

Fitting (Gaussian) Finite Mixtures using the EM-Algorithm

gustavoc@msu.edu

In a finite mixture model the density of a RV is modeled as the weighted sum of a finite number of densities. In this note we consider finite mixtures with Gaussian components. The density function of a mixture with 2 Gaussian components is:

$$p(x_i|\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \alpha_1) = \alpha_1 (2\pi\sigma_1^2)^{-\frac{1}{2}} e^{-\frac{(x_i-\mu_1)^2}{2\sigma_1^2}} + (1 - \alpha_1) (2\pi\sigma_2^2)^{-\frac{1}{2}} e^{-\frac{(x_i-\mu_2)^2}{2\sigma_2^2}}$$

Above, μ and σ^2 are the means and variances of each of the components and $0 < \alpha_1 < 1$ is a mixture proportion. The model can be naturally extended to K components.

Likelihood Function

Assuming IID data, the joint density of the data is

$$p(x_1, \dots, x_n|\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \alpha_1) = \prod_{i=1}^n \alpha_1 \text{dnorm}(x_i|\mu_1, \sigma_1^2) + (1 - \alpha_1) \text{dnorm}(x_i|\mu_2, \sigma_2^2)$$

Where $\text{dnorm}(x_i|\mu_*, \sigma_*^2) = (2\pi\sigma_*^2)^{-\frac{1}{2}} e^{-\frac{(x_i-\mu_*)^2}{2\sigma_*^2}}$.

The model parameters, $\theta = \{\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \alpha_1\}$, can be estimated via maximum likelihood. Maximization could be done using general purpose optimization algorithms (e.g., those implemented in `optim()`); alternatively, we can maximize the likelihood using the EM-algorithm.

Augmented likelihood

To facilitate the implementation of the EM-algorithm we introduce a latent variable $z_i \in \{1, 2\}$ which indicates whether the i th observation comes from 1st or 2nd component of the mixture. Parameter α_1 can be interpreted as the proportion of the observations coming from the first component; therefore $p(z_i = 1|\alpha_1) = \alpha_1$ and $p(z_i = 2|\theta) = 1 - \alpha_1$; thus $p(z_i = 1|\alpha_1) = \alpha_1^{1(z_i=1)}(1 - \alpha_1)^{1(z_i=2)}$.

The augmented (or complete-data) likelihood is the joint distribution of the observed (x) and the missing (z) data given the parameters (θ). For the i th-data point the augmented likelihood is:

$$\begin{aligned} p(x_i, z_i|\theta) &= p(x_i|z_i, \theta) \times p(z_i|\theta) \\ &= \text{dnorm}(x_i|\mu_1, \sigma_1^2)^{1(z_i=1)} \text{dnorm}(x_i|\mu_2, \sigma_2^2)^{1(z_i=2)} \times \alpha_1^{1(z_i=1)}(1 - \alpha_1)^{1(z_i=2)} \end{aligned}$$

Therefore, assuming IID data the complete-data likelihood becomes

$$p(\mathbf{x}, \mathbf{z} | \boldsymbol{\theta}) = \prod_{i=1}^n dnorm(x_i | \mu_1, \sigma_1^2)^{1(z_i=1)} dnorm(x_i | \mu_1, \sigma_1^2)^{1(z_i=2)} \times \alpha_1^{1(z_i=1)} (1 - \alpha_1)^{1(z_i=2)}$$

E-step

To perform the E-step we must drive the expected value of the logarithm of the complete-data likelihood with respect to the distribution of the missing data given the observed data and the parameters, that is $p(\mathbf{z} | \mathbf{x}, \boldsymbol{\theta})$. The logarithm of the complete likelihood takes the form

$$l(\mathbf{x}, \mathbf{z} | \boldsymbol{\theta}) = \sum_{i=1}^n 1(z_i = 1) \log[dnorm(x_i | \mu_1, \sigma_1^2)] + 1(z_i = 2) \log[dnorm(x_i | \mu_1, \sigma_1^2)] + 1(z_i = 1) \log[\alpha_1] + 1(z_i = 2) \log[1 - \alpha_1]$$

The expected value the above expression is

$$l(\mathbf{x}, \mathbf{z} | \boldsymbol{\theta}) = \sum_{i=1}^n w_i \log[dnorm(x_i | \mu_1, \sigma_1^2)] + (1 - w_i) \log[dnorm(x_i | \mu_1, \sigma_1^2)] + w_i \log[\alpha_1] + (1 - w_i) \log[1 - \alpha_1] \quad [1]$$

Where $w_i = E(z_i = 1 | x_i, \boldsymbol{\theta}) = p(z_i = 1 | x_i, \boldsymbol{\theta})$ is the success probability of the i th latent variable. This probability is given by

$$p(z_i = 1 | x_i, \boldsymbol{\theta}) = \frac{p(z_i=1|x_i,\boldsymbol{\theta})}{p(z_i=1|x_i,\boldsymbol{\theta}) + p(z_i=2|x_i,\boldsymbol{\theta})}$$

Using Bayes' rule

$$p(z_i = 1 | x_i, \boldsymbol{\theta}) = \frac{p(x_i | z_i=1)p(z_i=1)}{p(x_i | z_i=1)p(z_i=1) + p(x_i | z_i=2)p(z_i=2)} = \frac{A}{A+B} \quad [2]$$

Where $A = dnorm(x_i | \mu_1, \sigma_1^2) \times \alpha_1$ and $B = dnorm(x_i | \mu_1, \sigma_1^2) \times (1 - \alpha_1)$

M-Step:

In the M-step we maximize [1] with respect to each of the parameters of the mixture. Note that [1] is a weighted log-likelihood. It can be shown that the ML estimates of the parameters are given by the following weighted means and weighted variances:

$$\hat{\mu}_1 = \frac{\sum_{i=1}^n w_i y_i}{\sum_{i=1}^n w_i} ; \hat{\mu}_2 = \frac{\sum_{i=1}^n (1-w_i) y_i}{\sum_{i=1}^n (1-w_i)} ; \hat{\sigma}_1^2 = \frac{\sum_{i=1}^n w_i (y_i - \hat{\mu}_1)^2}{\sum_{i=1}^n w_i} ; \hat{\sigma}_2^2 = \frac{\sum_{i=1}^n (1-w_i) (y_i - \hat{\mu}_2)^2}{\sum_{i=1}^n (1-w_i)}$$