Gaussian Mixture Model

He He

Slides based on Lecture 13b from David Rosenberg's course materials
(https://github.com/davidrosenberg/mlcourse)

CDS, NYU

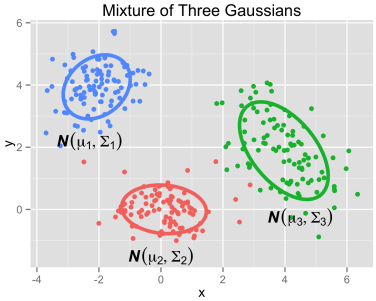
April 27, 2021

Probabilistic Model for Clustering

- Problem setup:
  - There are k clusters (or **mixture components**).
  - We have a probability distribution for each cluster.
- Generative story of a **mixture distribution**:
  1. Choose a random cluster $z \in \{1, 2, \ldots, k\}$.
  2. Choose a point from the distribution for cluster z.

Example:

1. Choose $z \in \{1, 2, 3\}$ with $p(1) = p(2) = p(3) = \frac{1}{3}$.
2. Choose $x \mid z \sim \mathcal{N}(X \mid \mu_z, \Sigma_z)$.



Gaussian mixture model (GMM)

Generative story of GMM with k mixture components:

1. Choose cluster $z \sim \text{Categorical}(\pi_1, \ldots, \pi_k)$.
2. Choose $x \mid z \sim \mathcal{N}(\mu_z, \Sigma_z)$.

Probability density of x:

- Sum over (marginalize) the **latent variable** z.

$$p(x) = \sum_z p(x, z) \tag{1}$$

$$= \sum_z p(x \mid z) p(z) \tag{2}$$

$$= \sum_k \pi_k \mathcal{N}(\mu_k, \Sigma_k) \tag{3}$$

Identifiability Issues for GMM

- Suppose we have found parameters

$$\begin{aligned} \text{Cluster probabilities}: &\quad \pi = (\pi_1, \ldots, \pi_k) \\ \text{Cluster means}: &\quad \mu = (\mu_1, \ldots, \mu_k) \\ \text{Cluster covariance matrices}: &\quad \Sigma = (\Sigma_1, \ldots \Sigma_k) \end{aligned}$$

  that are at a local minimum.

- What happens if we shuffle the clusters? e.g. Switch the labels for clusters 1 and 2.
- We'll get the same likelihood. How many such equivalent settings are there?
- Assuming all clusters are distinct, there are $k!$ equivalent solutions.
- Not a problem *per se*, but something to be aware of.

Learning GMMs

How to learn the parameters π_k, μ_k, Σ_k?

- MLE (also called maximize marginal likelihood).
- Log likelihood of data:

$$L(\theta) = \sum_{i=1}^{n} \log p(x_i; \theta) \tag{4}$$

$$= \sum_{i=1}^{n} \log \sum_{z} p(x, z; \theta) \tag{5}$$

- Cannot push log into the sum... z and x are coupled.
- No closed-form solution for GMM—try to compute the gradient yourself!

Gradient Descent / SGD for GMM

- What about running gradient descent or SGD on

$$J(\pi, \mu, \Sigma) \quad = \quad -\sum_{i=1}^{n} \log \left\{ \sum_{z=1}^{k} \pi_z \mathcal{N}(x_i \mid \mu_z, \Sigma_z) \right\} ?$$

- Can be done, in principle – but need to be clever about it.
- Each matrix $\Sigma_1, \ldots, \Sigma_k$ has to be positive semidefinite.
- How to maintain that constraint?
  - Rewrite $\Sigma_i = M_i M_i^T$, where M_i is an unconstrained matrix.
  - Then Σ_i is positive semidefinite.
- Even then, pure gradient-based methods have trouble.[1]

[1] See Hosseini and Sra's Manifold Optimization for Gaussian Mixture Models for discussion and further references.

Learning GMMs: observable case

Suppose we observe cluster assignments z. Then MLE is easy:

$$n_z = \sum_{i=1}^{n} 1(z_i = z) \qquad \text{\# examples in each cluster} \tag{6}$$

$$\hat{\pi}(z) = \frac{n_z}{n} \qquad \text{fraction of examples in each cluster} \tag{7}$$

$$\hat{\mu}_z = \frac{1}{n_z} \sum_{i:z_i=z} x_i \qquad \text{empirical cluster mean} \tag{8}$$

$$\hat{\Sigma}_z = \frac{1}{n_z} \sum_{i:z_i=z} (x_i - \hat{\mu}_z)(x_i - \hat{\mu}_z)^T. \qquad \text{empirical cluster covariance} \tag{9}$$

Learning GMMs: inference

The inference problem: observe x, want to know z.

$$p(z = j \mid x_i) = p(x, z = j)/p(x) \tag{10}$$

$$= \frac{p(x \mid z = j)p(z = j)}{\sum_k p(x \mid z = k)p(z = k)} \tag{11}$$

$$= \frac{\pi_j \mathcal{N}(x_i \mid \mu_j, \Sigma_j)}{\sum_k \pi_k \mathcal{N}(x_i \mid \mu_k, \Sigma_k)} \tag{12}$$

- $p(z \mid x)$ is a *soft assignment*.
- If we know the parameters μ, Σ, π, this would be easy to compute.

EM for GMM

Let's compute the cluster assignments and the parameters iteratively.

The expectation-minimization (EM) algorithm:

1. Initialize parameters μ, Σ, π randomly.
2. Run until convergence:
   1. E-step: fill in latent variables by inference.
      - compute soft assignments $p(z \mid x_i)$ for all i.
   2. M-step: standard MLE for μ, Σ, π given "observed" variables.
      - Equivalent to MLE in the observable case on data weighted by $p(z \mid x_i)$.

M-step for GMM

- Let $p(z \mid x)$ be the soft assignments:

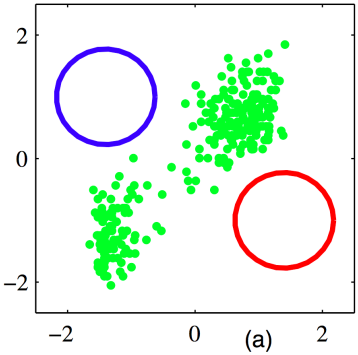
$$\gamma_i^j = \frac{\pi_j^{\text{old}} \mathcal{N}\left(x_i \mid \mu_j^{\text{old}}, \Sigma_j^{\text{old}}\right)}{\sum_{c=1}^{k} \pi_c^{\text{old}} \mathcal{N}\left(x_i \mid \mu_c^{\text{old}}, \Sigma_c^{\text{old}}\right)}.$$

- Exercise: show that

$$\begin{aligned}
\mu_c^{\text{new}} &= \frac{1}{n_c} \sum_{i=1}^{n} \gamma_i^c x_i \\
\Sigma_c^{\text{new}} &= \frac{1}{n_c} \sum_{i=1}^{n} \gamma_i^c \left(x_i - \mu_c^{\text{new}}\right)\left(x_i - \mu_c^{\text{new}}\right)^T \\
\pi_c^{\text{new}} &= \frac{n_c}{n}.
\end{aligned}$$

EM for GMM

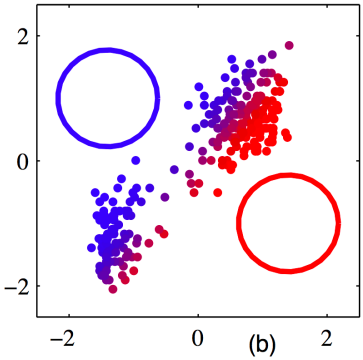
- Initialization



From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM

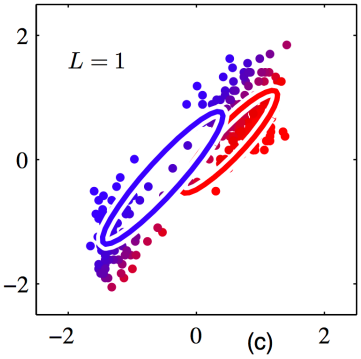
- First soft assignment:



From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM

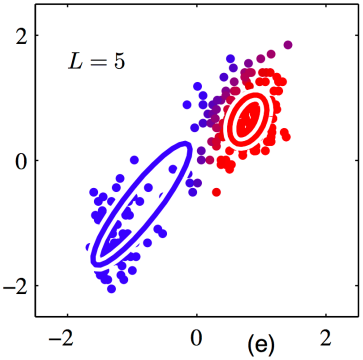
- First soft assignment:



From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM

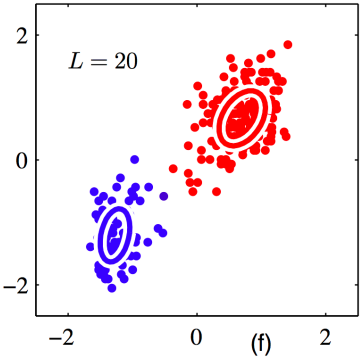
- After 5 rounds of EM:



From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM

- After 20 rounds of EM:



From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM: Summary

- EM is a general algorithm for learning latent variable models.
- *Key idea*: if data was fully observed, then MLE is easy.
  - E-step: fill in latent variables by computing $p(z \mid x, \theta)$.
  - M-step: standard MLE given fully observed data.
- Simpler and more efficient than gradient methods.
- Can prove that EM monotonically improves the likelihood and converges to a local minimum.
- k-means is a special case of EM for GMM with *hard assignments*, also called hard-EM.