Lecture 7: Clustering 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 clustering tendency using the Hopkins statistic
- 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

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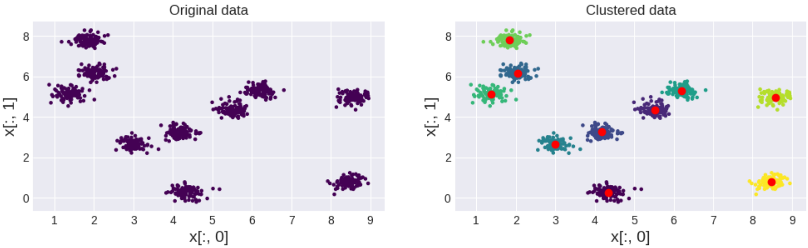

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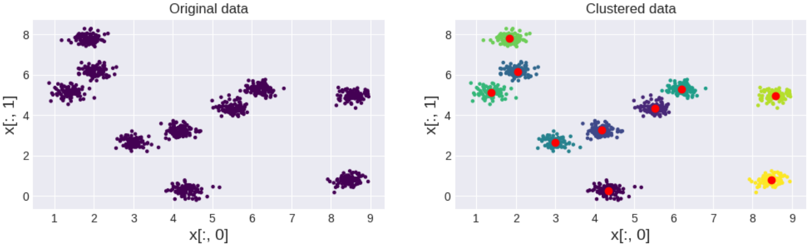

- The process of finding clusters is called **clustering**

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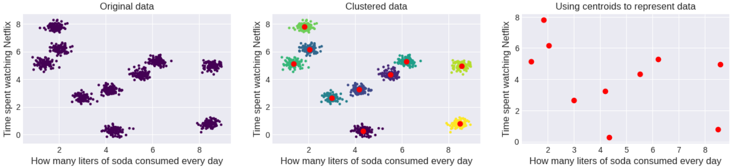

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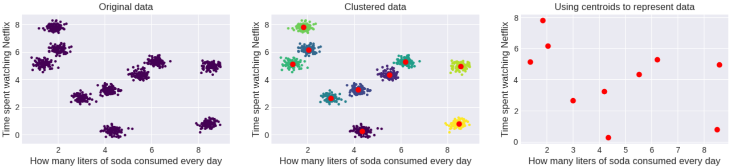

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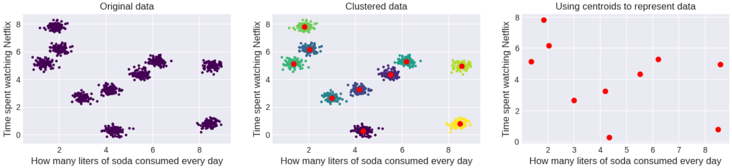

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   One important application is the **recommender system**
   - Task: find patterns of preferred items from a massive number of users
   - Challenge: there are too many users (all data points)
   - Solution: we recommend items to users on a cluster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

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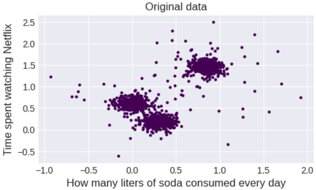

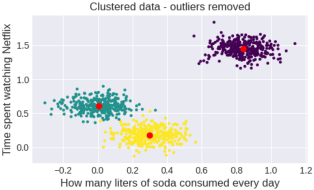

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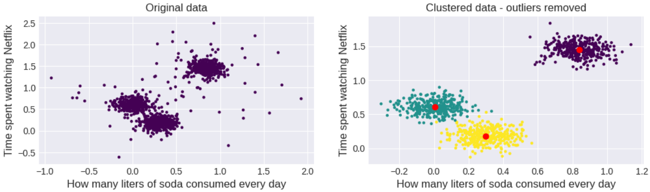

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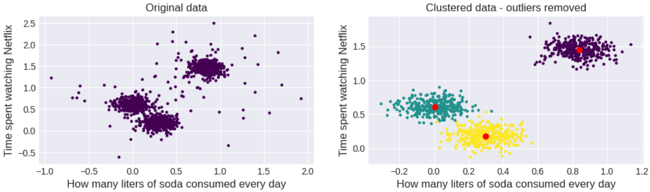

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Note: use with caution - some clustering methods are not robust enough for this type of use case

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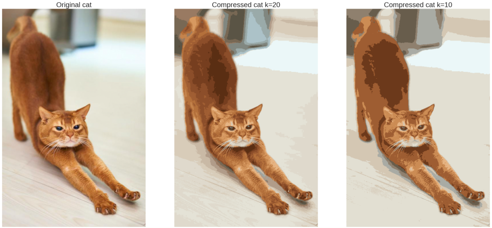

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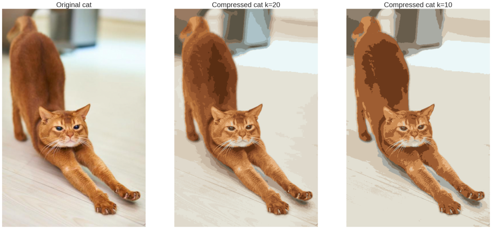

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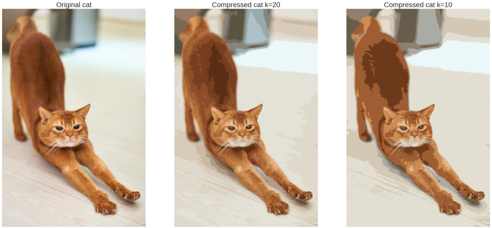

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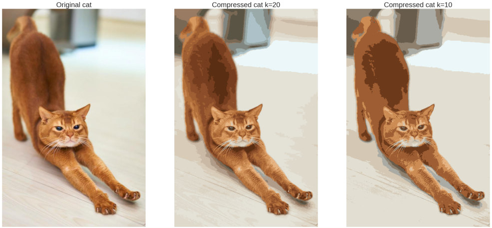

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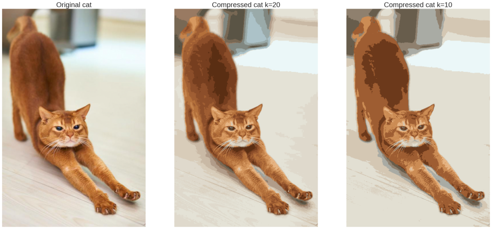

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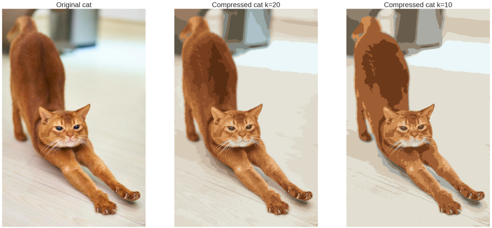

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- Now we only use $3 \times K$ unique values to represent the image instead of 3×256 values
- In this example, with $K = 10$ centroids, when we save the .png image, we have a reduction from 328.5 kB to 43.4 kB

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  - 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

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- 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
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- 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

Are there clusters in the data?

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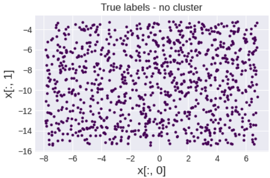

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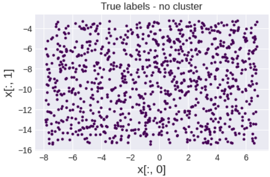

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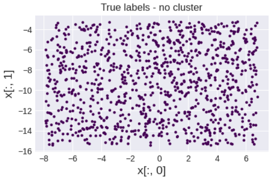

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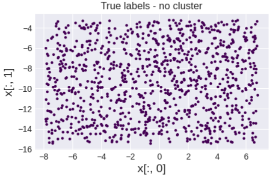

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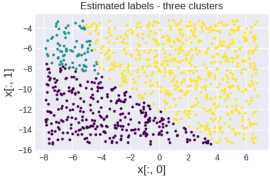

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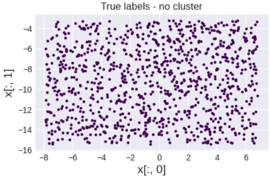

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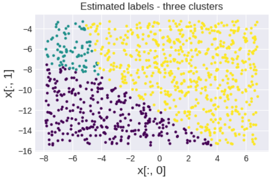

😭

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

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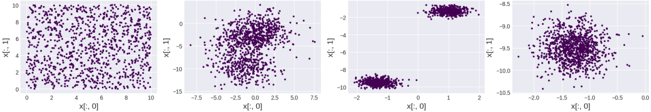

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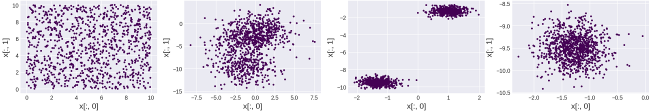

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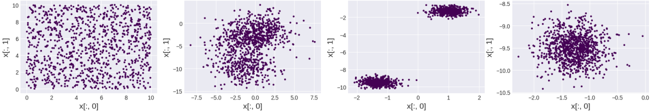

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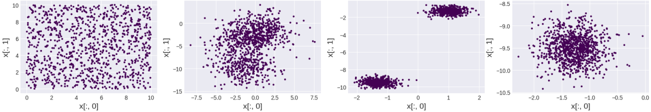

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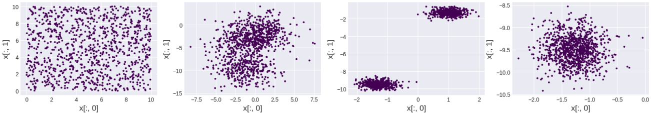

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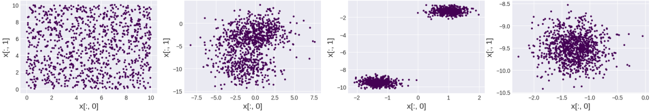

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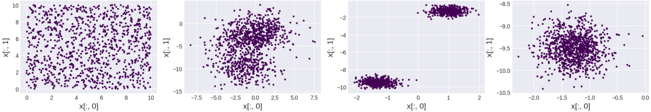

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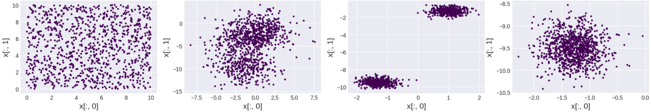

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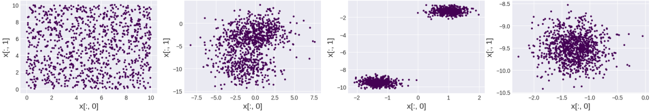

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- Now spend 30 secs staring at the plots and try to think how you can measure if the data set is clusterable

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- One solution: compute a **scalar** sample statistic instead

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Distance based approach (cont.)

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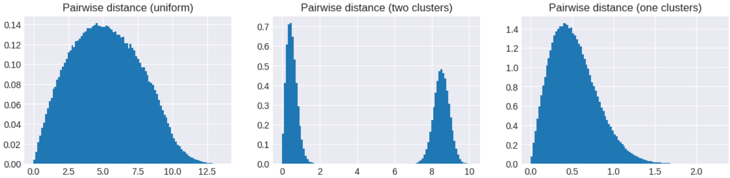

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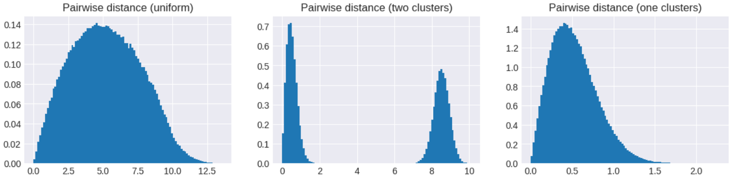

- Dissimilarity matrix
  - A matrix that contains pairwise distance $d(\boldsymbol{x}_i, \boldsymbol{y}_j)$ on its $(i, j)^{th}$ position

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

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- **Compute the Hopkins statistic**

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

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- Intuitively, we want to compare the distribution of $\sum_{i=1}^{M} u_i^d$ (sampled from uniform) and $\sum_{i=1}^{M} u_i^d + \sum_{i=1}^{M} w_i^d$ (data)

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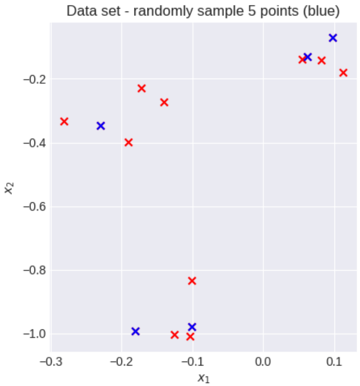
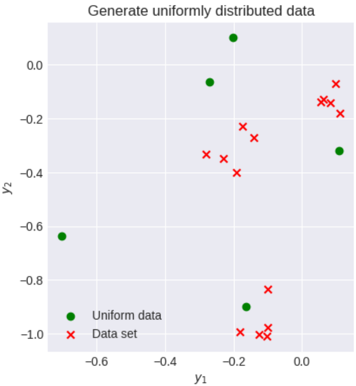
- We will revisit this topic in a later lecture (hypothesis testing)

Hypothesis testing using Hopkins statistic (cont.)





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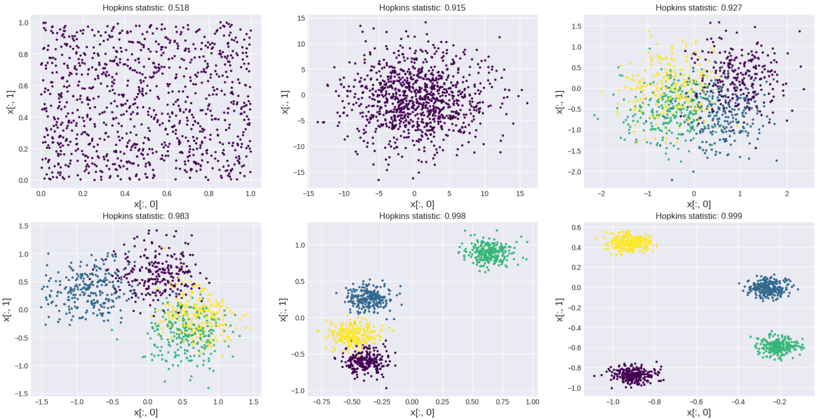

Histogram based technique

Histogram for high dimensional data

- High dimensional histogram - empirical joint distribution $f_{X_1,\cdots,X_d}(X_1,\cdots,X_d)$

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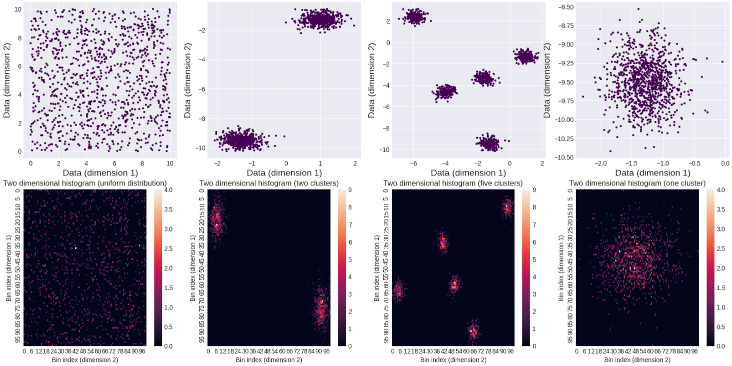
```

- Check out np.histogram2d

Histogram for high dimensional data (cont.)



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- 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**

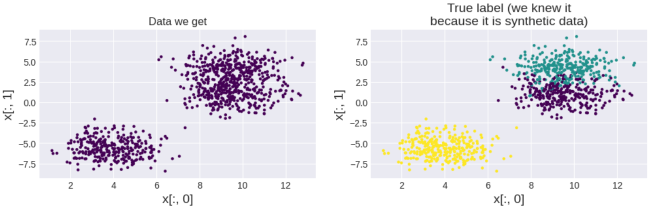
What we have seen so far

- Definition and modeling of clustering
- Example applications of clustering
    - Summarize data by its clusters, e.g. recommender systems
    - Outlier detection
    - Data compression
- Testing clustering tendency by comparing two distributions:
    - Pairwise distance
    - Hopkins statistic and
    - d dimensional histograms

Today

K-means

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



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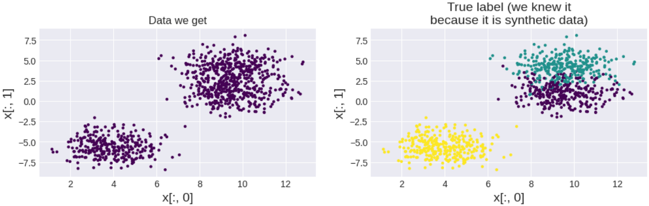

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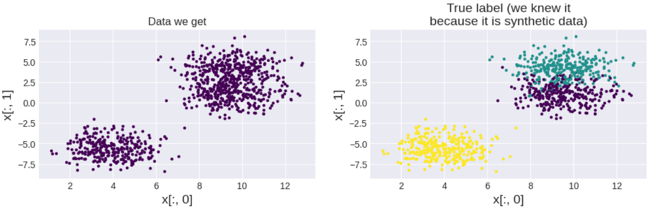

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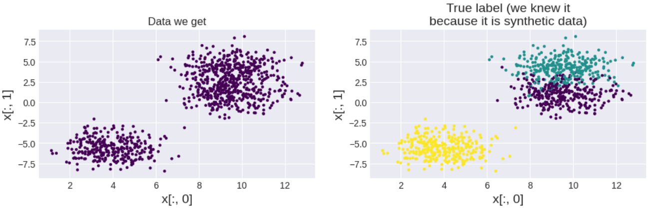

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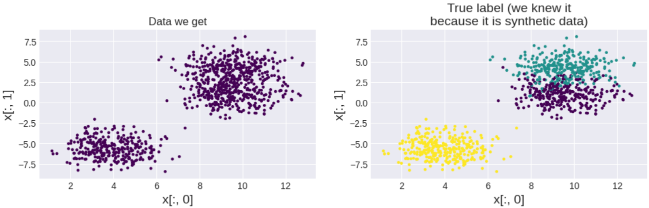

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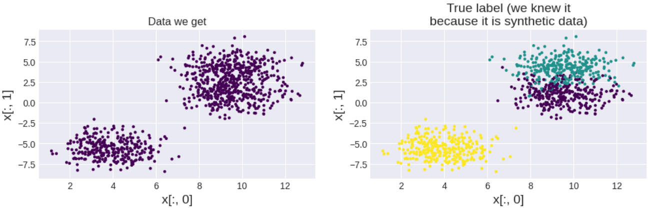

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  where $dist(\cdot, \cdot)$ is a distance measure; in this course, we use the Euclidean distance (cf. page 20)
- **Parameters**: K centroids $\hat{\boldsymbol{\mu}}_k$
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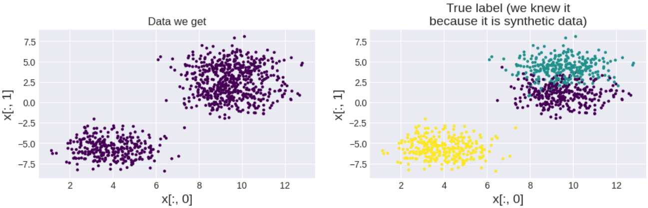
- **Parameter estimation**: an iterative method to update the centroids until convergence

K-means

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



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- 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 $\boldsymbol{\mu}_k$

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  - 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

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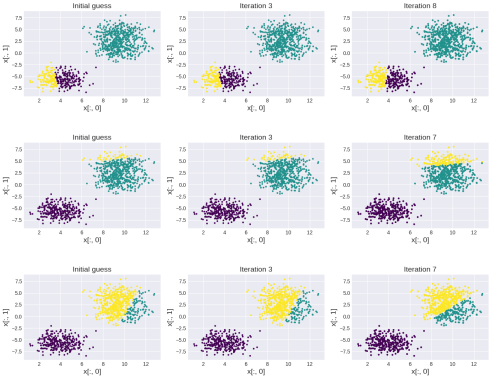
- There is some **randomness** in the algorithm - we should always be careful when there is randomness

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

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    - Not robust to outliers

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  - 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**

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- **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 $\hat{\boldsymbol{\mu}}_k$)

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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

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

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- 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

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   - **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

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

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   - **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

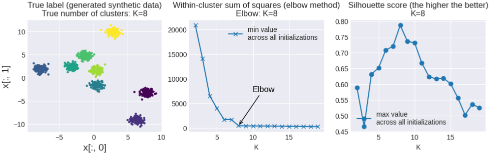
$$S = \frac{1}{N}\sum_{i=1}^{N} S_i, \quad S \in [-1, 1]$$

   - A large Silhouette score indicates a good clustering quality

Example - choose K

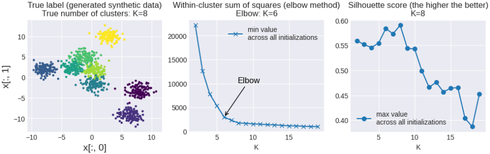
Clusters with equal variance ($K = 8$)

- 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

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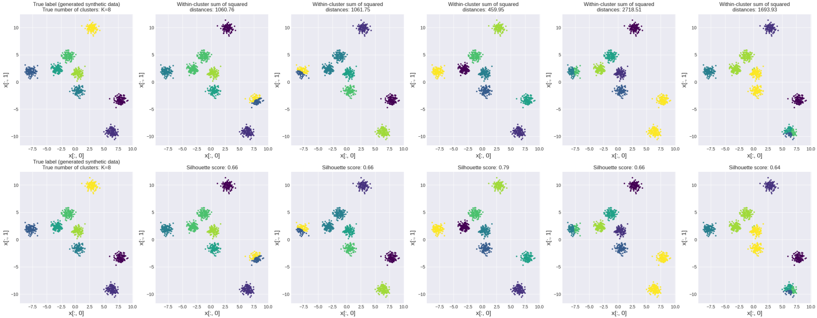

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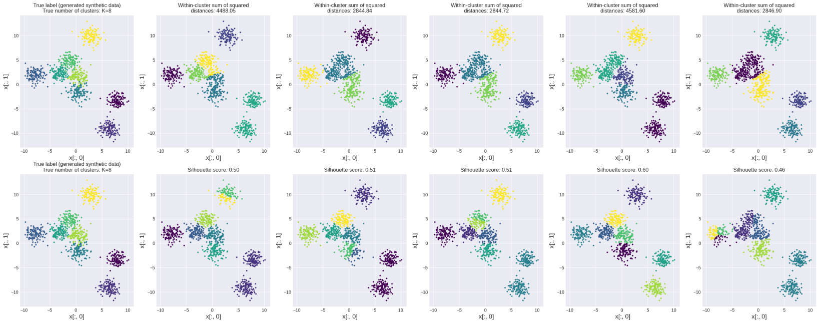

Today

1. Introduction
2. Modeling for clustering
3. Clustering tendency
4. Centroid clustering: K-means
5. Summary

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)
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Before next lecture:

- Gaussian distribution
- The Bayes' rule

You will never get rid of me!