Assignment 3: Clustering

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In [ ]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

from sklearn.preprocessing import StandardScaler, OneHotEncoder

from sklearn.cluster import KMeans, DBSCAN
from sklearn.metrics import silhouette_score, davies_bouldin_score
from sklearn.utils.random import sample_without_replacement
from sklearn.decomposition import PCA
from sklearn.manifold import TSNE

df_data = pd.read_csv('data/data.csv')
RANDOM_STATE = 420
```

In [ ]:
```
df_data.head()
```

Out[ ]:

	id	f_00	f_01	f_02	f_03	f_04	f_05	f_06	f_07	f_08	...	f_19	f_20	f_21
0	0	-0.389420	-0.912791	0.648951	0.589045	-0.830817	0.733624	2.258560	2	13	...	-0.478412	-0.757002	-0.763635
1	1	-0.689249	-0.453954	0.654175	0.995248	-1.653020	0.863810	-0.090651	2	3	...	-0.428791	-0.089908	-1.784204
2	2	0.809079	0.324568	-1.170602	-0.624491	0.105448	0.783948	1.988301	5	11	...	-0.413534	-1.602377	1.190984
3	3	-0.500923	0.229049	0.264109	0.231520	0.415012	-1.221269	0.138850	6	2	...	0.619283	1.287801	0.532837
4	4	-0.671268	-1.039533	-0.270155	-1.830264	-0.290108	-1.852809	0.781898	8	7	...	-1.628830	-0.434948	0.322505

5 rows × 30 columns

In [ ]:
```
df_data.describe()
```

Out[ ]:

	id	f_00	f_01	f_02	f_03	f_04	f_05	f_06	
count	98000.000000	98000.000000	98000.000000	98000.000000	98000.000000	98000.000000	98000.000000	98000.000000	98000.0
mean	48999.500000	0.001220	0.005580	-0.001042	-0.000700	-0.003522	-0.001612	-0.003042	5.5
std	28290.307527	1.002801	1.000742	1.001373	1.000422	1.003061	1.000532	0.997434	3.6
min	0.000000	-4.732235	-4.202795	-4.377021	-4.010826	-4.535903	-4.300767	-4.894525	0.0
25%	24499.750000	-0.675226	-0.670985	-0.672779	-0.672540	-0.682510	-0.675066	-0.680421	3.0
50%	48999.500000	0.002022	0.006650	-0.000324	-0.003185	-0.003307	0.001024	-0.002053	5.0
75%	73499.250000	0.677271	0.677746	0.677086	0.672097	0.677589	0.673344	0.668112	8.0
max	97999.000000	4.490521	4.324974	4.560247	4.399373	4.050549	4.710316	3.998595	32.0

8 rows × 30 columns

In [ ]:
```
cat_features = [
    'f_07',
    'f_08',
    'f_09',
    'f_10',
    'f_11',
    'f_12',
    'f_13'
]
df_cat = df_data[cat_features]

num_features = list(set(df_data.columns) - set(cat_features) - set('id'))
df_num = df_data[num_features]

columns = num_features
columns.extend(cat_features)

df_data = df_data[columns]
```

In [ ]:
```
df_cat.describe()
```

Out[ ]:

	f_07	f_08	f_09	f_10	f_11	f_12	f_13
count	98000.000000	98000.000000	98000.000000	98000.000000	98000.000000	98000.000000	98000.000000
mean	5.545918	6.763061	8.193163	8.057878	8.084990	7.076388	6.286102
std	3.691840	4.152348	5.904919	4.700226	4.197106	4.433308	4.120077
min	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
25%	3.000000	4.000000	4.000000	5.000000	5.000000	4.000000	3.000000
50%	5.000000	6.000000	7.000000	7.000000	8.000000	6.000000	6.000000
75%	8.000000	9.000000	11.000000	11.000000	11.000000	10.000000	9.000000
max	32.000000	30.000000	44.000000	36.000000	28.000000	38.000000	30.000000

Data Preprocessing

We change both categorical and numerical attributes to the same scale, since initially their scales are very different. Also K-means tends to prefer circular (not elongated) clusters, so we reduce the risk by transforming the space accordingly.

P.S. If we don't normalize the categorical features, the models completely neglect the numerical features due to scale

In [ ]:
```
num_schema = StandardScaler().fit(df_num)
cat_schema = StandardScaler().fit(df_cat)

df_scaled = pd.DataFrame(num_schema.transform(df_num), columns=df_num.columns)

if isinstance(cat_schema, OneHotEncoder):
    new_df_cat = pd.DataFrame(cat_schema.transform(df_cat).todense(), columns=cat_schema.get_feature_names_out())
    df_scaled = pd.concat([df_scaled, new_df_cat], axis=1)
elif cat_schema is None:
    df_scaled[df_cat.columns] = df_cat
else:
    df_scaled[df_cat.columns] = cat_schema.transform(df_cat)

df_scaled.drop(columns=['id'], inplace=True)
```

In [ ]:
```
df_scaled.head()
```

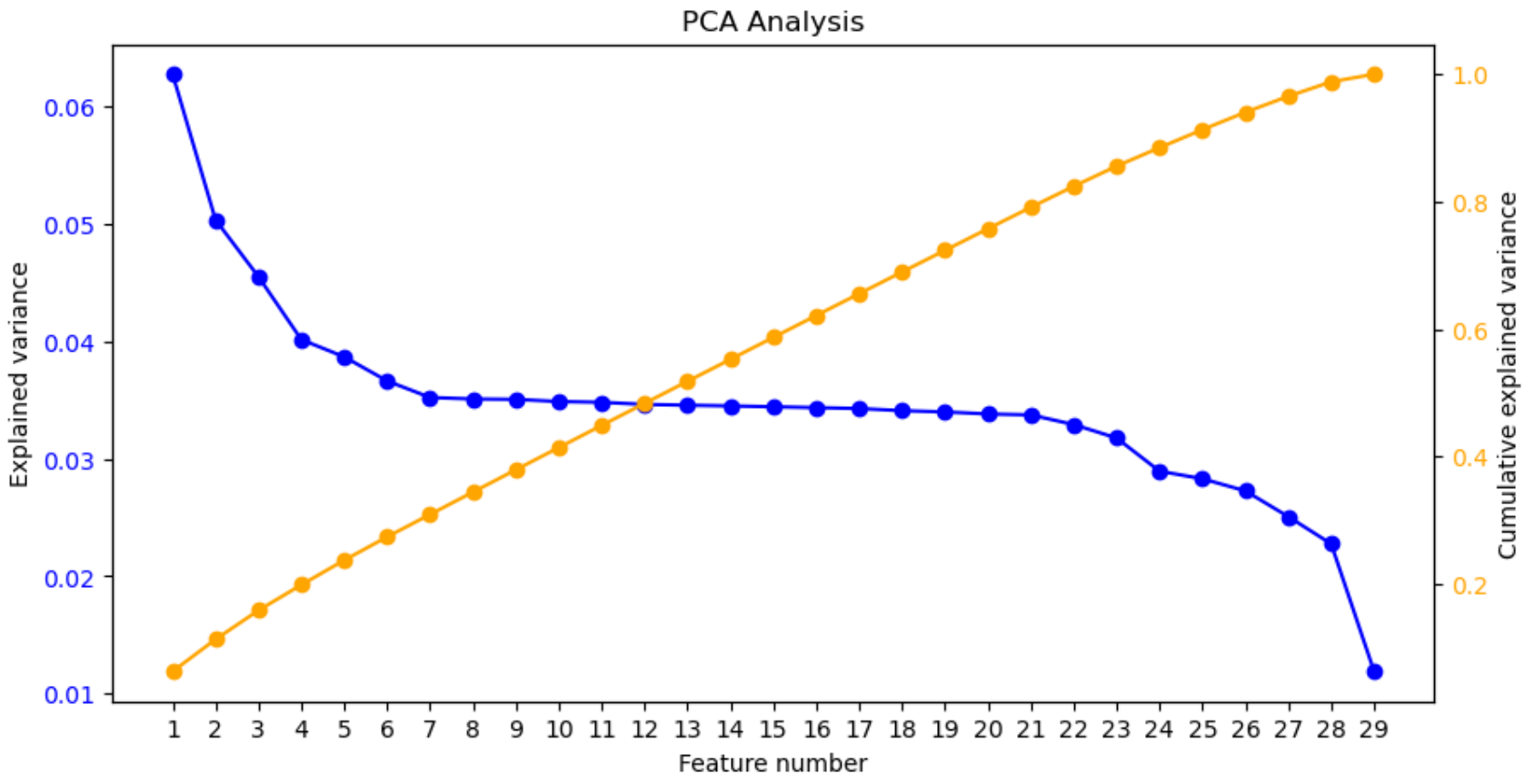
Out[ ]:

	f_05	f_20	f_04	f_28	f_18	f_26	f_27	f_06	f_19	f_21	...	f_03	
0	0.734849	-0.754257	-0.824775	0.683323	-0.362972	0.960482	1.045296	2.267432	-0.471839	-0.762195	...	0.589499	-0.4
1	0.864967	-0.089129	-1.644472	-1.602671	0.478499	-0.552942	0.355435	-0.087835	-0.422434	-1.783073	...	0.995533	0.5
2	0.785146	-1.597140	0.108638	-2.224327	0.298074	0.979171	-0.926250	1.996476	-0.407243	1.193015	...	-0.623531	-0.6
3	-1.219016	1.284518	0.417259	0.307002	-1.150052	-0.397908	-0.114228	0.142257	0.621083	0.534669	...	0.232124	-0.3
4	-1.850223	-0.433152	-0.285713	-1.149094	0.435485	1.166086	-0.385886	0.786963	-1.617255	0.324273	...	-1.828801	-0.1

5 rows × 29 columns

In [ ]:
```
max_components = 29
pca = PCA(n_components=max_components, random_state=RANDOM_STATE)
pca.fit(df_scaled)

fig, ax1 = plt.subplots(1, 1, figsize=(10, 5))
x_vals = range(1, max_components+1)
y_vals = pca.explained_variance_ratio_

color1="blue"
ax1.plot(x_vals, y_vals, c=color1)
ax1.scatter(x_vals, y_vals, c=color1)
ax1.set_xticks(x_vals)
ax1.tick_params(axis='y', labelcolor=color1)
ax1.set_xlabel("Feature number")
ax1.set_ylabel("Explained variance")
ax1.set_title("PCA Analysis")

ax2 = ax1.twinx()

color2 = "orange"
ax2.plot(x_vals, np.cumsum(y_vals), c=color2)
ax2.scatter(x_vals, np.cumsum(y_vals), c=color2)
ax2.tick_params(axis='y', labelcolor=color2)
ax2.set_ylabel("Cumulative explained variance")
```

Out[ ]:
```
Text(0, 0.5, 'Cumulative explained variance')
```



As we can see from the plot above, the features explain more or less the same variance, so we choose not to reduce the number of features (since we can't necessarily tell which ones are more informative)

In [ ]:
```
df_scaled.head()
```

Out[ ]:

	0	1	2	3	4	5	6	7	8	9
0	-0.690049	-0.065806	-1.152288	1.647112	1.049714	0.184268	0.122812	2.464091	-0.334974	1.365643
1	-0.962431	-0.926917	2.158420	-1.095303	-0.171867	-1.309496	0.237459	0.215473	1.332048	0.782343
2	-1.375477	0.695580	-1.117810	-0.932218	-0.286526	-0.266661	-0.075233	2.043526	-0.722874	0.470877
3	1.185497	0.147776	0.376840	-0.841213	0.574698	0.044402	-0.043146	-0.664526	-1.378243	-0.018358
4	-1.133003	-0.096996	1.399141	-2.320533	-0.824014	-0.075635	1.721909	-0.204940	-0.895963	-1.222530

In [ ]:
```
df_scaled.describe()
```

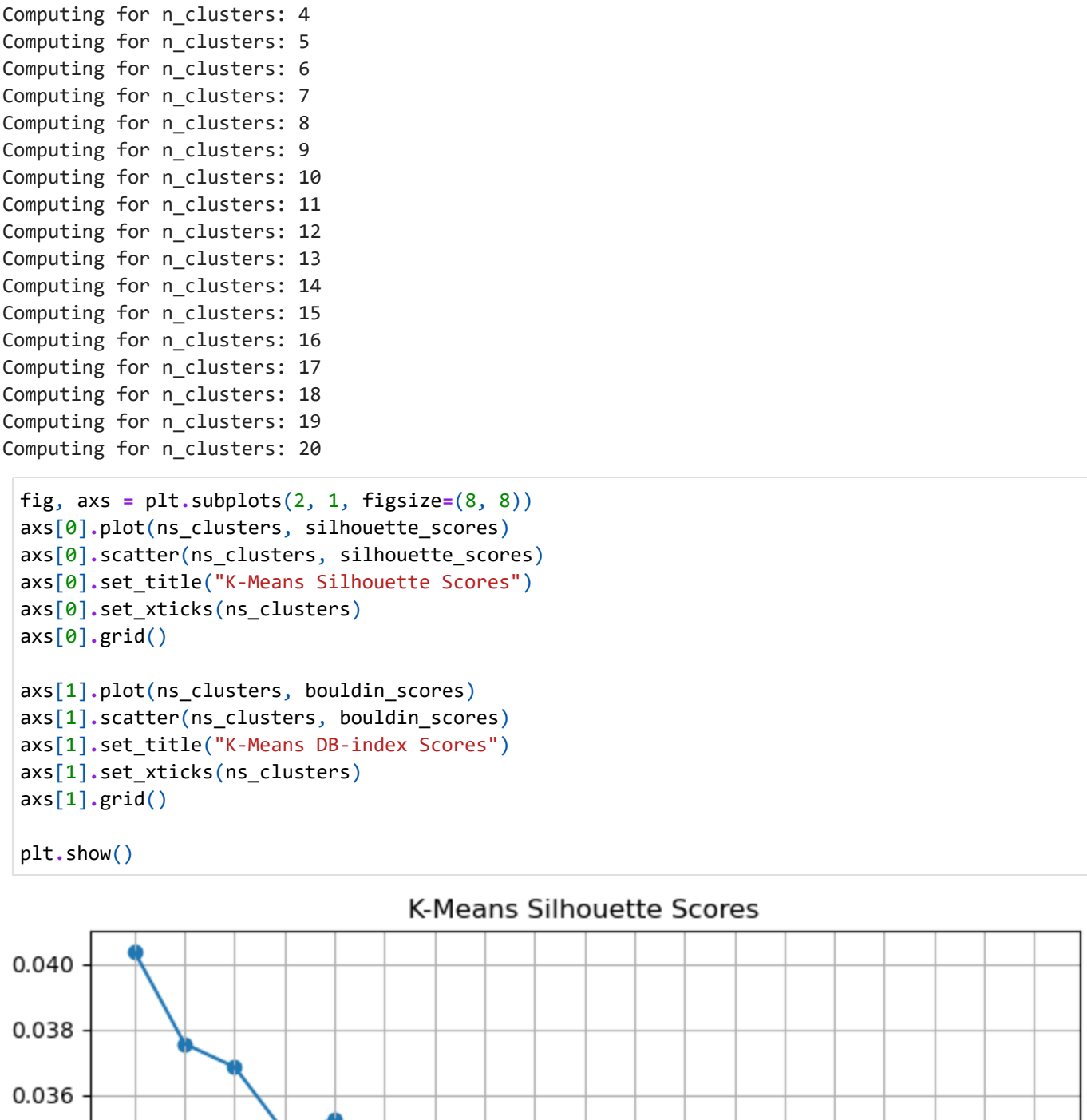
Out[ ]:

	0	1	2	3	4	5	6	7
count	9.800000e+04	9.800000e+04	9.800000e+04	9.800000e+04	9.800000e+04	9.800000e+04	9.800000e+04	9.800000e+04
mean	2.378143e-17	1.798108e-17	1.395709e-17	-3.429456e-17	2.465148e-18	2.146129e-17	-2.639159e-17	-1.392084e-17
std	1.348207e+00	1.207094e+00	1.141475e+00	1.061856e+00	1.049975e+00	1.022515e+00	1.008692e+00	1.003490e+00
min	-4.515005e+00	-5.251224e+00	-4.773852e+00	-4.594085e+00	-4.157578e+00	-4.236045e+00	-4.568747e+00	-4.437919e+00
25%	-9.152809e-01	-8.192529e-01	-7.800443e-01	-7.164679e-01	-7.139119e-01	-6.955284e-01	-6.787344e-01	-6.760083e-01
50%	-1.651001e-01	9.012007e-03	-1.230630e-02	-1.244448e-02	-7.563406e-03	-2.191989e-02	-4.365459e-04	-1.113340e-03
75%	7.823614e-01	8.325670e-01	7.687895e-01	7.105360e-01	6.997973e-01	6.826153e-01	6.795717e-01	6.757028e-01
max	5.967965e+00	5.304363e+00	5.479649e+00	4.972896e+00	4.418742e+00	4.935267e+00	4.673805e+00	4.460455e+00

In [ ]:
```
SAMPLE_SIZE = 10000

silhouette_scores = []
bouldin_scores = []
ns_clusters = list(range(2, 21, 1))

for n_clusters in ns_clusters:
    print(f"Computing for n_clusters: {n_clusters}")
    indices = sample_without_replacement(len(df_scaled), SAMPLE_SIZE, random_state=RANDOM_STATE)
    sampled_df_scaled = df_scaled.iloc[indices]

    kmeans = KMeans(n_clusters=n_clusters, random_state=RANDOM_STATE, n_init="auto", verbose=False)
    kmeans.fit(sampled_df_scaled)

    labels = kmeans.predict(sampled_df_scaled)
    silhouette_scores.append(silhouette_score(sampled_df_scaled, labels))
    bouldin_scores.append(davies_bouldin_score(sampled_df_scaled, labels))
```

```
Computing for n_clusters: 2
Computing for n_clusters: 3
Computing for n_clusters: 4
Computing for n_clusters: 5
Computing for n_clusters: 6
Computing for n_clusters: 7
Computing for n_clusters: 8
Computing for n_clusters: 9
Computing for n_clusters: 10
Computing for n_clusters: 11
Computing for n_clusters: 12
Computing for n_clusters: 13
Computing for n_clusters: 14
Computing for n_clusters: 15
Computing for n_clusters: 16
Computing for n_clusters: 17
Computing for n_clusters: 18
Computing for n_clusters: 19
Computing for n_clusters: 20
```

In [ ]:
```python
fig, axs = plt.subplots(2, 1, figsize=(8, 8))
axs[0].plot(ns_clusters, silhouette_scores)
axs[0].scatter(ns_clusters, silhouette_scores)
axs[0].set_title("K-Means Silhouette Scores")
axs[0].set_xticks(ns_clusters)
axs[0].grid()

axs[1].plot(ns_clusters, bouldin_scores)
axs[1].scatter(ns_clusters, bouldin_scores)
axs[1].set_title("K-Means DB-index Scores")
axs[1].set_xticks(ns_clusters)
axs[1].grid()

plt.show()
```



From the plot above, we see that according to Silhouette score, the quality goes down more with $k > 8$. And the Davies-Boulding score has potentially interesting "dips" at $k = 4, 6, 8$. Therefore we decided to set the range for K-means to $[2, 8]$

In [ ]:
```python
kmeans_ns = list(range(2, 9))
kmeans_names = [f"k={k}" for k in kmeans_ns]
kmeans_labels = []
for n_clusters in kmeans_ns:
    kmeans = KMeans(n_clusters=n_clusters, random_state=RANDOM_STATE, n_init="auto", verbose=False)
    kmeans.fit(df_scaled)

    labels = kmeans.predict(df_scaled)
    kmeans_labels.append(labels)
```

Unfortunately, when it comes to DBSCAN - no matter what parameters (eps & min_samples) we chose, it resulted in very poor clustering:

- either all examples labeled as *outliers*
- or all examples labeld as *one cluster*
- or one gigantic cluster with 99% of data, and lots of small ones of size < 10

In [ ]:
```
dbscan_epsilons = [2.8, 3.7, 5.0]
dbscan_min_samples = [5, 7, 4]
dbscan_names = [f"eps={eps}, minsamp={min_samples}" for eps, min_samples in zip(dbscan_epsilons, dbscan_min_samples)]
dbscan_labels = []
for i, (eps, min_samples) in enumerate(zip(dbscan_epsilons, dbscan_min_samples)):
    dbscan = DBSCAN(eps=eps, min_samples=min_samples)
    labels = dbscan.fit_predict(df_scaled)
    dbscan_labels.append(labels)
```

Cluster visualization

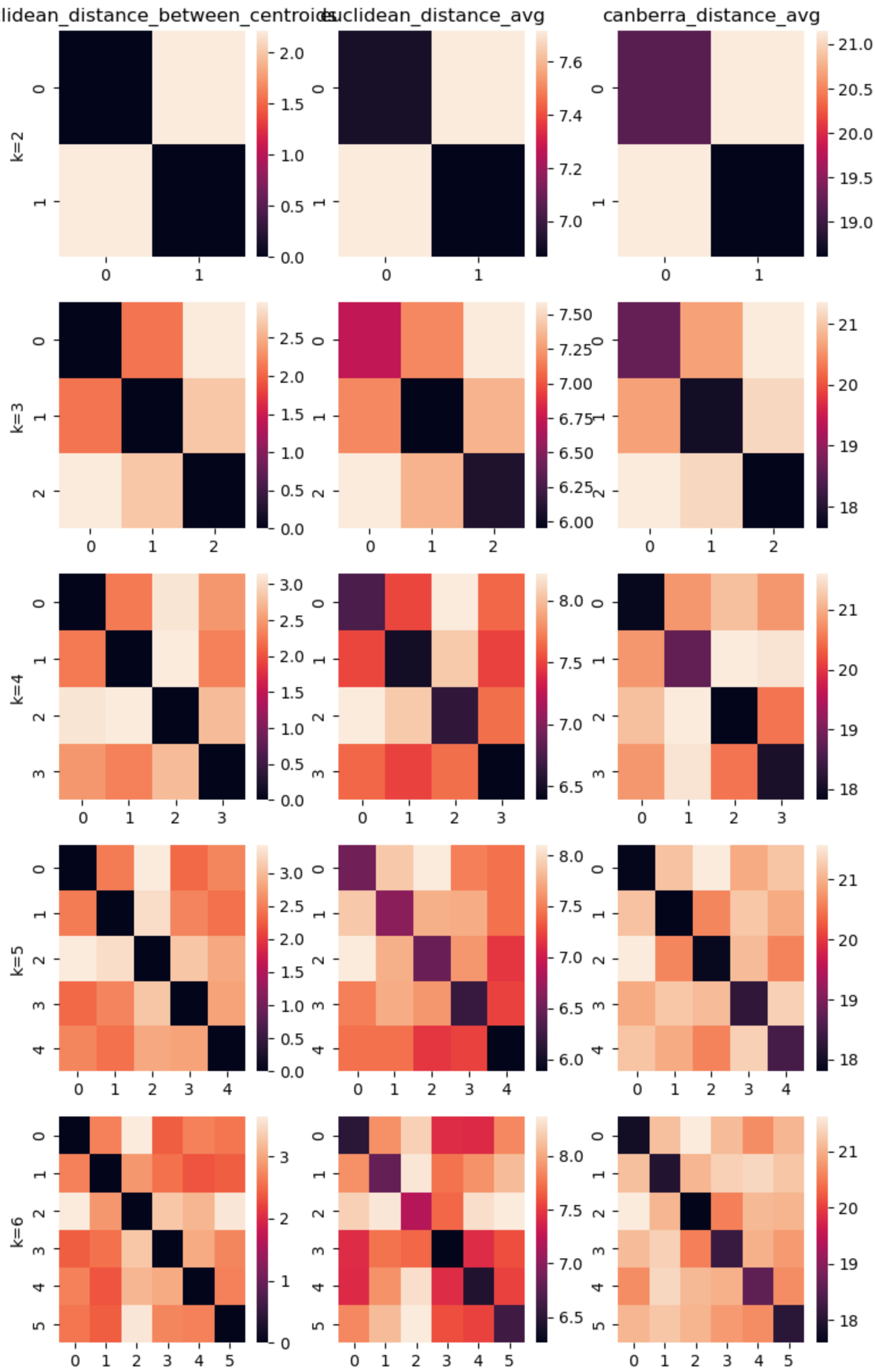
Since, as shown previously, PCA is more or less useless, we will be using a different visualization - **TSNE**

In [ ]:
```
def plot_clusters(X, labels_list, n_components=2, model_names=None, sample_size=5000):
    m = int(np.sqrt(len(labels_list)))
    n = int(np.ceil(len(labels_list) / m))
    fig, axs = plt.subplots(m, n, figsize=(5*n, 5*m))
    axs = np.reshape(axs, newshape=(m, n))

    if sample_size is not None:
        sample_inds = sample_without_replacement(len(X), sample_size)
        X = X.iloc[sample_inds, :]

    labels_list = list(labels_list)
    labels_list += [None]*(m*n-len(labels_list))
    labels_list = np.array(labels_list, dtype=object)
    labels_list = np.reshape(labels_list, newshape=(m, n))

    pca = TSNE(n_components=n_components)
    X_new = pca.fit_transform(X)
    for i in range(m):
        for j in range(n):
            labels = labels_list[i, j]
            ax = axs[i, j]

            if labels is None:
                ax.set_axis_off()
                continue

            scatter = ax.scatter(x=X_new[:, 0], y=X_new[:, 1], c=labels[sample_inds], alpha=0.5)
            if model_names is not None:
                ax.set_title(model_names[n*i+j])
            ax.legend(*scatter.legend_elements(), title="Clusters")

def plot_cluster_distances_heatmap(X, labels_list, dist_metrics_list, model_names=None):
    m, n = len(labels_list), len(dist_metrics_list)
    fig, axs = plt.subplots(m, n, figsize=(3*n, 3*m))
    axs = np.reshape(axs, newshape=(len(labels_list), len(dist_metrics_list)))

    for plot_i, labels in enumerate(labels_list):
        for plot_j, dist_metric in enumerate(dist_metrics_list):
            unique_labels = np.unique(labels)
            n_clusters = len(unique_labels)

            dist_matrix = np.zeros(shape=(n_clusters, n_clusters))

            for i, label1 in enumerate(unique_labels):
                for j, label2 in enumerate(unique_labels):
                    if i > j:
                        dist_matrix[i, j] = dist_matrix[j, i]
                        continue

                    dist_matrix[i, j] = dist_metric(X[labels==label1], X[labels==label2])

            sns.heatmap(dist_matrix, xticklabels=unique_labels, yticklabels=unique_labels, ax=axs[plot_i, plot_j])


            if plot_i == 0:
                axs[plot_i, plot_j].set_title(dist_metric.__name__)
            if model_names is not None and plot_j == 0:
                axs[plot_i, plot_j].set_ylabel(model_names[plot_i])
```

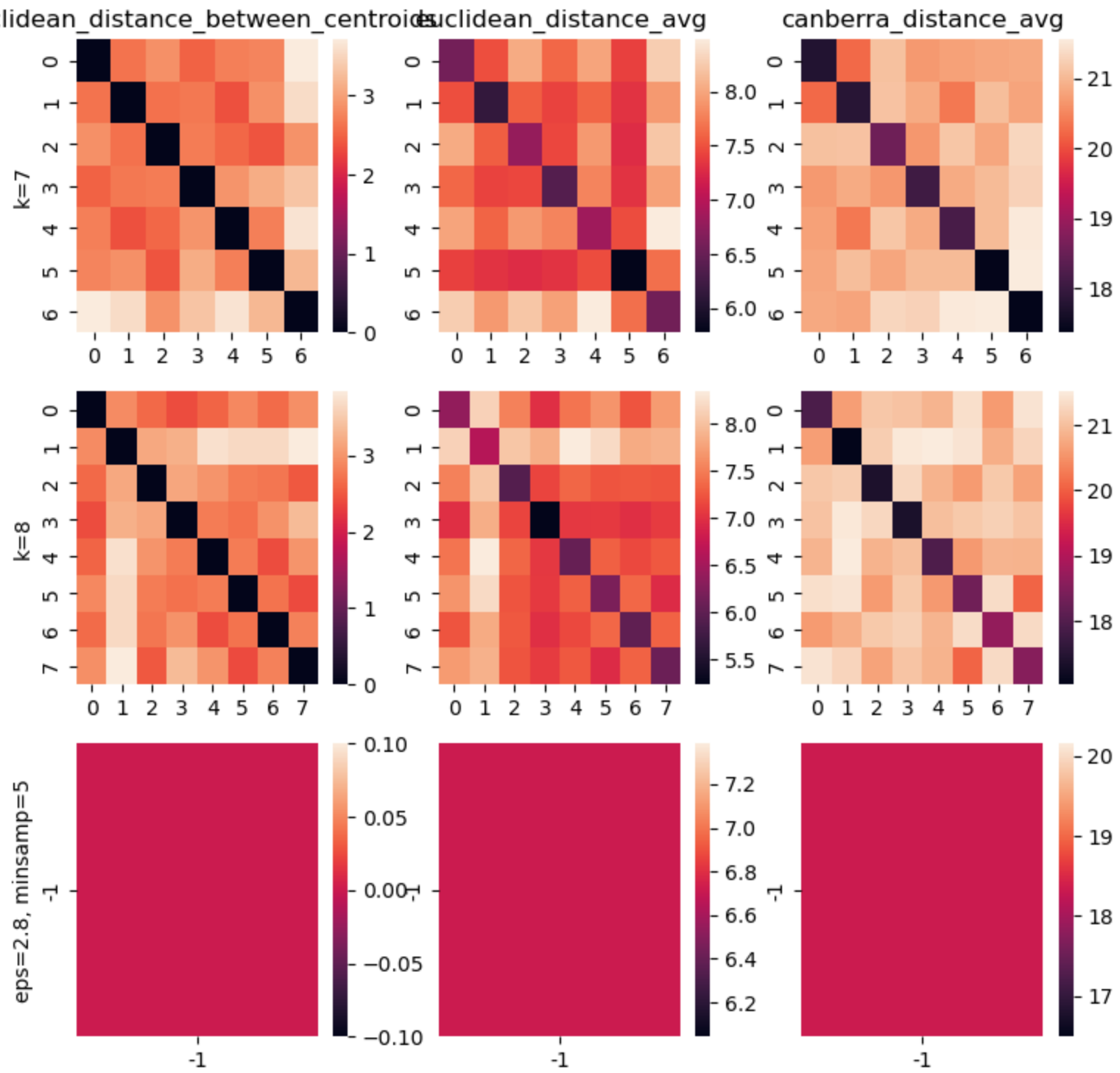
To inspect numerically the results of clusterization, we will use several distance metrics - visualized on the heatmaps below

In [ ]:
```
def euclidean_distance_between_centroids(X1: pd.DataFrame, X2: pd.DataFrame):
    centroid1, centroid2 = X1.mean(axis=0), X2.mean(axis=0)
    result = np.linalg.norm(centroid1-centroid2)
    return result

def euclidean_distance_avg(X1: pd.DataFrame, X2: pd.DataFrame, sample_size=10):
    X1_sample_inds = sample_without_replacement(len(X1), sample_size, random_state=RANDOM_STATE) if sample_size < ler
    X2_sample_inds = sample_without_replacement(len(X2), sample_size, random_state=RANDOM_STATE) if sample_size < ler
    dists = np.zeros(shape=(len(X1_sample_inds), len(X2_sample_inds)))
    for i, ind1 in enumerate(X1_sample_inds):
        for j, ind2 in enumerate(X2_sample_inds):
            dists[i, j] = np.linalg.norm(X1.iloc[ind1, :] - X2.iloc[ind2, :])

    return dists.mean()

def canberra_distance_avg(X1: pd.DataFrame, X2: pd.DataFrame, sample_size=10):
    X1_sample_inds = sample_without_replacement(len(X1), sample_size, random_state=RANDOM_STATE) if sample_size < ler
    X2_sample_inds = sample_without_replacement(len(X2), sample_size, random_state=RANDOM_STATE) if sample_size < ler
    dists = np.zeros(shape=(len(X1_sample_inds), len(X2_sample_inds)))
    for i, ind1 in enumerate(X1_sample_inds):
        for j, ind2 in enumerate(X2_sample_inds):
            row1, row2 = X1.iloc[ind1, :], X2.iloc[ind2, :]
            dists[i, j] = np.sum(np.abs(row1 - row2) / (np.abs(row1) + np.abs(row2)))
    return dists.mean()
```

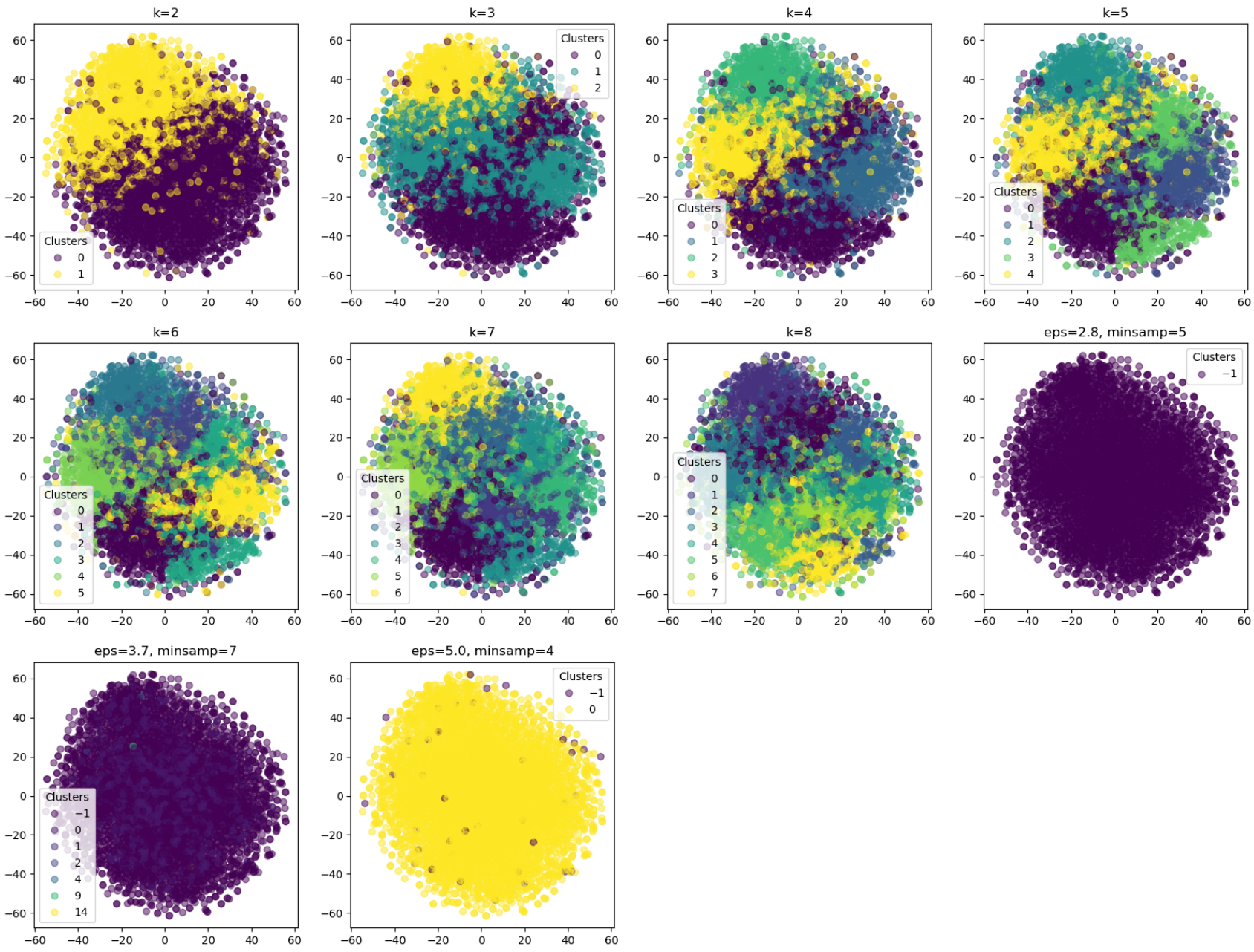
In [ ]:
```
plot_cluster_distances_heatmap(
    df_scaled,
    (kmeans_labels + dbscan_labels)[:5],
    [euclidean_distance_between_centroids, euclidean_distance_avg, canberra_distance_avg],
    model_names=(kmeans_names+dbscan_names)[:5]
)
```



In [ ]:
```
plot_cluster_distances_heatmap(
    df_scaled,
    (kmeans_labels + dbscan_labels)[-5:],
    [euclidean_distance_between_centroids, euclidean_distance_avg, canberra_distance_avg],
    model_names=(kmeans_names+dbscan_names)[-5:]
)
```



In [ ]:
```
plot_clusters(
    df_scaled,
    (kmeans_labels + dbscan_labels),
    model_names=(kmeans_names+dbscan_names)
)
```



Conclusions

As we can see from the results, none of our clustering models produced clean clusters for the data, however some appear to be better and some - worse.

The DBSCAN proved to be quite useless on this dataset. Perhaps, there could be something interesting in the very small clusters, but it seems quite unlikely considering the proportion of examples classified as "outliers".

When it comes to k-means, the best models appear to be those with $k = 2, 3 \text{ or } 4$, since the t-SNE plots of other appear more cluttered and the heatmaps have higher proportions of less-distance cells.