Lecture 9: Clustering, K-means and Gaussian Mixture Models (GMM) Part I

Statistical Methods for Data Science

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Today

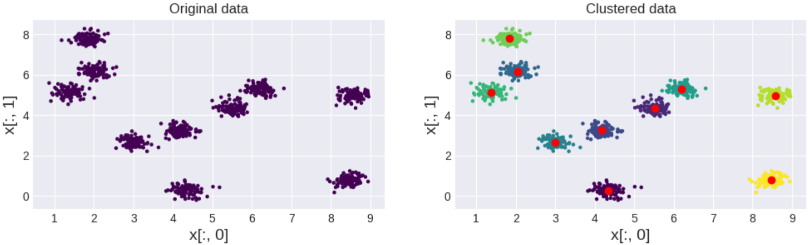
Learning outcome

- Understand the difference between supervised learning and unsupervised learning
- Understand how to apply clustering algorithms to the applications discussed in this lecture
- Be able to compute histograms for high dimensional data
- Be able to compute the dissimilarity matrix with the Euclidean distance
- Be able to explain how to identify clusterability using the Hopkins statistic
- Be able to implement the K-means algorithm

Today

Clustering

- We start with blobs of data
- We assign some semantics to each of these data points

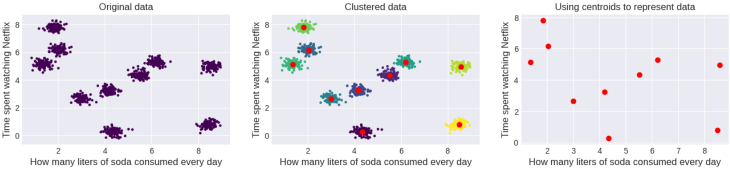


- Each of these semantics is called a **cluster**
- The process of finding clusters is called **clustering**

Application

Clustering is widely used in different applications - clustering algorithm development **does not require expensive annotations**

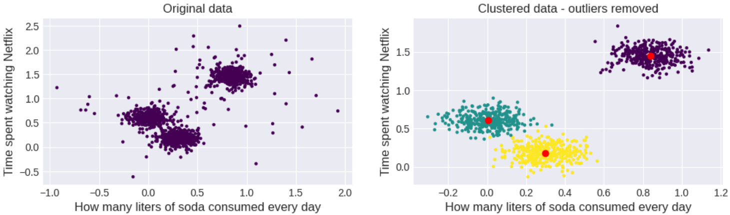
1. Clustering as a preprocessing method
   1.1 To summarize a large amount of data using their clusters
   Example: you have access to the time people spend on Netflix and the amount of soda they consume everyday; you want to make a more advanced summary from this data set



Group these people into clusters and correlate these patterns with other data sources

Application (cont.)

1. Clustering as a preprocessing method (cont.)
   1.2 To detect and remove **outliers** - data points that are far away from any clusters

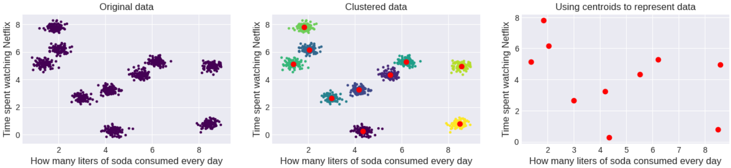


Without clustering, it is hard to define what should be considered outliers when the data distribution is **complex**:

- High dimensionality
- Data cannot be modeled with a single probability distribution

Application (cont.)

2. Clustering as a data reduction technique
    2.1 To reduce a large amount of data into fewer data points by, e.g., representing the data set with only the centroids - the set up is similar to 1.1

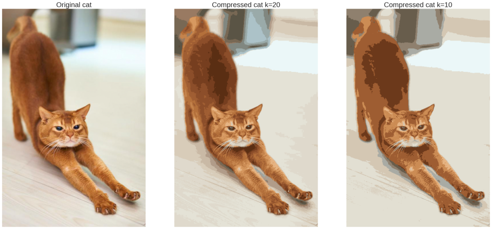


One important application is the **recommender system**

- Task: find patterns in preferred items from massive amount of users
- Challenge: there are too many users
- Solution: we recommend items to users on a cluster level

Application (cont.)

2. Clustering as a data reduction technique (cont.)
   2.2 Image compression



- Each data point is a pixel in the image, i.e. $\boldsymbol{x} = [red, green, blue] = [x_1, x_2, x_3]$, where $red, green, blue \in [0, 255]$ integers
- Run clustering algorithms in this RGB color space and find K centroids
- Replace each pixel by its closest centroid
- Now we only use $3 \times K$ unique values to represent the image instead of 3×256 values
- In this example, with $K = 10$ centroids, when we save the .png image, we have a reduction from 328.5 kB to 43.4 kB

Today

Clustering modeling

- Modeling for clustering

$$y = g(x; \theta \mid h)$$

- Clustering:
  - y: **categorical (nominal)**, scalar - each category is called a **cluster**
  - x: typically **continuous numerical**; feature vector $\boldsymbol{x} = [x_1, \cdots, x_d]$ (similar to classification problems in lecture 5)
  - g: **clustering model**, e.g. K-means, Gaussian mixture models, hierarchical clustering models, etc
    There are mainly four categories of clustering models
    - **Centroid clustering**
    - **Distribution clustering**
    - Density clustering
    - Hierarchical clustering
  - θ (parameters) and h (hyperparameters) depend on g

Parameter estimation

- Clustering models are **unsupervised learning** algorithms
- In unsupervised learning, the parameters are estimated from an **unlabeled data set**, that is, a data set contains only the feature vectors $\{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N\}$, e.g.

  $\{$  ,  , $\cdots$,  $\}$

  where $\boldsymbol{x}_i$ = pixel values in a picture and the task is to group **similar** ducks into the same cluster
- **Similarity** is not well defined
- Clustering tasks do not require annotations - it is cheaper, but also more difficult because there are no predefined clusters!
- In this course, we will look at one commonly used parameter estimation technique called the **Expectation-Maximization (EM)** algorithm

Models in this course

We are going to introduce various categories of clustering techniques; then we focus on two clustering models

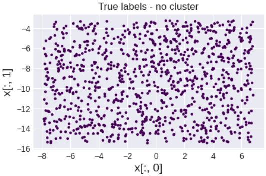
- K-means
    - **Parameters**: K centroids
    - **Hyperparameters**: K
    - **Parameter estimation**: an iterative method to update the centroids until convergence; this method can be interpreted as a simplified version of the Expectation-Maximization algorithm
- Gaussian mixture models
    - **Parameters**: K priors, K Gaussian likelihood (the big two!)
    - **Hyperparameters**: the number of Gaussian components K
    - **Parameter estimation**: the Expectation-Maximization algorithm

Today

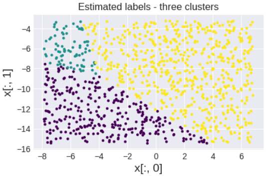
Are there clusters in the data?

Let's try something out!

- Generate some data $\{[x_1^1, x_1^2], \cdots, [x_N^1, x_N^2]\}$ from a uniform distribution for $i = 1, \cdots, N$, $j = 1, 2$ 😃



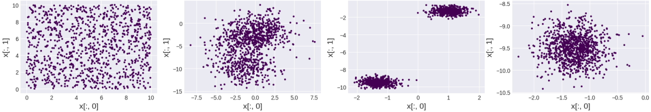
- Run a clustering algorithm - go you magical beast! 😋



😭

Take a step back: is the data "clusterable"?

- Do you see any clusters in the following plots?



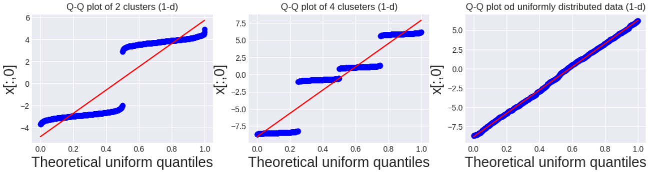
  - Figure 1: data is generated from a uniform distribution - no cluster
  - Figure 2: data is generated from three different Gaussian distributions - three clusters
  - Figure 3: data is generated from two different Gaussian distributions - two clusters
  - Figure 4: data is generated from one Gaussian distribution - one cluster
- How to decide if the data is culsterable
  - Need to define what a cluster is
  - Need to define the "null hypothesis", i.e. the situation where there are no clusters **Note: the "null hypothesis" is in quotes because it does not have to be described by a probabilistic distribution**
- There is no ground truth label - there are various ways of defining these prerequisites, which makes it a difficult task!
- Now spend 30 secs staring at the plots and try to think how you can measure if the data is clusterable

Cluster tendency

The general idea is to compare the data distribution with a theoretical distribution with no cluster tendency!

Let $\boldsymbol{x}_i = \left[x_1^i, \quad \cdots, \quad x_d^i\right]$ be a feature vector **when we need to index both the dimension and the data point, we use superscript to index the data point and use subscript to index the dimension**

- For example, we can make a qq-plot to compare the set $\{x_j^1, \cdots, x_j^N\}$ and a non-clusterable theoretical probability distribution, e.g. a uniform distribution



- We can repeat this for all dimensions $j = 1, \cdots, d$
- But then the question is how to aggregate all these d dimensions? - Not easy!
- **Comparing distributions gets trickier when $d > 1$!**

Cluster tendency (cont.)

- Luckily, we have some other techniques that can help us!
- In this course, we briefly introduce the following techniques
  - Distance based technique
    - Distance measure
    - Pairwise distance
    - Dissimilarity matrix
  - Hopkins statistic
  - Histogram based technique
    - Histogram for high dimensional data

Distance based approach

Distance based approach

- Distance measure
  - Defines how "similar" two items are
  - The most commonly used distance is the Euclidean distance
  - Example: let $\boldsymbol{x} = [x_1, x_2, x_3]$ and $\boldsymbol{y} = [y_1, y_2, y_3]$ be two feature vectors, the Euclidean distance is defined as

$$d(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + (x_3 - y_3)^2}$$

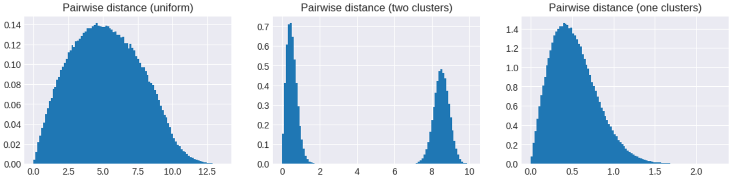
- Pairwise distance
  - Distances between all pairs of data points from two sets
  - Example: let $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3\}$ and $\{\boldsymbol{y}_1, \boldsymbol{y}_2\}$ be two sets, the pairwise distance is defined as

$$\{d(\boldsymbol{x}_1, \boldsymbol{y}_1), d(\boldsymbol{x}_1, \boldsymbol{y}_2), d(\boldsymbol{x}_2, \boldsymbol{y}_1), d(\boldsymbol{x}_2, \boldsymbol{y}_2), d(\boldsymbol{x}_3, \boldsymbol{y}_1), d(\boldsymbol{x}_3, \boldsymbol{y}_2)\}$$

- The general idea is to compare the **distribution of the pairwise distance computed from the data** to the one computed from a distribution without clustering tendency, e.g. a **uniform distribution**

Distance based approach (cont.)

- Pairwise distance (cont.)
  - A very simplistic example



- Dissimilarity matrix
  - A matrix that contains pairwise distance $d(\boldsymbol{x}_i, \boldsymbol{y}_j)$ on its $(i, j)^{th}$ position

$d(\boldsymbol{x}_1, \boldsymbol{y}_1)$	$d(\boldsymbol{x}_1, \boldsymbol{y}_2)$	$d(\boldsymbol{x}_1, \boldsymbol{y}_3)$
$d(\boldsymbol{x}_2, \boldsymbol{y}_1)$	$d(\boldsymbol{x}_2, \boldsymbol{y}_2)$	$d(\boldsymbol{x}_2, \boldsymbol{y}_3)$

  - It is very useful in many machine learning algorithms
  - **Ordered dissimilarity matrix**: reorder the similarity matrix to group similar items together

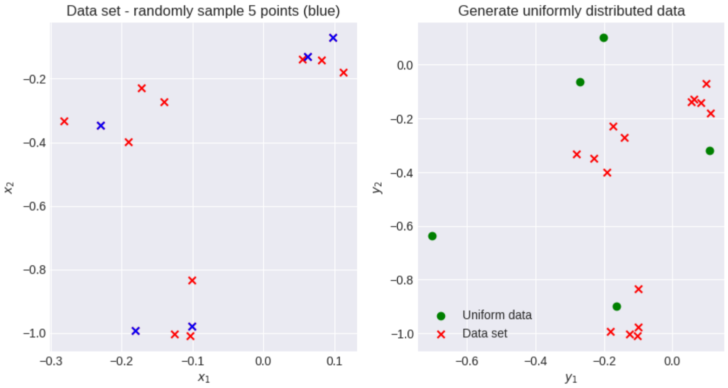
Hopkins statistic

Hopkins statistic for testing cluster tendency

- **Data**: $\mathcal{X} = \{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N\}$ from unknown distribution
- **Null hypothesis** H_0: there is no cluster tendency in the data set
- **Test statistic** h: Hopkins statistic **Just when you thought you'd never see hypothesis testing ever again... Bam!**
- **Computation**

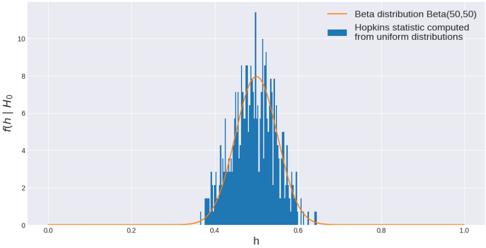
1: Choose an integer $M \ll N$ (sparse sampling)
2: Generate a sample of uniformly distributed data with sample size M: $\{\boldsymbol{y}_1, \cdots, \boldsymbol{y}_M\}$
3: Randomly choose M data points (without replacement) from $\mathcal{X}$: $\{\boldsymbol{x}_{m_1}, \cdots, \boldsymbol{x}_{m_M}\}$
4: **for** $i = 1$ to M **do**
5: Find the **nearest neighbor of $\boldsymbol{y}_i$** in $\mathcal{X}$: $\boldsymbol{y}$
6: Compute the distance between $\boldsymbol{y}_i$ and $\boldsymbol{y}$: $u_i = dist(\boldsymbol{y}_i, \boldsymbol{y})$
7: Find the **nearest neighbor of $\boldsymbol{x}_{m_i}$** in $\mathcal{X}$: x
8: Compute the distance between $\boldsymbol{x}_{m_i}$ and $\boldsymbol{x}$: $w_i = dist(\boldsymbol{x}_{m_i}, \boldsymbol{x})$
9: **end for**
10: $h_0 = \frac{\sum_{i=1}^M u_i^d}{\sum_{i=1}^M u_i^d + \sum_{i=1}^M w_i^d}$

Hypothesis testing using Hopkins statistic (cont.)



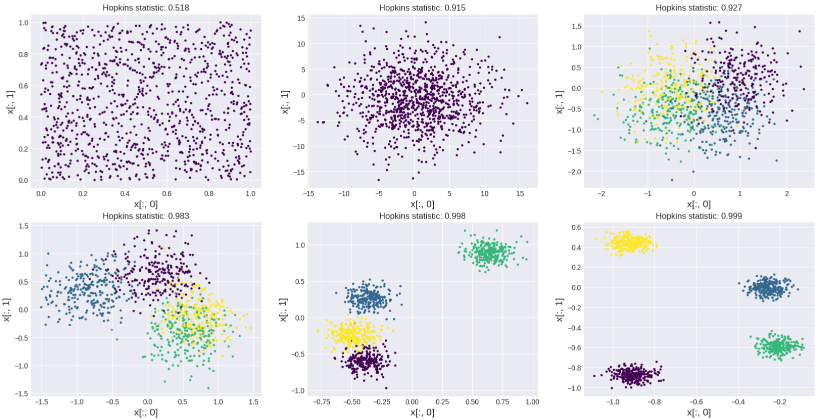
Hypothesis testing using Hopkins statistic (cont.)

- **Null distribution**:
  - PDF: Beta distribution with parameters $a = M$ and $b = M$
  - Python: stats.beta.pdf(x, M, M)



- Note: there are variations of the Hopkins statistic; in general, when the Hopkins statistic deviates from 0.5 significantly, it indicates cluster tendency

Hypothesis testing using Hopkins statistic (cont.)



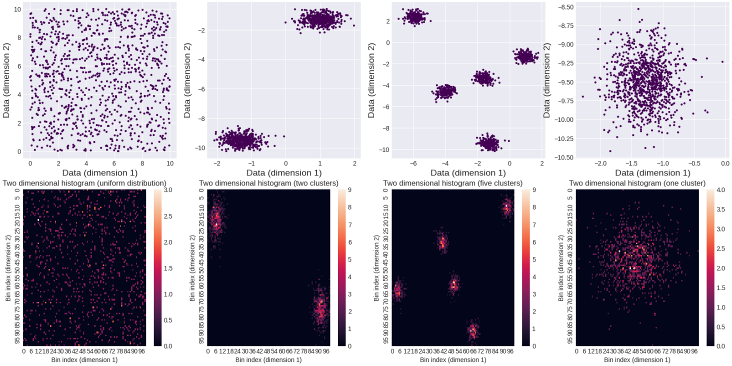
Histogram based technique

Histogram for high dimensional data

- High dimensional histogram - empirical joint distribution $f_{X_1,\cdots,X_d}(X_1,\cdots,X_d)$
- **Compute histogram for d dimensional data**

1: **for** $i = 1$ to d **do**
2: For dimension i, divide the range of data into n bins with the same size
3: **end for**
4: **for** $j = 1$ to n **do**
5: Count the number of points in each cell j - each cell is a d dimensional cell
6: **end for**

Histogram for high dimensional data (cont.)



Compare two distributions using d dimensional histograms

- Recall that our task here is to compare two distributions: a high dimensional data distribution and a theoretical distribution without cluster tendency, e.g. a uniform distribution - now we would like to compare this d dimensional histogram to a d dimensional theoretical distribution
- But high dimensional theoretical distribution can be hard to manipulate, for example, the area under the surface with integration is difficult
- We typically approximate high dimensional theoretical distributions using sampling techniques
- Pseudo-algorithm to illustrate the idea
  1: Given a data set $\mathcal{X} = \{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N\}$
  2: Compute the d dimensional histogram for $\mathcal{X}$
  3: Sample N data points from a d dimensional uniform distribution and compute the d dimensional histogram
  4: Compare these two histograms using, e.g. the **Kullback–Leibler divergence**

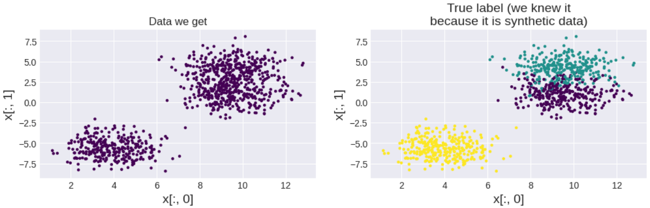
What we have seen so far

- Definition and modeling of clustering
- Applications of clustering
    - As a preprocessing technique, e.g. summarize data, detect outliers
    - As a data reduction technique, e.g. recommender system on a cluster level, image compression
- Testing cluster tendency test by comparing two distributions using 1) pairwise distance, 2) Hopkins statistic and 3) d dimensional histograms

Today

K-means

- **Data** x: d dimensional feature vector $\boldsymbol{x}$



- **Target** y:

$$y = \arg\min_{k \in \{1, \cdots, K\}} dist(\boldsymbol{x}, \boldsymbol{\mu}_k)$$

where $dist(\cdot, \cdot)$ is a distance measure; in this course, we use the Euclidean distance (cf. page 21)

- **Parameters**: K centroids
- **Hyperparameters**: K
- **Parameter estimation**: an iterative method to update the centroids until convergence
- It is a **hard clustering** technique - one data point is assigned to only one cluster

K-means parameter estimation algorithm

- Algorithm
  - **Randomly choose K centroids $\boldsymbol{\mu}_k$** for $k = 1, \cdots, K$, e.g. randomly choose K data points from $\mathcal{X}$
  - Repeat the two steps below until convergence, e.g. $\boldsymbol{\mu}_k$ does not change anymore
    - For all $i = 1, \cdots, N$, assign $\boldsymbol{x}_i$ to a cluster $\hat{k}_i$ by computing

$$\hat{k}_i = \arg \min_{k \in \{1, \cdots, K\}} dist(\boldsymbol{x}_i, \boldsymbol{\mu}_k)$$

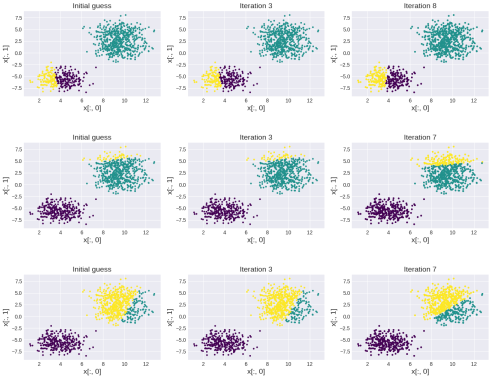
    - Let $\mathcal{X}_k$ be the set of all $\boldsymbol{x}_i$ assigned to cluster k and N_k be the size of $\mathcal{X}_k$, compute

$$\boldsymbol{\mu}_k \leftarrow \frac{1}{N_k} \sum_{\boldsymbol{x}_j \in \mathcal{X}_k} \boldsymbol{x}_j$$

- There is some **randomness** in the algorithm - we should always be careful when there is randomness

K-means initial guess

Different initializations result in different clusters



A typical solution is to run the algorithm multiple times with different initial points and aggregate the results

K-means parameter estimation pseudocode

Given a data set $\mathcal{X} = \{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N\}$
Randomly choose K data points from $\mathcal{X}$ as the centroids $\boldsymbol{\mu}_k$ for $k = 1, \cdots, K$
while true **do**
    Assign $\boldsymbol{x}_i$ to the closest $\boldsymbol{\mu}_k$ for all $i = 1, \cdots, N$
    For all $k = 1, \cdots, K$, compute $\boldsymbol{\mu}_k^{new}$ as the center of all $\boldsymbol{x}_i$ assigned to class k
    if $\boldsymbol{\mu}_k^{new} == \boldsymbol{\mu}_k$ for all k **then**
        break
    else
        $\boldsymbol{\mu}_k \leftarrow \boldsymbol{\mu}_k^{new}$
    end if
end while

K-means: pros and cons

- Pros:
  - Convergence guaranteed
  - Easy to implement
  - Scale to large data sets
- Cons - **potential improvement**:
  - Need to choose the hyperparameter K manually - **gradually increase K and monitor the loss during parameter estimation** - discussed in the next lecture
  - Dependence on random initial values - **multiple initial values**
  - Do not work well on very high dimensional data - **apply dimensionality reduction techniques before clustering**
  - Not robust to outliers - **try to remove outliers before clustering**

Today

Summary

So far:

- Data types and data containers
- Descriptive data analysis: descriptive statistics, visualization
- Probability distributions, events, random variables, PMF, PDF, parameters
- CDF, Q-Q plot, how to compare two distributions (data vs theoretical, data vs data)
- Modeling
- Parameter estimation: maximum likelihood estimation (MLE) and maximum a posteriori estimation (MAP)
- Classification, multinomial naive Bayes classifier, Gaussian naive Bayes classifier
- Central limit theorem, interval estimation
- Hypothesis tests, comparison of two classifiers
- Clustering, cluster tendency, k-means

Next:

- More clustering models

Before next lecture:

- Gaussian distribution
- The Bayes' rule