Introduction to Machine Learning

Lecture 9 Representation and Clustering - Gaussian Mixture Models and EM Algorithm

Hongteng Xu

中国人民大學 RENMIN UNIVERSITY OF CHINA

高瓴人工智能学院 Gaoling School of Artificial Intelligence

Outline

Review

- Kmeans
- Spectral clustering and its connections to Kmeans and manifold learning
- Evaluation of clustering results

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Today

- Generative modeling and Gaussian mixture model
- EM algorithm

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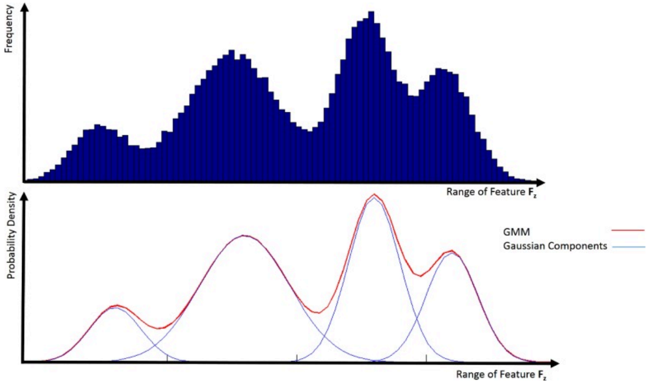
- How to categorize the models we learned before?
- Which one is harder?

Let's design the two modeling strategies in practice

- **Data:** Given $\{x_n, y_n\}_{n=1}^{N}$, where x's represent education years, and y's represent yearly incomes.
- **Task:** Learn an estimator predicting yearly incomes based on education years.

Gaussian Mixture Models

A generative model for the data with clustering structures



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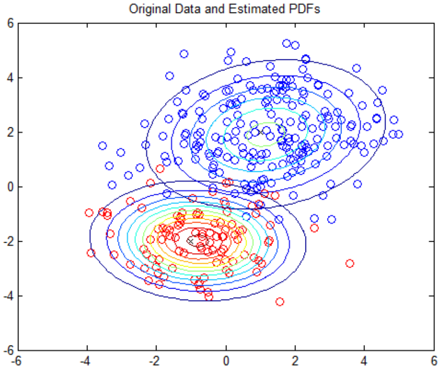

GMM: Generative Mechanism

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

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Generative process:

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How to achieve the above sampling processes?

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$$L(\boldsymbol{\theta}) = \prod_{n=1}^{N} p(\boldsymbol{x}_n; \boldsymbol{\theta}) \tag{2}$$

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- What if we know it?

Learning GMM: An EM Algorithm

In practice, we often apply an **expectation-maximization (EM)** algorithm to learn GMM.

- **E-step:** Given current parameters $\{w_k^{(t)}, \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)}\}_{k=1}^K$, calculate **responsibility** (the posterior distribution of clusters given a sample.)

$$p^{(t)}(k|\boldsymbol{x}_n) = \frac{w_k^{(t)} p(\boldsymbol{x}_n; \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)})}{\sum_{i=1}^K w_i^{(t)} p(\boldsymbol{x}_n; \boldsymbol{\mu}_i^{(t)}, \boldsymbol{\Sigma}_i^{(t)})}, \quad \forall n = 1, ..., N,\ k = 1, ..., K$$

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An Optimization Viewpoint of The EM Algorithm

Original MLE: Denote $\boldsymbol{\theta} = \{w_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$, the MLE of GMM corresponds to

$$\min_{\boldsymbol{\theta}} \sum_{n=1}^N -\log p(\boldsymbol{x}_n; \boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \underbrace{\sum_{n=1}^N -\log\left(\sum_{k=1}^K w_k p(\boldsymbol{x}_n; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right)}_{L(\boldsymbol{\theta})}.$$

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An Optimization Viewpoint of The EM Algorithm

The optimization problem in the t-th step:

$$\min_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}; \boldsymbol{\theta}^{(t)}) = \min_{\boldsymbol{\theta}} - \sum_{n=1}^{N} \sum_{k=1}^{K} p^{(t)}(k|\boldsymbol{x}_n) \log \frac{w_k p(\boldsymbol{x}_n; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{p^{(t)}(k|\boldsymbol{x}_n)}.$$

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- $w_k = p(k) = \frac{|\mathcal{C}_k|}{N}$, and

$$p(\boldsymbol{x}; \mathbf{c}_k) = \begin{cases} \frac{\Gamma(\frac{D}{2}+1)}{\pi^{D/2} r}, & \|\boldsymbol{x} - \mathbf{c}_k\|_2 \leq r, \\ 0, & \text{Otherwise.} \end{cases}$$

Revisit Kmeans from The Viewpoint of EM Algorithm

Kmeans learns K centroids, which also provides us with a **generative model**.

1. Initialize K centroids randomly from the observed data, e.g., $\{\mathbf{c}_k\}_{k=1}^K$.
2. Repeat the following steps till converge
   a. Assign each data to the nearest cluster: $\forall\, \boldsymbol{x}_n$

$$\boldsymbol{x}_n \in \mathcal{C}_k, \quad \text{if } k = \arg\min_{k\in\{1,\dots,K\}} d(\boldsymbol{x}_n, \mathbf{c}_k). \tag{10}$$

   b. Update the centriods:

$$\mathbf{c}_k = \frac{1}{|\mathcal{C}_k|} \sum\nolimits_{x_n\in\mathcal{C}_k} \boldsymbol{x}_n. \tag{11}$$

- $w_k = p(k) = \frac{|\mathcal{C}_k|}{N}$, and

$$p(\boldsymbol{x};\mathbf{c}_k) = \begin{cases} \frac{\Gamma(\frac{D}{2}+1)}{\pi^{D/2} r}, & \|\boldsymbol{x}-\mathbf{c}_k\|_2 \leq r, \\ 0, & \text{Otherwise}. \end{cases} \tag{12}$$

Recall nonparametric kernel functions:)

Revisit Kmeans from The Viewpoint of EM Algorithm

Original MLE: Denote $\boldsymbol{\theta} = \{w_k, \mathbf{c}_k, r_k\}_{k=1}^K$, the MLE of GMM corresponds to

$$\min_{\boldsymbol{\theta}} \sum_{n=1}^{N} -\log p(\boldsymbol{x}_n; \boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \underbrace{\sum_{n=1}^{N} -\log \left(\sum_{k=1}^{K} w_k p(\boldsymbol{x}_n; \mathbf{c}_k, r_k) \right)}_{L(\boldsymbol{\theta})}.$$

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EM Algorithm:

- **E-step:** $\exists r > 0$ for $\boldsymbol{x}_n$ and $k = 1, ..., K$

$$p^{(t)}(k|\boldsymbol{x}_n) = \frac{w_k^{(t)} p(\boldsymbol{x}_n; \mathbf{c}_k^{(t)}, r_k^{(t)})}{\sum_{i=1}^{K} w_i^{(t)} p(\boldsymbol{x}_n; \mathbf{c}_i^{(t)}, r_i^{(t)})} = \begin{cases} 1 & \|\boldsymbol{x}_n - \mathbf{c}_k^{(t)}\|_2 \leq r \\ 0 & \text{Otherwise} \end{cases}$$

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- **M-step:**

$$\min_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}; \boldsymbol{\theta}^{(t)}) = \min_{\boldsymbol{\theta}} -\sum_{n=1}^{N} \sum_{k=1}^{K} p^{(t)}(k|\boldsymbol{x}_n) \log \frac{w_k p(\boldsymbol{x}_n; \mathbf{c}_k)}{p^{(t)}(k|\boldsymbol{x}_n)}. \tag{15}$$

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\begin{aligned}
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Question: In GMM, what is Z? and what is $p(Z|\theta^{(t)})$?

In Summary

- Generative modeling and Gaussian mixture models
- EM algorithm
- Revisit K-means from a statistical viewpoint

Next...

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