Lecture 8: Clustering (Part I)

Statistical Methods for Data Science

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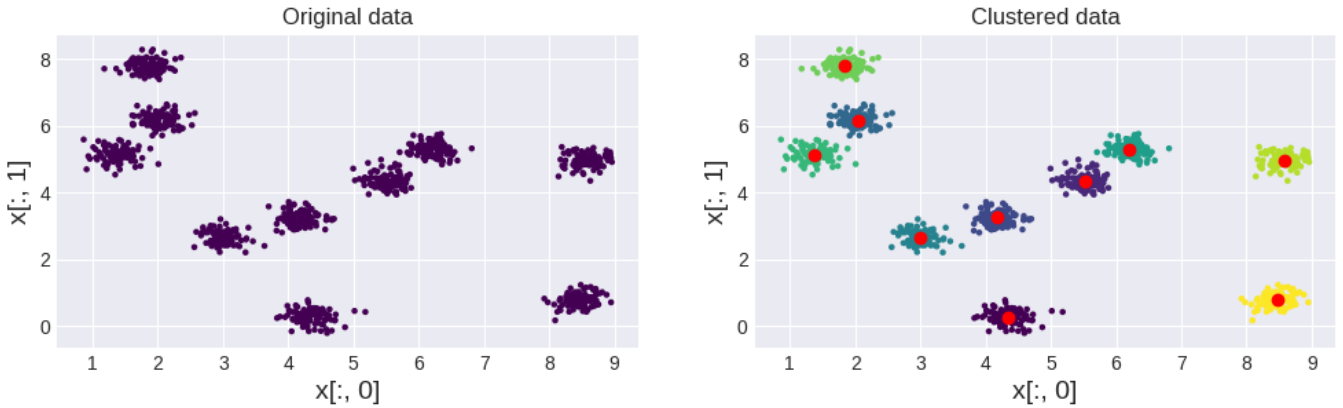
Learning outcome

- 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 implement the K-means algorithm
- Be able to explain the within-cluster sum of squared error (SSE) and the Silhouette score
- Be able to determine K and the best initial guesses using SSE and the Silhouette score

Today

Clustering

- Input (left): we start with blobs of data points (original data)



- Output (right): we assign each of these data points to a specific group
- Each group is called a **cluster**
- The process of finding these clusters is called **clustering**
- Clustering is widely used for different purposes; clustering algorithm development **does not require expensive annotations**; clustering is **unsupervised**

Application

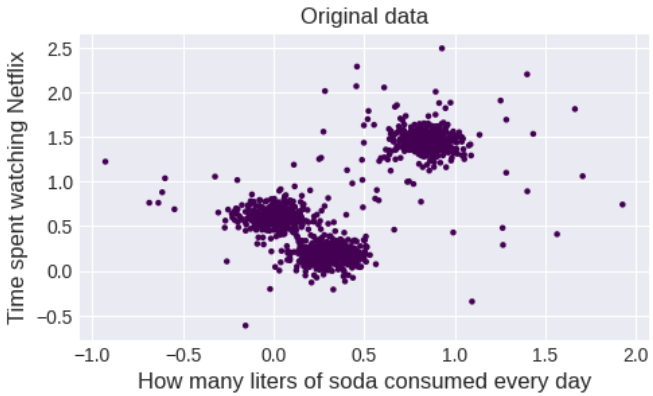
1. To reduce a large amount of data into fewer data points by, e.g., representing a data set with only a few centroids
   Example: you have access to the time people spend on Netflix and the amount of soda they consume everyday; you want to find patterns from this data set

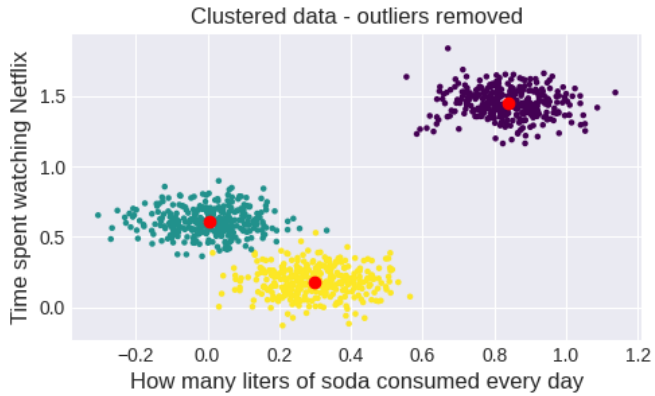
Group these people into clusters and only use the **centroids** for data exploration or as input data for downstream analysis
One important application is the **recommender system**

- Task: find patterns of preferred items from a massive number of users
- Challenge: there are too many users (all data points)
- Solution: we recommend items to users on a cluster level (only the centroids)

Application (cont.)

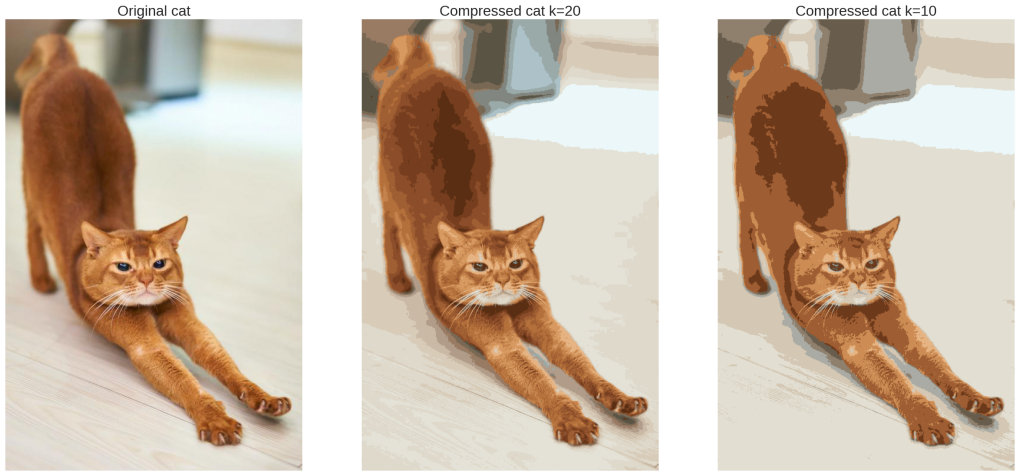
2. To detect and remove **outliers** - data points significantly distant from any of the clusters (here we assume that the clusters represent the underlying model)





Application (cont.)

3. 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 with 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** (geometry-based)
    - **Distribution clustering** (probability-based)
    - 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 containing only the feature vectors $\{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N\}$, e.g.

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

Models in this course

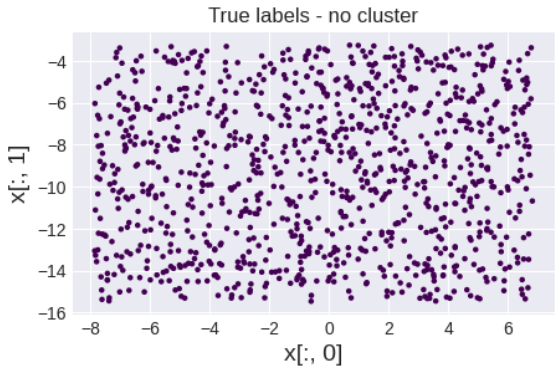
We are going to introduce various categories of clustering techniques; then we focus on two clustering models

- K-means (centroid clustering)
  - **Parameters**: K centroids
  - **Hyperparameters**: the number of centroids 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 (distribution clustering)
  - **Parameters**: K priors, K Gaussian likelihood (the big two!)
  - **Hyperparameters**: the number of Gaussian components K
  - **Parameter estimation**: the Expectation-Maximization algorithm

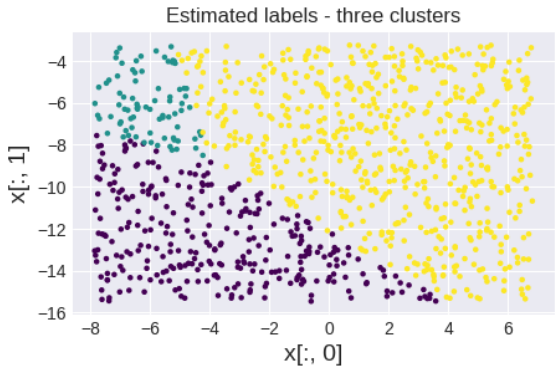
Today

Let's try something out!

- Generate some data $\{[x_1^1, x_2^1], \cdots, [x_1^N, x_2^N]\}$ from a uniform distribution (np.random.uniform) 😃 - there are **no clusters**



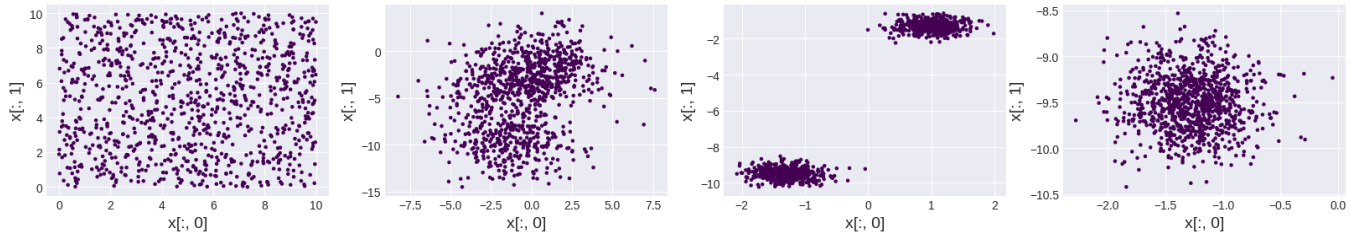
- Run a clustering algorithm



😭

Take one 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
- 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 set is clusterable

Clustering tendency

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

Let $\boldsymbol{x}_i = [x_1^i, \cdots, x_d^i]$ be a feature vector in this course, when we need to index both the dimension of the feature vector and the data point, we use a superscript to index the data point and a 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 $d >> 1$!**
- Approximation and sampling

Distance measure

- Measures how "similar" two data points 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

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

- A one dimensional value (scalar) computed from high dimensional data (here $d = 3$)
- 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

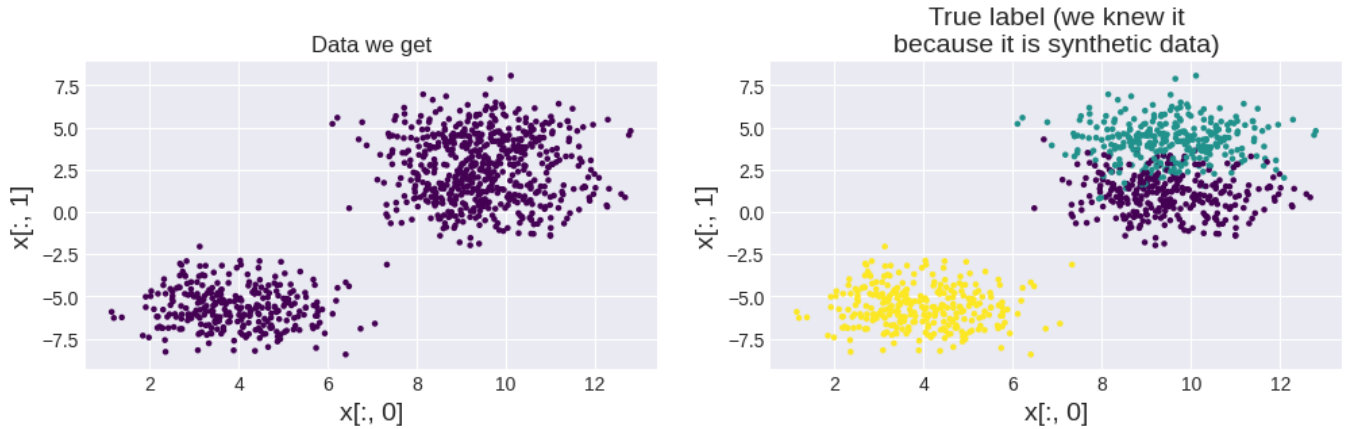
$$\{d(\boldsymbol{x}_1, \boldsymbol{y}_1), d(\boldsymbol{x}_1, \boldsymbol{y}_2), d(\boldsymbol{x}_2, \boldsymbol{y}_1), d(\boldsymbol{x}_2, \boldsymbol{y}_2), d(\boldsymbol{x}_3, \boldsymbol{y}_1), d(\boldsymbol{x}_3, \boldsymbol{y}_2)\}$$

- Generally useful concept
- Pairwise distance can be used to identify clustering tendency by comparing the **distribution of pairwise distances computed from data** to pairwise distances computed from a distribution without clustering tendency, e.g. a **uniform distribution**

Today

K-means

- **Data**: d dimensional feature vector $\boldsymbol{x}$ (in this example $d = 2$)



- **Target** (the coloring in this image - for each $\boldsymbol{x}$, we would like to assign a color to it):

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

  where $dist(\cdot, \cdot)$ is a distance measure; in this course, we use the Euclidean distance (cf. page 16)
- **Parameters**: K centroids $\hat{\boldsymbol{\mu}}_k$
- **Hyperparameters**: K
- **Parameter estimation**: an iterative method to update the centroids until convergence
- It is a **hard clustering** technique - one data point $\boldsymbol{x}$ is assigned to only one cluster y

K-means parameter estimation algorithm to find $\boldsymbol{\mu}_k$

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

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

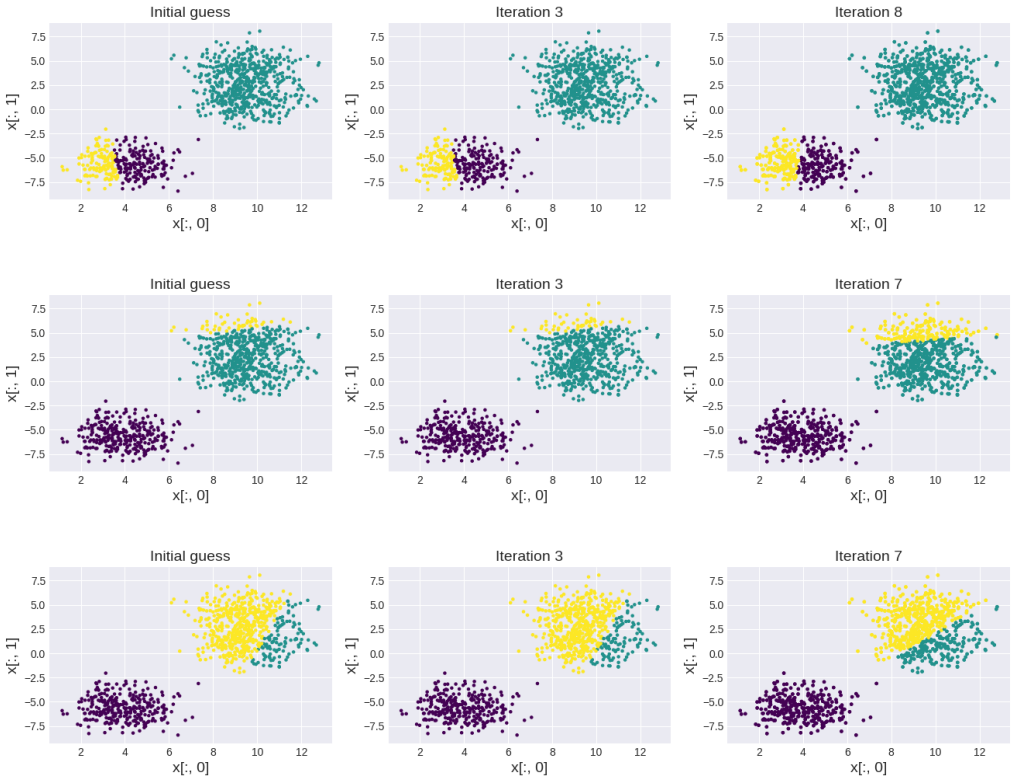
  - Step 2: Let $\mathcal{X}_k$ be the set of all $\boldsymbol{x}_i$ assigned to cluster k and N_k is the size of $\mathcal{X}_k$, compute

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

- 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 cluster 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**
  - 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 "obvious" outliers before clustering**

Two main challenges for K-means

- **Challenges**:
  - How to choose the hyperparameter K?
  - K-means is sensitive to the initialization of $\hat{\boldsymbol{\mu}}_k$ for $k = 1, \cdots, K$
- **Solution** (for both challenges):
  - Choose a set of **candidate values**, e.g. for the first problem, we can choose $K \in \{1, \cdots, 10\}$; for the second problem, we can randomly select 100 different initial guesses for $\hat{\boldsymbol{\mu}}_k$
  - For each of these **candidate values**, we run the K-means algorithm to estimate the parameters and evaluate the **quality** of the clusters produced by these parameters
  - Choose the **candidate value** that gives the best **quality**
- **Quality** evaluation criteria
  - Within-cluster sum of squared errors (SSE)
  - Silhouette score

Cluster quality evaluation criterion 1: SSE

1. **Within-cluster sum of squared errors (SSE)**: defied as the summation of the distances from all the data points to their closest centroid

$$SSE = \sum_{k=1}^{K} \sum_{\boldsymbol{x} \in C_k} dist(\boldsymbol{x}, \hat{\boldsymbol{\mu}}_k)^2 \tag{1}$$

where C_k denote cluster k; $dist(\cdot, \cdot)$ is a distance measure (**Euclidean distance**: $dist(\boldsymbol{x}, \hat{\boldsymbol{\mu}}_k)^2 = (\boldsymbol{x} - \hat{\boldsymbol{\mu}}_k)^T (\boldsymbol{x} - \hat{\boldsymbol{\mu}}_k)$ for column vectors $\boldsymbol{x}$ and $\hat{\boldsymbol{\mu}}_k$)
Example:

- Given $\boldsymbol{x}_1 = [x_1^1, x_2^1]$, $\boldsymbol{x}_2 = [x_1^2, x_2^2]$, $\boldsymbol{x}_3 = [x_1^3, x_2^3]$, $\boldsymbol{x}_4 = [x_1^4, x_2^4]$, where $\boldsymbol{x}_1, \boldsymbol{x}_2 \in$ cluster 1 with centroid $\boldsymbol{\mu}_1 = [\mu_1^1, \mu_2^1]$; $\boldsymbol{x}_3, \boldsymbol{x}_4 \in$ cluster 2 with centroid $\boldsymbol{\mu}_2 = [\mu_1^2, \mu_2^2]$
- The SSE is computed as

$$\begin{aligned} SSE &= \text{distance in cluster 1} + \text{distance in cluster 2} \\ &= \underbrace{(x_1^1 - \mu_1^1)^2 + (x_2^1 - \mu_2^1)^2}_{dist(\boldsymbol{x_1}, \boldsymbol{\mu_1})^2} + \underbrace{(x_1^2 - \mu_1^1)^2 + (x_2^2 - \mu_2^1)^2}_{dist(\boldsymbol{x_2}, \boldsymbol{\mu_1})^2} \\ &\quad + \underbrace{(x_1^3 - \mu_1^2)^2 + (x_2^3 - \mu_2^2)^2}_{dist(\boldsymbol{x_3}, \boldsymbol{\mu_2})^2} + \underbrace{(x_1^4 - \mu_1^2)^2 + (x_2^4 - \mu_2^2)^2}_{dist(\boldsymbol{x_4}, \boldsymbol{\mu_2})^2} \end{aligned}$$

Cluster quality evaluation criterion 1: SSE (cont.)

1. **Within-cluster sum of squared errors (SSE)** (cont.):

$$SSE = \sum_{k=1}^{K} \sum_{\boldsymbol{x} \in C_k} dist(\boldsymbol{x}, \hat{\boldsymbol{\mu}}_k)^2$$

- SSE is essentially an error term: we want SSE to be small - choose the K value that minimizes SSE?
- No can do! $SSE \to 0$ for $K \to N$, i.e. when every data point is their own centroid, $SSE = 0$, which is not optimal - we can't simply choose the K value that corresponds to the smallest SSE
- Instead, the best K is defined as the **elbow** point of the SSE (instead of the minimum), i.e. **the point with the maximum curvature** - find the largest K where the SSE does not go down significantly by further increasing K
- This method is also called the **elbow method** (in Python, you can find a library to compute the elbow point)

Cluster quality evaluation criterion 2: Silhouette score

2. **Silhouette score S**: the idea is that a good clustering should have **compact clusters** with a **large separation between different clusters**. This is characterized by the **within-cluster distance** and **between-cluster distance**

Cluster quality evaluation criterion 2: Silhouette score (cont.)

2. **Silhouette score** S (cont.):
   Example: given data $x_1, x_2, x_3 \in C_1$, $x_4, x_5 \in C_2$, $x_6, x_7 \in C_3$; $K = 3$; C_k denotes the set of cluster k; $|C_k|$ is the cardinality (size) of the set C_k
   - **Within-cluster distance**: measures how data points scatter in relation to $\boldsymbol{x}_i$ within its own cluster; let $\boldsymbol{x}_i$ be a data point from cluster k,

$$a_i = \frac{1}{|C_k| - 1} \sum_{\boldsymbol{x}_j \in C_k \text{ and } j \neq i} dist(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

     In this example, let $i = 1$, $x_1 \in C_1$; there are $|C_1| = 3$ data points in cluster 1

$$a_1 = \frac{1}{3 - 1} \left(dist(x_1, x_2) + dist(x_1, x_3) \right)$$

   - **Between-cluster distance**: measures how data points scatter in relation to $\boldsymbol{x}_i$ when these data points are from other clusters

$$b_i = \min_{k' \neq k, k' \in \{1, \cdots, K\}} \frac{1}{|C_{k'}|} \sum_{\boldsymbol{x}_j \in C_{k'}} dist(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

     In the example, $|C_2| = |C_3| = 2$

$$b_1 = \min \left(\frac{1}{2} \left(dist(x_1, x_4) + dist(x_1, x_5) \right), \frac{1}{2} \left(dist(x_1, x_6) + dist(x_1, x_7) \right) \right)$$

Cluster quality evaluation criterion 2: Silhouette score (cont.)

2. **Silhouette score** S (cont.):
   - Silhouette score for one data point $\boldsymbol{x}_i$:

$$S_i = \begin{cases} \frac{b_i - a_i}{\max(a_i, b_i)}, & \text{if } |C_k| > 1 \\ 0, & \text{if } |C_k| = 1 \end{cases}$$

     A large S_i indicates a compact cluster k in relation to $\boldsymbol{x}_i$ and a large distance from $\boldsymbol{x}_i$ to clusters other than k
   - Silhouette score for the data set

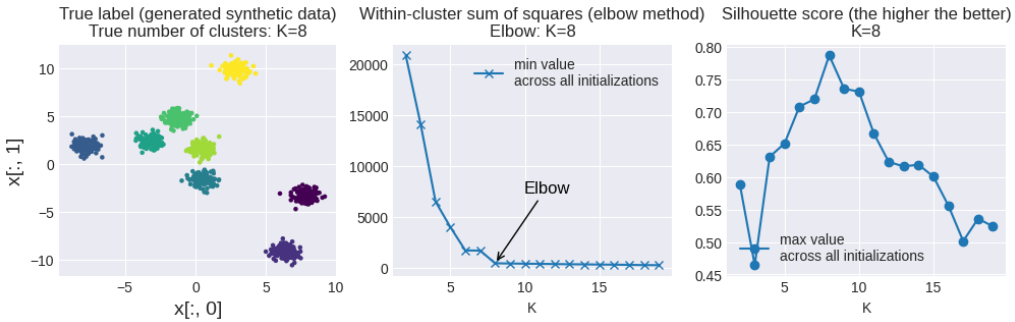
$$S = \frac{1}{N} \sum_{i=1}^{N} S_i, \quad S \in [-1, 1]$$

   - A large Silhouette score indicates a good clustering quality

Example - choose K

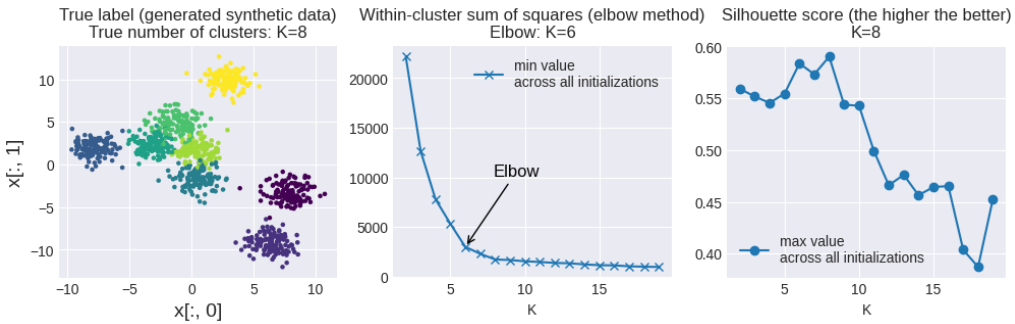
Clusters with equal variance ($K = 8$)

- SSE: $K = 8$
- Silhouette score: $K = 8$



Overlapping clusters with unequal variances ($K = 8$)

- SSE: $K = 6$
- Silhouette score: $K = 8$; but $K = 6$ and $K = 8$ have similar Silhouette scores

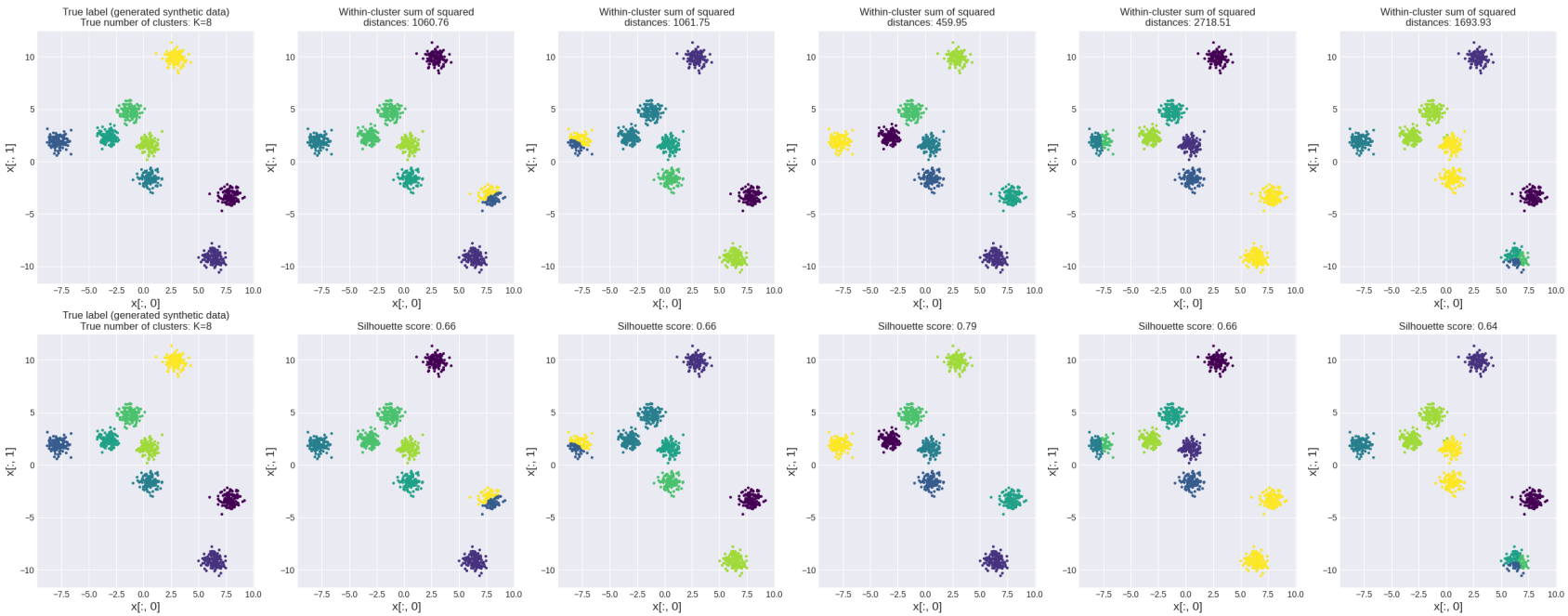


Example - choose initial guess

- Each column corresponds to a different initialization
- For a given K, choose the initialization that gives the smallest SSE or largest Silhouette score

Clusters with equal variance ($K = 8$)

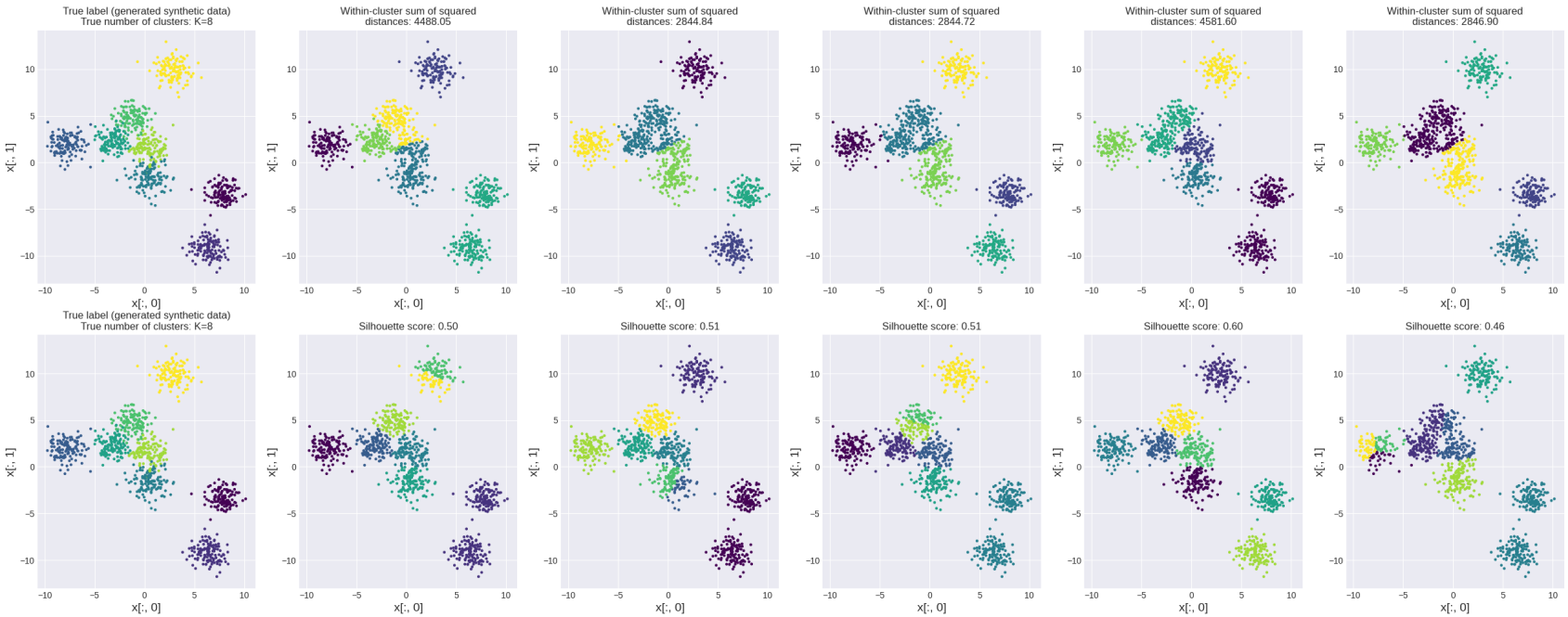
- SSE: $K = 8$
- Silhouette score: $K = 8$



Example - choose initial guess (cont.)

Overlapping clusters with unequal variances ($K = 8$)

- SSE: $K = 6$
- Silhouette score: $K = 8$



Today

Summary

So far:

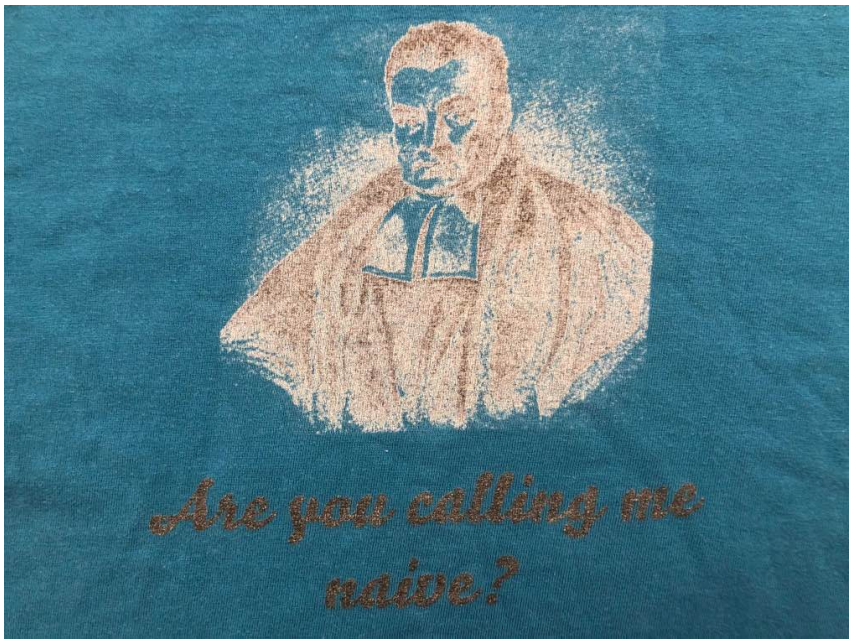
- Data types and data containers
- Descriptive data analysis: descriptive statistics, visualization
- Probability distributions, events, random variables, PMF, PDF, parameters
- CDF, Q-Q plot, how to compare two distributions (data vs theoretical, data vs data)
- Modeling
- Parameter estimation: maximum likelihood estimation (MLE) and maximum a posteriori estimation (MAP)
- Classification, multinomial naive Bayes classifier, Gaussian naive Bayes classifier
- Clustering, clustering tendency
- Centroid clustering, k-means, parameter estimation, SSE, Silhouette score

Next:

- Gaussian Mixture Models (GMMs)

Before next lecture:

- Gaussian distribution
- The Bayes' rule



You will never get rid of me!