Introduction to Machine Learning

Lecture 10　Representation and Clustering - Bayesian Gaussian Mixture Models and Mean Shift

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Outline

Review

- Generative modeling and Gaussian mixture model
- EM algorithm
- Revisit K-means from an EM viewpoint

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Today

- A Bayesian viewpoint of Gaussian mixture model and MCMC
- Nonparametric clustering and kernel density estimation
- Mean shift algorithm.

Revisit The Generative Mechanism of GMM

Suppose that there are K Gaussian distributions defined on the sample space $\mathcal{X} \subset \mathbb{R}^D$.

- $\boldsymbol{w} = [w_k] \in \Delta^{K-1}$
- $\{\mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\}_{k=1}^K$

Generative process:

1. Determine the cluster: $k \sim \text{Categorical}(\boldsymbol{w})$
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How to determine the number of clusters and the corresponding distributions?

Bayesian Inference of GMM

- Recall that a GMM is

$$p(x) = \sum_{k=1}^{K} w_k \underbrace{p_k(x; \boldsymbol{\mu}_k, \Sigma_k)}_{\text{Gaussian}}$$

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- **Bayesian GMM** sets the prior distributions for its parameters $\{w_k, \boldsymbol{\mu}_k, \boldsymbol{\Phi}_k\}_{k=1}^{K}$.

Bayesian Inference of GMM (1D)

Conjugate Priors

- $\boldsymbol{w} \sim \text{Dirichlet}(\delta_1, ..., \delta_K)$
- $\phi_k \sim \text{Gamma}(\frac{a}{2}, \frac{b}{2}), \forall k$
- $\mu_k|\phi \sim \mathcal{N}(m_k, \frac{1}{\alpha_k \phi_k}), \forall k$

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Posteriors given data x's and the latent code z's

- $\boldsymbol{w} | x, z \sim \text{Dirichlet}(\delta_1^*, \dots, \delta_K^*)$
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\begin{aligned}
&\delta_k^* = \delta_k + N_k, \quad a_k^* = a + N_k, \quad b_k^* = b + \sum\nolimits_{z_j = k} (x_j - \mu_k)^2 \\
&\alpha_k^* = \alpha_k + N_k, \quad m_k^* = \frac{1}{\alpha_k^*}(\alpha_k m_k + \sum\nolimits_{z_j = k} x_j)
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Compare to EM:

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- MCMC **samples** latent codes and parameters in a probabilistic way.

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- Generally, the complexity is high (due to the efficiency of sampling)

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- The distribution of data is constructed by the data itself.
- The inference is transductive.

Kernel Density Estimation (KDE)

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h is the bandwidth.

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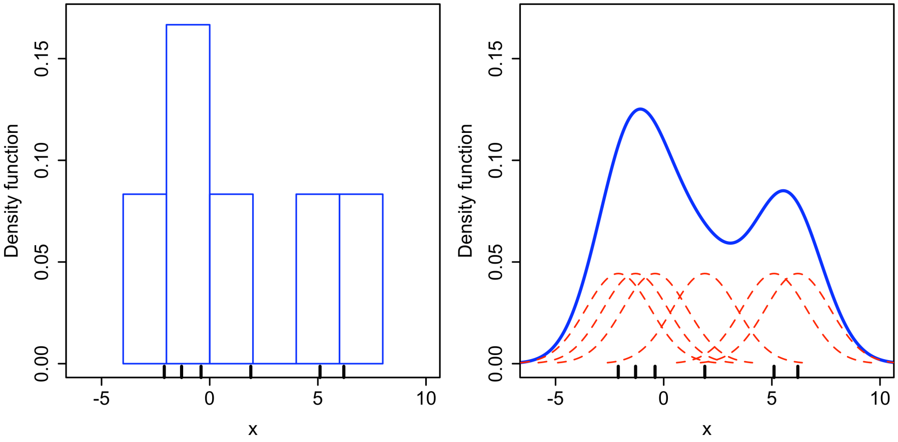
- For 1D data in general, $h = \mathcal{O}(N^{-0.2})$.

Histogram: The Simplest Kernel Density Estimation



Connections to What We Learned/Will Learn

Mixture Model:

- When K_h is a Gaussian kernel: $K_h(x, x') = \frac{1}{\sqrt{2\pi}h} \exp(-\frac{|x-x'|^2}{2h^2})$, KDE actually can be interpreted a GMM model with known parameters (See, the boundary of parametric and nonparametric modeling is not so strict:))

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Naïve Bayes Classifier:

- KDE is often used to estimate the class-conditional marginal densities of data, and thus, improve classification accuracy. (Next lecture)

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Principle:

- Given a set of samples $\{x_n \in \mathcal{X}\}_{n=1}^{N}$ and a kernel function $K : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}_+$, the mean of the samples in the neighborhood of x is

$$m(x) = \frac{\sum_{x_i \in \mathcal{N}(x)} K_h(x, x_i) x_i}{\sum_{x_i \in \mathcal{N}(x)} K_h(x, x_i)}.$$

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- **Why?**

The Rationality of (Gaussian) Mean-shift

- Suppose that $K_h(x, x') = \frac{1}{\sqrt{2\pi}h} \exp(-\frac{\|x-x'\|_2^2}{2h^2})$, derive $\frac{\partial \hat{p}(x)}{\partial x}$.

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- The curse of dimensionality is still a problem.

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- Update $x_n \leftarrow m(x_n)$.

(Gaussian) Mean-shift Is An EM Algorithm

E-step:

- Compute $m(x_n)\ \forall n$.

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Recall that EM learns the model with **observed data** and **latent variables**.

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- M-step: maximize $p(x) = \int p(x|m)p(m)\mathrm{d}m$. (What are $p(m)$ and $p(x|m)$?)

In Summary

- A Bayesian viewpoint of GMMs
- Kernel density estimation
- Mean-shift algorithm

Next...

- Classification problem and its challenges
- Linear classifiers (LDA and Logistic Regression)

HW 4: DDL May 12, 2022

Python Programming

1. Lab # 7 (4 Pts)
2. Lab # 8 (4 Pts)

Questions for Tech Report (6 Pts, ≤ 3 Pages)

1. **Gaussian mixture model with outliers.** Suppose that the observed data contains several outliers. The mixture model can be:

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} w_k p(\boldsymbol{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) + w_{K+1}, \quad \boldsymbol{w} = [w_1, ..., w_{K+1}] \in \Delta^K \tag{8}$$

and w_{K+1} is probability that the sample is an outlier. Modify the EM algorithm to learn this model. (2 Pts)

2. **Revisit mean-shift.** Derive the mean-shift as a maximum likelihood estimation method (refer to (7)). Derive a modified mean-shift as MAP if x owns a prior $\mathcal{N}(\mu, \sigma^2)$. What if the prior is a GMM $p_{\text{prior}}(x) = \frac{1}{K} \sum_k p(x; \mu_k, \sigma_k^2)$? (4 Pts)