

Lecture 9: Clustering Part I

Statistical Methods for Data Science

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Today

1 Introduction

2 Modeling for clustering

3 Cluster tendency

- Are there clusters in the data?
- Distance based approach
- Hopkins statistic
- Histogram based technique

4 Centroid clustering: 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 cluster 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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Clustering

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Clustering

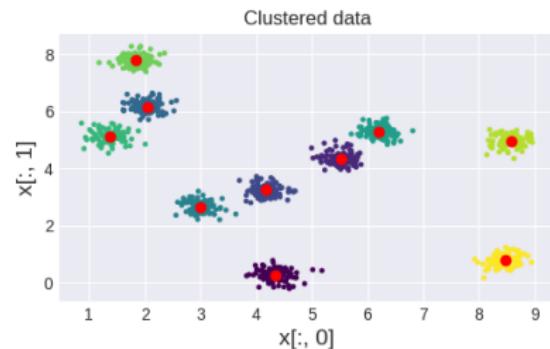
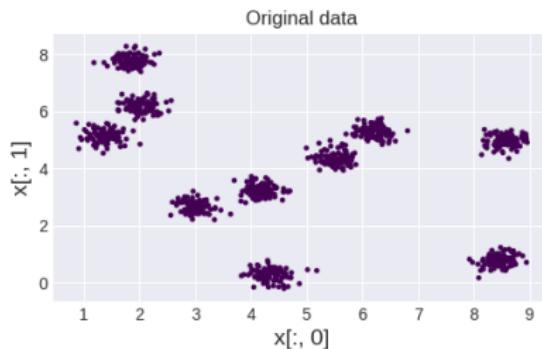
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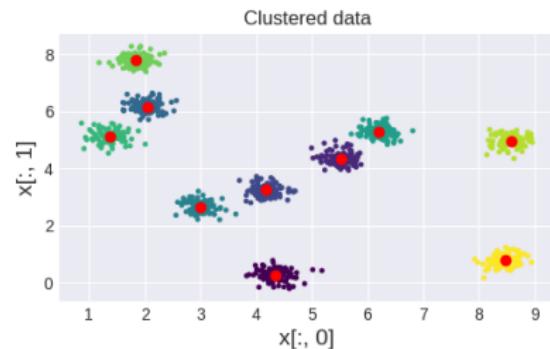
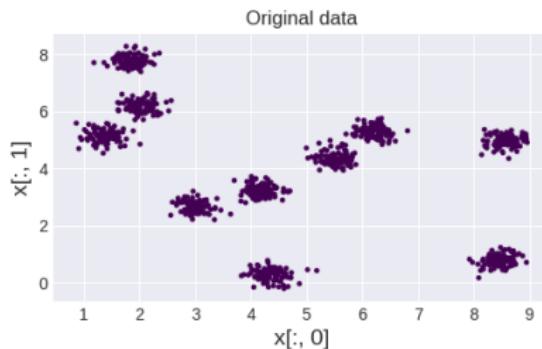
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- The process of finding clusters is called **clustering**

Application

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

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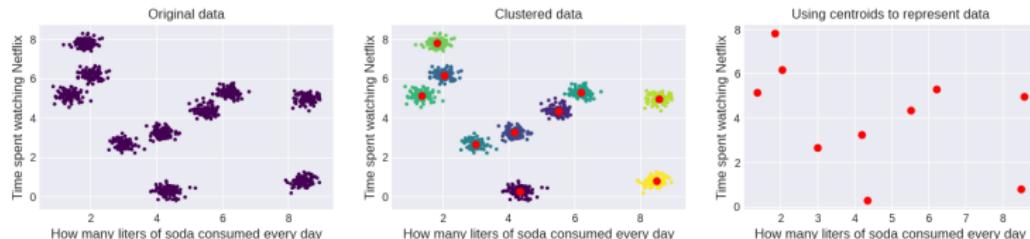
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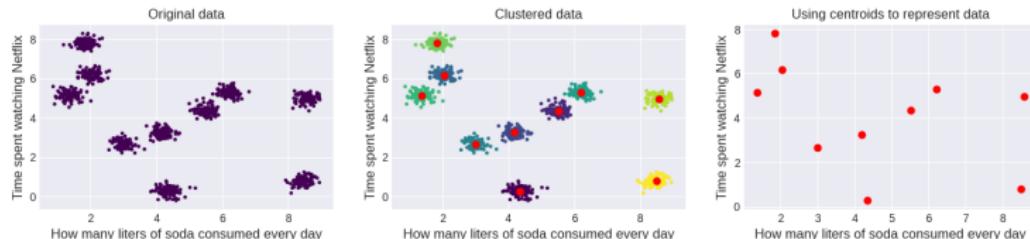
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Group these people into clusters and use the centroids for data exploration or as the input data for downstream analysis.

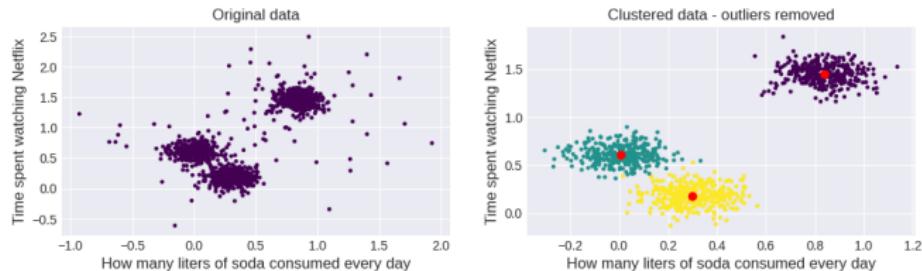
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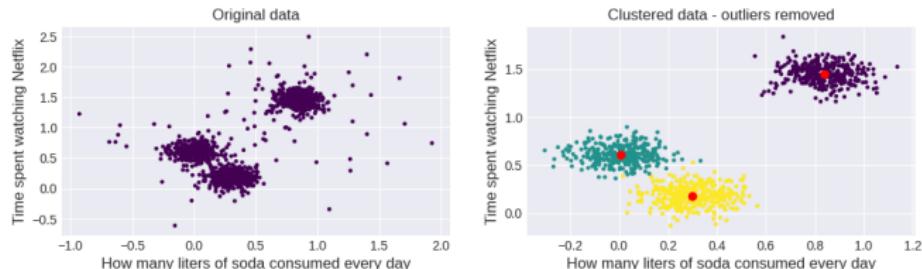
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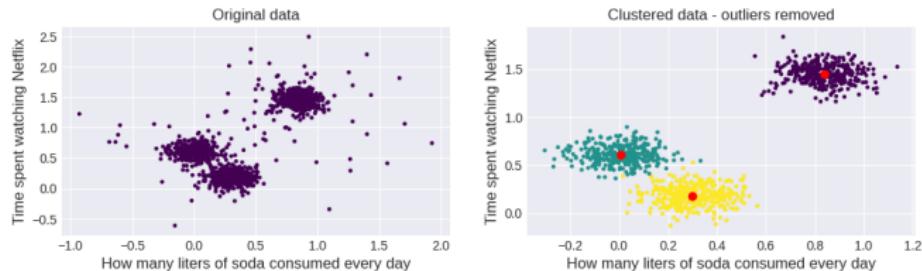
Without clustering, it is hard to define what should be considered outliers when the data distribution is **complex**:

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

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Note: use with caution - some clustering methods are not robust against outliers

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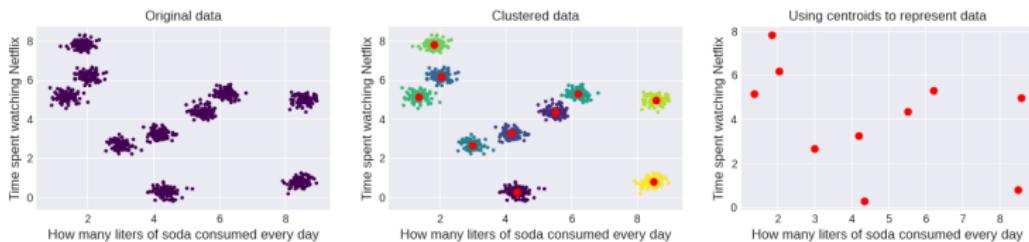
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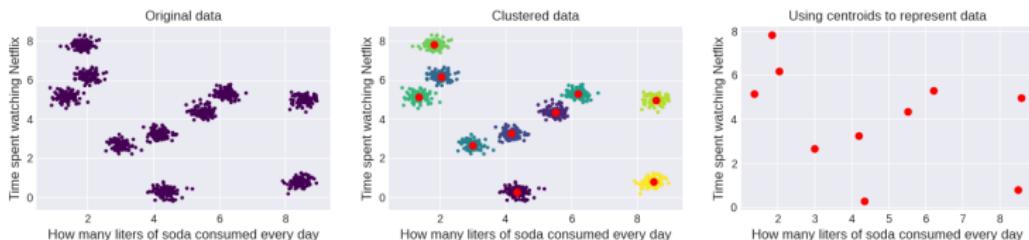
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One important application is the **recommender system**

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

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- 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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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
 - **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

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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

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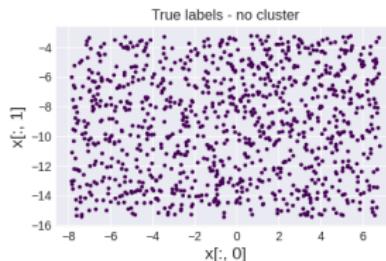
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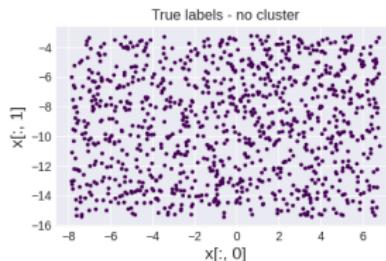
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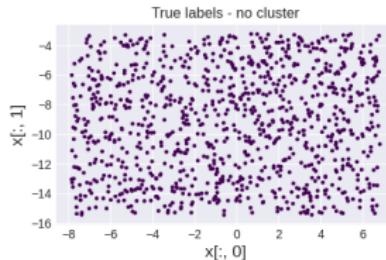
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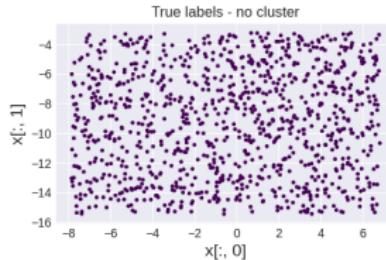
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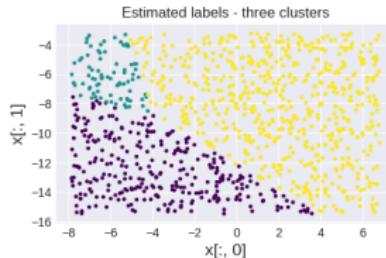
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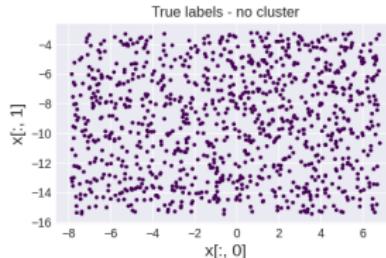


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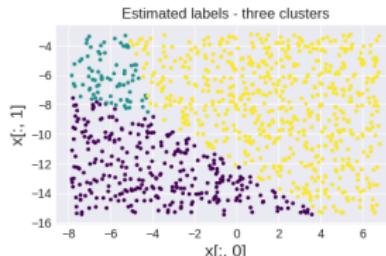


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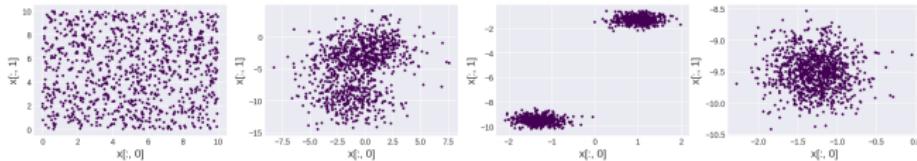


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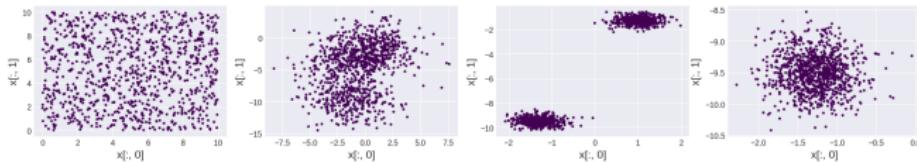
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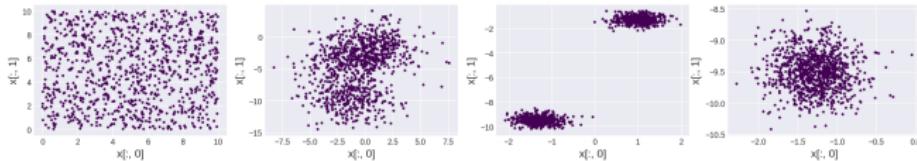
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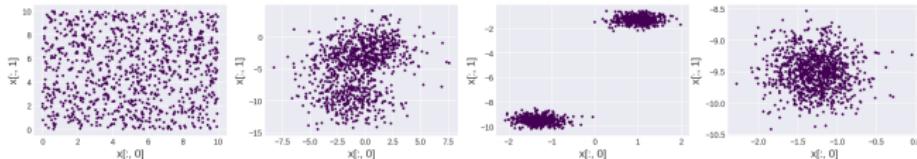
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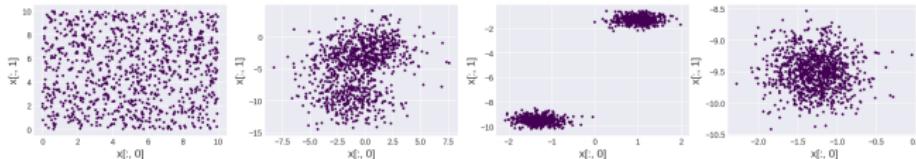
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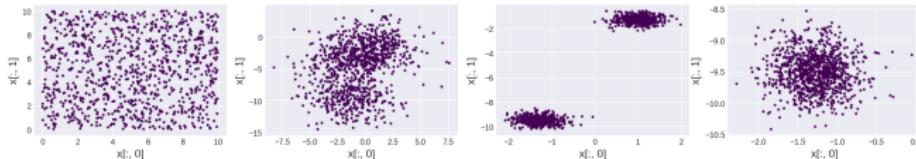
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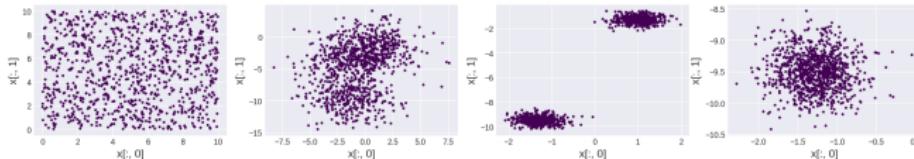
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- Now spend 30 secs staring at the plots and try to think how you can measure if the data set is clusterable

Cluster tendency

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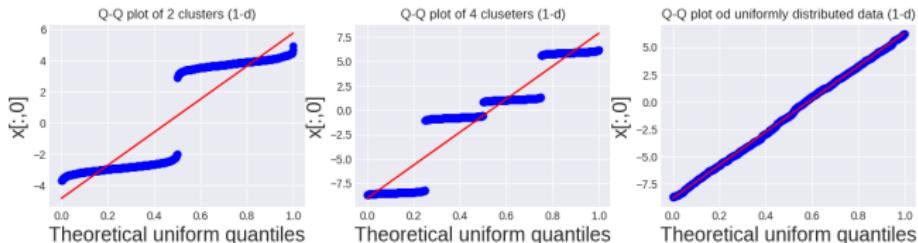
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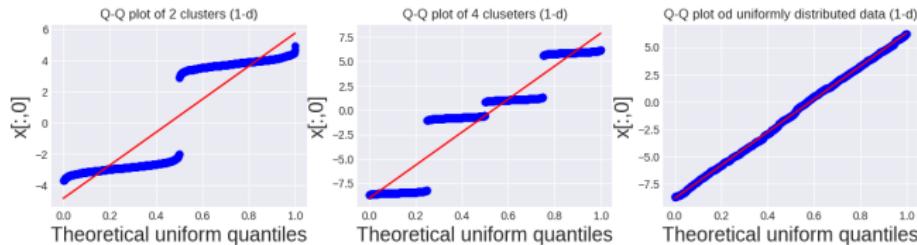


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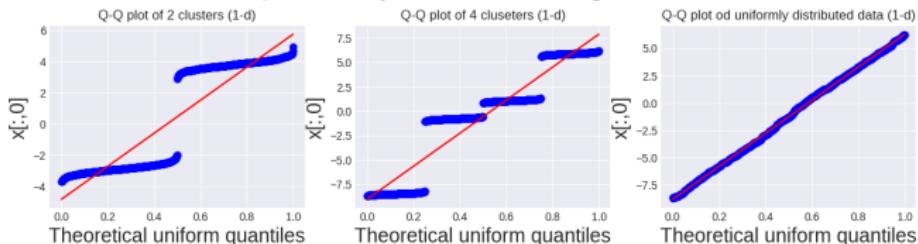
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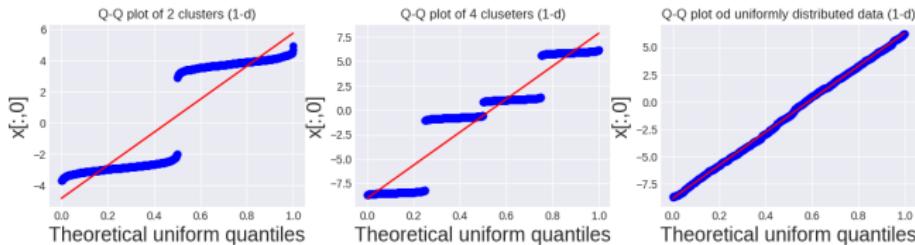
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- We can repeat this for all dimensions $j = 1, \dots, d$
- But then the question is how to aggregate all these d dimensions? - Not easy!
- Comparing distributions gets trickier when $d > 1$!

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 - Example: let $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ and $\{\mathbf{y}_1, \mathbf{y}_2\}$ be two sets, the pairwise distance is defined as

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

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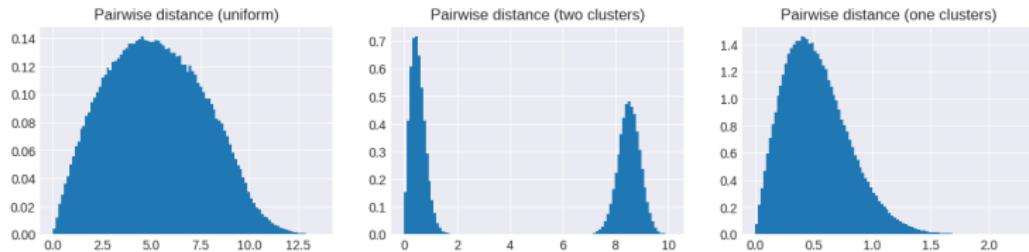
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- The general idea is to compare the **distribution of the pairwise distance computed from the data** to the one computed from a distribution without cluster tendency, e.g. a **uniform distribution**

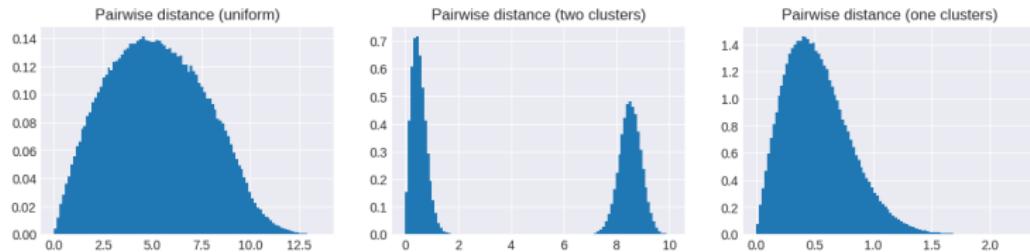
Distance based approach (cont.)

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

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

- 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:** $\mathcal{X} = \{x_1, \dots, x_N\}$ from unknown distribution
- **Null hypothesis H_0 :** there is no cluster tendency in the data set
- **Test statistic h :** Hopkins statistic

Hopkins statistic for testing cluster tendency

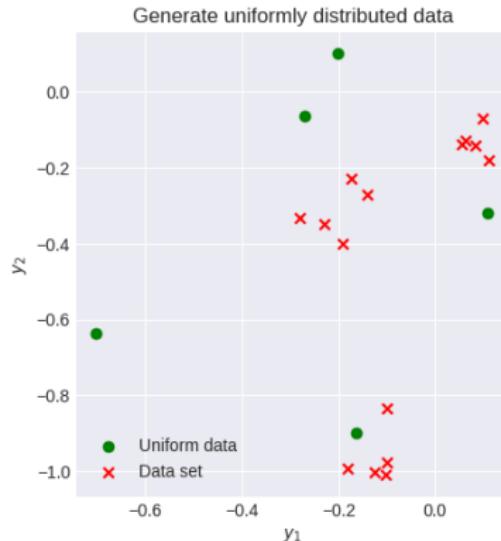
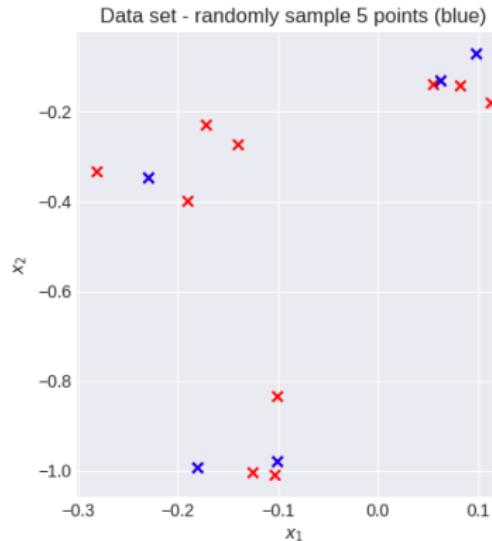
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- **Computation**

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

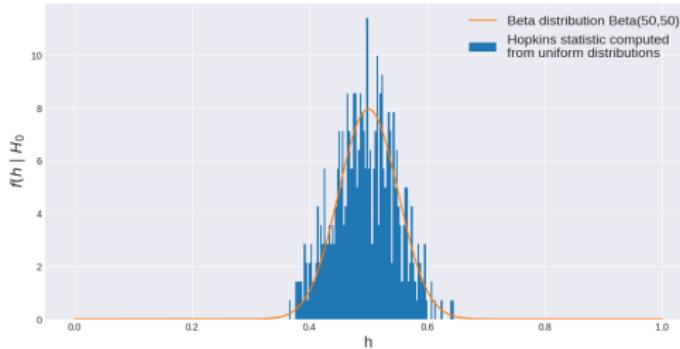
Hypothesis testing using Hopkins statistic (cont.)



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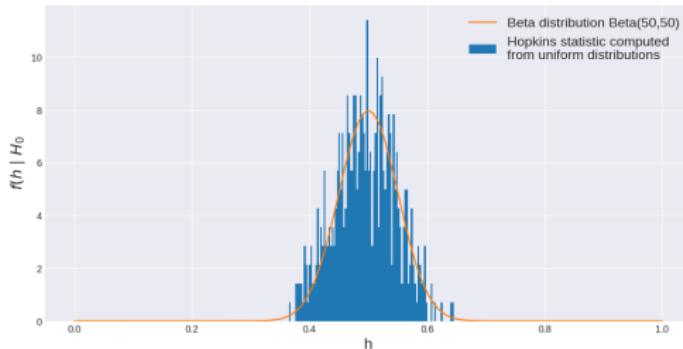
- PDF: Beta distribution with parameters $a = M$ and $b = M$
- Python: `stats.beta.pdf(x, M, M)`



Hypothesis testing using Hopkins statistic (cont.)

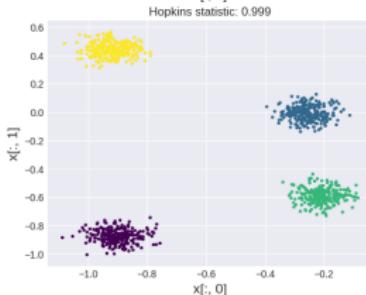
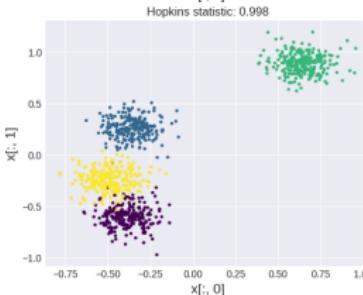
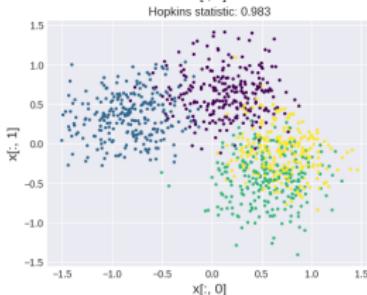
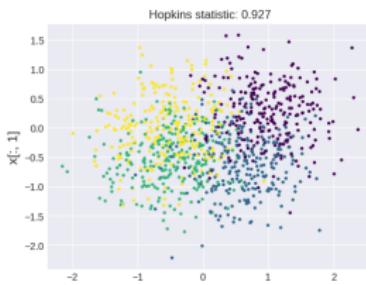
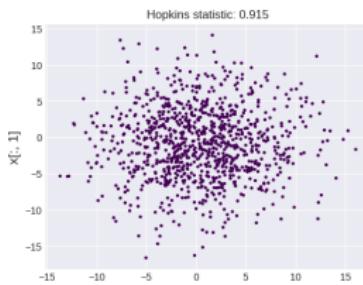
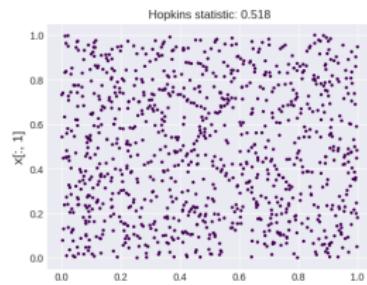
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- Note: there are variations of the Hopkins statistic; in this version, when the Hopkins statistic deviates from 0.5 significantly, it indicates cluster tendency

Hypothesis testing using Hopkins statistic (cont.)



Histogram based technique

Histogram for high dimensional data

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

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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**
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- 5: Count the number of points in each cell j - each cell is a d dimensional cell
- 6: **end for**

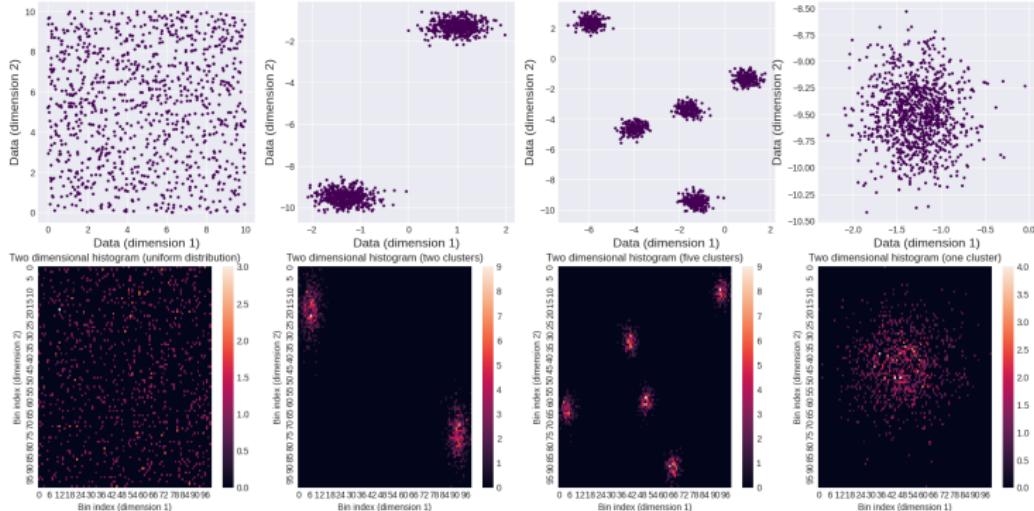
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- Check out np.histogram2d

Histogram for high dimensional data (cont.)



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- We typically approximate high dimensional theoretical distributions using sampling techniques
- Pseudo-algorithm to illustrate the idea
 - Given a data set $\mathcal{X} = \{x_1, \dots, x_N\}$
 - Compute the d dimensional histogram for \mathcal{X}
 - Sample N data points from a d dimensional uniform distribution and compute the d dimensional histogram
 - Compare these two histograms using, e.g. the **Kullback–Leibler divergence**

What we have seen so far

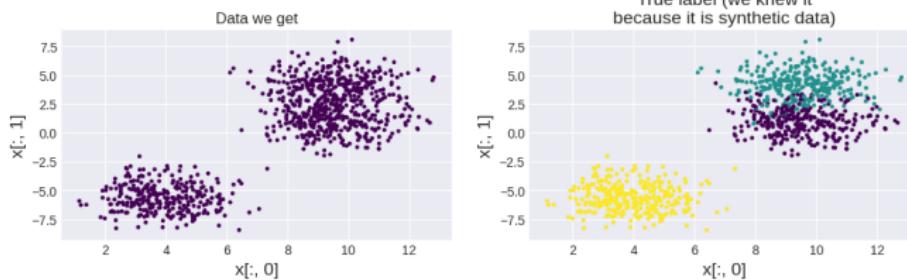
- Definition and modeling of clustering
- Applications of clustering
 - As a preprocessing technique, e.g. summarize data, detect outliers
 - As a reduction technique, e.g. recommender system on a cluster level, image compression
- Testing cluster tendency by comparing two distributions using 1) pairwise distance, 2) Hopkins statistic and 3) d dimensional histograms
- It is important to understand (conceptually) the objectives and methodology introduced in this section (for more details refer to the learning outcome)

Today

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

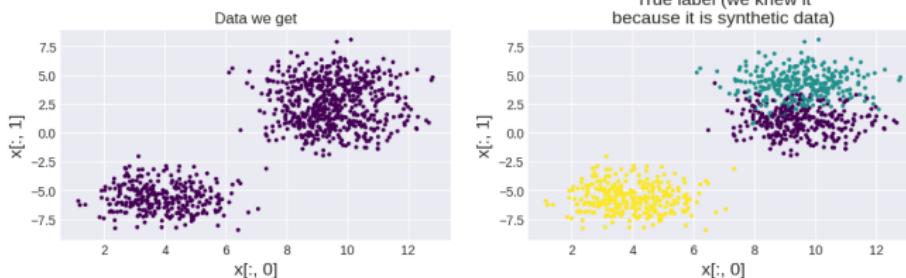
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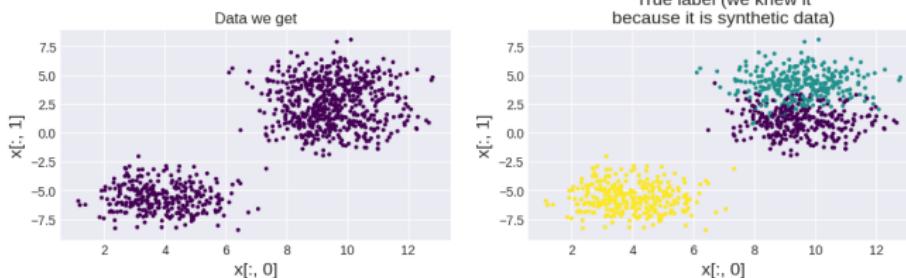
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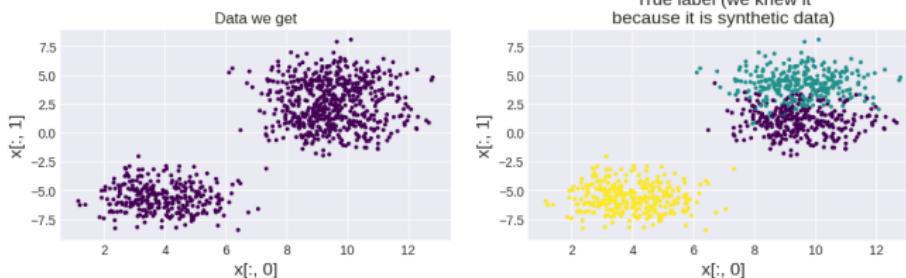
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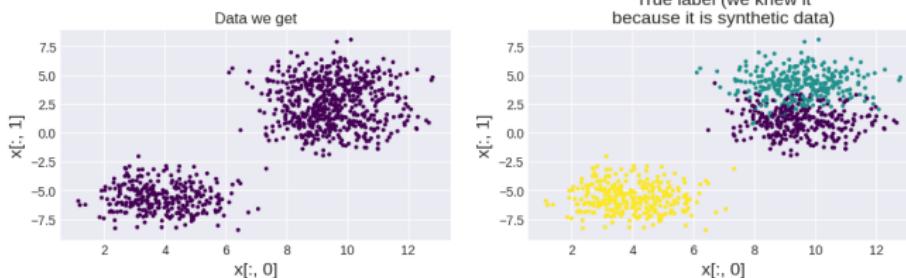
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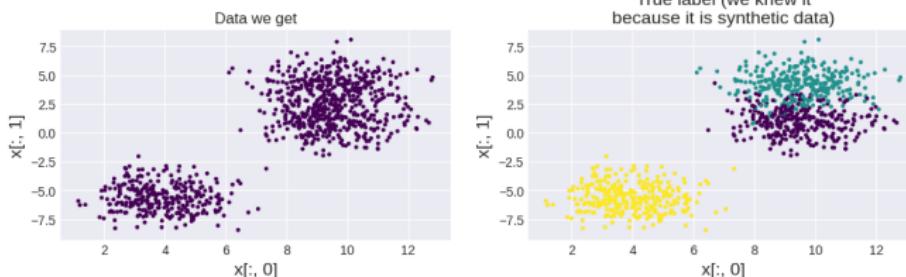
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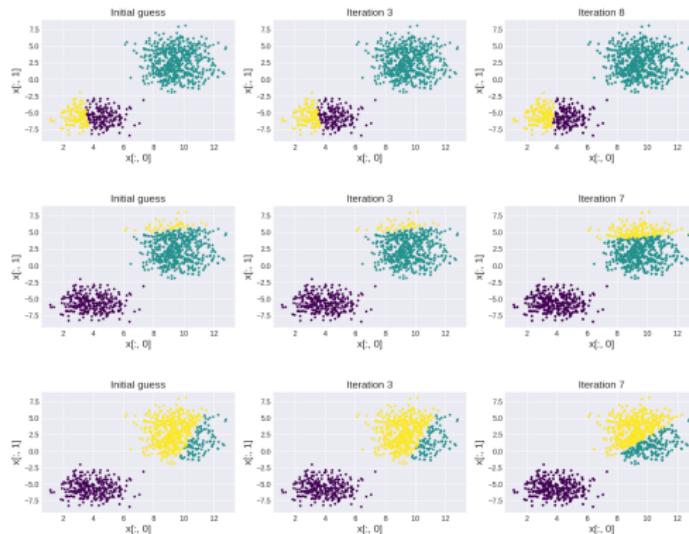
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- It is a **hard clustering** technique - one data point is assigned to only one cluster

K-means parameter estimation algorithm

- Algorithm
 - Randomly choose K centroids μ_k** for $k = 1, \dots, K$, e.g. randomly choose K data points from \mathcal{X}
 - Repeat the two steps below until convergence, e.g. $\hat{\mu}_k$ does not change anymore
 - For all $i = 1, \dots, N$, assign x_i to a cluster \hat{k}_i by computing
$$\hat{k}_i = \arg \min_{k \in \{1, \dots, K\}} dist(x_i, \hat{\mu}_k)$$
 - Let \mathcal{X}_k be the set of all x_i assigned to cluster k and N_k is the size of \mathcal{X}_k , compute
$$\hat{\mu}_k \leftarrow \frac{1}{N_k} \sum_{x_j \in \mathcal{X}_k} x_j$$
 - 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

```
1: Given a data set  $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ 
2: Randomly choose  $K$  data points from  $\mathcal{X}$  as the centroids  $\mu_k$  for
    $k = 1, \dots, K$ 
3: while true do
4:   Assign  $\mathbf{x}_i$  to the closest  $\mu_k$  for all  $i = 1, \dots, N$ 
5:   For all  $k = 1, \dots, K$ , compute  $\mu_k^{new}$  as the center of all  $\mathbf{x}_i$  assigned
      to cluster  $k$ 
6:   if  $\mu_k^{new} == \mu_k$  for all  $k$  then
7:     break
8:   else
9:      $\mu_k \leftarrow \mu_k^{new}$ 
10:  end if
11: end while
```

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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**

Two main challenges for K-means

- **Challenges:**
 - How to choose the hyperparameter K ?
 - K-means is sensitive to the initialization of $\hat{\mu}_k$ for $k = 1, \dots, K$
- **Solution:**
 - Choose a range of **candidate values**, e.g. for the first problem, we can choose $K \in \{1, \dots, 10\}$; for the second problem, we can randomly select 100 different initial guesses for $\hat{\mu}_k$
 - 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 criteria 1: SSE

Two commonly used alternative evaluation criteria

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

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

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

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Example:

- Given $x_1 = [x_1^1, x_1^2]$, $x_2 = [x_2^1, x_2^2]$, $x_3 = [x_3^1, x_3^2]$, $x_4 = [x_4^1, x_4^2]$, where $x_1, x_2 \in$ cluster 1 with centroid $\mu_1 = [\mu_1^1, \mu_1^2]$; $x_3, x_4 \in$ cluster 2 with centroid $\mu_2 = [\mu_2^1, \mu_2^2]$
- The SSE is computed as

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

Cluster quality evaluation criteria 1: SSE (cont.)

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

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

- SSE is essentially an error term: we want SSE to be small - choose the K value that minimizes SSE ?

Cluster quality evaluation criteria 1: SSE (cont.)

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- Note that $SSE \rightarrow 0$ for $K \rightarrow N$, 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

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- SSE is essentially an error term: we want SSE to be small - choose the K value that minimizes SSE ?
- Note that $SSE \rightarrow 0$ for $K \rightarrow N$, 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 , i.e. the point with the maximum curvature
- The elbow can be computed using, e.g. the kneed library in Python
- This method is also called the **elbow method**

Cluster quality evaluation criteria 2: Silhouette score

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

Cluster quality evaluation criteria 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

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

2. Silhouette score S (cont.):

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- **Within-cluster distance:** measures how data points scatter in relation to x_i within its own cluster; let x_i be a data point from cluster k ,

$$a_i = \frac{1}{|C_k| - 1} \sum_{x_j \in C_k \text{ and } j \neq i} dist(x_i, x_j)$$

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

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

Cluster quality evaluation criteria 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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- **Between-cluster distance:** measures how data points scatter in relation to x_i when these data points are from other clusters

$$b_i = \min_{k' \neq k, k' \in \{1, \dots, K\}} \frac{1}{|C_{k'}|} \sum_{x_j \in C_{k'}} dist(x_i, x_j)$$

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

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

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

2. Silhouette score S (cont.):

- Silhouette score for one data point:

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

A large S_i indicates a compact cluster k in relation to x_i and a large distance from x_i to clusters other than k

- Silhouette score for the data set

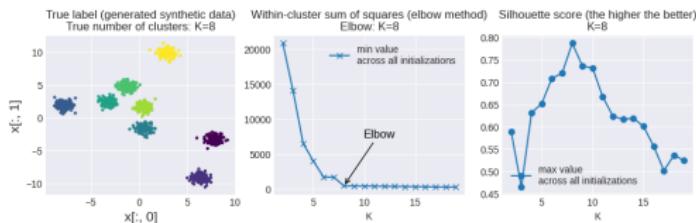
$$S = \frac{1}{N} \sum_{i=1}^N S_i, \quad S \in [-1, 1]$$

- A large Silhouette score indicates a good clustering quality

Example - choose K

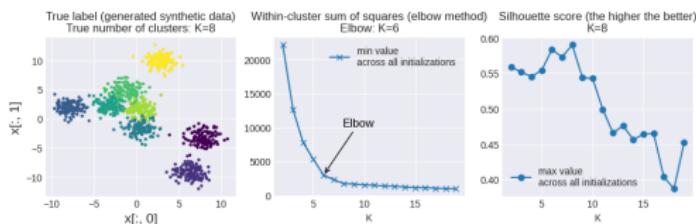
Clusters with equal variance ($K = 8$)

- 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

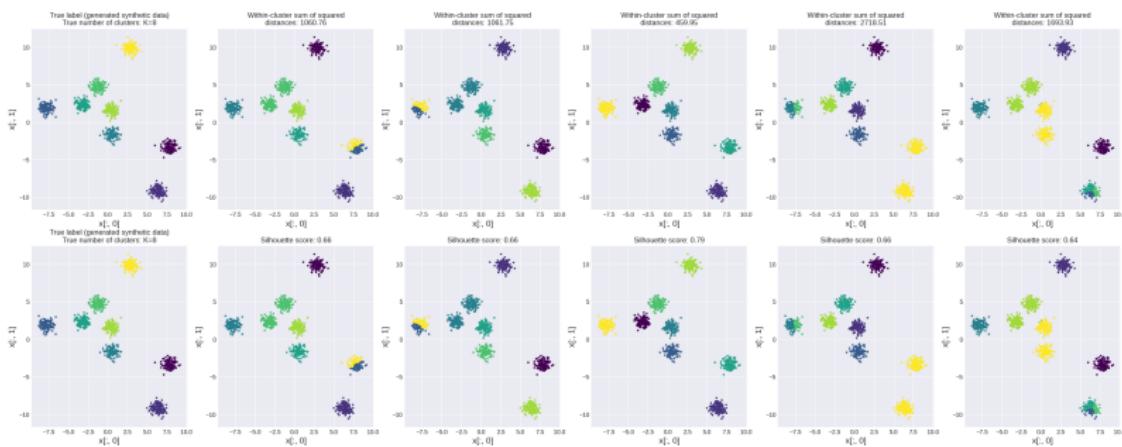


Example - choose initial guess

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

Clusters with equal variance ($K = 8$)

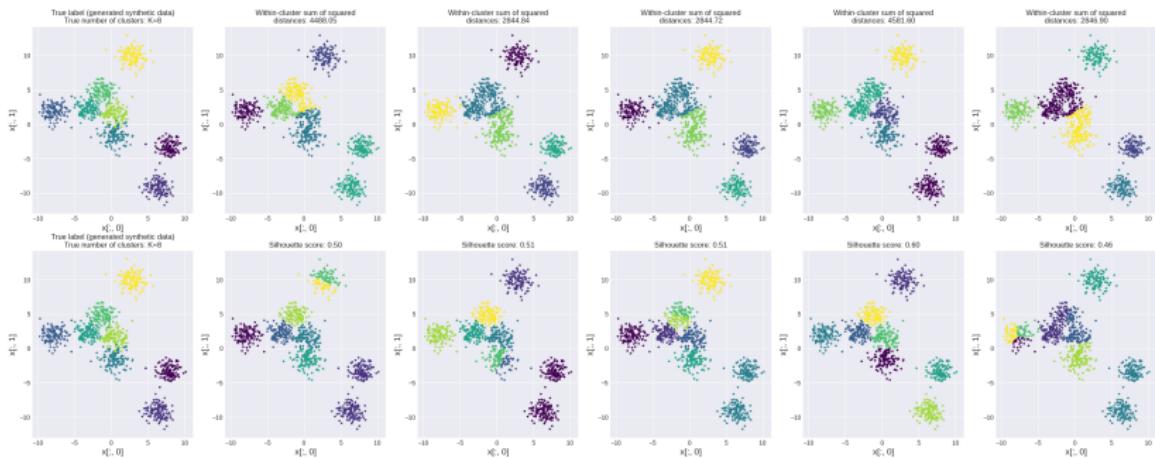
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- Silhouette score: $K = 8$



Example - choose initial guess (cont.)

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

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



Today

- 1 Introduction
- 2 Modeling for clustering
- 3 Cluster 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)
- Classification, multinomial naive Bayes classifier, Gaussian naive Bayes classifier
- Central limit theorem, interval estimation
- Hypothesis tests, comparison of two classifiers
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Next:

- More clustering models

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Before next lecture:

- Gaussian distribution
- The Bayes' rule