CSE 572: Lab 15

Cluster analysis seeks to partition the input data into groups of closely related instances so that instances that belong to the same cluster are more similar to each other than to instances that belong to other clusters. In this lab, you will practice implementing the K-means clustering technique.

To execute and make changes to this notebook, click File > Save a copy to save your own version in your Google Drive or Github. Read the step-by-step instructions below carefully. To execute the code, click on each cell below and press the SHIFT-ENTER keys simultaneously or by clicking the Play button.

When you finish executing all code/exercises, save your notebook then download a copy (.ipynb file). Submit the following **three** things:

1. a link to your Colab notebook,
2. the .ipynb file, and
3. a pdf of the executed notebook on Canvas.

To generate a pdf of the notebook, click File > Print > Save as PDF.

Load the dataset

We will start by loading the MNIST handwritten digits dataset. This dataset contains 8x8 grayscale images of handwritten digits from 0 to 9. Our goal in using clustering is to group images such that the handwritten digits on the images within each cluster are the same. Note: we do not split the dataset into train/val/test subsets because we are not doing classification.

```
import numpy as np
seed = 0
np.random.seed(seed)
from sklearn.datasets import load_digits

data, labels = load_digits(return_X_y=True)
```

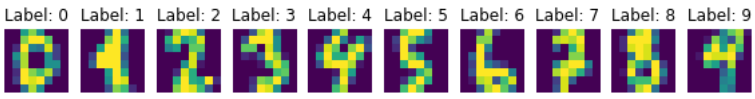
Print the number of samples and attributes in the dataset.

```
# YOUR CODE HERE
print(data.shape)
```

```
(1797, 64)
```

To get an idea of what is in our dataset, write code to visualize a random image from each class below.

```
# YOUR CODE HERE

import numpy as np
import matplotlib.pyplot as plt


unique_labels = np.unique(labels)

fig, ax = plt.subplots(1, len(unique_labels), figsize=(10, 4))
for i, label in enumerate(unique_labels):

    indices = np.where(labels == label)[0]


    idx = np.random.choice(indices)
    sample = data[idx].reshape(8, 8)

    ax[i].imshow(sample)
    ax[i].set_title(f"Label: {label}")
    ax[i].axis('off')

plt.show()
```



Next we standardize the data so that the mean of all attributes is 0 using the StandardScaler() class in scikit-learn to standardize the data.

```
from sklearn.preprocessing import StandardScaler

scaler = StandardScaler()
data = scaler.fit_transform(data)
```

K-means Clustering

The k-means clustering algorithm represents each cluster by its corresponding cluster centroid. The algorithm partitions the input data into *k* disjoint clusters by iteratively applying the following two steps:

1. Form *k* clusters by assigning each instance to its nearest centroid.
2. Recompute the centroid of each cluster.

We will first implement the standard K-means algorithm with randomly initialized centroids. We'll use 10 clusters because we have 10 classes and our goal is that each cluster contains mostly images from the same class.

```
from sklearn.cluster import KMeans

n_clusters = 10

k_means = KMeans(n_clusters=n_clusters, init='random', n_init=1, random_state=seed)
k_means.fit(data)
```

```
KMeans
KMeans(init='random', n_clusters=10, n_init=1, random_state=0)
```

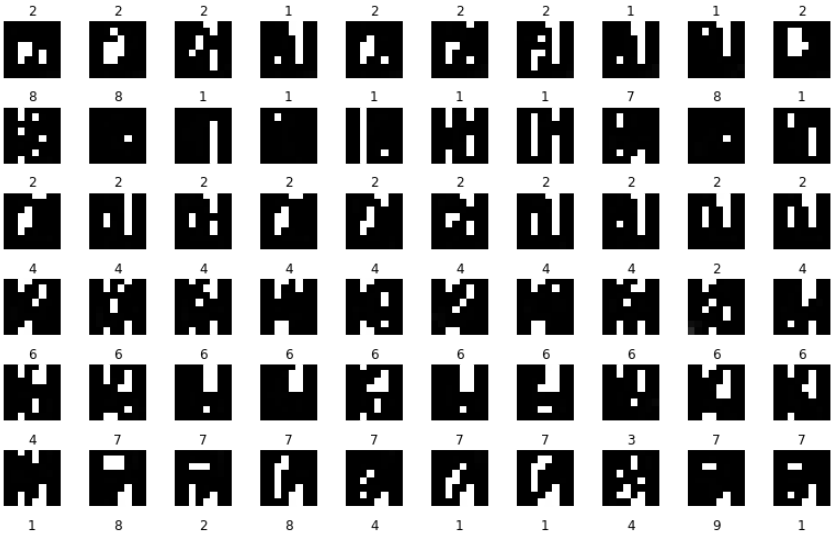
The `k_means.labels_` attribute contains the cluster labels assigned to each of our data samples. It is an array of integers representing the cluster number (starting from 0).

```
clusters = k_means.labels_

clusters
```

```
array([7, 1, 1, ..., 1, 8, 8], dtype=int32)
```

One way to evaluate how good our clustering was is to assess the homogeneity of classes in each cluster, since we know the class labels of this dataset. Below, we plot 10 examples randomly drawn from each of the 10 clusters. We plot the true class of each image in the title.

```
n_vis = 10
n_digits = n_clusters
data_rshp = data.reshape([1797, 8, 8])
fig, axes = plt.subplots(ncols=n_vis, nrows=n_clusters, figsize=(11,11))

for i in range(n_digits):
    rand_inds = np.random.randint(0, clusters[clusters==i].shape[0], size=n_vis)
    for j in range(n_vis):
        axes[i,j].imshow(data_rshp[clusters==i][rand_inds[j]].astype(np.uint8), cmap='gray')
        axes[i,j].set_title(labels[clusters==i][rand_inds[j]])
        axes[i,j].axis('off')

fig.tight_layout()
```



Looking at the homogeneity of classes in these sample subsets, we can see that the clustering was not perfect but appears to be pretty good. We can quantify this using the homogeneity score.

A clustering result satisfies homogeneity if all of its clusters contain only data points which are members of a single class. This metric is independent of the absolute values of the labels: a permutation of the class or cluster label values won't change the score value in any way.

We compute the homogeneity score below.


```
from sklearn.metrics import homogeneity_score

kmeans_homog = homogeneity_score(labels, clusters)
print('K-means homogeneity score: %f' % kmeans_homog)
```

```
K-means homogeneity score: 0.665576
```

We can also evaluate multiple algorithms by comparing the "inertia" aka "cohesiveness" aka sum of squared errors of the points within each resulting cluster. This is stored in the `inertia_` attribute.

```
print('K-means inertia: %f' % k_means.inertia_)
```

```
K-means inertia: 70668.011798
```

K-means++

K-means++ is a modified version of the K-means algorithm that chooses initial centroids to be far apart, instead of randomly choosing initial centroids. Read the scikit-learn documentation for K-means to figure out how to implement K-means++. Hint: this involves setting a specific argument.

Fit a K-means++ model for 10 clusters then compute the homogeneity score of the resulting clusters.

```
# YOUR CODE HERE
from sklearn.cluster import KMeans
from sklearn.datasets import load_digits
from sklearn.metrics import homogeneity_score

kmeans = KMeans(n_clusters=n_clusters, init='k-means++', random_state=seed)
kmeans.fit(data)

score = homogeneity_score(labels, kmeans.labels_)
print(f"Homogeneity score: {score:.3f}")
```

```
/usr/local/lib/python3.9/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarning: The default value of `n_init` will change fro
  warnings.warn(
Homogeneity score: 0.602
```

Additionally, print the inertia of the clustering resulting from K-means++.

```
# YOUR CODE HERE
print(f"K-means intertia: {kmeans.inertia_}")
```

```
K-means intertia: 69437.29782182128
```

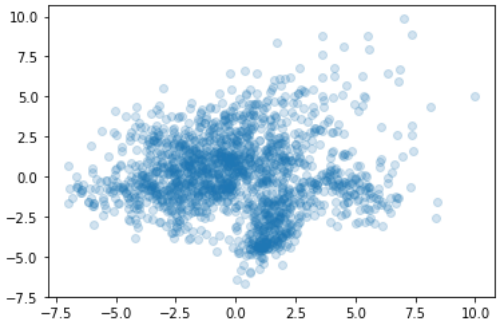
K-means + PCA

In previous lectures, we learned that dimensionality reduction techniques could be used for visualizing high-dimensional datasets in addition to being used to transform data into new features for classification. In this section, we will demonstrate using PCA for both purposes.

First, we demonstrate below how to use PCA to visualize our 64-dimensional dataset in two dimensions.

```
from sklearn.decomposition import PCA

data_pca = PCA(n_components=2).fit_transform(data)


plt.scatter(data_pca[:,0], data_pca[:,1], alpha=0.2)
```

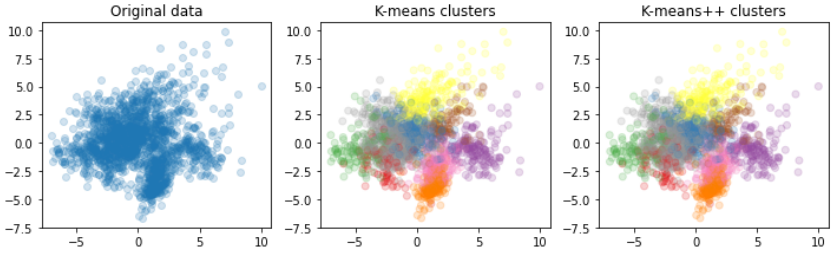
```
<matplotlib.collections.PathCollection at 0x7f42717f8760>
```



We can visualize the clusters learned by K-means and K-means++ by coloring the points in the above plot by their cluster ID from each algorithm.

```
fig, ax = plt.subplots(ncols=3, figsize=(10,3))
fig.tight_layout()

ax[0].scatter(data_pca[:,0], data_pca[:,1], alpha=0.2)
ax[0].set_title('Original data')

ax[1].scatter(data_pca[:,0], data_pca[:,1], alpha=0.2, c=clusters, cmap='Set1')
ax[1].set_title('K-means clusters')

ax[2].scatter(data_pca[:,0], data_pca[:,1], alpha=0.2, c=k_means.labels_, cmap='Set1')
ax[2].set_title('K-means++ clusters')
```

```
Text(0.5, 1.0, 'K-means++ clusters')
```



Note that even though we colored the points in PCA space by their cluster ID above, the points were clustered in the *original* feature space (not the PCA feature space).

Next, we will use PCA to reduce the data dimensionality and transform the data into new attributes **before** clustering. Fit a new K-means++ model to cluster the data in the principal subspace.

```
# YOUR CODE HERE

kmeansPCA = KMeans(n_clusters=n_clusters, init='k-means++', random_state=seed)
kmeansPCA.fit(data_pca)
```

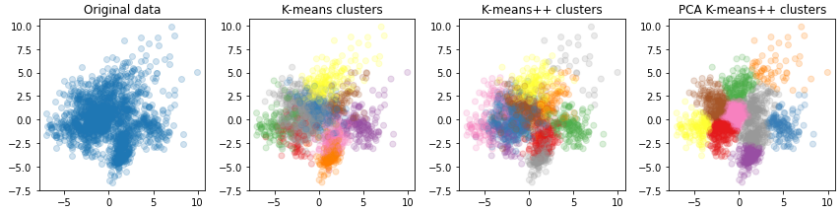
```
/usr/local/lib/python3.9/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarni
  warnings.warn(
```

```
KMeans(n_clusters=10, random_state=0)
```

Visualize the clusters by adding another subplot to the previous plot that visualizes the clustering from K-means++ after first applying PCA.

```
# YOUR CODE HERE
fig, ax = plt.subplots(ncols=4, figsize=(12,3))
fig.tight_layout()

ax[0].scatter(data_pca[:,0], data_pca[:,1], alpha=0.2)
ax[0].set_title('Original data')

ax[1].scatter(data_pca[:,0], data_pca[:,1], alpha=0.2, c=clusters, cmap='Set1')
ax[1].set_title('K-means clusters')

ax[2].scatter(data_pca[:,0], data_pca[:,1], alpha=0.2, c=kmeans.labels_, cmap='Set1')
ax[2].set_title('K-means++ clusters')

ax[3].scatter(data_pca[:,0], data_pca[:,1], alpha=0.2, c=kmeansPCA.labels_, cmap='Set1')
ax[3].set_title('PCA K-means++ clusters')
```

```
Text(0.5, 1.0, 'PCA K-means++ clusters')
```



Next, compute the homogeneity score and the inertia for the PCA + Kmeans++ clustering.

```
# YOUR CODE HERE

print(f"Homogeneity score: {homogeneity_score(labels, kmeansPCA.labels_):.3f}")
print(f"PCA K-means intertia: {kmeansPCA.inertia_}")
```

```
Homogeneity score: 0.458
PCA K-means intertia: 2816.2476898630694
```

Question 1: Which clustering had the best performance in terms of homogeneity score? Which clustering resulted in the lowest inertia (sum of squared distances of samples to their closest cluster center)?

Answer:

YOUR ANSWER HERE

We can say that Model 1 has a higher homogeneity score (0.602) than Model 2 (0.458), which suggests that Model 1 may be better at separating the data points by their class labels.

However, Model 2 has a much lower inertia (2816.247) than Model 1 (69437.298), which suggests that Model 2 has better separation of the data points overall.

Question 2: Is the homogeneity score or the inertia (SSE) a better metric for choosing the best clustering? Why?

Answer:

YOUR ANSWER HERE

A score of 1.0 indicates perfect homogeneity, and it measures how many data points from a single class are present in each cluster. In general, a greater homogeneity score is preferable because it shows that the clusters and class labels match up effectively. The homogeneity score is particularly useful in circumstances where the purpose is to find clusters that correspond to different groups or categories in the data.

The inertia, on the other hand, calculates the sum of the squared distances from each sample to the nearest cluster center, and a smaller inertia typically indicates greater clustering performance. For locating compact, clearly separated clusters in the data, the inertia is especially helpful.

If the goal is to identify clusters that correspond to different groups in the data, the homogeneity score may be more useful. If the goal is to identify well-separated clusters that capture the structure of the data, the inertia may be more useful.

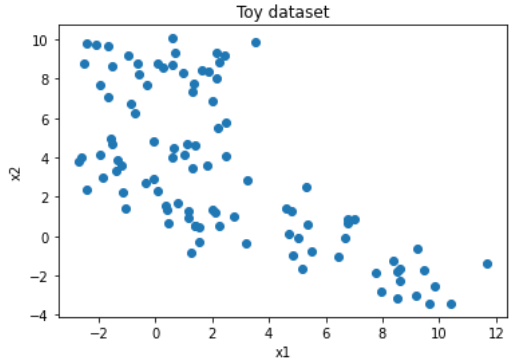
Choosing the number of clusters

In the previous examples, we used 10 clusters because we knew there were 10 classes in the dataset. However, in many use cases for clustering, we don't know which classes or how many classes are in the data, so we need a way of choosing the number of clusters to use.

To demonstrate these techniques, we will create a toy 2-dimensional dataset of blobs.

```
from sklearn.datasets import make_blobs

np.random.seed(seed)
X, _ = make_blobs(n_samples=100, centers=np.random.randint(2, 11), n_features=2, random_state=seed)


# Visualize the dataset

plt.scatter(X[:,0], X[:,1])
plt.title('Toy dataset')
plt.xlabel('x1')
plt.ylabel('x2')
```

```
Text(0, 0.5, 'x2')
```



Question 3: How many clusters do you think is the ideal number of clusters for this dataset? Restrict your answer to numbers between 1 and 10.

Answer:

YOUR ANSWER HERE 4

To determine the number of clusters in the data, we can apply k-means with varying number of clusters from 1 to 10 and compute their corresponding sum-of-squared errors (SSE) as shown in the example below. The "elbow" in the plot of SSE versus number of clusters can be used to estimate the number of clusters.

```
num_clusters = range(1, 11)
sse = []

for k in num_clusters:
    kmeans = KMeans(n_clusters=k)
    kmeans.fit(X)
    sse.append(kmeans.inertia_)

plt.plot(num_clusters, sse)
plt.xlabel('Number of Clusters')
plt.ylabel('SSE')
```

```
/usr/local/lib/python3.9/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarni
  warnings.warn(
/usr/local/lib/python3.9/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarni
  warnings.warn(
/usr/local/lib/python3.9/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarni
  warnings.warn(
/usr/local/lib/python3.9/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarni
  warnings.warn(
/usr/local/lib/python3.9/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarni
  warnings.warn(
```

Fit a K-means++ classifier to this dataset. Choose k based on the "elbow" location in the plot above. Note that scikit-learn initializes centroids using the K-means++ algorithm by default, so this was used in the previous cell too. In practice, K-means is used to describe random and K-means++ initialization of centroids interchangeably, so we will continue referring to both as simply "K-means".

```
# YOUR CODE HERE

kmeansScatter = KMeans(n_clusters=3, init='k-means++', random_state=seed)
kmeansScatter.fit(X)
```

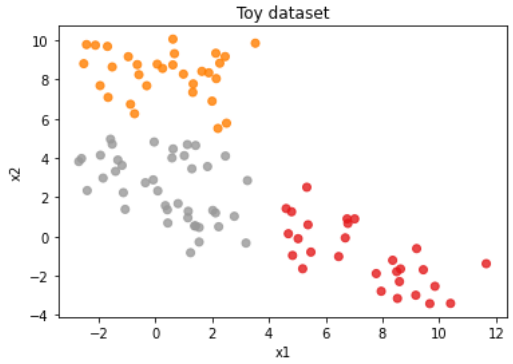
```
/usr/local/lib/python3.9/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarni
  warnings.warn(
```

```
KMeans
KMeans(n_clusters=3, random_state=0)
```

Finally, plot the toy dataset colored by the resulting clusters.

```
# Visualize the dataset

plt.scatter(X[:,0], X[:,1], alpha=0.8, c=kmeansScatter.labels_, cmap='Set1')
plt.title('Toy dataset')
plt.xlabel('x1')
plt.ylabel('x2')
```

```
Text(0, 0.5, 'x2')
```



Question 4: Was your guess from Question 3 the same as the number of clusters you chose based on the SSE plot? Why or why not?

Answer:

YOUR ANSWER HERE

No, I guessed it 4 but the elbow graph shows as 3. I particularly guess it as 4 because if you see the red cells above there is a huge gap between the two close clusters and I thought those can be broken down into two.

✓ 0s completed at 6:12 AM