CSE 412: Machine Learning Lab
Lab Activity 5: K-Means Clustering

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October 28, 2023

1 Objective

The k-means clustering method is an **unsupervised machine learning** technique used to identify clusters of data objects in a dataset. There are many different types of clustering methods, but k-means is one of the oldest and most approachable techniques. These traits make implementing k-means clustering in Python reasonably straightforward, even for new machine programmers.

In this lab activity, you will learn:

- What k-means clustering is
- When to use k-means clustering to analyze your data
- How to implement k-means clustering in Python with scikit-learn
- How to select a meaningful number of clusters

2 What Is Clustering?

Clustering is a set of techniques used to partition data into groups, or clusters. Clusters are loosely defined as groups of data objects that are more similar to other objects in their cluster than they are to data objects in other clusters. In practice, clustering helps identify two qualities of data:

- Meaningfulness
- Usefulness

Meaningful clusters expand domain knowledge. For example, in the medical field, researchers applied clustering to gene expression experiments. The clustering results identified groups of patients who respond differently to medical treatments.

Useful clusters, on the other hand, serve as an intermediate step in a data pipeline. For example, businesses use clustering for customer segmentation. The clustering results segment customers into groups with similar purchase histories, which businesses can then use to create targeted advertising campaigns.

There are many other applications of clustering, such as document clustering and social network analysis. These applications are relevant in nearly every industry, making clustering a valuable skill for professionals working with data in any field.

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3 Overview of Clustering Techniques

You can perform clustering using many different approaches–so many, in fact, that there are entire categories of clustering algorithms. Each of these categories has its own unique strengths and weaknesses. This means that certain clustering algorithms will result in more natural cluster assignments depending on the input data.

4 Mathematics behind K-Mean Clustering algorithm

K-Means is one of the simplest unsupervised clustering algorithm which is used to cluster our data into K number of clusters. The algorithm iteratively assigns the data points to one of the K clusters based on how near the point is to the cluster centroid.

1. K number of cluster centroids
2. Data points classified into the clusters

4.1 Outline of the algorithm

Assuming we have input data points $x_1, x_2, x_3, \ldots, x_n$ and value of K (the number of clusters needed). We follow the below procedure:

1. Pick K points as the initial centroids from the dataset, either randomly or the first K.
2. Find the Euclidean distance of each point in the dataset with the identified K points (cluster centroids).
3. Assign each data point to the closest centroid using the distance found in the previous step.
4. Find the new centroid by taking the average of the points in each cluster group.
5. Repeat 2 to 4 for a fixed number of iteration or till the centroids don't change.

4.2 Euclidean Distance between two points in space

We use euclidean distance to measure the distance between two points in space which is expressed as follows:

$$d(\mathbf{p}, \mathbf{q}) = \sqrt{(q_1 - p_1)^2 + (q_2 - p_2)^2}.$$

If $\mathbf{p} = (p_1, p_2)$ and $\mathbf{q} = (q_1, q_2)$ then the distance function can be implemented in Python as follows:

```
def euclidean_distance(pt1, pt2):
    return math.sqrt((pt1[0]-pt2[0])**2+(pt1[1]-pt2[1])**2)
```

4.3 Assigning each point to the nearest cluster

If each cluster centroid is denoted by c_i, then each data point x is assigned to a cluster based on

$$\arg\min_{c_i \in C} dist(c_i, x)$$

here $dist()$ is the euclidean distance. We implement this in Python as follows:

```
#find the distance between the points and the centroids
for point in data:
    distances = []
    for index in self.centroids:
         distances.append(self.distance(point,self.centroids[index]))

         #find which cluster the datapoint belongs to by finding
         #the minimum ex: if distances are 2.03,1.04,5.6,1.05
         #then point belongs to cluster 1 (zero index)
         cluster_index = distances.index(min(distances))
         self.classes[cluster_index].append(point)
```

4.4 Finding the new centroid from the clustered group of points

$$c_i = \frac{1}{|S_i|} \sum_{x_i \epsilon S_i} x_i.$$

S_i is the set of all points assigned to the ith cluster. The following function can be used to perform this task.

```
#find new centroid by taking the centroid of the points in the
#cluster class
for index in self.classes:
    self.centroids[index]=np.average(self.classes[index], axis = 0)
```

5 What is Scikit-Learn (Sklearn)

Scikit-learn (Sklearn) is the most useful and robust library for machine learning in Python. It provides a selection of efficient tools for machine learning and statistical modeling including classification, regression, clustering and dimensionality reduction via a consistence interface in Python. This library, which is largely written in Python, is built upon NumPy, SciPy and Matplotlib.

5.1 Dataset Loading

A collection of data is called dataset. It is having the following two components:

Features – The variables of data are called its features. They are also known as predictors, inputs or attributes.

- *Feature matrix* – It is the collection of features, in case there are more than one.
- *Feature Names* – It is the list of all the names of the features.

Response – It is the output variable that basically depends upon the feature variables. They are also known as target, label or output.

- *Response Vector* – It is used to represent response column. Generally, we have just one response column.
- *Target Names* – It represent the possible values taken by a response vector.

Scikit-learn have few example datasets like **iris** and **digits** for classification and the **Boston house prices** for regression.

Following is an example to load iris dataset:

```
from sklearn.datasets import load_iris
iris = load_iris()
X = iris.data
y = iris.target
feature_names = iris.feature_names
target_names = iris.target_names
print("Feature␣names:", feature_names)
print("Target␣names:", target_names)
print("\nFirst␣10␣rows␣of␣X:\n", X[:10])
```

Output:

```
Feature names: ['sepal length (cm)', 'sepal width (cm)', 'petal length (cm)',
'petal width (cm)']
Target names: ['setosa' 'versicolor' 'virginica']
First 10 rows of X:
[
[5.1 3.5 1.4 0.2]
[4.9 3. 1.4 0.2]
[4.7 3.2 1.3 0.2]
[4.6 3.1 1.5 0.2]
[5. 3.6 1.4 0.2]
[5.4 3.9 1.7 0.4]
[4.6 3.4 1.4 0.3]
[5. 3.4 1.5 0.2]
[4.4 2.9 1.4 0.2]
[4.9 3.1 1.5 0.1]
]
```

6 K-Means on Iris Dataset

Now K-Means algorithm will be applied on Iris dataset to classify our 3 classes of flowers, Iris setosa, Iris versicolor, Iris virginica (our classess) using the features collected from flowers sepal-length, sepal-width, petal-length and petal-width.

Importing libraries:

```
import pandas as pd
import numpy as np
from sklearn import datasets
from sklearn.cluster import KMeans
import matplotlib.pyplot as plt
import matplotlib.patches as mpatches
import sklearn.metrics as sm
%matplotlib inline
```

Loading dataset:

```
iris = datasets.load_iris()
```

Prining the first 5 data:

```
print (iris.data[0:5])
```

Output:

```
[[5.1 3.5 1.4 0.2]
 [4.9 3.  1.4 0.2]
 [4.7 3.2 1.3 0.2]
 [4.6 3.1 1.5 0.2]
 [5.  3.6 1.4 0.2]]
```

Prining traget names:

```
print (iris.target_names)
```

Output:

```
['setosa' 'versicolor' 'virginica']
```

Prining data labels:

```
print (iris.target)
```

Output:

```
[0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2
 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 2 2]
```

Pandas is a popular python library useful for data scientiest. Pandas data structure *DataFrame* is a way to represent and work with tabular data. It can be seen as a table that organizes data into rows and columns, making it a two-dimensional data structure. A DataFrame can be either created from scratch or you can use other data structures like **Numpy** arrays.

Converting iris data into Pandas DataFrames:

```
# assigning column labels SL, SW, PL, PW for SL: Sepal Length,
# SW: Sepal Width, PL: Petal Length and PW: Petal Width.
x = pd.DataFrame(iris.data, columns=['SL','SW','PL','PW'])
y = pd.DataFrame(iris.target, columns=['Target'])
```

Prining Data in data frames:

```
x.head()
```

Output:

	SL	SW	PL	PW
0	5.1	3.5	1.4	0.2
1	4.9	3.0	1.4	0.2
2	4.7	3.2	1.3	0.2
3	4.6	3.1	1.5	0.2
4	5.0	3.6	1.4	0.2

Prining target:

```
y.head()
```

Output:

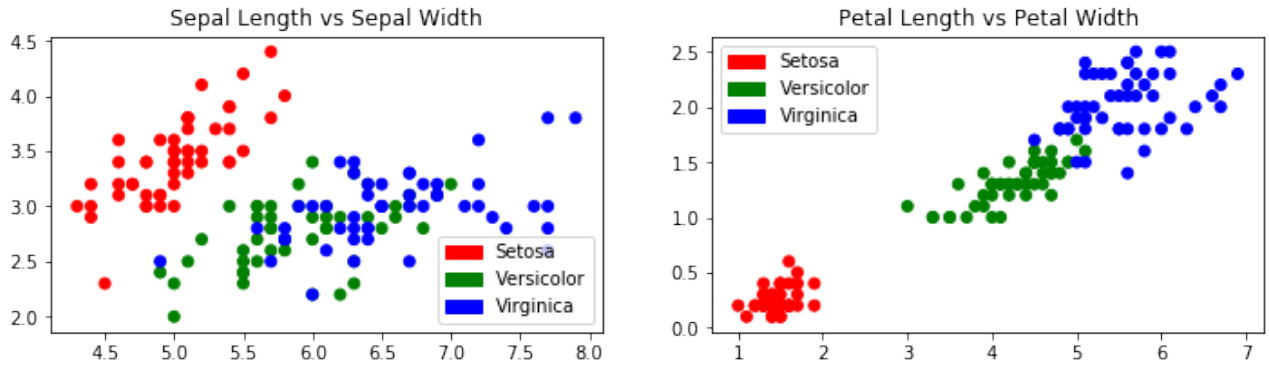
	Target
0	0
1	0
2	0
3	0
4	0

Now, lets visualize the data using scatter plots. It would be the best if we could generate a 4D scatter plot. Since it is not possible, we can visualize the relationship between any two features using a 2D scatter plot. In the following, we generated two diagrams representing Sepal Length vs Sepal Width, and Petal Length vs Petal Width respectively.

```
plt.figure(figsize=(12,3))
colors = np.array(['red', 'green', 'blue'])
iris_targets_legend = np.array(iris.target_names)
red_patch = mpatches.Patch(color='red', label='Setosa')
```

```
green_patch = mpatches.Patch(color='green', label='Versicolor')
blue_patch = mpatches.Patch(color='blue', label='Virginica')

plt.subplot(1, 2, 1)
plt.scatter(x['SL'], x['SW'], c=colors[y['Target']])
plt.title('Sepal Length vs Sepal Width')
plt.legend(handles=[red_patch, green_patch, blue_patch])

plt.subplot(1,2,2)
plt.scatter(x['PL'], x['PW'], c= colors[y['Target']])
plt.title('Petal Length vs Petal Width')
plt.legend(handles=[red_patch, green_patch, blue_patch])
```

Output:



Next, let us create a KMeans model to cluster the data. We use the entire dataset for training. Please note that, we have not split the dataset into training and test set here. However, if we want to do that, how it can be done?

```
iris_k_mean_model = KMeans(n_clusters=3)  # we set K = 3
iris_k_mean_model.fit(x) # trained using the entire dataset
```

Output:

```
KMeans(algorithm='auto', copy_x=True, init='k-means++', max_iter=300,
    n_clusters=3, n_init=10, n_jobs=None, precompute_distances='auto',
    random_state=None, tol=0.0001, verbose=0)
```

We test the model performance using the entire dataset that was used for training the model. Although, this is not an standard parctice, we are doing it to gain an insight about the KMeans algorithm.

```
print(iris_k_mean_model.predict(x))
```

Output:

```
[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 0 2 2 2 2 0 2 2 2 2
 2 2 0 0 2 2 2 2 0 2 0 2 0 2 2 0 0 2 2 2 2 2 0 2 2 2 2 0 2 2 2 0 2 2 2 0 2
 2 0]
```

The computed cluster centers can be examined using the following piece of code. Please have a careful look on the data and identify which cluster center belongs which class of iris flower. UNDERSTANDING THIS IS IMPORTANT.

```
print (iris_k_mean_model.cluster_centers_)
```

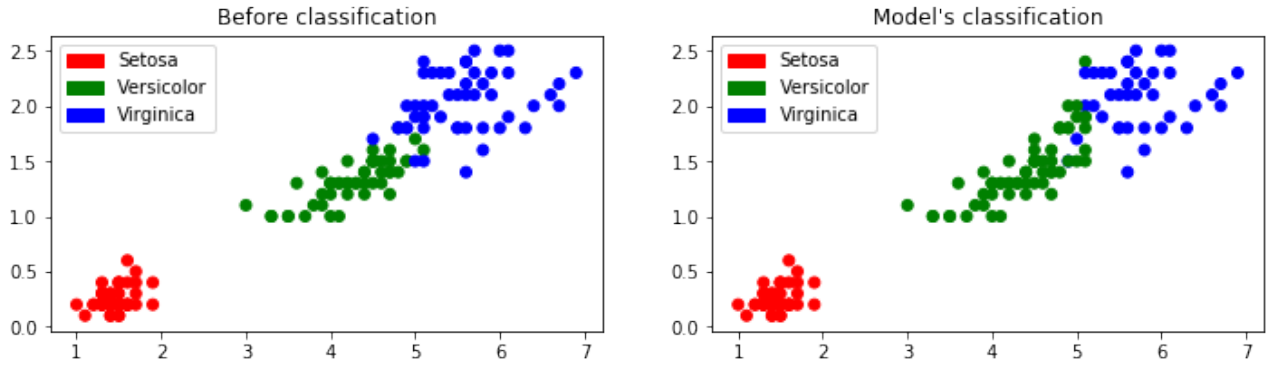
Output:

```
[[5.9016129  2.7483871  4.39354839 1.43387097]
 [5.006      3.428      1.462      0.246     ]
 [6.85       3.07368421 5.74210526 2.07105263]]
```

Now, we are interested to check the classification performance of the trained model. The following piece of code visualizes the data before classification and the classification made by the model.

```
plt.figure(figsize=(12,3))

colors = np.array(['red', 'green', 'blue'])

predictedY=np.choose(iris_k_mean_model.labels_,[1,0,2]).astype(np.int64)

plt.subplot(1, 2, 1)
plt.scatter(x['PL'], x['PW'], c=colors[y['Target']])
plt.title('Before classification')
plt.legend(handles=[red_patch, green_patch, blue_patch])

plt.subplot(1, 2, 2)
plt.scatter(x['PL'], x['PW'], c=colors[predictedY])
plt.title("Model's classification")
plt.legend(handles=[red_patch, green_patch, blue_patch])
```

Output:



At this stage, we would like to know the accuracy of the trained model. We do it using the following piece of code.

```
sm.accuracy_score(predictedY, y['Target'])
```

Output:

```
0.8933333333333333
```

And finally, we generate the confusion matrix using the following piece of code. As it can be seen, 50 out of 50 setosa has been classified successfully. However, 2 versicolor and 14 virginica flowers have be failed to detect correctly by the trained model.

```
sm.confusion_matrix(predictedY, y['Target'])
```

Output:

```
array([[50,  0,  0],
       [ 0, 48, 14],
       [ 0,  2, 36]])
```

7 Lab Exercises

Please code yourself and write a report based on your findings:

1. Split the dataset into training and testing set and evaluate their performance.
2. Evaluate the model performance using Sepal Length vs Petal Width.
3. Use your own dataset (done previously) to perform K-means clustering.