Data Science Lab
Lab #10

Politecnico di Torino

Intro

In this laboratory, you will learn more about clustering techniques. You will first implement your own version of the K-means algorithm. Then you will apply it to different datasets and evaluate the performance achieved. In the last part of the laboratory you will work on textual data, a domain where the data preparation phase is crucial to any subsequent task. Specifically, you will try to detect topics out of a set of real-world news data. Then, you will describe each cluster through frequent itemset mining.

1 Preliminary steps

1.1 NumPy

As you may have already understood, the Python language comes with many handy functions and third-party libraries that you need to master to avoid boilerplate code. In many cases, you should leverage them to focus on the analysis process rather than its implementation.
That said, we listed a series of libraries you can make use of in this laboratory:

- NumPy
- scikit-learn
- Natural Language Toolkit
- SciPy

We will point out their functions and classes when needed. In many cases, their full understanding decreases significantly your programming effort: take your time to explore their respective documentations. Make sure you have this library installed. As usual, if not available, you need to install it with `pip install wordcloud` (or any other package manager you may be using). The `wordcloud` library is a word cloud generator. You can read more about it on its official website.

1.2 Datasets

For this lab, three different datasets will be used. Here, you will learn more about them and how to retrieve them.
The firsts two are synthetic datasets, i.e. they contain data that has been generated by hand to match a specific scientific need. Synthetic data are often used to test machine learning algorithms under conditions that are unlikely to occur with real-world data. Both datasets have been used in Fränti and Sieranoja 2018. You can find them and many more (eventually, more complex) on their official web page.
The third dataset instead is a real-world dataset containing textual news belonging to different topics.

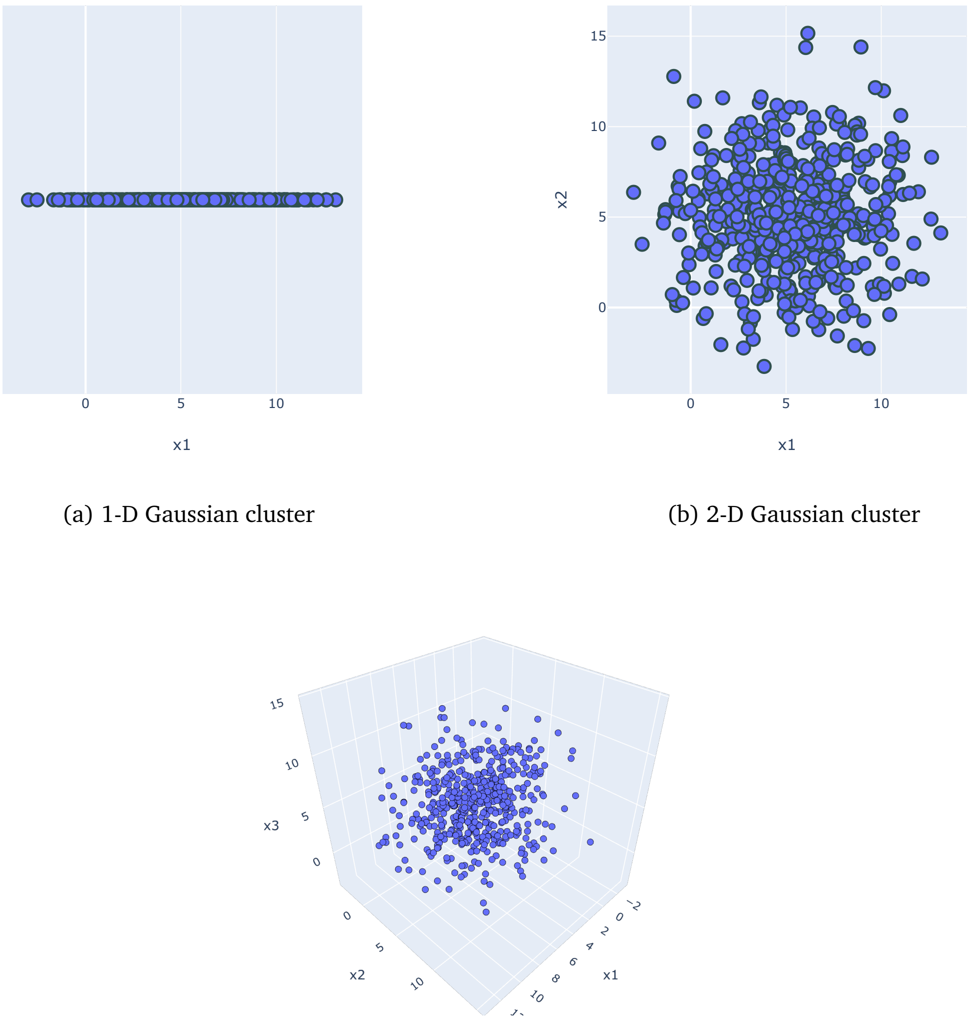
1.2.1 Synthetic 2-D Gaussian clusters

The first dataset contains several two-dimensional points distributed among separated globular clusters.

Globular clusters are also known as Gaussian clusters. In a Gaussian cluster, points coordinates follow a Gaussian distribution that share the same mean. In the context of probability theory, a Gaussian cluster is a specific case of a mixture of probability distributions, where every component follows a normal distribution. Remember that, given a mean μ and a standard deviation σ, the probability density function of a normal variable is:

$$N(x;\mu;\sigma) = \sqrt{\frac{1}{2\pi\sigma^2}} exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$

A comprehensive description of mixtures of distributions can be found in the Probability and Information Theory chapter of Goodfellow, Bengio, and Courville 2016. Figure 1 shows some examples of N-dimensional clusters.



(a) 1-D Gaussian cluster

(b) 2-D Gaussian cluster

(c) 3-D Gaussian cluster

Figure 1: Gaussian clusters obtained from $\{x1, x2, x3\} \sim N(x;5;3)$

For your convenience, we generated a 2D dataset and saved it as a `txt` file. You can download it at:

`https://raw.githubusercontent.com/dbdmg/data-science-lab/master/datasets/2D_gauss_clusters.txt`

Each of the 5,000 rows contains the x and y coordinates of a single point. These points are grouped in the Euclidean space in 15 different globular clusters.

1.2.2 Chameleon

This synthetic dataset was originally introduced in Karypis, Han, and Kumar 1999. It contains again two-dimensional data points distributed along interleaved clusters with different shapes. For your convenience, we parsed the original dataset and saved it as a `txt` file. You can download it at:

```
https://raw.githubusercontent.com/dbdmg/data-science-lab/master/datasets/chameleon_clusters.txt
```

Each of the 8,000 rows contains the x and y coordinates of a single point. These points are grouped in the Euclidean space in 6 different clusters.

1.2.3 20 Newsgroups

The 20 Newsgroups dataset was originally collected in Lang 1995. It includes approximately 20,000 documents, partitioned across 20 different newsgroups, each corresponding to a different topic.

For the sake of this laboratory, we chose $T \leq 20$ topics and sampled uniformly only documents belonging to them. As a consequence, you have $K \leq 20,000$ documents uniformly distributed across T different topics. You can download the dataset at:

```
https://github.com/dbdmg/data-science-lab/blob/master/datasets/T-newsgroups.zip?raw=true
```

Each document is located in a different file, which contains the raw text of the news. The name of the file in an integer number and corresponds to its ID.

2 Exercises

Note that exercises marked with a (*) are optional, you should focus on completing the other ones first.

2.1 K-means design and implementation

This exercise will focus on the K-means clustering technique. You will implement your own version of the algorithm and then you will test it on the two synthetic datasets.

1. Load the synthetic 2-D dataset containing Gaussian clusters.

2. Plot the data points as a scatter chart using the Matplotlib library. At first sight, you should see 15 different globular clusters. Given this distribution, which could be the most suitable clustering technique among the ones that you known? Why?

3. Focus now on the K-means technique. You can find a thorough explanation of the algorithm on the course slides on clustering (slides 16-22).

   Later in this laboratory you will use the `scikit-learn` package. Many of its functionalities are exposed via an object-oriented interface. With this paradigm in mind, implement now the K-means algorithm and expose it as a Python class. **Try to solve this exercise by using `numpy` APIs.** The bare skeleton of your class should look like this (you are free to add as many functions as you want):

   ```
   class KMeans:
       def __init__(self, n_clusters, max_iter=100):
           self.n_clusters = n_clusters
           self.max_iter = max_iter
           self.centroids = None
           self.labels = None

       def fit_predict(self, X):
           """Run the K-means clustering on X.

           :param X: input data points, array, shape = (N,C).
           :return: labels : array, shape = N.
           """
           pass
   ```

   The core method is `fit_predict`. It should execute the K-means with `K=self.n_clusters` finding the centroids and assigning the label to each data point. Note that the class is intended to be stateful: it must keep track of the obtained centroids and labels. The `max_iter` parameter should be used to specify how many iterations are allowed for the main loop of the algorithm.

4. Once you get to a fully functional version of your class, load also the Chameleon data (see Section 1.2.2) and run the K-means algorithm on both the datasets. Feel free to run multiple times the algorithm varying `n_clusters` (i.e. K). For each run, you will get two list of labels. In the next points you will try to inspect the results you obtained.

5. (*) Since you are working with two-dimensional data, you are able to visualize them and inspect the results after an algorithm run. Specifically, using the Matplotlib package, create a figure containing a scatter plot with you original data points. Then, draw onto the figure itself the centroids you obtained with a different marker and color (e.g. `marker="*", color="red"`). Create this chart for both your datasets. Where are your centroids located? Based on this, can you assess which clustering was successful and which not (or, in other words, which dataset the K-means was more efficient on)? Can you figure why?

6. (*) Let's improve your K-means class with an additional visualization tool. Add two parameters to your `fit_predict` method: `plot_clusters=False` and `plot_step=5`. If `plot_clusters` is set to True, the intermediate positions of your centroids should be displayed every `plot_step` loop iterations. Also, choose a different color for each cluster and assign it to every point belonging to it. Figure 2 shows one of such intermediate charts.

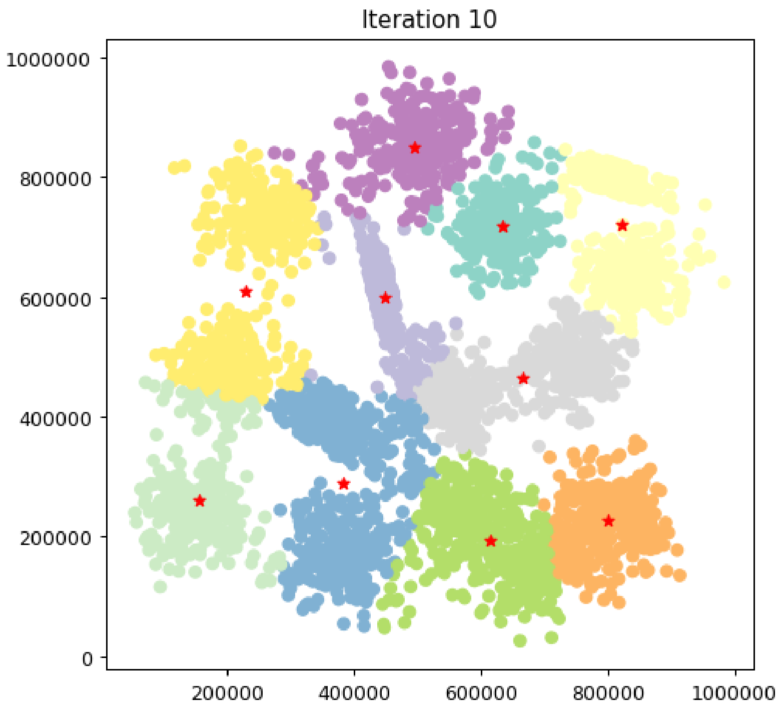


Figure 2: 2-D Gaussian synthetic dataset: clusters found at the 10*th* iteration with k=10.

2.2 Evaluate clustering performance

In this exercise you will evaluate the clustering performance of your K-means implementation. To do so, you will exploit the Silhouette measure. You can read more about it on Wikipedia.

1. Design and implement two different functions to compute the Silhouette. One should compute the metric for each sample, the other should compute the average silhouette score (you will find several evaluation scores like this in scikit-learn). **Try to solve this exercise by using `numpy` APIs.** You can start from this structure:

   ```
   def silhouette_samples(X, labels):
       """Evaluate the silhouette for each point and return them as a list.

       :param X: input data points, array, shape = (N,C).
       :param labels: the list of cluster labels, shape = N.
       :return: silhouette : array, shape = N
       """
       pass

   def silhouette_score(X, labels):
       """Evaluate the silhouette for each point and return the mean.

       :param X: input data points, array, shape = (N,C).
       :param labels: the list of cluster labels, shape = N.
       :return: silhouette : float
       """
       pass
   ```

   Note that the array `labels` is the one you generated in the previous exercise, point 4.

2. Implement a function to plot the silhouette values sorted in ascending order. This kind of chart is particularly useful to inspect the overall performance of a clustering technique. In an ideal case, the curve is heavily shifted towards the value 1 on the y-axis, i.e. most of the points have been assigned

coherently. Create the chart for both your datasets and discuss the results. Do these plots match the clustering performance that you expected looking at the scatter plots from the previous exercise, point 5? Again, can you identify on which dataset the K-Means is performing better?

3. (*) Until now, knowing in advance the number of clusters included in our datasets (either via specifications or by visualizing them) has made us able to chose the number K accordingly. This is typically not the case in real situations, either because there are more than two or three dimensions in your data or worse, a clear cluster subdivision does not exist at all. Turning the problem around, the most common task becomes choosing the K value that leads to the best possible clustering division. For what concerns the silhouette measure, the higher is the average silhouette the better are the intra-cluster cohesion and the inter-cluster separation.

   > **Warning:** the silhouette, like several other indices, is based on a geometrical distance. Maximizing such indices assures the best *geometrical* solution. However, the semantical meaning of the clusters could not be reflected. Can you imagine a way to address the problem?

   Define a function that, given a set of K values and a dataset, plots a line chart with the values of the average silhouette obtained for each K. By simply looking at it, you should be able to identify the best K for the task. Is it the one that you expected beforehand? Can you spot a trend (e.g. the higher the K value the higher the average silhouette)? Discuss this especially for the Chameleon dataset.

2.3 Newsgroups clustering

In this exercise you will build your first complete data analytics pipeline. More specifically, you will load, analyze and prepare the newsgroups dataset to finally identify possible clusters based on topics. Then, you will evaluate your process through any clustering quality measure.

1. Load the dataset from the root folder. Here the Python's os module comes to your help. You can use the `os.listdir` function to list files in a directory.

2. Focus now on the data preparation step. As you have learned in laboratory 2, textual data needs to be processed to obtain a numerical representation of each document. This is typically achieved via the application of a weighting schema.
   Choose now one among the weighting schema that you know and transform each news into a numerical representation. The Python implementation of a simple *TFIDF* weighting schema is provided in section 2.3.1, you can use it as starting point.

   This preprocessing phase is likely going to influence the quality of your results the most. Pay enough attention to it. You could try to answer the following questions:

   - Which weigthing schema have you used?
   - Have you tried to remove stopwords?
   - More generally, have you ignored words with a document frequency lower than or higher than a given threshold?
   - Have you applied any dimensionality reduction strategy? This is not mandatory, but in some cases it can improve your results. You can find more details in Appendix 2.4.

3. Once you have your vector representation, choose one clustering algorithm of those you know and apply it to your data.

4. You can now evaluate the quality of the cluster partitioning you obtained. There exists many metrics based on distances between points (e.g. the Silhouette or the Sum of Squared Errors (SSE)) that you can explore. Choose one of those that you known and test your results on your computer.

5. Consider now that our online system will evaluate your cluster quality based on the real cluster labels (a.k.a. the *ground truth*, that you do not have). Consequently, it could happen that a cluster subdivision achieves an high Silhouette value (i.e. *geometrically* close points were assigned to the same cluster) while the matching with the real labels gives a poor score (i.e. real labels are heterogeneous within your clusters).
   In order to understand how close you came to the real news subdivision, upload your results to our online verification system (you can perform as many submission as you want for this laboratory, the only limitation being a time limit of 5 minutes between submissions). Head to Section **??** to learn more about it.

2.3.1 A basic TFIDF implementation

The transformation from texts to vector can be simplified by means of ad-hoc libraries like Natural Language Toolkit and scikit-learn (from now on, `nltk` and `sklearn`). If you plan to use the *TFIDF* weighting schema, you might want to use the sklearn's `TfidfVectorizer` class. Then you can use its `fit_transform` method to obtain the *TFIDF* representation for each document. Specifically, the method returns a SciPy sparse matrix. You are encouraged to exhaustively analyze TfidfVectorizer's constructor parameters since they can significantly impact the results. Note for now that you can specify a custom `tokenizer` object and a set of stopwords to be used.

For the sake of simplicity, we are providing you with a simple tokenizer class. Note that the TfidfTokenizer's tokenizer argument requires a callable object. Python's callable objects are instances of classes that implement the `__call__` method. The class makes use of two nltk functionalities: word_tokenize and the class WordNetLemmatizer. The latter is used to lemmatize your words after the tokenization. The *lemmatization* process leverages a morphological analysis of the words in the corpus with the aim to remove the grammatical inflections that characterize a word in different contexts, returning its base or dictionary form (e.g. {am, are, is} ⇒ be; {car, cars, car's, cars'} ⇒ car).
For what concerns the stop words, you can use again a nltk already-available function: stopwords.
The following is a snippet of code including everything you need to get to a basic *TFIDF* representation:

```python
from sklearn.feature_extraction.text import TfidfVectorizer
from nltk.tokenize import word_tokenize
from nltk.stem.wordnet import WordNetLemmatizer
from nltk.corpus import stopwords as sw


class LemmaTokenizer(object):
    def __init__(self):
        self.lemmatizer = WordNetLemmatizer()

    def __call__(self, document):
        lemmas = []
        for t in word_tokenize(document):
            t = t.strip()
            lemma = self.lemmatizer.lemmatize(t)
            lemmas.append(lemma)
        return lemmas


lemmaTokenizer = LemmaTokenizer()
vectorizer = TfidfVectorizer(tokenizer=lemmaTokenizer, stop_words=sw.words('english'))
tfidf_X = vectorizer.fit_transform(corpus)
```

2.4 Cluster characterization by means of word clouds and itemset mining

In many real cases, the *real* clustering subdivision is not accessible at all[1]. Indeed, it is what you want to discover by clustering your data. For this reason, it is commonplace to add a further step to the pipeline and try to characterize the clusters by inspecting their points' characteristics. This is especially true while working with news, where the description can lead to the identification of a topic shared among all the documents assigned to it (e.g. one of your clusters may contain news related to sports).

In this exercise you will exploit word clouds and frequent itemset algorithms to characterize the clusters obtained in the previous exercise.

1. Split your initial data into separate chunks accordingly to the cluster labels obtained in the previous exercise. For each of them, generate a Word Cloud image using the `wordcloud` library. Take a look at the library documentation to learn how to do it. Can you figure out the topic shared among all the news of each cluster?

2. Let's adopt frequent itemset mining algorithms to further characterize your clusters. Choose one algorithm and run it for each cluster of news. Try to identify the most distinctive set of words playing around with different configurations of the chosen algorithm. Based on the results, can you identify any topic in any of your clusters?

[1] Or worse, it might not exist at all.

Appendix

Notions on linear transformations and dimensionality reduction

In many real cases, your data comes with a large number of features. However, there is often a good chance that some of them are uninformative or redundant and have the only consequence of making your analysis harder. The simplest example could be features that are linearly dependent with each other (e.g. a feature that describes the same information with different, yet correlated units, like degrees Celsius and Fahrenheit).

One additional detail can be addressed in your preprocessing step, other than the dimensionality reduction. There might be cases where the distribution of your data has hidden underlying dynamics that could be enhanced by choosing different features (i.e. dimensions). Figure 3 shows several points distributed in a Gaussian cluster (see Laboratory 4). Let's make now an assumption: quantitatively we assess that directions with largest variances in our space contain the dynamics of interest. In Figure 3 the direction with the largest variance is not (1,0) nor (0,1), but the direction along the long axis of the cluster.

As you will soon learn, in the known literature there is a proven method that addresses the aforementioned problems: the *Principal Component Analysis* (PCA). This technique frames the problem as a linear change of basis. The final basis vector are commonly termed *principal components*. Let's qualitatively understand why and how it is made by means of a few algebraic notions.

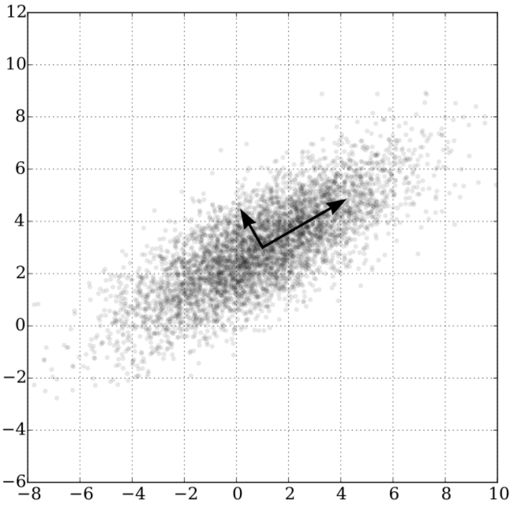


Figure 3: Points distributed in a Gaussian cluster with mean (1,3) and standard deviation 3. Source: Wikipedia

In PCA we assume that there exist a more meaningful basis to re-express our data. The hope is that this new basis will filter out the noise and reveal hidden dynamics. Following the assumption presented beforehand, the new basis must align the directions with the highest variance. Also, the change of basis follows another strict, yet powerful assumption: it is assumed that the new basis is a linear combination of the original one (studies expanded on this to non linear domains). In Figure 3 PCA would likely identify a new basis in the directions of the two black arrows.

In other words, if we call **X** the original set of data, in PCA we are interested in finding a matrix **P** that stretches and rotates our initial space to obtain a more convenient representation **Y**:

$$PX = Y \tag{1}$$

Now that foundations are laid, we know that we are looking for a new basis that highlights the inner dynamics and we assume that the change of basis can be achieved with a simple linear transformation. This linearity assumption let us solve analytically the problem with matrix decomposition techniques. Even if the simpler eigendecomposition can be used, the state-of-the-art solution is obtained through the *Singular Value Decomposition* (SVD).

Many, many theoretical and technical details have been left behind in this short summary. If you are willing to learn more, you can find a thorough tutorial about PCA, SVD and their relationship in Shlens 2014.

The use of the PCA algorithm via SVD decomposition in Python is straightforward. The following lines show how you can apply the change of basis transforming your data.

```python
from sklearn.decomposition import TruncatedSVD

# X: np.array, shape (1000, 20)
svd = TruncatedSVD(n_components=5, random_state=42)
red_X = svd.fit_transform(X)    # red_X will be: np.array, shape (1000, 5)
```

Note that the `TruncatedSVD` class lets you choose how many top-principal components to retain (they are ranked by explained variance). Doing so, you will be applying the dimensionality reduction at the same time.

References

[1] Pasi Fränti and Sami Sieranoja. *K-means properties on six clustering benchmark datasets*. 2018. URL: http://cs.uef.fi/sipu/datasets/.

[2] Ian Goodfellow, Yoshua Bengio, and Aaron Courville. *Deep Learning*. http://www.deeplearningbook.org. MIT Press, 2016.

[3] George Karypis, Eui-Hong Sam Han, and Vipin Kumar. “Chameleon: Hierarchical clustering using dynamic modeling”. In: *Computer* 8 (1999), pp. 68–75.

[4] Ken Lang. “Newsweeder: Learning to filter netnews”. In: *Proceedings of the Twelfth International Conference on Machine Learning*. 1995, pp. 331–339.

[5] Jonathon Shlens. “A Tutorial on Principal Component Analysis”. In: *CoRR* abs/1404.1100 (2014). arXiv: 1404.1100. URL: http://arxiv.org/abs/1404.1100.