

# Variational Bayesian Inference for a Mixture of Mixtures

## A Finite Mixture of Finite Gaussian Mixtures

Let  $\mathbf{y} = (y_1, y_2, \dots, y_N)$  be a sample from a finite mixture of finite Gaussian mixtures. We use shared kernels by letting  $\mu_{bk} = \mu_k$  and  $\sigma_{bk}^2 = \sigma_k^2$  for all  $k = 1, 2, \dots, K$  and  $b = 1, 2, \dots, B$ . Then their joint density is given by

$$\begin{aligned} p(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \{\mathbf{p}\}_{b=1}^B, \boldsymbol{\phi}) &= \prod_{i=1}^N \sum_{b=1}^B \phi_b \sum_{k=1}^K p_{bk} N(y_i \mid \mu_{bk}, \sigma_{bk}^2) \\ &= \prod_{i=1}^N \sum_{b=1}^B \phi_b \sum_{k=1}^K p_{bk} N(y_i \mid \mu_k, \sigma_k^2). \end{aligned}$$

where  $\boldsymbol{\phi} = (\phi_1, \phi_2, \dots, \phi_B)'$  with  $\sum_{b=1}^B \phi_b = 1$  and  $\{\mathbf{p}\}_{b=1}^B = \{\mathbf{p}_1, \dots, \mathbf{p}_B\}$  and  $\mathbf{p}_b = (p_{b1}, p_{b2}, \dots, p_{bK})'$  with  $\sum_{k=1}^K p_{bk} = 1$ .

Let the weights  $\boldsymbol{\phi}$  and  $\mathbf{p}_b$  have a  $\text{Dirichlet}(\alpha_\phi \mathbf{1})$  and  $\text{Dirichlet}(\alpha_p \mathbf{1})$  prior respectively. For each  $y_i$  we can introduce auxiliary variable vectors  $\mathbf{w} = (\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_N)$  for the “parent” distribution where  $\sum_{b=1}^B w_{ib} = 1$  and  $p(w_{ib} = 1) = \phi_b$ . Then given the “parent” distribution we can introduce another set of auxiliary variable vectors  $\mathbf{z}_b = (\mathbf{z}_{b1}, \mathbf{z}_{b2}, \dots, \mathbf{z}_{bN})$  for the “child” distribution where  $\sum_{k=1}^K z_{ibk} = 1$  and  $p(z_{ibk} = 1) = p_{bk}$ . Then,  $\mathbf{w} \mid \boldsymbol{\phi} \sim \text{Multinomial}(N, \boldsymbol{\phi})$  and  $\mathbf{z}_b \mid \mathbf{w}, \mathbf{p}_b \sim \text{Multinomial}(N, \mathbf{p}_b)$ .

Now the joint density can be written as

$$p(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mathbf{w}, \{\mathbf{z}_b\}_{b=1}^B) = \prod_{i=1}^N \prod_{b=1}^B \prod_{k=1}^K p(y_i \mid \mu_k, \sigma_k^2)^{w_{ib} z_{ibk}} p(\mathbf{z}_b \mid \mathbf{w}, \mathbf{p}_b) p(\mathbf{w} \mid \boldsymbol{\phi})$$

## A Finite Mixture of Infinite Gaussian Mixtures

Extending this to a finite mixture of infinite Gaussian mixtures model using the Stick-breaking representation of a Dirichlet Process.

$$\begin{aligned} p(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mathbf{w}, \{\mathbf{z}_b\}_{b=1}^B) &= \prod_{i=1}^N \prod_{b=1}^B \prod_{k=1}^{\infty} p(y_i \mid \mu_k, \sigma_k^2)^{w_{ib} z_{ibk}} p(\mathbf{z}_b \mid \mathbf{w}, \mathbf{p}_b) p(\mathbf{w} \mid \boldsymbol{\phi}) \\ p(\mathbf{z}_b \mid \mathbf{w}, \mathbf{p}_b) &= \text{Multinomial}(N, \mathbf{p}_b) \quad \text{where} \quad \mathbf{p}_b = (p_{b1}, p_{b2}, \dots) \\ p_{bk} &= V_{bk} \prod_{k=1}^{k-1} (1 - V_{bk}) \quad \text{where} \quad V_{bk} \sim \text{Beta}(1, \beta_b) \quad b = 1, 2, \dots, B \\ p(\mathbf{w} \mid \boldsymbol{\phi}) &= \text{Multinomial}(N, \boldsymbol{\phi}) \\ p(\boldsymbol{\phi}) &= \text{Dirichlet}(\alpha_\phi \mathbf{1}) \\ p(\mu_k) &= N(\mu_0, \sigma_0^2) \\ p(\sigma_k^2) &= \text{inverse-gamma}(A, B) \end{aligned}$$

## Posterior

$$p(\boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mathbf{w}, \{\mathbf{z}_b\}_{b=1}^B \mid \mathbf{y}) \propto \prod_{i=1}^N \prod_{b=1}^B \prod_{k=1}^{\infty} p(y_i \mid \mu_k, \sigma_k^2)^{w_{ib} z_{ibk}} p(z_{ibk} \mid \mathbf{w}, \mathbf{p}_b) p(w_{ib} \mid \phi) p(p_{bk}) p(\phi_b) p(\mu_k) p(\sigma_k^2)$$

## Full Conditionals

$$p(w_{ib} = 1 \mid \cdot) \propto \phi_b \prod_{k=1}^{\infty} p_{bk} N(y_i \mid \mu_k, \sigma_k^2) \quad \text{for } b = 1, 2, \dots, B, \quad i = 1, 2, \dots, N$$

$$p(z_{ibk} = 1 \mid \cdot) \propto p_{bk} N(y_i \mid \mu_k, \sigma_k^2) \prod_{b=1}^B \phi_b \quad \text{for } k = 1, 2, \dots, \infty, \quad i = 1, 2, \dots, N$$

$$p(V_{bk} \mid \cdot) = \text{Beta}\left(1 + n_{bk}, \beta + \sum_{j=k+1}^{\infty} n_{bj}\right) \quad \text{where } n_{bk} = \sum_{i=1}^N z_{ibk} w_{ib} \quad k = 1, 2, \dots$$

$$p(\phi \mid \cdot) = \text{Dirichlet}(\boldsymbol{\alpha}) \quad \alpha_j = \alpha_{\phi_j} + \sum_{i=1}^N y_i w_{ib}$$

$$p(\mu_k \mid \cdot) = N(a^{-1}b, a^{-1}) \quad \text{where } a = \frac{1}{\sigma_0^2} + \frac{\sum_{b=1}^B n_{bk}}{\sigma_k^2} \quad \text{and } b = \frac{\mu_0}{\sigma_0^2} + \frac{\sum_{i=1}^N \sum_{b=1}^B y_i z_{ibk} w_{ib}}{\sigma_k^2} \quad k = 1, 2, \dots$$

$$p(\sigma_k^2 \mid \cdot) = \text{inverse-gamma}\left(A + \frac{\sum_{b=1}^B n_{bk}}{2}, B + \frac{\sum_{i=1}^N \sum_{b=1}^B (y_i - \mu_k)^2 z_{ibk} w_{ib}}{2}\right) \quad k = 1, 2, \dots$$

## Optimal Densities

The optimal densities are given by

$$q_i^*(\theta_i) \propto \exp\{E_{-\theta_i} \log p(\theta_i \mid \cdot)\}.$$

### Optimal density for $w_{ib}$

$$\begin{aligned} \log q_w^*(w_{ib}) &\propto E_{\phi, \mu_k, \sigma_k^2} \log p(w_{ik} = 1 \mid \cdot) \\ &= E_{\phi} [\log \phi_b] + \sum_{k=1}^{\infty} [E_{\mathbf{p}} [\log p_{bk}] - \frac{1}{2} \log(2\pi) - \frac{1}{2} E_{\sigma_k^2} [\log \sigma_k^2] - \frac{1}{2E_{\sigma_k^2} [\sigma_k^2]} E_{\mu_k} [(y_i - \mu_k)^2]] \\ &= \log \tilde{\phi}_{ib_{q(\phi)}} \end{aligned}$$

It follows that

$$q_w^*(w_i) = \text{categorical}(\boldsymbol{\phi}_{q(\phi)}) \quad \text{where } \phi_{ib_{q(\phi)}} = \frac{\tilde{\phi}_{ib_{q(\phi)}}}{\sum_{b=1}^B \tilde{\phi}_{ib_{q(\phi)}}}$$

### Optimal density for $z_{ibk}$

$$\begin{aligned} \log q_z^*(z_{ibk}) &\propto E_{\mathbf{p}, \mu_k, \sigma_k^2} \log p(z_{ibk} = 1 \mid \cdot) \\ &= E_{\mathbf{p}} [\log p_{bk}] - \frac{1}{2} \log(2\pi) - \frac{1}{2} E_{\sigma_k^2} [\log \sigma_k^2] - \frac{1}{2E_{\sigma_k^2} [\sigma_k^2]} E_{\mu_k} [(y_i - \mu_k)^2] + \sum_{b=1}^B E_{\phi} \log(\phi_b) \\ &= \log \tilde{p}_{ib_{k_{q(p)}}} \end{aligned}$$

It follows that

$$q_z^*(z_{ib}) = \text{categorical}(\mathbf{p}_{q(p)}) \quad \text{where} \quad p_{ibk_{q(p)}} = \frac{\tilde{p}_{ibk_{q(p)}}}{\sum_{k=1}^{\infty} \tilde{p}_{ibk_{q(p)}}}$$

**Optimal density for  $V_{bk}$**

$$q_V^*(V_{bk}) = \text{Beta}(\alpha_{q(V_{bk})}, \beta_{q(V_{bk})}) \quad \text{where} \quad \alpha_{q(V_{bk})} = 1 + E_{w,z}[n_{bk}], \quad \beta_{q(V_{bk})} = \beta + \sum_{j=k+1}^{\infty} E_{w,z}[n_{bj}]$$

**Optimal density for  $\phi$**

$$q_{\phi}^*(\phi) = \text{Dirichlet}(\boldsymbol{\alpha}_{q(\phi)}) \quad \text{where} \quad \alpha_{q(\phi_j)} = \alpha_{\phi_j} + \sum_{i=1}^N y_i E_w[w_{ib}]$$

**Optimal density for  $\mu_k$**

$$\begin{aligned} q_{\mu_k}^*(\mu_k) &= N(\mu_{q(\mu_k)}, \sigma_{q(\mu_k)}^2) \\ \sigma_{q(\mu_k)}^2 &= \left( \frac{1}{\sigma_0^2} + \frac{E_{w,z}[n_{bk}]}{E_{\sigma_k^2}[\sigma_k^2]} \right)^{-1} \\ \mu_{q(\mu_k)} &= \sigma_{q(\mu_k)}^2 * \left( \frac{\mu_0}{\sigma_0^2} + \frac{\sum_{i=1}^N \sum_{b=1}^B y_i E_z[z_{ibk}] E_w[w_{ib}]}{E_{\sigma_k^2}[\sigma_k^2]} \right) \end{aligned}$$

**Optimal density for  $\sigma_k^2$**

$$\begin{aligned} q_{\sigma_k^2}^*(\sigma_k^2) &= \text{inverse-gamma}(A_{q(\sigma_k^2)}, B_{q(\sigma_k^2)}) \\ A_{q(\sigma_k^2)} &= A + \frac{E_{w,z}[n_{bk}]}{2}, \\ B_{q(\sigma_k^2)} &= B + \frac{\sum_{i=1}^N \sum_{b=1}^B E_{w,z,\mu_k}[(y_i - \mu_k)^2 z_{ibk} w_{ib}]}{2} \end{aligned}$$

**Expectations**

$$\begin{aligned} E_{\phi}[\log \phi_b] &= \psi(\alpha_{q(\phi_b)}) + \psi\left(\sum_{b=1}^B \alpha_{q(\phi_b)}\right) \\ E_p[\log p_{bk}] &= E_V[\log V_{bk}] + \sum_{j=1}^{k-1} E_V[\log(1 - V_{bj})] \\ &= \psi(\alpha_{q(V_{bk})}) - \psi(\alpha_{q(V_{bk})} + \beta_{q(V_{bk})}) + \sum_{j=1}^{k-1} [\psi(\beta_{q(V_{bj})}) - \psi(\alpha_{q(V_{bj})} + \beta_{q(V_{bj})})] \\ E_{\sigma_k^2}[\log \sigma_k^2] &= \log(B_{q(\sigma_k^2)}) - \psi(A_{q(\sigma_k^2)}) \\ E_{\sigma_k^2}[\sigma_k^2] &= \frac{B_{q(\sigma_k^2)}}{A_{q(\sigma_k^2)}} \\ E_{\mu_k}[\mu_k] &= \mu_{q(\mu_k)} \\ E_{\mu_k}[(y_i - \mu_k)^2] &= (y_i - \mu_{q(\mu_k)})^2 + \sigma_{q(\mu_k)}^2 \end{aligned}$$