

# Lecture 11: Clustering Part III

## Statistical Methods for Data Science

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# Today

- 1 Clustering models
  - Centroid clustering
  - Distribution clustering
  - Hierarchical clustering
  - Density clustering
- 2 Cluster validation
- 3 Summary



# Learning outcome

- Be able to explain the EM algorithm for one dimensional GMM
- Be able to explain the difference between K-means and the EM algorithm in terms of parameter estimation

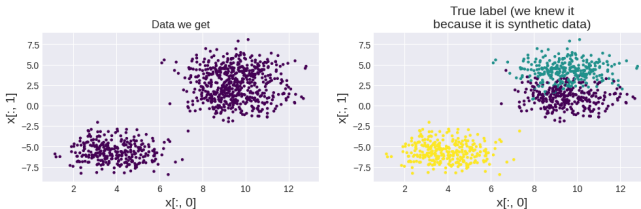
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## Centroid clustering

# Recall: K-means

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



- **Target**  $\mathbf{y}$ :

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

where  $\text{dist}(\cdot, \cdot)$  is a distance measure; in this course, we use the Euclidean distance (cf. lecture 9)

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

# K-means: pros and cons

- Pros:
  - Convergence guaranteed
  - Easy to implement
  - Scale to large data sets
- Cons:
  - Need to choose the hyperparameter  $K$  manually
  - Dependence on random initial values
  - Do not work well on very high dimensional data
  - Not robust to outliers

## Distribution clustering



# Recall: Gaussian Mixture Models (GMM) - overview

- **Data  $\mathbf{x}$** : a  $d$  dimensional feature vector  $\mathbf{x} = [x_1, \dots, x_d]$  with PDF  $f(\mathbf{x}) = \sum_{k=1}^K \pi_k f(\mathbf{x} | k)$
- **Target  $y$** :  $y$  is a set of  $K$  posterior probabilities; for  $k = 1, \dots, K$

$$\underbrace{P(k | \mathbf{x})}_{\text{posterior}} = \frac{\underbrace{P(k)}_{\text{prior}} \underbrace{f(\mathbf{x} | k)}_{\text{likelihood of } k}}{\sum_{c=1}^K P(c) f(\mathbf{x} | c)}$$

It is **soft clustering** -  $\mathbf{x}$  is assigned to **all clusters** with a probability - the posterior  $P(k | \mathbf{x})$ ;  
**alternatively**,  $y$  can be defined as the cluster index with the highest posterior probability, i.e.

$$y = \arg \max_{k \in \{1, \dots, K\}} P(k | \mathbf{x}) = \arg \max_{k \in \{1, \dots, K\}} P(k) f(\mathbf{x} | k)$$

- **Parameter**: the parameters of the mixture distribution  $f(\mathbf{x})$ 
  - The parameters for each Gaussian likelihood  $f(\mathbf{x} | k)$
  - The prior  $P(k)$ , typically denoted as  $\pi_k$

## Recall: two challenges for parameter estimation

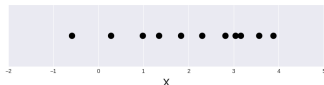
Compared to the Gaussian naive Bayes classifier parameter estimation

- Cluster labels unknown
- High dimensional features not independent - joint probability distribution

Let's address the first issue by looking at one dimensional Gaussian Mixture models

# Recall: parameter estimation for 1-d GMM

- **Data:**  $x_1, \dots, x_N$



- **Random variable:**  $X_1, \dots, X_N$  i.i.d. with PDF

$$f(x) = \sum_{k=1}^K \pi_k f(x | k)$$

The joint probability distribution of all data points is defined as

$$f_{X_1, \dots, X_N}(x_1, \dots, x_N) \stackrel{i.i.d.}{=} \prod_{i=1}^N f(x_i) = \prod_{i=1}^N \sum_{k=1}^K \pi_k f(x_i | k) \quad (1)$$

This is the **likelihood** of the **mixture distribution** given data  $x_1, \dots, x_N$ .

- **Parameter of interest:**  $\pi_k, \mu_k, \sigma_k$  for all  $k = 1, \dots, K$
- **Parameter estimation method:** maximum likelihood estimation

# Recall: parameter estimation for 1-d GMM (cont.)

- The **log likelihood** (cf. Eq. (1) on page 11) is defined as:

$$\begin{aligned} Q(\theta) &= \log L(\theta \mid x_1, \dots, x_N) = \log f_{X_1, \dots, X_N}(x_1, \dots, x_N) \\ &= \sum_{i=1}^N \log \left( \sum_{k=1}^K \pi_k f(x_i \mid k) \right) \end{aligned} \quad (2)$$

where  $\theta = (\mu_1, \dots, \mu_K, \sigma_1, \dots, \sigma_K, \pi_1, \dots, \pi_K)$

- The parameters are estimated by **maximizing the log likelihood**

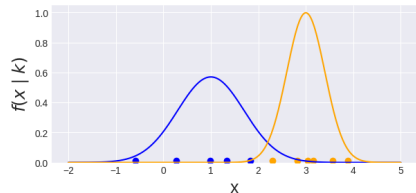
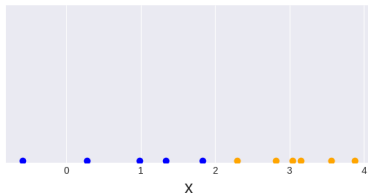
$$\hat{\theta} = \arg \max_{\theta} Q(\theta)$$

- There is no closed-form solution due to the summation inside the log!
- We need to apply an iterative method to find the solution - the **EM algorithm**

# Intuition behind EM

**Scenario 1:** if we knew the label of each data point, the task would be to estimate the parameters

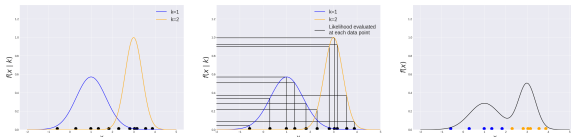
- $\pi_k = P(k) = \frac{N_k}{N}$ , where  $N_k$  is the count of data points that belong to cluster  $k$ , i.e.  
 $\pi_1 = P(\text{blue}) = \frac{5}{11}$  and  $\pi_2 = P(\text{orange}) = \frac{6}{11}$
- $\mu_k = \frac{1}{N_k} \sum_{i=1}^{N_k} x_i$
- $\sigma_k^2 = \frac{1}{N_k} \sum_{i=1}^{N_k} (x_i - \mu_k)^2$



Scenario 1  $\approx$  **maximization** step in the EM algorithm

# Intuition behind EM (cont.)

**Scenario 2:** if we knew the two priors  $P(1)$ ,  $P(2)$  and the two Gaussian distributions  $f(x | 1)$ ,  $f(x | 2)$ , the task would be to compute the posterior probability  $P(k | x)$  for  $k \in \{\text{orange}, \text{blue}\}$ ; then we can assign each data point  $x$  to a cluster  $y$  by the maximum a posteriori estimation  $y = \begin{cases} \text{blue}, & P(\text{orange} | x) < P(\text{blue} | x) \\ \text{orange}, & P(\text{orange} | x) \geq P(\text{blue} | x) \end{cases}$



- **Prior:**  $\pi_1 = P(z_1) = P(\text{blue})$ ,  $\pi_2 = P(z_2) = P(\text{orange})$
- **Likelihood:**  $f(x | \text{blue}) = \text{blue}$ ,  $f(x | \text{orange}) = \text{orange}$
- **Posterior:**

$$P(\text{blue} | x) = \frac{P(\text{blue})f(x | \text{blue})}{P(\text{blue})f(x | \text{blue}) + P(\text{orange})f(x | \text{orange})}$$

$$P(\text{orange} | x) = \frac{P(\text{orange})f(x | \text{orange})}{P(\text{blue})f(x | \text{blue}) + P(\text{orange})f(x | \text{orange})}$$

Scenario 2  $\approx$  **expectation** step in the EM algorithm

## Intuition behind EM (cont.)

- In reality, we don't know any of these!
- The idea here is that we alternate scenario 1 and 2 **iteratively** until convergence
- This is essentially how the **Expectation-Maximization (EM) algorithm** works
  - **E-step (expectation)**: estimate the posterior for all data points given each cluster (scenario 2)
  - **M-step (maximization)**: estimate the parameters for each cluster (scenario 1)
- Disclaimer: the purpose of the scenario 1 and 2 is to build up some intuitions only; for details of the EM algorithm, please refer to the description in the next few slides

# The EM algorithm: two main steps

Two main steps in the EM algorithm

- **E-step (expectation)**: compute the **posterior probability** of the cluster for each data point  $x_i$

$$\gamma_{ik} = P(k | x_i) = \frac{\pi_k f(x_i | k)}{\sum_{c=1}^K \pi_c f(x_i | c)}, \text{ for all } k = 1, \dots, K$$

This posterior is also called the **responsibility**, denoted as  $\gamma_{ik}$

- **M-step (maximization)**: estimate the parameters
  - $\pi_k = P(k) = \frac{N_k}{N}$ , where  $N_k = \sum_{i=1}^N \gamma_{ik}$  - **soft clustering**
  - $\mu_k = \frac{1}{N_k} \sum_{i=1}^N \gamma_{ik} x_i$
  - $\sigma_k^2 = \frac{1}{N_k} \sum_{i=1}^N \gamma_{ik} (x_i - \mu_k)^2$
 for each cluster  $k = 1, \dots, K$



# K-means as a special case of the EM algorithm

## Expectation Step

- EM: **soft clustering** - posterior

$$\gamma_{ik} = P(k | x_i)$$

Why soft? - It is a probability, i.e.  $\gamma_{ik} \in [0, 1]$

- K-means: **hard clustering** - equivalent to

$$\gamma_{ik} = \begin{cases} 1, & \text{if the centroid of cluster } k \text{ is the closest to } x_i \\ 0, & \text{otherwise} \end{cases}$$

Why hard? - It is a binary decision, i.e.  $\gamma_{ik} \in \{0, 1\}$

## Maximization Step

- EM: need to estimate  $\mu_k, \sigma_k$ , where

$$\mu_k = \frac{1}{N_k} \sum_{i=1}^K \gamma_{ik} x_i, \quad \sigma_k^2 = \frac{1}{N_k} \sum_{i=1}^K \gamma_{ik} (x_i - \mu_k)^2, \quad N_k = \sum_{i=1}^N \gamma_{ik}, \quad \text{for } \gamma_{ik} \in [0, 1]$$

- K-means: only need to estimate  $\mu_k$ , where

$$\mu_k = \frac{1}{N_k} \sum_{i=1}^N \gamma_{ik} x_i = \frac{1}{N_k} \sum_{x \in \text{cluster } k} x, \quad N_k = \sum_{i=1}^N \gamma_{ik}, \quad \text{for } \gamma_{ik} \in \{0, 1\}$$

# The complete EM algorithm

- These two steps are the core of the EM algorithm
- Besides that, there are some extra steps involved
- The EM algorithm is an **iterative method**
- There are three important components in an iterative method:
  - 1) Initialization step
  - 2) Update the parameters in a while loop (the core, i.e. the maximization step and the expectation step)
  - 3) Stopping criteria

## The complete EM algorithm (cont.)

- **1) Initialization step:** initialize  $\pi_k$ ,  $\mu_k$ ,  $\sigma_k$  manually or using, e.g. the K-means algorithm  $\mu_k$ , for all  $i = 1, \dots, N$ ,  $k = 1, \dots, K$

## The complete EM algorithm (cont.)

- **1) Initialization step:** initialize  $\pi_k$ ,  $\mu_k$ ,  $\sigma_k$  manually or using, e.g. the K-means algorithm  $\mu_k$ , for all  $i = 1, \dots, N$ ,  $k = 1, \dots, K$
- **2) Update the parameters in a while loop:** repeat the expectation step and the maximization step until the stopping criteria are met; each repetition of this process is called **one iteration**

## The complete EM algorithm (cont.)

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- **2) Update the parameters in a while loop:** repeat the expectation step and the maximization step until the stopping criteria are met; each repetition of this process is called **one iteration**
- **3) Stopping criteria:** something you check (using e.g. a conditional statement) inside the while loop; if the stopping criteria are true, the loop shall be escaped - then you are done! There are two alternative stopping criteria for the EM algorithm:
  - Has the objective function, i.e. the log likelihood (cf. Eq. (2)), changed since the last iteration?
  - Have any of the parameters, i.e.  $\pi_k$ ,  $\mu_k$ ,  $\sigma_k$ , changed since the last iteration?

# High dimensional GMM

- The second problem on page 10 is the high dimensional joint probability distribution of the correlated feature vectors
- In this course, we will not go into details of multivariate Gaussian distributions; nevertheless, the EM steps for  $d > 1$  is presented as follows

## Expectation Step

$$\gamma_{ik} = P(k | \mathbf{x}_i) = \frac{\pi_k f(\mathbf{x}_i | k)}{\sum_{c=1}^K \pi_c f(\mathbf{x}_i | c)}, \text{ for all } k = 1, \dots, K$$

## Maximization Step

- $\pi_k = P(k) = \frac{N_k}{N}$ , where  $N_k = \sum_{i=1}^N \gamma_{ik}$
- $\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{i=1}^N \gamma_{ik} \mathbf{x}_i$
- $\boldsymbol{\Sigma}_k = \frac{1}{N_k} \sum_{i=1}^N \gamma_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T$  - note that  $\mathbf{x}_i$  is a column vector here

The covariance matrix  $\boldsymbol{\Sigma}_k$  captures the dependence between features

# Recap: GMM

- Gaussian Mixture Models (GMM) is a mixture distribution characterized by a mixture PDF

$$f(\mathbf{x}) = \sum_{k=1}^K \pi_k f(\mathbf{x} | k)$$

where each  $f(\mathbf{x} | k)$  is a multivariate Gaussian PDF for each Gaussian component  $k$  **multivariate**  
because  $\mathbf{x} \in \mathbb{R}^d$  is a  $d$  dimension feature vector

- $f(\mathbf{x})$  is the PDF of the mixture model with **parameters**  $\theta = \{\mu_1, \dots, \mu_K, \Sigma_1, \dots, \Sigma_K\}$
- $f(\mathbf{x})$  is the **likelihood** of  $\theta$  given data  $\mathbf{x}$
- **Parameter estimation**: maximum **likelihood** estimation - given  $\mathbf{x}_1, \dots, \mathbf{x}_N$

$$\hat{\theta} = \arg \max_{\theta} \sum_{i=1}^N \log(f(\mathbf{x}_i))$$

- No closed form solution - iterative algorithm for finding  $\hat{\theta}$  - the EM algorithm
- Comparison to other techniques
  - Gaussian naive Bayes classifiers vs GMM
  - K-means vs the EM algorithm for parameter estimation

# GMM: pros and cons

- Pros:
  - Relatively simple compared to other mixture models **we love Gaussians!**
  - Flexibility due to the soft clustering criterion
- Cons:
  - Might get stuck on local optimum of the objective function
  - Convergence can be slow
  - Covariance matrix estimate might lead to divergence in case of small data set
  - Need to choose the hyperparameter  $K$  manually
  - Gaussian mixture assumption might not be true



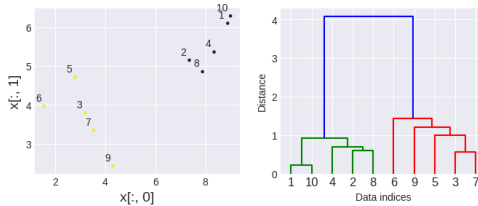
# Hierarchical clustering

# Agglomerative vs divisive

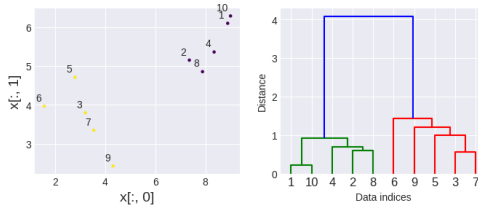
Two types of hierarchical clustering

- Agglomerative (bottom-up):
  - Start with each data point being its own cluster
  - Merge the closest clusters until there is only one cluster
- Divisive (top-down):
  - Start with one cluster
  - Split until each cluster contains only one data point

# Agglomerative hierarchical clustering using a dendrogram

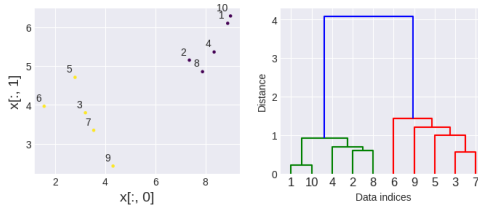


# Agglomerative hierarchical clustering using a dendrogram



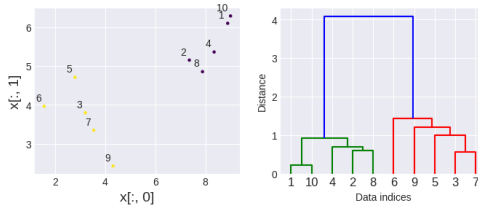
- Step 1: consider each data point as its own cluster; find the closest clusters - 1 and 10; group 1 and 10 into one cluster; the height of the dendrogram indicates the Euclidean distance

# Agglomerative hierarchical clustering using a dendrogram



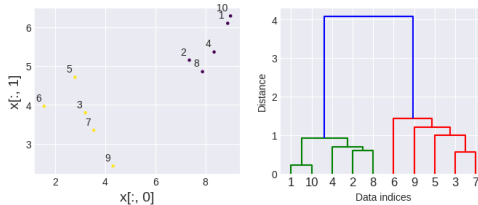
- Step 1: consider each data point as its own cluster; find the closest clusters - 1 and 10; group 1 and 10 into one cluster; the height of the dendrogram indicates the Euclidean distance - now we have 9 clusters in total

# Agglomerative hierarchical clustering using a dendrogram



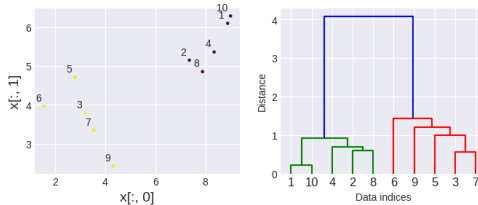
- Step 1: consider each data point as its own cluster; find the closest clusters - 1 and 10; group 1 and 10 into one cluster; the height of the dendrogram indicates the Euclidean distance - now we have 9 clusters in total
- Step 2: find the closest clusters - 3 and 7 - group 3 and 7 into one cluster

# Agglomerative hierarchical clustering using a dendrogram



- Step 1: consider each data point as its own cluster; find the closest clusters - 1 and 10; group 1 and 10 into one cluster; the height of the dendrogram indicates the Euclidean distance - now we have 9 clusters in total
- Step 2: find the closest clusters - 3 and 7 - group 3 and 7 into one cluster
- Step 3: repeat until there is only one cluster left

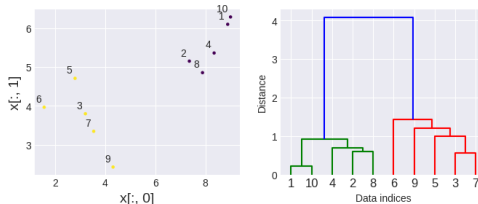
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- Step 1: consider each data point as its own cluster; find the closest clusters - 1 and 10; group 1 and 10 into one cluster; the height of the dendrogram indicates the Euclidean distance - now we have 9 clusters in total
- Step 2: find the closest clusters - 3 and 7 - group 3 and 7 into one cluster
- Step 3: repeat until there is only one cluster left
- Step 4: draw a horizontal line to split data into different clusters



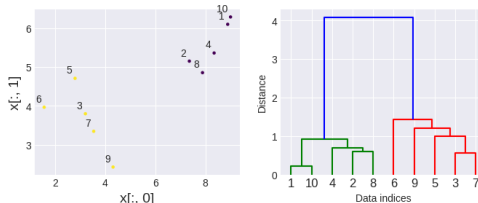
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Divisive hierarchical clustering has a similar process (but top-down)

# Distance between clusters - alternative linkages



- The height of the dendrogram shows the distance between two clusters
- We need to choose how to compute the distance on the cluster level when there are more than one point in each cluster
- There are different alternatives to defined the distance between two clusters, e.g. the distance between cluster  $\{1, 10\}$  and cluster  $\{4, 2, 8\}$ 
  - **Single-linkage**: the distance between the closest pair, i.e.  $dist(1, 4)$
  - **Complete-linkage**: the distance between the farthest pair, i.e.  $dist(10, 8)$
  - **Centroid**: the distance between two centroids, i.e.

$$dist(\text{centroid}(\{1, 10\}), \text{centroid}(\{4, 2, 8\}))$$

Here,  $dist(\cdot, \cdot)$  is the Euclidean distance

# Hierarchical clustering: pros and cons

- Pros:
  - No need to choose  $K$
  - Easy to implement
  - Might give meaningful taxonomies
- Cons:
  - Once two clusters are grouped, the action cannot be undone
  - Does not scale well with large data set
  - No well defined objective function

## Density clustering

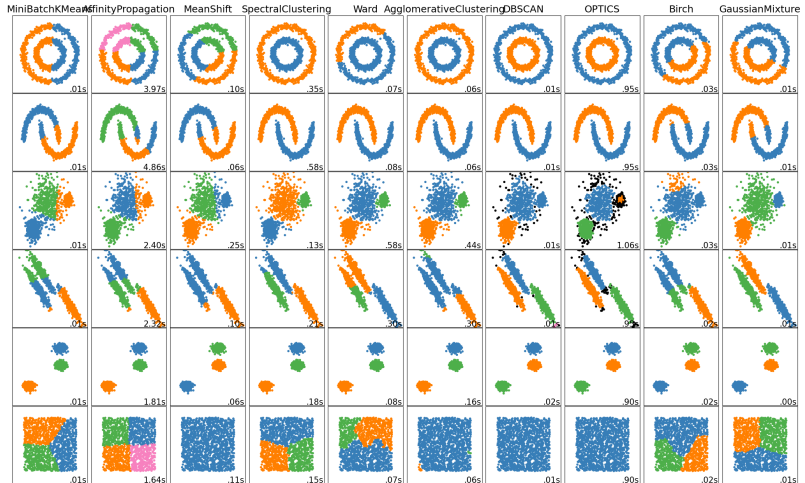
# Introduction

- Idea: cluster data based on their closest points, i.e. the neighborhood
- Hyperparameter
  - Radius of the neighborhood  $\epsilon$
  - Minimum number of points  $n$  in its  $\epsilon$  neighborhood

# Density clustering: pros and cons

- Pros:
  - Handles clusters with arbitrary shapes
  - Handles noise explicitly
- Cons:
  - Sensitive to the sampling technique in the neighborhood
  - Need to choose the hyperparameters  $\epsilon$  and  $n$
  - Not optimal for clusters with varying density

# Comparison (from Python scikit-learn)



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# Validation criteria

Cluster validation is to evaluate the quality of clusters; there are two types of criteria:

- Internal criteria: unsupervised; cluster labels are unknown
  - Algorithms that assume clusters with spherical shapes
    - Silhouette score
    - SSE
    - Many other indices, e.g. Davies–Bouldin index, Dunn index, etc
  - Algorithms that assume mixture distributions
    - AIC
    - BIC
  - Distance based criteria; more generic
    - Similarity matrix with data ordered by cluster indices
- External criteria: supervised; ground truth labels are given
  - Purity
  - F1-score
  - Entropy and mutual information

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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
- Clustering, cluster tendency, k-means
- SSE and Silhouette score for cluster evaluation, one dimensional Gaussian Mixture Models, AIC/BIC, the EM algorithm, clustering validation

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Next:

- Hypothesis testing, review for exam



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Before next lecture:

- Slides of lecture 8

