EM for Gaussian Mixtures using MapReduce

Andrea Mannocci, Giuseppe Portaluri, Lucia Vadicamo

Suppose we have a data set of observations $X = \{x_1, \ldots, x_n\}, x_j \in \mathbb{R}^d$, and we wish to model this data using a mixture of Gaussians. We can estimate the parameters of a Gaussian Mixture Model (GMM) using the Expectation-Maximization (EM) algorithm [1] to optimize a Maximum Likelihood (ML) criterion. We denote the parameters of a k-component GMM by $\Theta = \{w_i \in \mathbb{R}, \mu_i \in \mathbb{R}^d, \Sigma_i \in \mathbb{R}^{d \times d}; i = 1, \ldots, k\}$, where w_i, μ_i, Σ_i are respectively the mixture weight, mean vector and covariance matrix of Gaussian i. The Gaussian mixture distribution can be written as:

$$p_{\Theta}(x) = \sum_{i=1}^{k} w_i p_i(x), \tag{1}$$

where

$$p_i(x) = \frac{\exp\{-\frac{1}{2}(x-\mu_i)^T \Sigma_i^{-1}(x-\mu_i)\}}{(2\pi)^{\frac{d}{2}} |\Sigma_i|^{\frac{1}{2}}}$$
(2)

and

$$\sum_{i=1}^{k} w_i = 1, \quad w_k \ge 0 \qquad \forall i = 1, \dots, k.$$
 (3)

If we assume that the data points are drawn independently from the distribution, then we can express the log of the likelihood function as:

$$\ln p(X|\Theta) = \sum_{s=1}^{n} \ln \left\{ \sum_{i=1}^{k} w_i p_i(x_t|\Theta) \right\}. \tag{4}$$

1 EM for Gaussian mixtures

Given a data set X and a Gaussian Mixture Model, the goal is to maximize the likelihood function with respect to the parameters (comprising the means and covariances of the components and the mixing weight).

1. Initialize the means μ_i , covariances Σ_i and mixing coefficient w_i . K-means algorithm can be used to find a suitable initialization.

2. Expectation step (E-step) Use the current values for the parameters to calculate the posterior probabilities $\gamma_s(i)$

$$\gamma_s(i) := p(i|x_s, \Theta) = \frac{w_i p_i(x_s|\Theta)}{\sum_{j=1}^k w_j p_j(x_s|\Theta)} \qquad \forall i = 1, \dots, k.$$
 (5)

3. Maximization step (M-step) Use the posterior probabilities $\gamma_s(i)$ to re-estimate the means, variances, and mixing coefficient:

$$w_i^{\text{new}} = \frac{n_i}{n} \tag{6}$$

$$\mu_i^{\text{new}} = \frac{1}{n_i} \sum_{s=1}^n \gamma_s(i) x_s \tag{7}$$

$$\Sigma_i^{\text{new}} = \frac{1}{n_i} \sum_{s=1}^n \gamma_s(i) (x_s - \mu_i^{\text{new}}) (x_s - \mu_i^{\text{new}})^T$$
 (8)

where $n_i = \sum_{s=1}^n \gamma_s(i)$, for all $i = 1, \dots, k$.

4. Check for convergence of either the parameters or the log likelihood. If the convergence criterion is not satisfied return to step 2.

Each update to the parameters resulting from an E-step followed by an M-step is guaranteed to increase the likelihood function. The algorithm is deemed to have converged when the change in the likelihood function, or alternatively in the parameters, falls below some threshold.

In our experiments we are interested to fit a GMM on a dataset of image local features, such as SIFTs [2]. We assume diagonal covariances matrices and we denote $\sigma_i^2 \in \mathbb{R}^d$ the variance vectors, i.e. the diagonal of Σ_i . This is a suitable assumption for most computer vision applications, where estimating a full covariance matrix would be prohibitive due to the relative high dimensionality of the data. For example, when clustering SIFT features, each data vector has dimension 128, and each full covariance matrix would contain more than 8k distinct parameters.

Note also that the equations 6-8 can be computed in terms of the following 0-order, 1st-order and 2nd-order statistics:

$$S_0(i) = \sum_{s=1}^n \gamma_s(i), \quad S_1(i) = \sum_{s=1}^n \gamma_s(i)x_s, \quad S_2(i) = \sum_{s=1}^n \gamma_s(i)x_s^2, \quad i = 1, \dots k$$

where $S_0(i) \in \mathbb{R}$, $S_1(i) \in \mathbb{R}^d$ and $S_2(i) \in \mathbb{R}^d$. The square of a vector must be understood as a term-by-term operation. We have:

$$w_i^{\text{new}} = \frac{S_0(i)}{n}, \qquad \mu_i^{\text{new}} = \frac{S_1(i)}{S_0(i)}, \qquad (\sigma_i^2)^{\text{new}} = \frac{S_2(i)}{S_0(i)} - \frac{S_1(i)^2}{S_0(i)^2}.$$
 (9)

2 MapReduce implementation

Input: a data set of observations $X = \{x_1, \ldots, x_n\}$, such as the local descriptors of several images.

Map Key in: -, Value in: $x_s \in \mathbb{R}^d$

- read Gaussian parameters $\Theta = \{w_i \in \mathbb{R}, \mu_i \in \mathbb{R}^d, \sigma_i^2 \in \mathbb{R}^d; i = 1, \dots, k\}$ from HDFS.
- E-step: compute $\gamma_s(i), \forall i = 1, \ldots, k$.
- precompute statistics:

$$S_0(i) = \gamma_s(i),$$
 $S_1(i) = \gamma_s(i)x_s,$ $S_2(i) = \gamma_s(i)x_s^2$

for(i = 1, ..., k) { Key out: i, Value out: $(S_0(i), S_1(i), S_2(i), 1)$ }

Combine Key in: int i, Value in: List($S_0(i)_j, S_1(i)_j, S_2(i)_j, m_j \mid j = 1, ... t$)

- compute statistics: $S_h(i) = \sum_{j=1}^t S_h(i)_j$, for h = 0, 1, 2.
- compute $m = \sum_{j=1}^{t} m_j$

Key out: i, Value out: $(S_0(i), S_1(i), S_2(i), m)$

Reduce Key in: int i, Value in: List($S_0(i)_j, S_1(i)_j, S_2(i)_j, m_i \mid j = 1, ... t$)

- compute statistics: $S_h(i) = \sum_{j=1}^t (S_h(i))_j$, for h = 0, 1, 2.
- compute $n = \sum_{j=1}^{t} m_j$
- M-step: compute new GMM parameters

$$w_i^{\text{new}} = \frac{S_0(i)}{n}, \quad \mu_i^{\text{new}} = \frac{S_1(i)}{S_0(i)}, \quad (\sigma_i^2)^{\text{new}} = \frac{S_2(i)}{S_0(i)} - (\mu_i^{\text{new}})^2.$$

Key out: i, Value out: $(w_i^{\text{new}}, \mu_i^{\text{new}}, (\sigma_i^2)^{\text{new}})$

At the end of the Map-Reduce phase, the algorithm tests for the convergence of μ parameters

$$\|\mu_i^{\text{new}} - \mu_i^{\text{old}}\|_2 < \epsilon$$

and it stops when the above condition is satisfied or the maximum number of iterations is reached.

2.1 Implementation notes: computation in the log domain

When the data points are high-dimensional (as in the case of low-level descriptors of images), the likelihood values $p_i(x)$ and the posterior probabilities $\gamma_i(x)$ can be extremely small. Hence for a stable implementation we

perform all the computation in the log domain, as suggested in [3]. In the log domain we have:

$$\log p_i(x_s|\Theta) = -\frac{1}{2} \sum_{l=1}^d \left[\log(2\pi) + \log((\sigma_i^2)_l) + \frac{((x_s)_l - (\mu_i)_l)^2}{(\sigma_i^2)_l} \right]$$
(10)

$$\log \gamma_s(i) = \log \left(w_i p_i(x_s | \Theta) \right) - \log \left(\sum_{j=1}^k w_j p_j(x_s | \Theta) \right). \tag{11}$$

Given $\log(w_i p_i(x_s|\Theta))$ for all i = 1, ..., k, we can compute $\log\left(\sum_{j=1}^k w_j p_j(x_s|\Theta)\right)$ using the fact that $\log(a+b) = \log(a) + \log(1 + \exp(\log b - \log a))$.

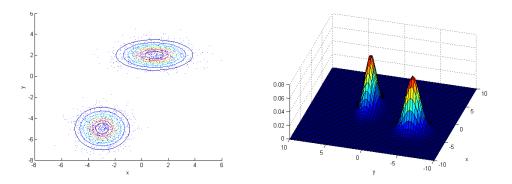


Figure 1: Example of GMM with k = 2, estimated on 2000 points of dimension d=2.

References

- [1] C. M. Bishop, Pattern Recognition and Machine Learning, Information Science and Statistics, Springer, 2006.
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