Gaussian Mixture Models (GMM) and ML Estimation Examples
Mean and Variance of Gaussian

• Consider the Gaussian PDF:

\[ f(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left\{ -\frac{(x - \mu)^2}{2\sigma^2} \right\}, \]

Given the observations (sample) \( X_1, \cdots, X_n \).

Form the log-likelihood function

\[ l(\mu, \sigma) = \sum_{i=1}^{n} \left[ -\log \sigma - \frac{1}{2} \log 2\pi - \frac{1}{2\sigma^2}(X_i - \mu)^2 \right] = -n \log \sigma - \frac{n}{2} \log 2\pi - \frac{1}{2\sigma^2} \sum_{i=1}^{n} (X_i - \mu)^2 \]

Take the derivatives \( \text{wrt} \ \mu \ \text{and} \ \sigma \) and set it to zero
Solution

• Sample mean and variance:

\[
\frac{\partial l(\mu, \sigma)}{\partial \mu} = \frac{1}{\sigma^2} \sum_{i=1}^{n} (X_i - \mu) = 0
\]

\[
\frac{\partial l(\mu, \sigma)}{\partial \sigma} = -\frac{n}{\sigma^3} + \sigma^{-3} \sum_{i=1}^{n} (X_i - \mu)^2 = 0
\]

Solving these equations will give us the MLE for \( \mu \) and \( \sigma \):

\[
\hat{\mu} = \bar{X} \quad \text{and} \quad \hat{\sigma} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (X_i - \bar{X})^2}
\]
Gaussian Mixture Model

• GMM

\[
Pr(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k)
\]

where

\[
\sum_{k=1}^{K} \pi_k = 1, \quad 0 \leq \pi_k \leq 1.
\]

\(X\) is multidimensional.
Ref: https://people.eecs.berkeley.edu/~jordan/courses/294-fall09/lectures/clustering/slides.pdf
Can we use the ML estimation method to estimate the unknown parameters, $\mu_k, \sigma_k, \pi_k$?

• It is not easy:
  
  • Loss function is the negative log likelihood

  $$-\log \Pr(x|\pi, \mu, \Sigma) = -\sum_{i=1}^{n} \log \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k) \right\}$$

  • Why is this function difficult to optimize?
    • Notice that the sum over the components appears inside the log, thus coupling all the parameters.

However, it is possible to obtain an iterative solution!
We can estimate the parameters using iterative Expectation-Maximization (EM) algorithm

• Given the observations $x_i, i=1,2,...,n$
  
  • Each $x_i$ is associated with a latent variable $z_i = (z_{i1}, \ldots, z_{iK})$.
  
  • Given the complete data $(x, z) = (x_i, z_i), i = 1, \ldots, n$
    
    • We can estimate the parameters by maximizing the complete data log likelihood.
    
    $$
    \log \Pr(x, z|\pi, \mu, \Sigma) = \sum_{i=1}^{N} \sum_{k=1}^{K} z_{ik} \{ \log \pi_k + \log \mathcal{N}(x_i|\mu_k, \Sigma_k) \}
    $$
    
    • Notice that the $\pi_k$ and $(\mu_k, \Sigma_k)$ decouple. Trivial closed-form solution exists.

The latent variable parameter $z_{ik}$ represents the contribution of $k$-th Gaussian to $x_i$

Take the derivative of the log-likelihood wrt $\mu_k, \sigma_k, \pi_k$ and set it to zero to get equations to be used in EM algorithm.
Iterate for \( k=1,2,\ldots \)

- Initialize with \( \mu_o, \sigma_o I, \pi_o \)
- Update equations at the \( k \)-th iteration:

  - **E-step**: Given parameters, compute
    \[
    r_{ik} \triangleq E(Z_{ik}) = \frac{\pi_k \mathcal{N}(x_i | \mu_k, \Sigma_k)}{\sum_{k'=1}^{K} \pi_k \mathcal{N}(x_i | \mu_k, \Sigma_k)}
    \]
  - **M-step**: Maximize the expected complete log likelihood
    \[
    E[\log \Pr(x, z | \pi, \mu, \Sigma)] = \sum_{i=1}^{n} \sum_{k=1}^{K} r_{ik} \{ \log \pi_k + \log \mathcal{N}(x_i | \mu_k, \Sigma_k) \}
    \]

  By updating the parameters
  \[
  \pi_{k+1} = \frac{\sum_{i} r_{ik}}{n}, \quad \mu_{k+1} = \frac{\sum_{i} r_{ik} x_i}{\sum_{i} r_{ik}}, \quad \Sigma_{k+1} = \frac{\sum_{i} r_{ik} (x_i - \mu_k)(x_i - \mu_k)^T}{\sum_{i} r_{ik}}
  \]
  - Iterate till likelihood converges.
  - Converges to local optimum of the log likelihood.

It may not converge to the global optimum!
Example

GMM example

- Training set: $n = 900$ examples from a uniform pdf inside an annulus
- Model: GMM with $C = 30$ Gaussian components
- Training procedure
  - Gaussians centers initialized by choosing 30 arbitrary training examples
  - Covariance matrices initialized to be diagonal, with large variance compared to that of the training data
  - To avoid singularities, at every iteration the covariance matrices computed with EM were regularized with a small multiple of the identity matrix
  - Components whose mixing coefficients fell below a threshold are removed

Illustrative results are provided in the next slide
Observations: blue dots

Ellipses represent 2-D Gaussians
Vector quantization = K-means clustering

**k-means clustering**

- The k-means algorithm is a simple procedure that attempts to group a collection of unlabeled examples $X = \{x_1 \ldots x_n \}$ into one of $C$ clusters
  - k-means seeks to find compact clusters, measured as
    $$J_{MSE} = \sum_{c=1}^{C} \sum_{x \in \omega_c} \|x - \mu_c\|^2; \mu_c = \frac{1}{n_c} \sum_{x \in \omega_c} x$$
  - It can be shown that k-means is a special case of the GMM-EM algorithm

- Procedure
  1. Define the number of clusters
  2. Initialize clusters by
     a) an arbitrary assignment of examples to clusters or
     b) an arbitrary set of cluster centers (i.e., use some examples as centers)
  3. Compute the sample mean of each cluster
  4. Reassign each example to the cluster with the nearest mean
  5. If the classification of all samples has not changed, stop, else go to step 3

You may initialize the GMM algorithm from K-means cluster centers!
Fig. 3. Comparison of distribution modeling: (a) Histogram of a single cepstral coefficient from a 25 second utterance by a male speaker; (b) maximum likelihood unimodal Gaussian model; (c) GMM and its 10 underlying component densities; (d) histogram of the data assigned to the VQ centroid locations of a 10-element codebook.
Speaker Identification

- Feature extractions from data using mel-cepstrum

- Extract feature vectors for each speaker (e.g., 90 sec long data)
- Frame length 10ms
Speaker model  GMM

A Gaussian mixture density is a weighted sum of $M$ component densities, as depicted in Fig. 2 and given by the equation

$$p(\vec{x} \mid \lambda) = \sum_{i=1}^{M} p_i b_i(\vec{x})$$

(1)

where \(\vec{x}\) is a \(D\)-dimensional random vector, \(b_i(\vec{x}), i = 1, \ldots, M\), are the component densities and \(p_i, i = 1, \ldots, M\), are the mixture weights. Each component density is a \(D\)-variate Gaussian function of the form

$$b_i(\vec{x}) = \frac{1}{(2\pi)^{D/2}|\Sigma_i|^{1/2}} \exp\left\{-\frac{1}{2}(\vec{x} - \vec{\mu}_i)' \Sigma_i^{-1} (\vec{x} - \vec{\mu}_i)\right\}$$

(2)

with mean vector \(\vec{\mu}_i\) and covariance matrix \(\Sigma_i\). The mixture weights satisfy the constraint that \(\sum_{i=1}^{M} p_i = 1\).

\Lambda represents a person (speaker)
GMM Model

Mixture weights $\sum_i p_i = 1$

Train the model from observations using the iterative algorithm for each speaker
How do we decide?

\[ P(\mathcal{X} | \text{She}) > P(\mathcal{X} | \text{He}) \]

She is the person!
For speaker identification, a group of $S$ speakers $S = \{1, 2, \ldots, S\}$ is represented by GMM's $\lambda_1, \lambda_2, \ldots, \lambda_S$. The objective is to find the speaker model which has the maximum a posteriori probability for a given observation sequence. Formally,

$$\hat{S} = \arg \max_{1 \leq k \leq S} \Pr(\lambda_k | X) = \arg \max_{1 \leq k \leq S} \frac{p(X | \lambda_k) \Pr(\lambda_k)}{p(X)}$$  \hspace{1cm} (9)

where the second equation is due to Bayes’ rule. Assuming equally likely speakers (i.e., $\Pr(\lambda_k) = 1/S$) and noting that $p(X)$ is the same for all speaker models, the classification rule simplifies to

$$\hat{S} = \arg \max_{1 \leq k \leq S} p(X | \lambda_k).$$  \hspace{1cm} (10)

Using logarithms and the independence between observations, the speaker identification system computes

$$\hat{S} = \arg \max_{1 \leq k \leq S} \sum_{t=1}^{T} \log p(\bar{x}_t | \lambda_k)$$  \hspace{1cm} (11)

in which $p(\bar{x}_t | \lambda_k)$ is given in (1).
Speaker Identification result

16 speakers

TABLE I
GMM IDENTIFICATION PERFORMANCE FOR DIFFERENT AMOUNTS OF TRAINING DATA AND MODEL ORDERS

<table>
<thead>
<tr>
<th>Amount of Training Speech</th>
<th>Model Order</th>
<th>Test Length</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>M = 8</td>
<td>1 sec 5 sec 10 sec</td>
</tr>
<tr>
<td>30 sec</td>
<td>54.6</td>
<td>79.8 85.6</td>
</tr>
<tr>
<td></td>
<td>63.7</td>
<td>87.3 90.5</td>
</tr>
<tr>
<td></td>
<td>64.6</td>
<td>85.3 88.4</td>
</tr>
<tr>
<td>60 sec</td>
<td>66.1</td>
<td>91.5 97.3</td>
</tr>
<tr>
<td></td>
<td>74.9</td>
<td>95.7 98.8</td>
</tr>
<tr>
<td></td>
<td>78.6</td>
<td>95.6 98.3</td>
</tr>
<tr>
<td>90 sec</td>
<td>71.5</td>
<td>95.5 98.8</td>
</tr>
<tr>
<td></td>
<td>79.0</td>
<td>98.0 99.7</td>
</tr>
<tr>
<td></td>
<td>84.7</td>
<td>98.8 99.6</td>
</tr>
</tbody>
</table>
Exponential Distribution Example

Example 2: Suppose $X_1, X_2, \ldots, X_n$ are i.i.d. random variables with density function $f(x|\sigma) = \frac{1}{2\sigma} \exp\left(-\frac{|x|}{\sigma}\right)$, please find the maximum likelihood estimate of $\sigma$.

Solution: The log-likelihood function is

$$l(\sigma) = \sum_{i=1}^{n} \left[-\log 2 - \log \sigma - \frac{|X_i|}{\sigma}\right]$$

Let the derivative with respect to $\theta$ be zero:

$$l'(\sigma) = \sum_{i=1}^{n} \left[-\frac{1}{\sigma} + \frac{|X_i|}{\sigma^2}\right] = -\frac{n}{\sigma} + \frac{\sum_{i=1}^{n} |X_i|}{\sigma^2} = 0$$

and this gives us the MLE for $\sigma$ as

$$\hat{\sigma} = \frac{\sum_{i=1}^{n} |X_i|}{n}$$

You get a different estimate for the standard deviation.
References

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