
plt.plot(cluster_num_list, list(silhouette_avg_kmeans.
 ↪values()),'gv-',label="Kmeans clustering")
plt.plot(cluster_num_list, list(silhouette_avg_spectral.
 ↪values()),'rv-',label='Spectral clustering')
plt.legend(loc="upper left")
plt.show()
```



[40]:
```
# ============================================================================
# Calinski Harabasz
# ============================================================================

calinski_harabasz_mapping={}

for n_cluster in cluster_num_list:
    calinski_harabasz_mapping[n_cluster] = metrics.calinski_harabasz_score(X,␣
 ↪clusters[n_cluster])

calinski_harabasz_mapping_spectral={}

for n_cluster in cluster_num_list:
    calinski_harabasz_mapping_spectral[n_cluster] = metrics.
 ↪calinski_harabasz_score(X, clusters_spectral[n_cluster])
```

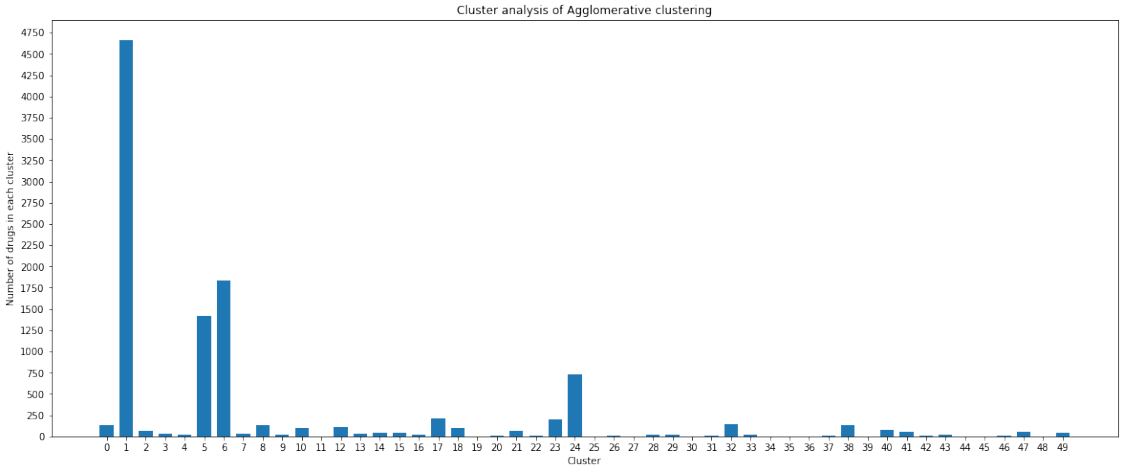
```
calinski_harabasz_mapping_kmeans={}

for n_cluster in cluster_num_list:
    calinski_harabasz_mapping_kmeans[n_cluster] = metrics.
 ↪calinski_harabasz_score(X, clusters_kmeans[n_cluster])

plt.figure(figsize=(8,5))
plt.xlabel('Number of Clusters')
plt.ylabel('Calinski Harabasz Score')
plt.title('Calinski Harabasz Score for Agglomerative clustering')
plt.plot(cluster_num_list, list(calinski_harabasz_mapping.
 ↪values()),'bo-',label="Agglomerative clustering")
plt.plot(cluster_num_list, list(calinski_harabasz_mapping_kmeans.
 ↪values()),'gv-',label="Kmeans clustering")
plt.plot(cluster_num_list, list(calinski_harabasz_mapping_spectral.
 ↪values()),'rv-',label='Spectral clustering')
plt.legend(loc="upper right")
plt.show()
```



2 agglomerative bar graph

[41]:
```
# ================================================================================
# cluster sizes
# ================================================================================


bindingDB_data['Cluster'] = clusters[n_clusters]
by_clusters = bindingDB_data.groupby(['Cluster'])

cluster_count = bindingDB_data.groupby(['Cluster'])['Drug'].count()
cluster_count_mapping = {k:v for k,v in enumerate(cluster_count)}

fig = plt.subplots(figsize=(20,8))

plt.bar(range(len(cluster_count_mapping)), cluster_count_mapping.values(),␣
 ↪align='center', width=0.7)
plt.xlabel('Cluster')
plt.xticks(np.arange(n_clusters))
plt.yticks(np.arange(0, max(cluster_count_mapping.values()) + 100, step=250))
plt.ylabel('Number of drugs in each cluster')
plt.title('Cluster analysis of Agglomerative clustering')
```

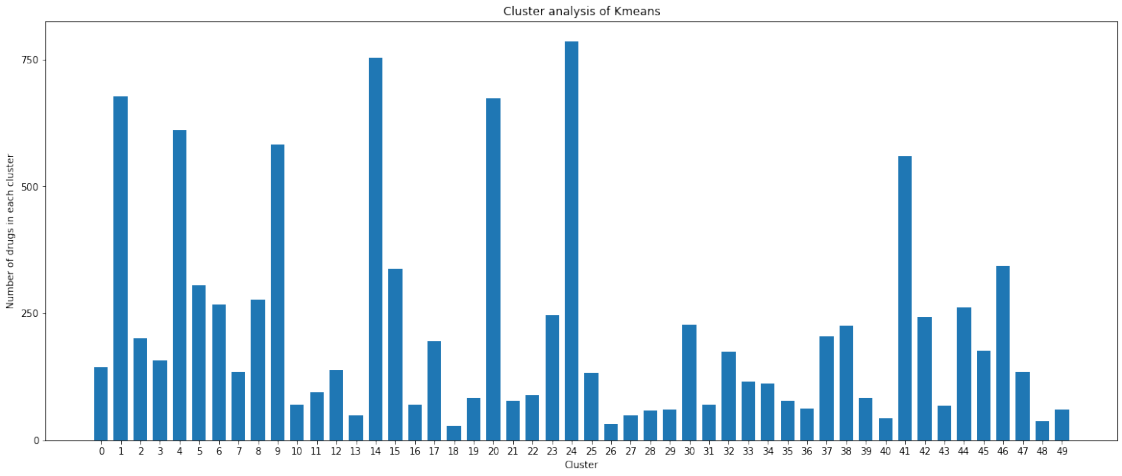
[41]:
```
Text(0.5, 1.0, 'Cluster analysis of Agglomerative clustering')
```



3 Kmeans bar graph

[42]:
```
bindingDB_data['Cluster'] = clusters_kmeans[n_clusters]
kmeans_count = bindingDB_data.groupby(['Cluster'])['Drug'].count()
kmeans_count_mapping = {k:v for k,v in enumerate(kmeans_count)}

fig = plt.subplots(figsize=(20,8))

plt.bar(range(len(kmeans_count_mapping)), kmeans_count_mapping.values(),␣
↪align='center', width=0.7)
plt.xlabel('Cluster')
plt.xticks(np.arange(n_clusters))
plt.yticks(np.arange(0, max(kmeans_count_mapping.values()) + 100, step=250))
plt.ylabel('Number of drugs in each cluster')
plt.title('Cluster analysis of Kmeans')
```

[42]:
```
Text(0.5, 1.0, 'Cluster analysis of Kmeans')
```

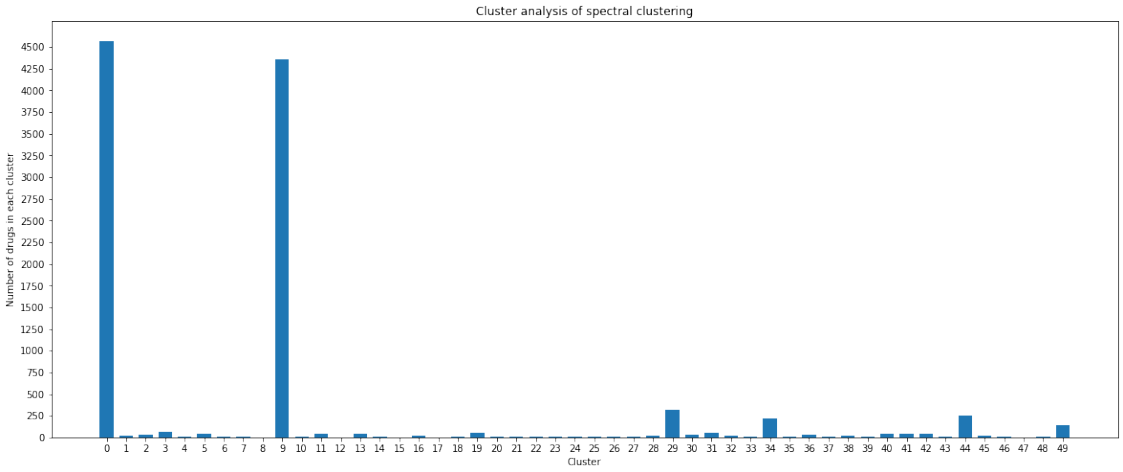


4 spectral bar graph

[43]:
```
bindingDB_data['Cluster'] = clusters_spectral[n_clusters]
spectral_count = bindingDB_data.groupby(['Cluster'])['Drug'].count()
spectral_count_mapping = {k:v for k,v in enumerate(spectral_count)}

fig = plt.subplots(figsize=(20,8))

plt.bar(range(len(spectral_count_mapping)), spectral_count_mapping.values(),␣
↪align='center', width=0.7)
plt.xlabel('Cluster')
plt.xticks(np.arange(n_clusters))
```

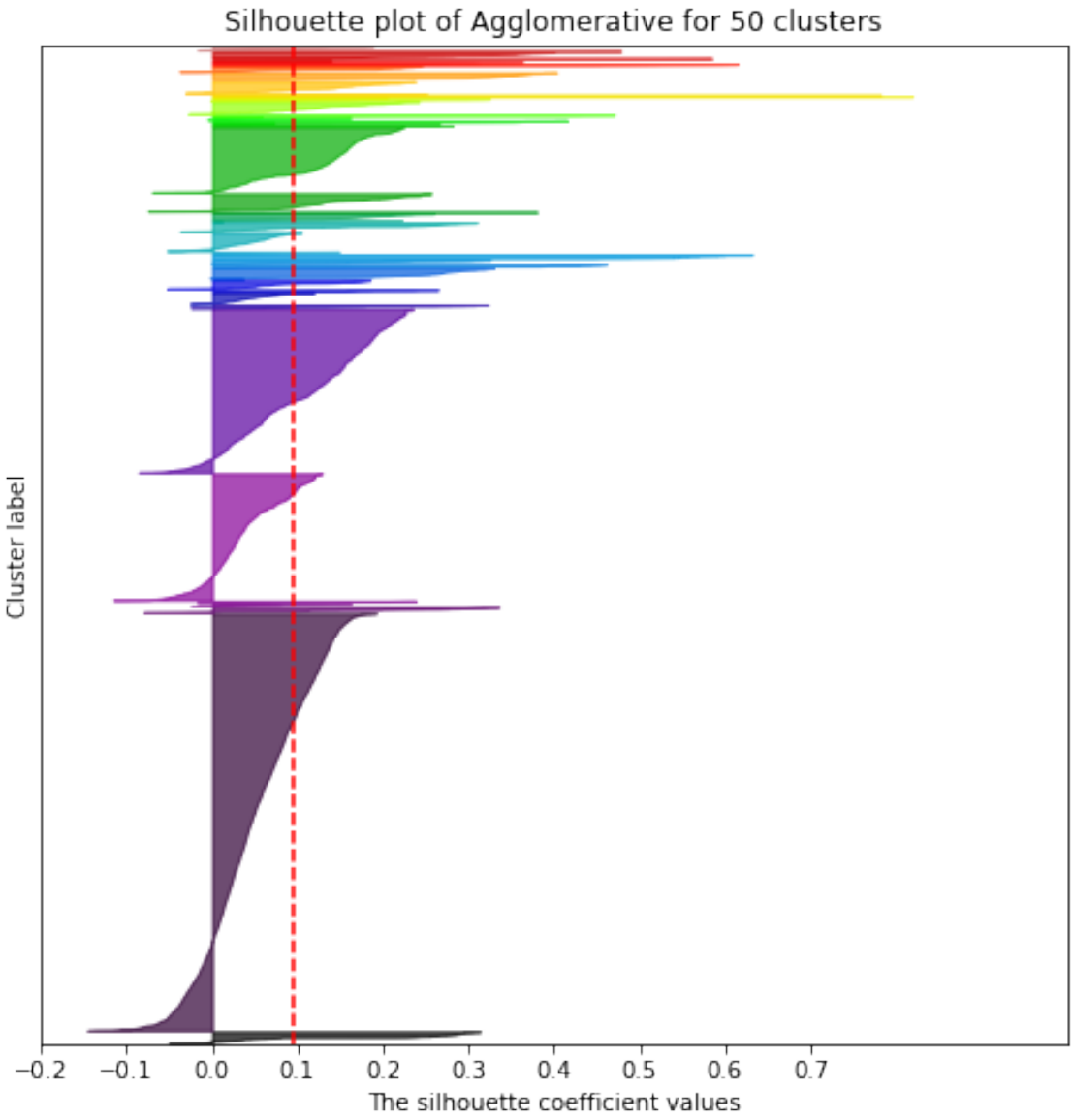
```
plt.yticks(np.arange(0, max(spectral_count_mapping.values()) + 100, step=250))
plt.ylabel('Number of drugs in each cluster')
plt.title('Cluster analysis of spectral clustering')
```

[43]: Text(0.5, 1.0, 'Cluster analysis of spectral clustering')



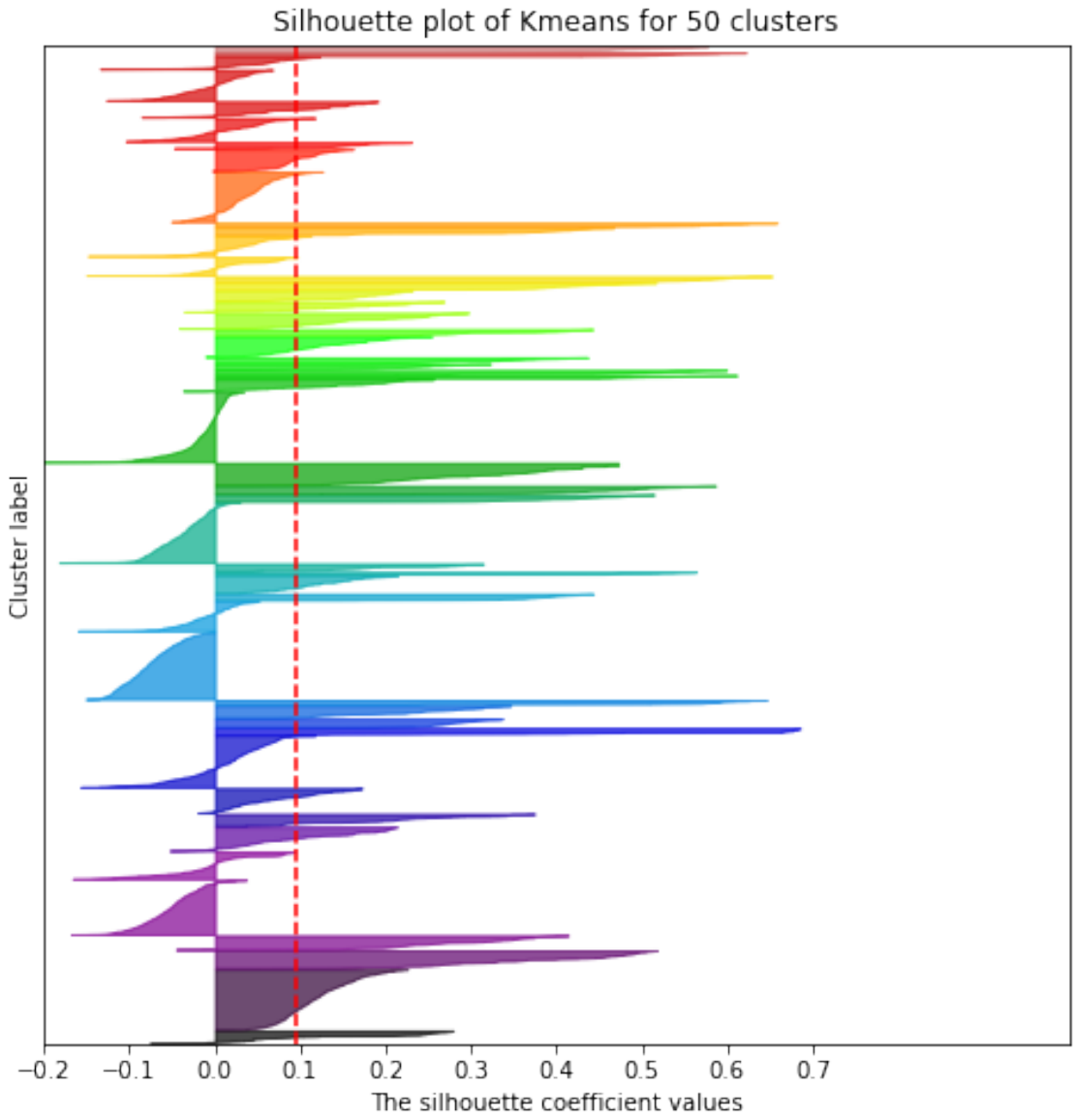
[44]:
```
X = torch_data
y = clusters[n_clusters]
sample_silhouette_values = silhouette_samples(X, y)

fig, ax1 = plt.subplots(figsize=(8,8))

ax1.set_xlim([-0.1, 1])
ax1.set_ylim([0, len(X) + (n_clusters + 1) * 10])
y_lower = 10

for i in range(n_clusters):
    ith_cluster_silhouette_values = \
        sample_silhouette_values[y == i]

    ith_cluster_silhouette_values.sort()

    size_cluster_i = ith_cluster_silhouette_values.shape[0]
    y_upper = y_lower + size_cluster_i

    color = cm.nipy_spectral(float(i) / n_clusters)
    ax1.fill_betweenx(np.arange(y_lower, y_upper),
                      0, ith_cluster_silhouette_values,
                      facecolor=color, edgecolor=color, alpha=0.7)
    #ax1.text(-0.05, y_lower + 0.5 * size_cluster_i, str(i))
    y_lower = y_upper + 10  # 10 for the 0 samples
```

```
ax1.set_title("Silhouette plot of Agglomerative for " + str(n_clusters) + '␣
↪clusters')
ax1.set_xlabel("The silhouette coefficient values")
ax1.set_ylabel("Cluster label")
ax1.axvline(x=silhouette_avg[60], color="red", linestyle="--")

ax1.set_yticks([])  # Clear the yaxis labels / ticks
ax1.set_xticks([-0.2, -0.1, 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6,0.7])

cluster_33_torch_data = bindingDB_data[bindingDB_data['Cluster'] == 33]
```



[45]:
```
bindingDB_data['Cluster'] = clusters_kmeans[n_clusters]

X = torch_data
y = clusters_kmeans[n_clusters]
sample_silhouette_values = silhouette_samples(X, y)

fig, ax1 = plt.subplots(figsize=(8,8))

ax1.set_xlim([-0.1, 1])
ax1.set_ylim([0, len(X) + (n_clusters + 1) * 10])
y_lower = 10

for i in range(n_clusters):
    ith_cluster_silhouette_values = \
        sample_silhouette_values[y == i]

    ith_cluster_silhouette_values.sort()

    size_cluster_i = ith_cluster_silhouette_values.shape[0]
    y_upper = y_lower + size_cluster_i

    color = cm.nipy_spectral(float(i) / n_clusters)
    ax1.fill_betweenx(np.arange(y_lower, y_upper),
                      0, ith_cluster_silhouette_values,
                      facecolor=color, edgecolor=color, alpha=0.7)
    #ax1.text(-0.05, y_lower + 0.5 * size_cluster_i, str(i))
    y_lower = y_upper + 10  # 10 for the 0 samples

ax1.set_title("Silhouette plot of Kmeans for " + str(n_clusters) + ' clusters')
ax1.set_xlabel("The silhouette coefficient values")
ax1.set_ylabel("Cluster label")
ax1.axvline(x=silhouette_avg[60], color="red", linestyle="--")

ax1.set_yticks([])  # Clear the yaxis labels / ticks
ax1.set_xticks([-0.2, -0.1, 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6,0.7])
```

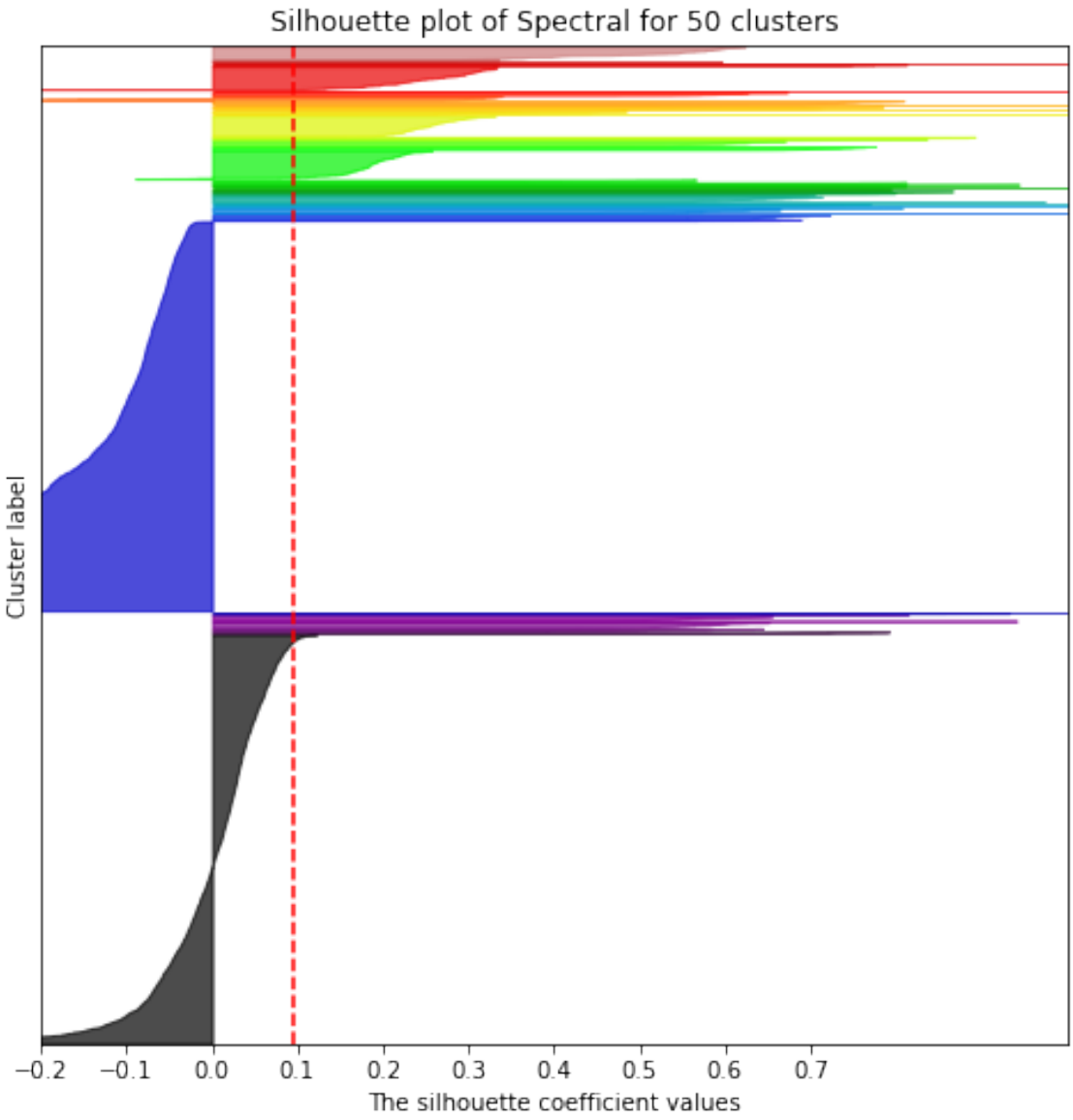
[45]:
```
[<matplotlib.axis.XTick at 0x13ff019a0>,
 <matplotlib.axis.XTick at 0x13ff01970>,
 <matplotlib.axis.XTick at 0x13fef84f0>,
 <matplotlib.axis.XTick at 0x14009f100>,
 <matplotlib.axis.XTick at 0x14009f610>,
 <matplotlib.axis.XTick at 0x14009fb20>,
 <matplotlib.axis.XTick at 0x1400ab070>,
 <matplotlib.axis.XTick at 0x1400ab580>,
 <matplotlib.axis.XTick at 0x1400aba90>,
 <matplotlib.axis.XTick at 0x1400abfa0>]
```



[46]:
```
bindingDB_data['Cluster'] = clusters_spectral[n_clusters]

X = torch_data
y = clusters_spectral[n_clusters]
sample_silhouette_values = silhouette_samples(X, y)

fig, ax1 = plt.subplots(figsize=(8,8))

ax1.set_xlim([-0.1, 1])
ax1.set_ylim([0, len(X) + (n_clusters + 1) * 10])
y_lower = 10
```

```
for i in range(n_clusters):
    ith_cluster_silhouette_values = \
        sample_silhouette_values[y == i]

    ith_cluster_silhouette_values.sort()

    size_cluster_i = ith_cluster_silhouette_values.shape[0]
    y_upper = y_lower + size_cluster_i

    color = cm.nipy_spectral(float(i) / n_clusters)
    ax1.fill_betweenx(np.arange(y_lower, y_upper),
                      0, ith_cluster_silhouette_values,
                      facecolor=color, edgecolor=color, alpha=0.7)
    #ax1.text(-0.05, y_lower + 0.5 * size_cluster_i, str(i))
    y_lower = y_upper + 10  # 10 for the 0 samples

ax1.set_title("Silhouette plot of Spectral for " + str(n_clusters) + '␣
 ↪clusters')
ax1.set_xlabel("The silhouette coefficient values")
ax1.set_ylabel("Cluster label")
ax1.axvline(x=silhouette_avg[60], color="red", linestyle="--")

ax1.set_yticks([])  # Clear the yaxis labels / ticks
ax1.set_xticks([-0.2, -0.1, 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6,0.7])
```

[46]:
```
[<matplotlib.axis.XTick at 0x1400e2d90>,
 <matplotlib.axis.XTick at 0x1400e2d60>,
 <matplotlib.axis.XTick at 0x1400dc9a0>,
 <matplotlib.axis.XTick at 0x13eca4ac0>,
 <matplotlib.axis.XTick at 0x13eca4fd0>,
 <matplotlib.axis.XTick at 0x13eca9520>,
 <matplotlib.axis.XTick at 0x13eca9a30>,
 <matplotlib.axis.XTick at 0x13eca9f40>,
 <matplotlib.axis.XTick at 0x13ecac490>,
 <matplotlib.axis.XTick at 0x13ecac9a0>]
```


Silhouette plot of Spectral for 50 clusters
Cluster label
−0.2
−0.1
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
The silhouette coefficient values

[ ]: