Lecture 9: Clustering Part I

Statistical Methods for Data Science

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December 3, 2020

Today

1. Introduction
2. Modeling for clustering
3. Clustering tendency
   - Are there clusters in the data?
   - Distance based approach
   - Hopkins statistic
   - Histogram based technique
4. First clustering model: K-means
5. Summary

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

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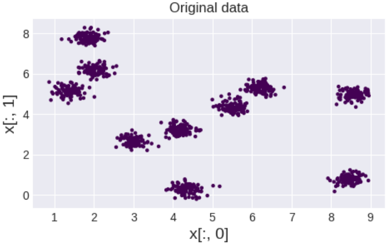

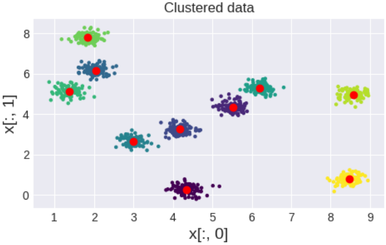

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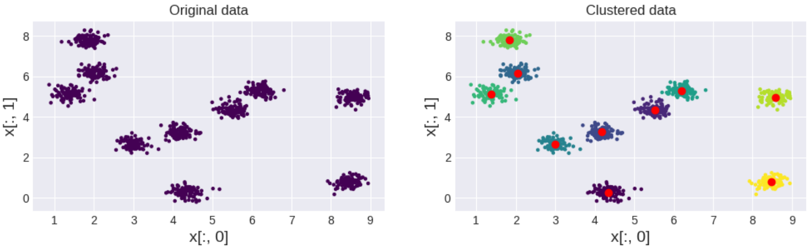

- Each of these semantics is called a **cluster**
- The process of finding clusters is called **clustering**

Application

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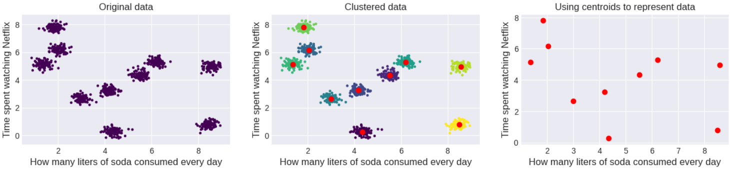
1. Clustering as a preprocessing method

   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.)

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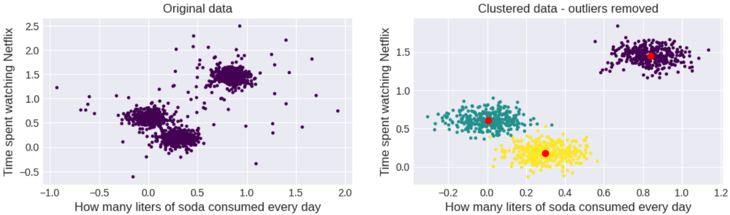

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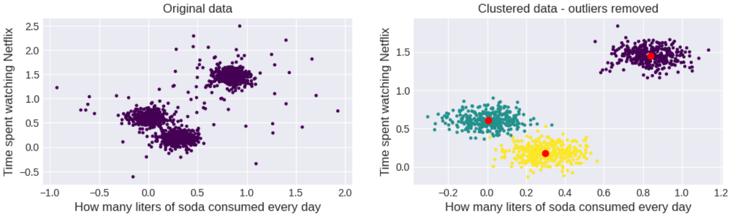

Without clustering, it is hard to define what should be considered outliers when the data distribution is **complex**:

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

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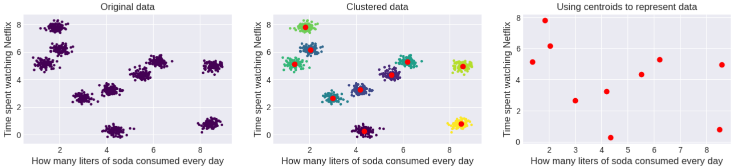

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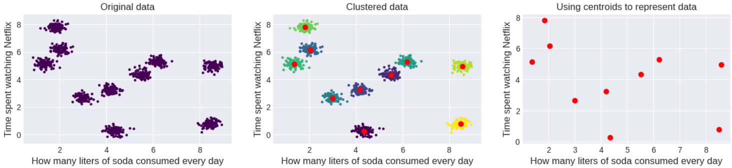

One important application is the **recommender system**

- 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

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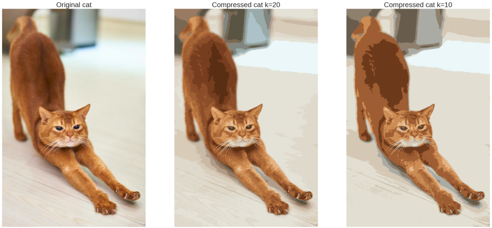

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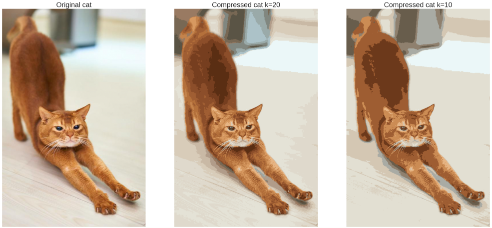

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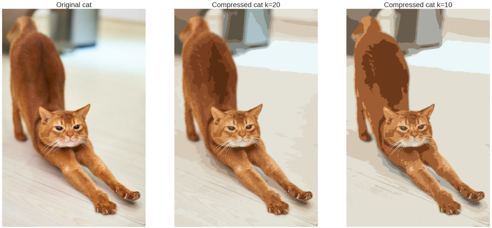

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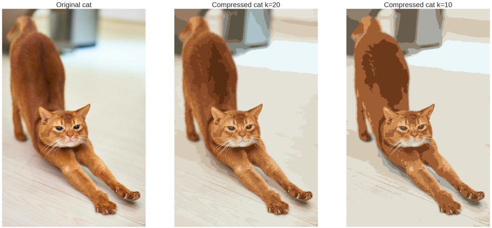

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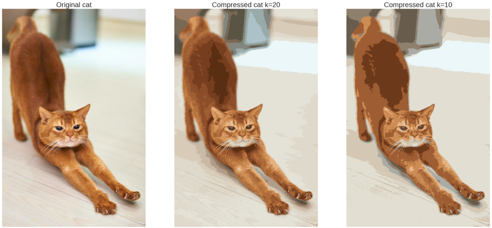

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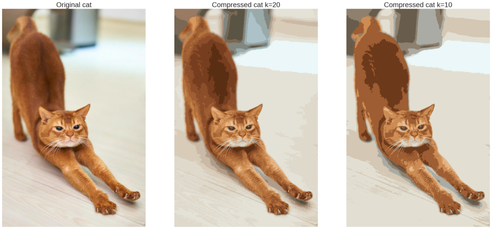

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- Now we only use $3 \times K$ unique values to represent the image instead of 3×256 values
- In this example, with $K = 10$ centroids, when we save the .png image, we have a reduction from 328.5 kB to 43.4 kB

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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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- 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
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  - **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

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- 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

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Are there clusters in the data?

Let's try something out!

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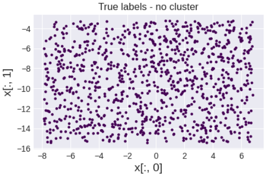

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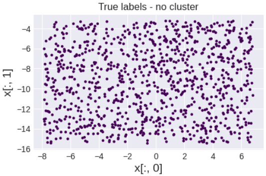

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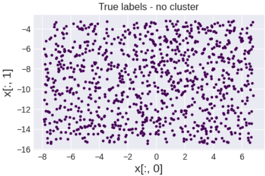

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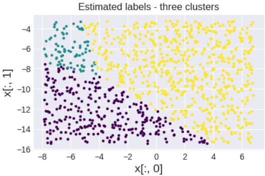

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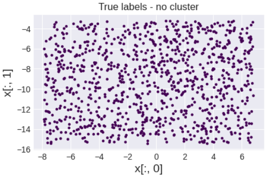

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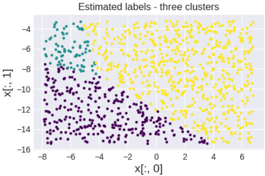

😭

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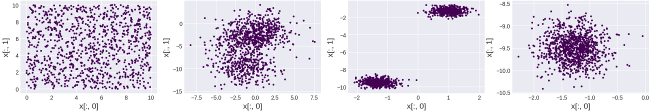

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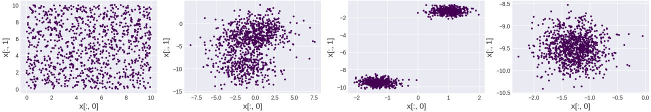

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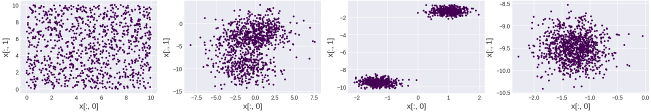

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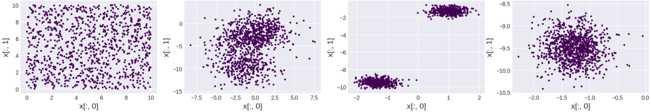

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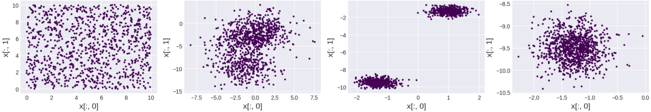

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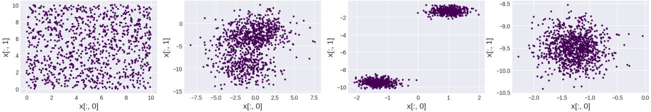

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  - Need to define what a cluster is
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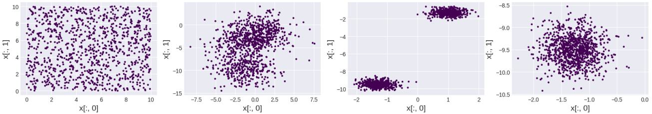

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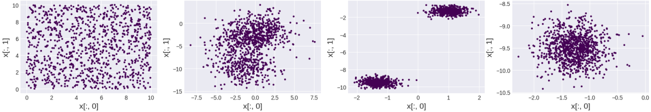

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- There is no ground truth label - there are various ways of defining these prerequisites, which makes it a difficult task!
- Now spend 30 secs staring at the plots and try to think how you can measure if the data is clusterable

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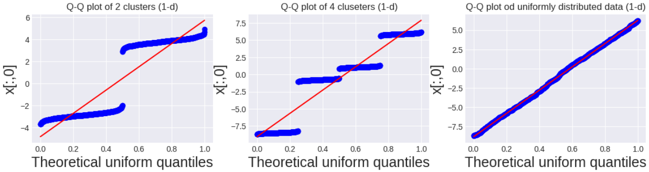

- We can repeat this for all dimensions $j = 1, \cdots, d$

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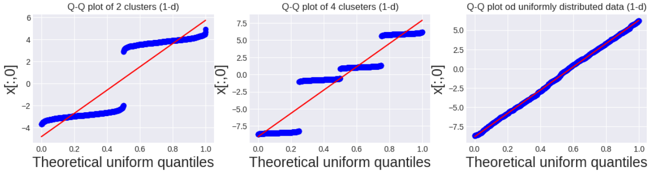

- We can repeat this for all dimensions $j = 1, \cdots, d$
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- **Comparing distributions gets trickier when $d > 1$!**

Cluster tendency (cont.)

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  - Histogram based technique
    - Histogram for high dimensional data

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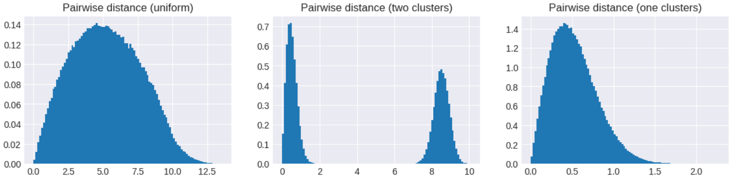
- The general idea is to compare the **distribution of the pairwise distance computed from the data** to the one computed from a distribution without clustering tendency, e.g. a **uniform distribution**

Distance based approach (cont.)

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



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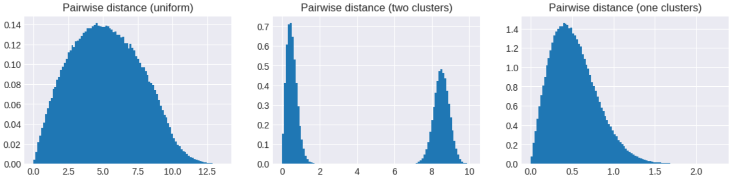

- Dissimilarity matrix
    - A matrix that contains pairwise distance $d(\boldsymbol{x}_i, \boldsymbol{y}_j)$ on its $(i, j)^{th}$ position

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

    - 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

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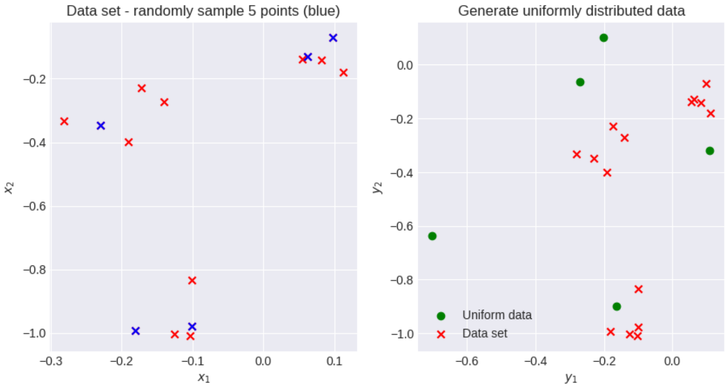
- **Computation**

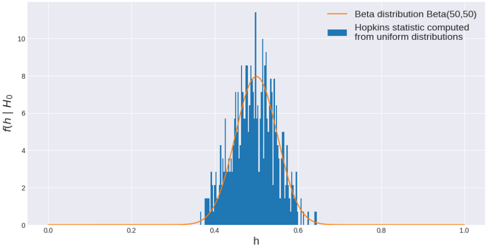
1: Choose an integer $M \ll N$ (sparse sampling)
2: Generate a sample of uniformly distributed data with sample size M: $\{\boldsymbol{y}_1, \cdots, \boldsymbol{y}_M\}$
3: Randomly choose M data points (without replacement) from $\mathcal{X}$: $\{\boldsymbol{x}_{m_1}, \cdots, \boldsymbol{x}_{m_M}\}$
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)



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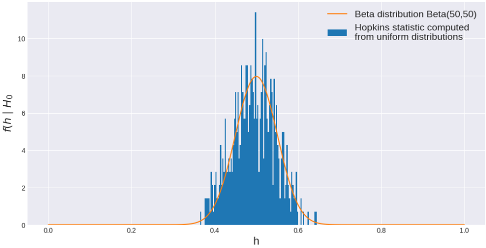
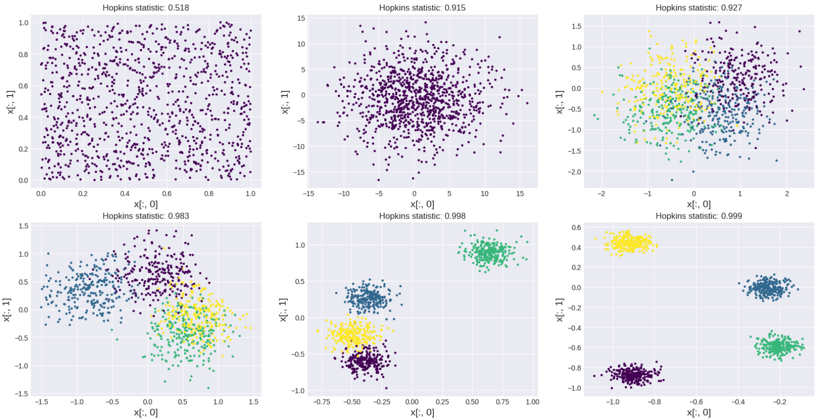


- Note: there are variations of the Hopkins statistic; in general, when the Hopkins statistic deviates from 0.5 significantly, it indicates cluster tendency

Hypothesis testing using Hopkins statistic (cont.)



Histogram based technique

Histogram for high dimensional data

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

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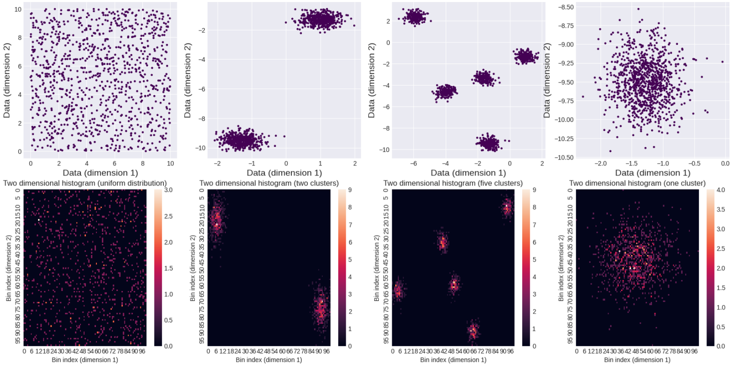
- **Compute histogram for d dimensional data**

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

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- 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

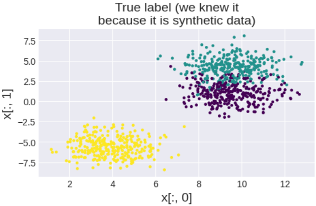
- Definition and modeling of clustering
- Applications of clustering
  - As a preprocessing technique, e.g. summarize data, detect outliers
  - As a data reduction technique, e.g. recommender system on a cluster level, image compression
- Testing cluster tendency by comparing two distributions using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

Today

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

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

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

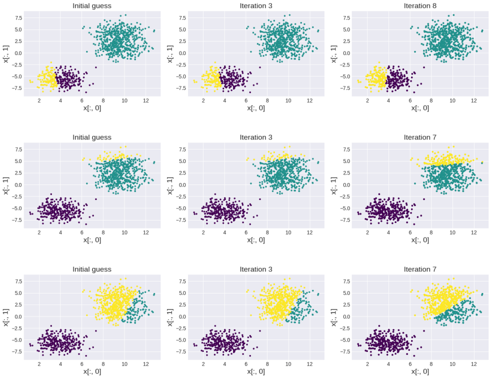
    - Let $\mathcal{X}_k$ be the set of all $\boldsymbol{x}_i$ assigned to cluster k and N_k be the size of $\mathcal{X}_k$, compute

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

- 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

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  - 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**

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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
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Before next lecture:

- Gaussian distribution
- The Bayes' rule