INF554 - MACHINE LEARNING I
ÉCOLE POLYTECHNIQUE
Lab 9: Unsupervised Learning

1 k-Means Algorithm

k-means is one of the simplest unsupervised learning algorithms that solves the well known clustering problem. The algorithm defines an iterative process, where the following two steps take part at each iteration: (i) take each instance belonging to the dataset and assign it to the nearest centroid, and (ii) re-calculate the centroids of each of the k clusters. Thus, the k centroids change their location step by step until no more changes are done.

More formally, suppose that we are given a dataset $\mathbf{X} = \{\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_m}\}$, where each $\mathbf{x}_i \in \mathbb{R}^n$. The goal of the k-means algorithm is to group the data into k cohesive clusters, where k in as input parameter of the algorithm. Algorithm 1 gives the pseudocode of k-means.

Algorithm 1 k-Means Clustering Algorithm

Input: Dataset $\mathbf{X} = \{\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_m}\}$, where each $x_i \in \mathbb{R}^n$ and parameter k
Output: Clusters $\mathbf{C}_1, \mathbf{C}_2, \ldots, \mathbf{C}_k$ (i.e., cluster assignments of each instance $C = \{c_1, c_2, \ldots, c_m\}$)

1: Initialize cluster centroids $\mu_1, \mu_2, \ldots, \mu_k$ by choosing k instances of $\mathbf{X}$ randomly
2: **repeat**
3: Assign each instance $\mathbf{x}_i \in \mathbf{X}$ to the closest centroid, i.e., $c_i = \arg\min_j \|\mathbf{x}_i - \mu_j\|$
4: Re-compute the centroids $\mu_1, \mu_2, \ldots, \mu_k$ of each cluster based on $\mu_j = \frac{1}{|\mathbf{C}_j|} \sum_{\mathbf{x} \in \mathbf{C}_j} \mathbf{x}$, where $\mathbf{C}_j, j = 1, \ldots, k$ the j-th cluster and $|\mathbf{C}_j|$ the size of the j-th cluster
5: **until** Centroids do not change (convergence)

In the algorithm above, k is a parameter of the algorithm and corresponds to the number of clusters we want to find; the cluster centroids μ_j represent our current guesses for the positions of the centers of the clusters. To initialize the cluster centroids (in step 1 of the algorithm), we could choose k training examples randomly, and set the cluster centroids to be equal to the values of these k examples. Of course, other initialization methods are also possible, such as the kmeans++ technique[1]. To find the closest centroid, a distance (or similarity) function should be defined, and typically the Euclidean distance is used.

Based on this notion of similarity, the problem of clustering can be reduced to the problem of finding appropriate centroids. This, in turn, can be expressed as the task of minimizing the following objective

[1] Wikipedias lemma for *k-means++*: `http://en.wikipedia.org/wiki/K-means++`.

function:

$$E(k) = \sum_{j=1}^{k} \sum_{\mathbf{x}_i \in \mathbf{C}_j} \|\mathbf{x}_i - \mu_j\|. \quad (1)$$

Thus, minimizing Eq. (1) is to determine suitable centroids μ_j such that, if the data is partitioned into corresponding clusters $\mathbf{C}_j$, distances between data points and their closest cluster centroid become as small as possible.

The convergence of k-means algorithm is highly dependent on the initialization of the centroids. Although the algorithm can converge, this may be to a local minimum of the objective function of Eq. (1). One way to overcome this problem is by executing the algorithm several times, with different initializations of the centroids.

Another issue is how to set parameter k, i.e., how to determine the number of clusters of the dataset. Intuitively, increasing k without penalty, will always reduce the amount of error in the resulting clustering, to the extreme case of zero error if each data point is considered its own cluster (i.e., when k equals the number of data points, m). One such method is known as the *elbow rule*[2]. The idea is to examine and compare the sum of squared error (SSE) given in Eq. (1) for a number of cluster solutions. In general, as the number of clusters increases, the SSE should decrease because clusters are, by definition, smaller. A plot of the SSE against a series of sequential cluster levels (i.e., different values) can be helpful here. That is, an appropriate cluster solution could be defined as the one where the reduction in SSE slows dramatically. This produces an "elbow" in the plot of SSE against the different values of k.

1.1 Tasks to be done

The goal here is to apply k-means on two datasets. The first one is an artificial dataset where the data points form four distinct clusters, similar to the one shown in Fig. 1. The second one is the MNIST handwritten digits dataset that has been also used in the supervised learning labs. The basic difference here is that we do not take into account the class labels. We have applied PCA on the data and we keep the first 8 principal components. We also keep a sample of the data consisting of 1000 instances. Thus, the size of dataset $\mathbf{X}$ is 1000×8. Our goal is to apply k-means clustering on $\mathbf{X}$.

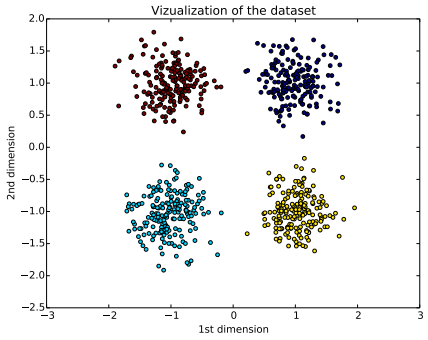


Figure 1: Example of artificial dataset.

- Fill in the code of the `kmeans()` function in the `kmeans.py` file, based on Algorithm 1.
- Run the k-means algorithm for different values of k for the two datasets and examine the quality of the produced clusters.

2 Spectral Clustering

Spectral clustering techniques make use of the *spectrum* (eigenvalues) of the similarity matrix of the data to perform dimensionality reduction before clustering in fewer dimensions. The similarity matrix

[2]Description of the *elbow rule* can be found in `http://www.mattpeeples.net/kmeans.html`.

is provided as an input and consists of a quantitative assessment of the relative similarity of each pair of points in the dataset.

Given a set of data points $\mathbf{x}_1, \ldots, \mathbf{x}_m, \forall \mathbf{x}_i \in \mathbb{R}^n$ and some notion of similarity s_{ij} between all pairs of data points $\mathbf{x}_i$ and $\mathbf{x}_j$, the intuitive goal of clustering is to divide the data points into several groups such that points in the same group are similar and points in different groups are dissimilar to each other. If we do not have more information than similarities between data points, a nice way of representing the data is in form of the similarity graph $G = (V, E)$. Each vertex v_i in this graph represents a data point $\mathbf{x}_i$. Two vertices are connected if the similarity s_{ij} between the corresponding data points $\mathbf{x}_i$ and $\mathbf{x}_j$ is positive or larger than a certain threshold, and the edge is weighted by s_{ij}. The problem of clustering can now be reformulated using the similarity graph: we want to find a partition of the graph such that the edges between different groups have very low weights (which means that points in different clusters are dissimilar from each other) and the edges within a group have high weights (which means that points within the same cluster are similar to each other).

How to create a similarity graph

There are several popular constructions to transform a given set $\mathbf{x}_1, \ldots, \mathbf{x}_m, \forall \mathbf{x}_i \in \mathbb{R}^n$ of data points with pairwise similarities s_{ij} or pairwise distances d_{ij} into a graph. When constructing similarity graphs the goal is to model the local neighborhood relationships between the data points.

- **k-Nearest Neighbors graph.** Here the goal is to connect vertex $\mathbf{x}_i$ with vertex $\mathbf{x}_j$ if $\mathbf{x}_j$ is among the k-nearest neighbors of $\mathbf{x}_i$. However, this definition leads to a directed graph, as the neighborhood relationship is not symmetric. The most common way to deal with this, is to simply ignore the directions of the edges; that is, we connect $\mathbf{x}_i$ and $\mathbf{x}_j$ with an undirected edge if $\mathbf{x}_i$ is among the k-nearest neighbors of $\mathbf{x}_j$ or if $\mathbf{x}_j$ is among the k-nearest neighbors of $\mathbf{x}_i$. The resulting graph is what is usually called the k-nearest neighbors graph.

- **The fully connected graph.** Here we simply connect all points with positive similarity with each other, and we weight all edges by s_{ij}. As the graph should represent the local neighborhood relationships, this construction is only useful if the similarity function itself models local neighborhoods. An example for such a similarity function is the Gaussian similarity function $s(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/(2\sigma^2))$, where parameter σ controls the width of the neighborhood.

The algorithm

Algorithm 2 gives the pseudocode of the spectral clustering algorithm. In spectral clustering, the data is projected into a lower-dimensional space (the spectral/eigenvector domain) where they are easily separable, say using k-means.

So, what is the reason to apply spectral clustering (in the similarity data matrix) and not applying directly k-means to the initial data? Typically, k-means algorithm is good at finding compact clusters of convex shape, while on the other hand spectral clustering methods tend to identify connectivity patterns in the similarity graph. In many cases, we are interested in finding clusters that are non-convex and in this case the k-means algorithm does not behave well. Figure 2 shows an example of a dataset where the "natural" clusters in $\mathbb{R}^2$ do not correspond to convex compact regions. Applying k-means to this dataset will extract the clusters shown in Fig. 3 (a). On the other hand, as shown in Fig. 3 (b), applying spectral clustering, we are able to find non-convex clusters with good connectivity properties.

Algorithm 2 Spectral Clustering

Input: Dataset $\mathbf{X} = \{\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_m}\}$, where each $\mathbf{x}_i \in \mathbb{R}^n$ and parameter k
Output: Clusters $\mathbf{C}_1, \mathbf{C}_2, \ldots, \mathbf{C}_k$ (i.e., cluster assignments of each instance $C = \{c_1, c_2, \ldots, c_m\}$)

1: Construct the similarity graph G using one of the ways described above. Let $\mathbf{W}$ be the adjacency matrix of this graph.
2: Compute the Laplacian matrix $\mathbf{L} = \mathbf{D} - \mathbf{W}$. Matrix $\mathbf{D}$ corresponds to the diagonal degree matrix of graph G (i.e., degree of each node v_i (= number of neighbors) in the main diagonal).
3: Apply eigenvalue decomposition to the Laplacian matrix $\mathbf{L}$ and compute the eigenvectors that correspond to k smallest eigenvalues. Let $\mathbf{U} = [\mathbf{u}_1|\mathbf{u}_2|\ldots|\mathbf{u}_k] \in \mathbb{R}^{m \times k}$ be the matrix containing these eigenvectors as columns.
4: For $i = 1, \ldots, m$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the i-th row of $\mathbf{U}$. Apply k-means to the points $(y_i)_{i=1,\ldots,m}$ (i.e., the rows of $\mathbf{U}$) and find clusters $\mathbf{C}_1, \mathbf{C}_2, \ldots, \mathbf{C}_k$.

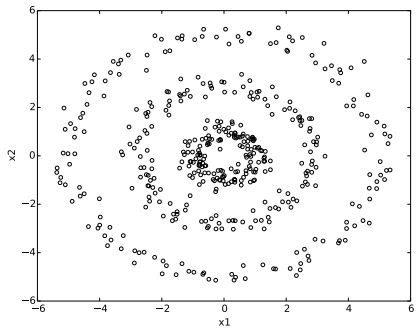


Figure 2: Example of a dataset.

2.1 Tasks to be done

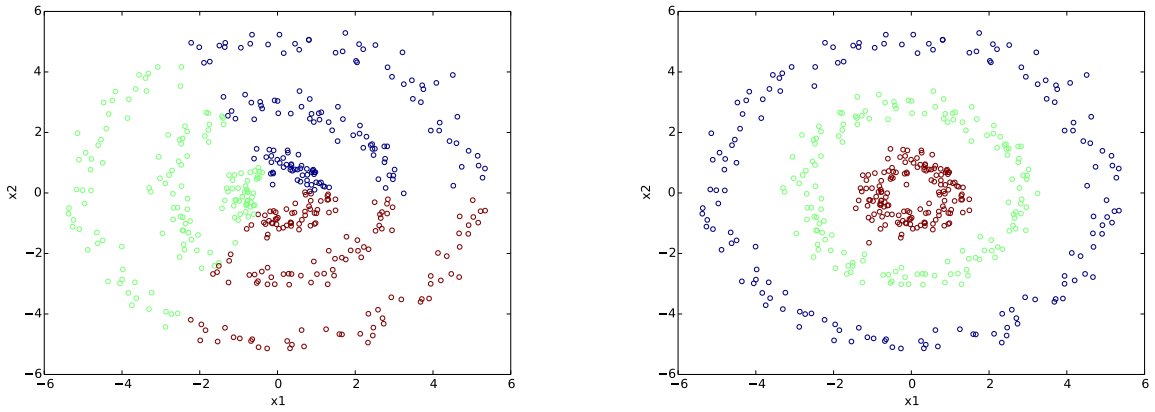
- Fill in the code of the `findClosestNeighbours` function in the `findClosestNeighbours.py` file, to find the N nearest neighbors (based on the Euclidean distance) for each instance of the dataset.
- Fill in the code of the `spectralClustering()` function in the `spectralClustering.py` file to implement the spectral clustering algorithm as described in Algorithm 2. Note that, the adjacency matrix $\mathbf{W}$ (step 1 of the algorithm) has been already created.
- Run the algorithm and reproduce the clustering results shown in Fig. 3 (b).

3 Auto Encoders

You will find `main.py` in the folder `autoencoder` which loads in the MNIST data, similarly to in the k-means task. This time, we will not apply PCA first, and we will aim to produce only 2 components, i.e., a representation $\mathbf{z}_i \in \mathbb{R}^2$ for each instance $\mathbf{x}_i$, so that we can visualize the dataset in a 2D plot.

3.1 Tasks to be done

- Using the KERAS library, build a simple auto encoder: a multi-layer perceptron, with one hidden layer of size 2 (for the encoding). Enter this code where marked `TODO` in `main.py`, after the dataset has been loaded. A suggested starting point is



(a) k-means (b) Spectral clustering

Figure 3: Results using k-means and spectral clustering algorithms.

  - `relu` and `sigmoid` activations
  - `adadelta` optimizer
  - `binary_crossentropy` loss
  - 100 epochs, batch size 32

  but you may find better values after some experimentation.

- Run the algorithm and visualize the data points in the embedded (2D) space; colours are respective of original class labels (even though these labels are not used in the learning process). The goal is to see at least some indication of *clusters* that correspond to the true classes.

References

[1] Christopher M. Bishop. "Pattern Recognition and Machine Learning". Springer-Verlag New York, Inc., 2006.

[2] Tom M. Mitchell. "Machine learning". Burr Ridge, IL: McGraw Hill 45, 1997.

[3] Ulrike Von Luxburg."A tutorial on spectral clustering". Statistics and computing, Springer, 2007.