Assignment 3 (DAT340) - AI tools

February 6, 2024

1 Assignment 3 - AI tools

- Student 1 Luca Modica
- Student 2 Hugo Manuel Alves Henriques E Silva

1.1 Import libraries

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

sns.set_style('darkgrid')
%matplotlib inline
```

/tmp/ipykernel_5908/3608931809.py:2: DeprecationWarning:

Pyarrow will become a required dependency of pandas in the next major release of pandas (pandas 3.0),

(to allow more performant data types, such as the Arrow string type, and better interoperability with other libraries)

but was not found to be installed on your system.

If this would cause problems for you,

please provide us feedback at https://github.com/pandas-dev/pandas/issues/54466

import pandas as pd

1.2 Reading data

```
for file in csv_files:
             file_path = os.path.join(directory, file)
             df = pd.read_csv(file_path)
            key = file.replace('_labeled.csv', '')
             data[key] = df
        return [file.replace('_labeled.csv', '') for file in csv_files], data
[3]: # with this method we will return an object
     # with as property name the city and as
     # property value the related dataframe
    cities_names, dfs = read_csv_files('./')
    print(f'Data from the following cities: {", ".join(cities_names)}.')
    Data from the following cities: Shenyang, Guangzhou, Shanghai, Chengdu, Beijing.
[4]: city = 'Beijing'
    print(f'Data from {city}: ')
    dfs[city].head()
    Data from Beijing:
[4]:
       season DEWP HUMI
                             PRES TEMP
                                            Iws precipitation cbwd_NE
                                                                         cbwd NW \
            4 -8.0 79.0 1026.0 -5.0
                                          23.69
                                                           0.0
                                                                      0
                                                                               0
            4 -11.0 85.0 1021.0 -9.0 105.93
                                                                               0
    1
                                                           1.1
                                                                      0
    2
            4 -21.0 43.0 1030.0 -11.0 117.55
                                                           0.0
                                                                      0
                                                                               1
            4 -25.0 33.0 1034.0 -12.0
                                                           0.0
                                                                               0
    3
                                          39.35
                                                                      1
            4 -24.0 30.0 1034.0 -10.0
                                          59.00
                                                           0.0
                                                                      1
                                                                               0
               PM_HIGH
       cbwd_SE
    0
             1
                    1.0
    1
             1
                    0.0
    2
             0
                    0.0
    3
             0
                    0.0
                    0.0
             0
[5]: city = 'Chengdu'
    print(f'Data from {city}: ')
    dfs[city].head()
    Data from Chengdu:
[5]:
                              PRES TEMP
       season DEWP
                      HUMI
                                          Iws precipitation cbwd_NE cbwd_NW \
    0
            2 20.0 88.45
                            1007.1 22.0
                                                         0.0
                                                                    0
                                                                             0
                                          1.0
    1
            2 17.0 54.39
                            1008.1 27.0
                                          5.0
                                                         0.0
                                                                    0
                                                                             0
                                                         0.0
    2
            2 20.0 78.39
                            1008.1 24.0
                                          2.0
                                                                    0
                                                                             0
    3
            2 19.0 65.41
                                                         0.0
                                                                    0
                                                                             0
```

1006.1 26.0 2.0

```
4
            2 20.0 61.90 1003.1 28.0 2.0
                                                         0.0
                                                                    0
                                                                             0
       cbwd_SE PM_HIGH
    0
             0
                    1.0
    1
             0
                    0.0
    2
             0
                    0.0
                    0.0
    3
             0
    4
             0
                    0.0
[6]: city = 'Guangzhou'
    print(f'Data from {city}: ')
    dfs[city].head()
    Data from Guangzhou:
[6]:
       season DEWP HUMI
                                             precipitation cbwd_NE
                             PRES TEMP
                                         Iws
                                                                      cbwd_NW \
          3.0 15.2 62.0 1013.9 22.9 7.3
                                                        0.0
    0
                                                                   1
                                                                            0
    1
          3.0 10.7 43.0 1013.7 24.0 5.2
                                                        0.0
                                                                   1
                                                                            0
    2
               8.8 42.0 1014.4 22.3 9.2
                                                                            0
          3.0
                                                        0.0
                                                                   1
    3
          3.0 12.1 51.0 1013.2 22.7 9.5
                                                        0.0
                                                                   1
                                                                            0
          3.0 15.3 76.0 1011.5 19.6 3.0
                                                        0.0
                                                                   0
                                                                            1
       cbwd_SE PM_HIGH
             0
                    0.0
    0
    1
             0
                    0.0
    2
             0
                    0.0
    3
             0
                    0.0
    4
                    0.0
             0
[7]: city = 'Shanghai'
    print(f'Data from {city}: ')
    dfs[city].head()
    Data from Shanghai:
[7]:
                              PRES
       season DEWP
                      HUMI
                                    TEMP
                                            Iws precipitation cbwd_NE
                                                                         cbwd_NW \
                            1030.1
    0
                3.0 57.77
                                    11.0
                                           66.0
                                                           0.0
                                                                      1
                                                                               0
            4
              -2.0 49.22
                            1032.9
                                          194.0
                                                           0.0
                                                                      1
                                                                               0
    1
                                     8.0
    2
            4 -1.0 49.51
                            1029.1
                                     9.0
                                            2.0
                                                           0.0
                                                                      1
                                                                               0
    3
            4 -4.0 42.40
                            1029.1
                                     8.0
                                            7.0
                                                           0.0
                                                                      1
                                                                               0
    4
            4 -4.0 45.40
                                                                      0
                            1028.1
                                     7.0
                                            2.0
                                                           0.0
                                                                               1
       cbwd_SE PM_HIGH
    0
             0
                    0.0
             0
                    0.0
    1
                    0.0
    2
             0
    3
             0
                    0.0
```

```
4 0 0.0
```

```
[8]: city = 'Shenyang'
print(f'Data from {city}: ')
dfs[city].head()
```

Data from Shenyang:

```
[8]:
       season DEWP
                      HUMI
                              PRES TEMP
                                           Iws precipitation cbwd_NE
                                                                        cbwd_NW
                            1010.0 16.0
            1 -3.0 26.98
                                          31.0
                                                          0.0
                                                                     0
    1
            1
                6.0 58.54
                            1008.0 14.0
                                          51.0
                                                          0.0
                                                                     0
                                                                              0
                0.0 43.60
                                           7.0
                                                          0.0
                                                                     0
            1
                            1006.0 12.0
                                                                              1
    3
                2.0 41.43
                            1011.0 15.0
                                          23.0
                                                          0.0
                                                                     0
                                                                              1
            1 -5.0 18.06 1013.0 20.0 28.0
                                                          0.0
       cbwd_SE PM_HIGH
    0
             0
                    0.0
             0
                    0.0
    1
    2
             0
                    0.0
    3
             0
                    0.0
             1
                    0.0
```

1.3 Model implementation

The Python class below will implement the KMeans algorithm.

```
[9]: import warnings
     from sklearn.metrics import normalized_mutual_info_score, silhouette_score,_
      →adjusted_rand_score
     from sklearn.base import BaseEstimator, ClusterMixin, check_array
     class KMeans(BaseEstimator, ClusterMixin):
         def __init__(self,
             n_centers=2,
             max_iter=200,
             init_centroids='random',
             random_seed=None,
             distance_metric="euclidean"
             ):
             self.n_centers = n_centers
             self.max_iter = max_iter
             self.init_centroids = init_centroids
             self.random_seed = int(random_seed) if random_seed is not None else None
             self.distance_metric = distance_metric
```

```
# ***private methods***
  def _set_distance_func(self, distance_metric):
       if distance_metric == "euclidean":
           self.distance_func_ = euclidean_distance
       elif distance_metric == "manhattan":
           self.distance_func_ = manhattan_distance
       else:
           raise ValueError(f"Unknown distance metric: {self.distance_metric}")
  def _initialize_centroids(self, X):
       if self.init centroids == 'random':
           if X.shape[0] < self.n_centers:</pre>
               warnings.warn(
                    "Number of samples in X is less than the number of centers. \Box
→\
                       The number of clusters has changed to number of \sqcup
⇔datapoints.", UserWarning)
               self.n_centers = X.shape[0]
           # sample "n_centers" datapoints as first centroids positions
           indices = np.random.choice(range(X.shape[0]), size=self.n_centers)
           self.centroids_ = X[indices]
       elif self.init_centroids == 'kmeans++':
           self.centroids_ = self._kmeans_plus_plus(X)
           # self.centroids_, = kmeans_plusplus(X=X, n_clusters=self.
\rightarrow n_centers)
       else:
           raise ValueError(f"Unknown centroid initialization method: {self.
→init centroids}")
  def _kmeans_plus_plus(self, X):
       centroids = np.empty((self.n_centers, self.n_features_in_))
       # sample a datapoint as first centroid
       index = np.random.choice(range(X.shape[0]), size=1)
       first_centroid = X[index]
       centroids[0] = first_centroid
       for i in range(1, self.n_centers):
           # Calculate distances from each point to its nearest centroid
           distances = np.array(
               [np.min([self.distance_func_(x, c) for c in centroids[:i]]) for_
\rightarrow x in X])
           # Normalize the square of these distances to create a probability_
\hookrightarrow distribution
```

```
squared_distances = distances**2
           probabilities = squared_distances / np.sum(squared_distances)
           # Randomly select the next centroid based on the probability
\hookrightarrow distribution
           next centroid index = np.random.choice(range(X.shape[0]),
→p=probabilities, size=1)
           centroids[i] = X[next_centroid_index]
      return centroids
  # ***public methods***
  def fit(self, X, y=None):
      np.random.seed(self.random_seed)
      X = check_array(X)
      self.n_features_in_ = X.shape[1]
      self._set_distance_func(self.distance_metric)
      self._initialize_centroids(X)
      n_iter = 0
      while n_iter < self.max_iter:</pre>
           # calculate distance from each point to each centroid
           distances = np.zeros((X.shape[0], self.n_centers))
          for i in range(self.n_centers):
               for j in range(X.shape[0]):
                   distances[j, i] = self.distance_func_(X[j], self.
⇔centroids_[i])
           # assign each point to the closest centroid
           self.labels_ = np.argmin(distances, axis=1)
           # calculate new centroids
          new_centroids = np.zeros((self.n_centers, X.shape[1]))
           for i in range(self.n_centers):
               cluster_points = X[self.labels_ == i]
               if cluster_points.size > 0:
                   new_centroids[i] = np.mean(cluster_points, axis=0)
               else:
                   # Handle the empty cluster case
                   new_centroids[i] = X[np.random.choice(range(X.shape[0]),__
⇔size=1)]
```

```
# if centroids have not changed, stop
           if np.allclose(self.centroids_, new_centroids):
               break
           # otherwise, update centroids and continue
           self.centroids_ = new_centroids
          n_{iter} += 1
      self.n_iter_ = n_iter
      return self
  def transform(self, X):
       """In this custom KMeans implementation, X wont't be changed.
      The implementaion of the method is for consitency puroposes
      with the sklearn APIs and pipeline purposes to extract the
      data tranformed by previous steps (for example)"""
      X = check\_array(X)
      if X.shape[1] != self.n_features_in_:
           raise ValueError("The number of features in transform is different ⊔

¬from the number of features in fit.")

      return check_array(X)
  def fit_transform(self, X, y=None):
       """In this custom KMeans implementation, after .fit() X wont't be_{\sqcup}
\hookrightarrow changed.
       The implementaion of the method is for consitency puroposes
      with the sklearn APIs and pipeline purposes to extract the
      data tranformed by previous steps (for example)"""
      return self.fit(X).transform(X)
  def predict(self, X):
      X = check_array(X, accept_sparse=True)
      pred_labels = np.zeros(X.shape[0], dtype=np.dtype("int64"))
      distances = np.zeros((X.shape[0], self.n_centers))
      for i in range(self.n_centers):
           for j in range(X.shape[0]):
               distances[j, i] = self.distance_func_(X[j], self.centroids_[i])
      pred_labels = np.argmin(distances, axis=1)
      return pred_labels
```

```
def score(self, X=None, y=None, score_metric='inertia'):
        # raise value error if "y" is none for score
        # metrics that require ground truth labels
        if y is None and score_metric in ['nmi', 'ari']:
            raise ValueError(
                f"To compute the this score ({score_metric}), 'y' cannot be_
 →None.")
        # raise value error if "X" is none for score
        # metrics that measures the internal clusters
        # quality
        if X is None and score_metric in ['inertia', 'silhouette']:
            raise ValueError(
                f"To compute the this score ({score_metric}), 'X' cannot be_
 ⊸None.")
        if score_metric == 'inertia':
            return inertia_score(X, self.centroids_, self.labels_)
        elif score_metric == 'silhouette':
            return effcient_silhouette_score(X, self.labels_, self.

¬distance_metric)
        elif score metric == 'nmi':
            return nmi_score(y, self.labels_)
        elif score_metric == 'ari':
            return adjusted_rand_score(y, self.labels_)
        else:
            raise ValueError(f"Unknown score metrix: {score_metric}")
# distance functions
def euclidean_distance(x, y):
    return np.sqrt(np.sum((x - y) ** 2))
def manhattan_distance(x, y):
    return np.sum(np.abs(x - y))
# scoring functions
def inertia score(X, centroids, labels):
    """Inertia measures the sum of squared distances between each sample and \Box
 \hookrightarrow its
    closest centroid. A lower inertia indicates better clustering."""
    return np.sum((X - centroids[labels]) ** 2)
def custom_silhouette_score(X, labels, n_centers, distance_func):
    """Silhouette score measures how similar an object is to its own cluster
```

```
(cohesion) compared to other clusters (separation). The silhouette ranges
    from -1 to 1, where a high value indicates that the object is well matched
    to its own cluster and poorly matched to neighboring clusters."""
    silhouette_scores = np.zeros(X.shape[0])
    for i in range(X.shape[0]):
        #get label of the current point
        label = labels[i]
        intra_distances = [distance_func(X[i], X[j]) for j in range(X.shape[0])
 →if labels[j] == label and i != j]
        average_intra_cluster_distance = np.mean(intra_distances) if_
 →intra_distances else 0
        #distance to points in other clusters
        min_distance_other_clusters = np.min([np.mean([distance_func(X[i]],__
 →X[j]) for j in range(X.shape[0]) if labels[j] == k]) for k in_
 →range(n_centers) if k != label])
        if average_intra_cluster_distance or min_distance_other_clusters:
            silhouette_scores[i] = (min_distance_other_clusters -_
 →average_intra_cluster_distance) / max(min_distance_other_clusters,
 →average_intra_cluster_distance)
        else:
            silhouette_scores[i] = 0
    return np.mean(silhouette_scores)
def effcient_silhouette_score(X, labels, metric):
    return silhouette_score(X=X, labels=labels, metric=metric)
def nmi_score(labels_true, labels_pred):
    """Normalized Mutual Information between the true labels and the predicted_{\sqcup}
 \hookrightarrow clusters
    divided by the average entropy of the true labels and the predicted \Box
    return normalized_mutual_info_score(labels_true, labels_pred)
def ari_score(labels_true, labels_pred):
    """The Adjusted Rand index is a function that measures the
    similarity of true and predicted assignments, ignoring permutations.
    return adjusted_rand_score(labels_true, labels_pred)
```

1.4 Sanity check

Usage of check_estimator to make sure the pattern "fit(), predict(), score()" is followed, alongside the good practises for a new custom cluster algorithm:

```
[10]: from sklearn.utils.estimator_checks import check_estimator

# Check if estimator adheres to scikit-learn conventions.
check_estimator(KMeans(random_seed=0))
```

Down below will define the sklarn pipline that will be used for checking for the usability of our class in there.

Function to train and then visualize a 2D dataset. It will return the trained k-means model.

```
[12]: from sklearn.base import clone
      def k means_visualization(k, X, title, init_centroids='random'):
          # k-means training
          pipeline = clone(pipe)
          pipeline.set_params(kmeans__n_centers=k,_
       ⇒kmeans__init_centroids=init_centroids,
              kmeans__random_seed=None)
          X_scaled = pipeline.fit_transform(X)
          # Visualize the K-Means clusters
          kmeans = pipeline.named_steps['kmeans']
          plt.figure(figsize=(8, 6))
          sns.scatterplot(x=X_scaled[:, 0], y=X_scaled[:, 1], hue=kmeans.labels_,u
       ⇔palette='viridis')
          plt.scatter(kmeans.centroids_[:,0], kmeans.centroids_[:,1], marker="X",_
       ⇔c="r", s=80, label="centroids")
          plt.title(title)
          plt.grid(True)
          plt.legend(title='Cluster')
          # highlight clusters' centroids
          plt.scatter(kmeans.centroids_[:,0], kmeans.centroids_[:,1], marker="X",_

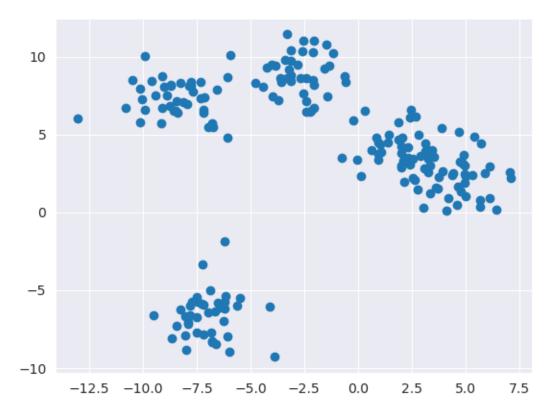
c="r", s=80, label="centroids")
```

```
plt.show()
return kmeans, X_scaled
```

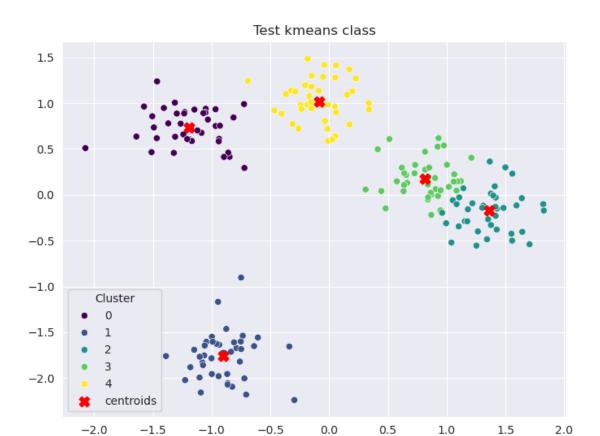
```
[13]: from sklearn.datasets import make_blobs

# generate 2D data set
k = 5
X, y = make_blobs(
    n_samples=200,
    centers=k,
    cluster_std=1.3,
    random_state=42
)

# plot the data set
plt.scatter(X[:,0], X[:,1])
plt.show()
```



```
[14]: kmeans, X_scaled = k_means_visualization(k=k, X=X, init_centroids='kmeans++', u title="Test kmeans class")
```



Check for the internal quality of the clusters themselves.

```
[15]: print(f'Inertia score: {kmeans.score(X=X_scaled)}')
print(f'Silhouette score: {kmeans.score(X=X_scaled, u

→score_metric="silhouette")}')
```

Inertia score: 20.33513776553783
Silhouette score: 0.5859707207927123

Check for the for the scoring that cehck similarity with ground truth labels.

```
[16]: print(f'Normalized Mutual Info score: {kmeans.score(y=y, score_metric="nmi")}') print(f'Adjusted Rand Index score: {kmeans.score(y=y, score_metric="ari")}')
```

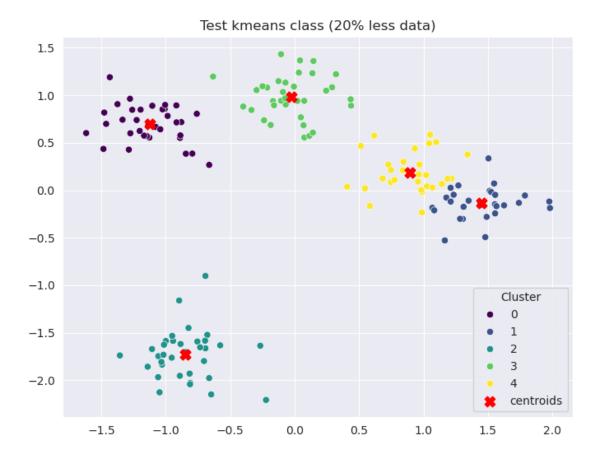
Normalized Mutual Info score: 0.9337944107790918 Adjusted Rand Index score: 0.9292019230769231

Test printing KMeans main information: the centroids coordinates and the label assignments.

```
[17]: print(f"kmeans centroids coordinates: \n {kmeans.centroids_}")
print(f"kmeans labels for each datapoint: \n {kmeans.labels_}")
```

```
kmeans centroids coordinates:
  [[-1.19021388    0.73434046]
  [-0.90010829 -1.76121708]
  [ 1.35835139 -0.17462223]
  [ 0.81516133    0.17952727]
  [-0.08319055    1.02197158]]
kmeans labels for each datapoint:
  [1 4 3 0 2 0 3 3 1 2 2 1 1 1 0 3 4 3 3 0 0 0 2 4 0 4 4 2 4 1 0 0 0 1 4 0 0
2 0 4 1 3 4 1 1 0 0 3 3 3 3 2 0 4 3 2 4 4 2 0 2 3 1 2 0 3 3 1 3 4 3 4 4 2
4 0 2 1 3 4 0 4 4 1 1 0 0 0 3 4 1 0 1 2 2 1 2 1 3 4 2 4 2 1 2 2 0 2 1 3 1
0 4 2 0 4 3 2 3 3 4 4 4 0 0 2 3 2 1 1 4 0 1 0 4 3 3 2 1 1 2 0 2 4 3 2 1 4
2 3 0 0 4 3 1 3 1 3 3 3 1 2 4 1 1 2 4 3 1 2 2 0 1 0 2 1 0 2 0 2 4 2 0 4 1
3 3 0 4 2 1 1 4 4 1 3 3 4 3 2]
```

Clustering validation: we will randomly remove 20% and then 40% of the data, to make sure the cluster will approximately maintain the same shapes.





1.5 Evaluation

Beijing and Shenyang will be the train and validation set: we can do training on a city and then validate it, and viceversa. Then, Guangzhou and Shanghai are 2 test sets.

```
[20]: train_data = pd.concat([dfs['Beijing'], dfs['Shenyang']])
X = train_data.drop('PM_HIGH', axis=1)
y = train_data['PM_HIGH']

X.head()
```

```
[20]:
         season
                 DEWP
                       HUMI
                                PRES
                                      TEMP
                                                Iws
                                                     precipitation
                                                                    cbwd_NE
                                                                              cbwd_NW \
      0
              4 -8.0
                       79.0
                              1026.0
                                      -5.0
                                             23.69
                                                               0.0
                                                                           0
                                                                                    0
      1
              4 -11.0
                       85.0
                              1021.0 -9.0
                                             105.93
                                                               1.1
                                                                           0
                                                                                    0
      2
              4 -21.0
                       43.0
                              1030.0 -11.0
                                                               0.0
                                                                           0
                                                                                    1
                                             117.55
              4 -25.0
                       33.0
                              1034.0 -12.0
                                                               0.0
      3
                                              39.35
                                                                           1
                                                                                    0
      4
              4 -24.0 30.0
                              1034.0 -10.0
                                             59.00
                                                               0.0
                                                                           1
                                                                                    0
```

cbwd_SE 0 1

```
1 1
2 0
3 0
4 0
```

[21]: KMeans(init_centroids='kmeans++', random_seed=42)

assessing the quality of the clustering with the internal cluster scoring:

Inertia score: 17196.824183523437
Silhouette score: 0.26843214299414797

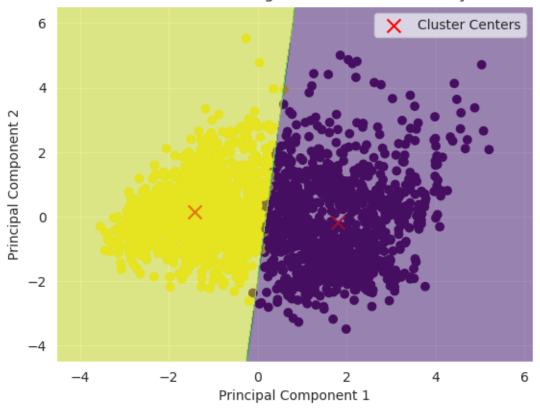
Plot of the boundaries by applying PCA dimensionality reduction, to justify the score obtained from the Silhouette score.

```
# Plot the decision boundary
h = 0.02 # step size of the meshgrid
x_min, x_max = X_pca[:, 0].min() - 1, X_pca[:, 0].max() + 1
y_min, y_max = X_pca[:, 1].min() - 1, X_pca[:, 1].max() + 1
xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))
Z = kmeans.predict(pca.inverse_transform(np.c_[xx.ravel(), yy.ravel()]))
Z = Z.reshape(xx.shape)
plt.contourf(xx, yy, Z, alpha=0.5, cmap='viridis')

# Add labels and title
plt.xlabel('Principal Component 1')
plt.ylabel('Principal Component 2')
plt.title('K-Means Clustering with Decision Boundary')

# Display the plot
plt.legend()
plt.show()
```

K-Means Clustering with Decision Boundary



Asses the similarity with the ground-truth using external cluster scoring:

Normalized Mutual Info score: 0.0028264788660817075 Adjusted Rand Index score: -0.003225155254636967

classification scoring metrics on train set:

```
[25]: y_pred_train = kmeans.predict(X_train_scaled)
print(classification_report(y_train, y_pred_train))
```

	precision	recall	f1-score	support
0.0	0.76	0.46	0.57	1687
1.0	0.30	0.61	0.40	629
accuracy			0.50	2316
macro avg	0.53	0.53	0.48	2316
weighted avg	0.63	0.50	0.52	2316

scoring metrics on validation set:

```
[26]: y_pred_val = kmeans.predict(X_test_scaled)
print("Classification scores:")
print(classification_report(y_test, y_pred_val))
```

Classification scores:

	precision	recall	f1-score	support
0.0	0.74	0.45	0.56	412
1.0	0.31	0.61	0.41	167
accuracy			0.50	579
macro avg	0.53	0.53	0.49	579
weighted avg	0.62	0.50	0.52	579

Now KMeans will be evaluated on the 2 test set (Guangzhou and Shanghai).

```
[27]: X_guangzhou = dfs['Guangzhou']
   X_guangzhou = X_guangzhou.drop('PM_HIGH', axis=1)
   X_guangzhou_scaled = scaler.transform(X_guangzhou)
   y_guangzhou = dfs['Guangzhou']['PM_HIGH']
   y_pred_guangzhou = kmeans.predict(X_guangzhou_scaled)
   print(classification_report(y_guangzhou, y_pred_guangzhou))
```

precision recall f1-score support

```
0.0
                   0.95
                             0.10
                                       0.18
                                                 1266
                   0.07
                             0.93
         1.0
                                       0.12
                                                   86
                                       0.15
                                                 1352
   accuracy
                                       0.15
                                                 1352
   macro avg
                   0.51
                             0.52
weighted avg
                   0.90
                             0.15
                                       0.18
                                                 1352
```

```
[28]: X_shanghai = dfs['Shanghai']
X_shanghai = X_shanghai.drop('PM_HIGH', axis=1)
X_shanghai_scaled = scaler.transform(X_shanghai)
y_shanghai = dfs['Shanghai']['PM_HIGH']
y_pred_shanghai = kmeans.predict(X_shanghai_scaled)
print(classification_report(y_shanghai, y_pred_shanghai))
```

	precision	recall	f1-score	support
0.0	0.80	0.27	0.41	1218
1.0	0.05	0.36	0.09	133
accuracy			0.28	1351
macro avg	0.42	0.32	0.25	1351
weighted avg	0.72	0.28	0.38	1351