Distribution clustering Hierarchical clustering Density clustering Cluster validation Summary

Lecture 8: Clustering Part II Statistical Methods for Data Science

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Today

- Distribution clustering
 - Gaussian Mixture Models (GMM)
 - Parameter estimation: the EM algorithm
 - Hyperparameter K: AIC and BIC
- 2 Hierarchical clustering
- 3 Density clustering
- Cluster validation
- Summary





Learning outcome

- Be able to explain the difference between Gaussian naive Bayes classifier and GMM in terms of parameter estimation
- ullet Be able to explain the objective function Q(heta) for GMM
- Understand what EM algorithm is used for and why we need it
- Be able to calculate AIC/BIC and use them to determine K for GMM
- 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 their assumptions and parameter estimation



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Distribution clustering
Hierarchical clustering
Density clustering
Cluster validation

Gaussian Mixture Models (GMM)
Parameter estimation: the EM algorithm
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Gaussian Mixture Models (GMM)





Four categories

Clustering models

- Centroid clustering (lecture 7)
- Distribution clustering
- Density clustering
- Hierarchical clustering





Distribution clustering:

- Each cluster is modeled using a probability distribution
- Each data point is modeled using a "combination of all clusters"



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Gaussian Mixture Models:

• Data x: a d dimensional feature vector $\mathbf{x} = [x_1, \dots, x_d]$

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

where

- f(x) is the PDF of x ("multivariate");
- $\pi_k = P(k) > 0$ and $\sum_{k=1}^K \pi_k = 1$;
- f(x | k) is a d dimensional multivariate Gaussian PDF describing cluster k.





Gaussian Mixture Model:

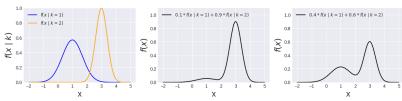
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- ullet Examples of the mixture distribution with d=1
 - Example 1: $\pi_1 = 0.1$, $\pi_2 = 0.9$

$$f(\mathbf{x}) = 0.1 \times f(\mathbf{x} \mid \mathbf{k} = 1) + 0.9 \times f(\mathbf{x} \mid \mathbf{k} = 2) = 0.1 \times f(\mathbf{x} \mid \mu_1, \sigma_1) + 0.9 \times f(\mathbf{x} \mid \mu_2, \sigma_2)$$

• Example 2: $\pi_1 = 0.4$, $\pi_2 = 0.6$

$$f(\mathbf{x}) = 0.4 \times f(x \mid k = 1) + 0.6 \times f(x \mid k = 2) = 0.4 \times f(x \mid \mu_1, \sigma_1) + 0.6 \times f(x \mid \mu_2, \sigma_2)$$



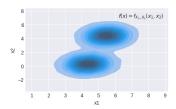




• Examples of the mixture distribution with d=2: $\pi_1=0.5$, $\pi_2=0.5$

$$f(\mathbf{x}) = 0.5 \times f(\mathbf{x} \mid k = 1) + 0.5 \times f(\mathbf{x} \mid k = 2) = 0.5 \times f(\mathbf{x} \mid \mu_1, \Sigma_1) + 0.5 \times f(\mathbf{x} \mid \mu_2, \Sigma_2)$$

where $\mu_k \in \mathbb{R}^2$ is the mean and $\Sigma_k \in \mathbb{R}^{2 \times 2}$ is the covariance matrix



Gaussian Mixture Models (GMM)

Parameter estimation: the EM algorithm Hyperparameter K: AIC and BIC

Gaussian Mixture Models (GMM) - overview (cont.)





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- Target y: y is a set of K posterior probabilities; for $k = 1, \dots, K$

likelihood of k

$$\underbrace{P(k \mid x)}_{posterior} = \underbrace{\frac{P(k)}{F(k)}}_{c=1} \underbrace{\frac{given data}{f(x \mid k)}}_{f(x \mid c)}$$

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- Parameter:
 - The parameters for each Gaussian likelihood $f(x \mid k)$
 - The prior P(k), typically denoted as π_k





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Hyperparameter K: AIC and BIC

Parameter estimation: the EM algorithm





Parameter estimation





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- Let's discuss the key differences between these two algorithms



Parameter estimation

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- Let's discuss the key differences between these two algorithms
- Set up: given a data set $\mathcal{X} = \{x_1, \cdots, x_N\}$, we need to estimate the parameter of interest from \mathcal{X}

	Gaussian naive Bayes classifier	Gaussian Mixture Models
Parameter of interest	$P(k)$, Gaussian PDF $f(x \mid k)$, for $k = 1, \dots, K$	
Training data (labels) available?	Yes	No
Probabilistic model	One Gaussian for each x;	A linear combination of K Gaussians for each x_i
Interpretation	One label for each x_i (hard assignment)	K probabilities for each x_i (soft assignment)
Assumption	x_i and x_j independent for $i \neq j$	
	x_m^i and x_n^i independent for dimensions $m \neq n$ (NAIVE!)	x_m^i and x_n^i NOT necessarily independent for dimensions $m \neq n$

Note: the subscripts here are the indices for the dimensions of the feature space; they are not the indices for the data points - data points are still independent!





Parameter estimation for GMM (cont.)

In summary, we have the following additional challenges compared to the Gaussian naive Bayes classifier:

- 1. We do not have the labels we cannot easily estimate P(k) and $f(x \mid k)$
- 2. The distribution $f(\mathbf{x} \mid k)$ is a multivariate Gaussian PDF and the features are not necessarily independent now we need to explicitly work with joint probability distributions $f_{X_1, \dots, X_d}(x_1, \dots, x_d \mid k)$ and covariance matrices (ugh!!)



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Let's focus on the first issue by working with one dimensional feature vectors so we don't get overwhelmed by dealing with all the problems at once Note: in this lecture, sometimes we simply use θ to denote the estimate (instead of $\hat{\theta}$) in order to reduce clutter since the notations are already quite complex

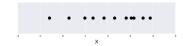


Data: x₁, · · · , x_N





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• Random variable: X_1, \dots, X_N i.i.d. with PDF

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The joint probability distribution of all data points is defined as

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

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- Parameter estimation method: maximum likelihood estimation





• The log likelihood (cf. Eq. (1) on page 14) is

$$Q(\theta) = \log L(\theta \mid x_1, \dots, x_N) = \log f_{X_1, \dots, X_N}(x_1, \dots, x_N)$$

$$= \sum_{i=1}^N \log \left(\sum_{k=1}^K \pi_k f(x_i \mid k) \right)$$
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where
$$\theta = (\mu_1, \cdots, \mu_K, \sigma_1, \cdots, \sigma_K, \pi_1, \cdots, \pi_K)$$



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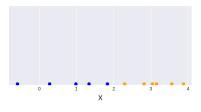
- There is no closed-form solution due to the summation inside the log!
- We need to apply an iterative method to find the solution the EM algorithm

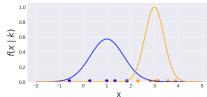




Intuition behind (simplified) EM

Scenario 1: if we knew the label of each data point, the task would be to estimate the parameters (similar to Gaussian Naive Bayes)

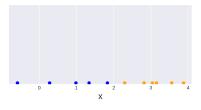


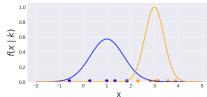




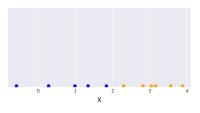
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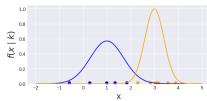
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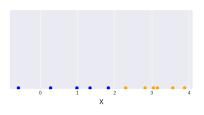


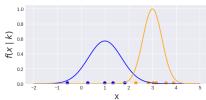


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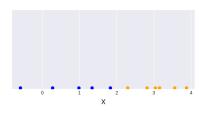


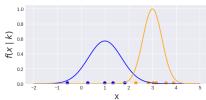


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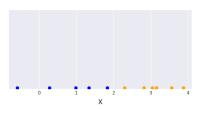
Lecture 8: Clustering Part II

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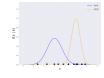
Scenario $1 \approx \text{maximization}$ step in the EM algorithm





Scenario 2: if we knew the two priors P(1), P(2) and the two Gaussian distributions $f(x \mid 1)$, $f(x \mid 2)$, the task would be to compute the posterior probability $P(k \mid x)$ 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
$$y = \begin{cases} \text{blue}, & P(\text{orange} \mid x) < P(\text{blue} \mid x) \\ \text{orange}, & P(\text{orange} \mid x) \ge P(\text{blue} \mid x) \end{cases}$$



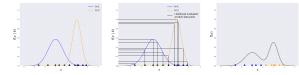






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- Prior: $\pi_1 = P(z_1) = P(blue)$, $\pi_2 = P(z_2) = P(orange)$
- Likelihood: $f(x \mid blue) = blue$, $f(x \mid orange) = orange$
- Posterior:

$$P(\mathsf{blue} \mid x) = \frac{P(\mathsf{blue})f(x \mid \mathsf{blue})}{P(\mathsf{blue})f(x \mid \mathsf{blue}) + P(\mathsf{orange})f(x \mid \mathsf{orange})}$$

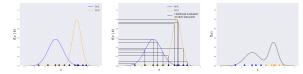
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Scenario $2 \approx \text{expectation}$ step in the EM algorithm





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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

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

This posterior is also called the **responsibility**, denoted as γ_{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

$$\bullet \ \mu_k = \frac{1}{N_k} \sum_{i=1}^N \frac{\gamma_{ik}}{\gamma_{ik}} x_i$$

$$\bullet \ \sigma_k^2 = \frac{1}{N_k} \sum_{i=1}^N \frac{\gamma_{ik}}{\gamma_{ik}} (x_i - \mu_k)^2$$

for each cluster $k = 1, \dots, K$





K-means as a special case of the EM algorithm

Expectation Step

EM: soft clustering - posterior

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

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 μ_k , σ_k , where

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

ullet K-means: only need to estimate μ_k , where

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

The complete EM algorithm

- These two steps are the core of the EM algorithm
- 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 π_k , μ_k , σ_k manually (randomly) or using, e.g. the K-means algorithm μ_k , for all $i=1,\cdots,N$, $k=1,\cdots,K$



The complete EM algorithm (cont.)

- 1) Initialization step: initialize π_k , μ_k , σ_k manually (randomly) or using, e.g. the K-means algorithm μ_k , for all $i=1,\cdots,N$, $k=1,\cdots,K$
- 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.)

- 1) Initialization step: initialize π_k , μ_k , σ_k manually (randomly) or using, e.g. the K-means algorithm μ_k , for all $i=1,\cdots,N$, $k=1,\cdots,K$
- 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**
- 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)), stopped changing since the last iteration?
 - Have any of the parameters, i.e. π_k , μ_k , σ_k , stopped changing since the last iteration?





Take away

- GMM: weighted summation of PDFs
- GMM vs K-means?
- GMM vs Gaussian naive Bayes?
- EM implementation (what does each step do)?



Gaussian Mixture Models (GMM)
Parameter estimation: the EM algorithm
Hyperparameter K: AIC and BIC

Hyperparameter K: AIC and BIC





How to choose hyperparameter K

- ullet For a given data set, we need to choose the number of clusters ${\cal K}$
- Similar to K-means, we first estimate $\hat{\theta}$ and then we choose the K value that gives the best clustering quality
- We introduce two alternative criteria for this task: Akaike Information Criterion (AIC) and Bayesian Information Criterion (BIC)
- Principle: low error + low model complexity





How to choose hyperparameter K (cont.)

Let c_K be the number of parameters to be estimated:

$$c_K = \overbrace{K \times d \times (d+1)/2}^{\text{covariance matrices}} + \overbrace{(K-1)}^{\text{priors}} + \overbrace{d \times K}^{\text{means}}$$

Note: the covariance matrix is symmetric \Rightarrow (d diagonal elements + d^2 all elements)/2



How to choose hyperparameter K (cont.)

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Note: the covariance matrix is symmetric \Rightarrow (d diagonal elements + d^2 all elements)/2

Akaike Information Criterion (AIC)

$$\begin{array}{lll} & & & \text{How well the model explains data ("error")} & & \text{Complexity of the model} \\ AIC(K) & = & & -\log(\text{likelihood}) & + & & \\ & = & -Q(\hat{\theta}) + c_K & & & \\ \end{array}$$

How to choose hyperparameter K (cont.)

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Bayesian Information Criterion (BIC)

$$BIC(K) = \frac{\text{How well the model explains data ("error")}}{-\log(\text{likelihood})} + \frac{1}{2}c_K\log N$$

$$= -Q(\hat{\theta}) + \frac{1}{2}c_K\log N$$

Lecture 8: Clustering Part II

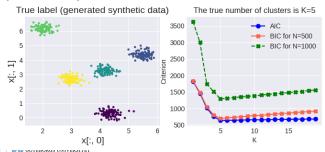
Note: an alternative definition is to multiply this definition of AIC and BIC by 2





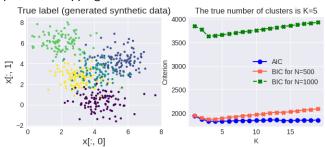
AIC vs BIC

- The idea is to find the best K that balances the "error" and the complexity of the model - Occam's Razor (cf. lecture 5) - if two models explain the data equally well, we choose the simpler one!
- ullet BIC penalizes the complexity more than AIC BIC increases more as ${\cal K}$ gets larger
- Example 1: well separated clusters



AIC vs BIC (cont.)

• Example 2: overlapping clusters



High dimensional GMM

- The second problem on page 13 is the high dimensional joint (multivariate) probability distribution of the correlated features
- The EM steps for d > 1 is presented as follows

Expectation Step

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

Maximization Step

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

The covariance matrix Σ_k captures the dependence between features

Note: you should be able to calculate the two dimensional case





Recap: GMM

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

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

where each $f(x \mid k)$ is a multivariate Gaussian PDF for each Gaussian component k multivariate because $x \in \mathbb{R}^d$ is a $d \geq 1$ dimensional 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(x) is the **likelihood** of θ given data x
- Parameter estimation: maximum likelihood estimation given x_1, \dots, x_N

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

- ullet No closed form solution iterative algorithm for finding $\hat{ heta}$ 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!
 - Flexible 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



Today

- 1 Distribution clustering
- 2 Hierarchical clustering
- 3 Density clustering
- 4 Cluster validation
- Summary



Agglomerative vs divisive

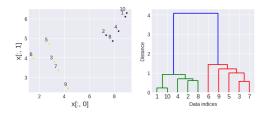
Two types of hierarchical clustering

- 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



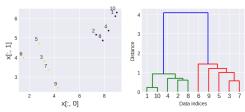
- Step 1: consider each data point as its own cluster; find the closest clusters 1 and 10; group 1 and 10 into one cluster; the height of the dendrogram indicates the Euclidean distance - now we have 9 clusters in total
- Step 2: find the closest clusters 3 and 7 group 3 and 7 into one cluster
- Step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

Divisive hierarchical clustering has a similar process but top-down; split can be done using, e.g., K-means





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 a cluster level when there are more than one point in a 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.

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

In this example, $dist(\cdot, \cdot)$ is the Euclidean distance





Hierarchical clustering: pros and cons

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



Today

- Distribution clustering
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Introduction

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



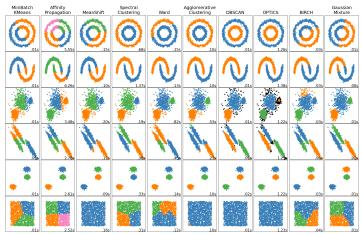
Density clustering: pros and cons

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





Comparison (from Python scikit-learn)







Today

- Distribution clustering
- 2 Hierarchical clustering
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Distribution clustering Hierarchical clustering Density clustering Cluster validation Summary

Validation criteria

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





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

- 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



Validation criteria

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 - 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





Today

- Distribution clustering
- 2 Hierarchical clustering
- 3 Density clustering
- 4 Cluster validation
- **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
- Clustering, cluster tendency
- Centroid clustering, k-means, parameter estimation, SSE, Silhouette score
- Gaussian Mixture Models, AIC/BIC
- The EM algorithm





Summary

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Next:

- Recap: probability distributions, likelihood function, MLE, MAP, the Bayes' rule, CLT
- Hypothesis testing



