DPGMM Variational Inference (Isotropic)

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This document contains the evidence lower bound and updates for variational inference in a Dirichlet Process isotropic Gaussian mixture model, as well as their derivations.

1 Setup

1.1 Variables

X: data

N: number of datapoints

D: dimensionality of data

i: datapoint index

T: truncation parameter, i.e., number of clusters in variational distribution

k: cluster index

 ϕ_k : cluster stick-breaking proportion

 μ_k : cluster mean τ_k : cluster precision

 $z_i = k$: assignment of datapoint i to cluster k

1.2 Model, *P*

We use the 'rate' or 'inverse-scale' parametrization of the Gamma distribution, and the stick breaking process view of the Dirichlet process.

$$\begin{split} \phi_k &\sim Beta(1,\alpha) \\ \mu_k &\sim Gaussian(0,\mathbf{I}) \\ \tau_k &\sim Gamma(\mathrm{shape} = 1, \mathrm{rate} = 1) \\ z_i &\sim SBP(\phi) \\ x_i &\sim Gaussian(\mu_{z_i}, \frac{1}{\tau_{z_i}}\mathbf{I}) \end{split}$$

1.3 Variational distribution, Q

We use the truncated mean-field variational approximation set out in Blei and Jordan, with the variational distribution factorising as:

$$\begin{split} Q(\boldsymbol{\phi}, \boldsymbol{\mu}, \boldsymbol{\tau}, \mathbf{z}) &= \prod_{k=1}^{T} Q_{\phi_k}(\phi_k) Q_{\mu_k}(\mu_k) Q_{\tau_k}(\tau_k) \prod_{i=1}^{N} Q_{z_i}(z_i) \\ \phi_k &\sim Beta(\lambda_{k,1}, \lambda_{k,2}) \\ \mu_k &\sim Gaussian(\nu_k, \mathbf{I}) \\ \tau_k &\sim Gamma(a_k, b_k) \\ z_i &\sim Discrete(\boldsymbol{\zeta}_i) \end{split}$$

Where the distribution is clear from context, we omit the subscript on Q and write simply $Q(\phi_k)$ or $\mathbb{E}_{\phi_k \sim Q}[\ldots]$

2 Evidence lower bound

Maximizing the evidence lower bound provides the variational updates.

$$\begin{split} \log P(X) &\geq \sum_{k=1}^{T} \underset{\phi_k \sim Q}{\mathbb{E}} \left[\log P(\phi_k) - \log Q(\phi_k) \right] \\ &+ \sum_{k=1}^{T} \underset{\mu_k \sim Q}{\mathbb{E}} \left[\log P(\mu_k) - \log Q(\mu_k) \right] \\ &+ \sum_{k=1}^{T} \underset{\tau_k \sim Q}{\mathbb{E}} \left[\log P(\tau_k) - \log Q(\tau_k) \right] \\ &+ \sum_{i=1}^{N} \underset{\phi, z_i \sim Q}{\mathbb{E}} \left[\log P(z_i | \phi) - \log Q(z_i) \right] \\ &+ \sum_{i=1}^{N} \underset{z, \mu, \tau \sim Q}{\mathbb{E}} \left[\log P(x_i | \mu_{z_i}, \tau_{z_i}) \right] \end{split}$$

2.1 ϕ_k term

This bound is equal to the negative KL divergence between Beta distributions.

$$\begin{split} \underset{\phi_k \sim Q}{\mathbb{E}} \left[\log P(\phi_k) - \log Q(\phi_k) \right] &= -D_{KL}(Q_{\phi_k} || P_{\phi_k}) \\ &= \log \Gamma(1+\alpha) - \log \Gamma(\alpha) \\ &+ (\alpha-1)(\Psi(\lambda_{k,2}) - \Psi(\lambda_{k,1} + \lambda_{k,2})) \\ &- \log \Gamma(\lambda_{k,1} + \lambda_{k,2}) + \log \Gamma(\lambda_{k,1}) + \log \Gamma(\lambda_{k,2}) \\ &- (\lambda_{k,1} - 1)(\Psi(\lambda_{k,1}) - \Psi(\lambda_{k,1} + \lambda_{k,2})) \\ &- (\lambda_{k,2} - 1)(\Psi(\lambda_{k,2}) - \Psi(\lambda_{k,1} + \lambda_{k,2})) \end{split}$$

2.2 μ_k term

The bound is equal to the negative KL divergence between isotropic Gaussians.

$$\mathbb{E}_{\mu_k \sim Q} \left[\log P(\mu_k) - \log Q(\mu_k) \right] = -D_{KL}(Q_{\mu_k} || P_{\mu_k})$$

$$= -\frac{1}{2} || \nu_k ||^2$$

2.3 τ_k term

The bound is equal to the negative KL divergence between Gamma distributions.

$$\begin{split} \underset{\tau_k \sim Q}{\mathbb{E}} \left[\log P(\tau_k) - \log Q(\tau_k) \right] &= -D_{KL}(Q_{\tau_k} || P_{\tau_k}) \\ &= \log \Gamma(a_k) - (a_k - 1) \Psi(a_k) - \log(b_k) + a_k - \frac{a_k}{b_k} \end{split}$$

2.4 z_i term

$$\mathbb{E}_{\phi, z_i \sim Q} \left[\log P(z_i | \phi) - \log Q(z_i) \right] = \sum_{k=1}^{T} \zeta_{i,k} \left[-\log(\zeta_{i,k}) + \Psi(\lambda_{1,k}) - \Psi(\lambda_{1,k} + \lambda_{2,k}) + \sum_{j=1}^{k-1} \left(\Psi(\lambda_{j,2}) - \Psi(\lambda_{1,j} + \lambda_{2,j}) \right) \right]$$

For convenience later, we define:

$$\eta_{z_{i,k}} = \Psi(\lambda_{1,k}) - \Psi(\lambda_{1,k} + \lambda_{2,k}) + \sum_{i=1}^{k-1} \left(\Psi(\lambda_{j,2}) - \Psi(\lambda_{1,j} + \lambda_{2,j}) \right)$$

2.4.1 Derivation

The stick breaking process gives:

$$P(z_i = k) = \phi_k \prod_{j=1}^{k-1} 1 - \phi_j$$

To derive the bound, we use the following properties of a Beta-distributed variable $B \sim Beta(b_1, b_2)$: 1) $\mathbb{E}[\log B] = \Psi(b_1) - \Psi(b_1 + b_2)$, 2) $1 - B \sim Beta(b_2, b_1)$.

$$\begin{split} \underset{\phi, z_i \sim Q}{\mathbb{E}} \left[\log P(z_i | \phi) - \log Q(z_i) \right] &= \underset{z_i \sim Q}{\mathbb{E}} \left[\underset{\phi \sim Q}{\mathbb{E}} \left[\log \phi_{z_i} + \sum_{j=1}^{z_i - 1} \log(1 - \phi_j) - \log(\zeta_i) \right] \right] \\ &= \underset{z_i \sim Q}{\mathbb{E}} \left[\underset{\phi \sim Q}{\mathbb{E}} [\log \phi_{z_i}] + \sum_{j=1}^{z_i - 1} \underset{\phi \sim Q}{\mathbb{E}} [\log(1 - \phi_j)] - \log(\zeta_i) \right] \\ &= \underset{z_i \sim Q}{\mathbb{E}} \left[\Psi(\lambda_{z_i, 1}) - \Psi(\lambda_{z_i, 1} + \lambda_{z_i, 2}) + \sum_{j=1}^{z_i - 1} (\Psi(\lambda_{z_j, 1}) - \Psi(\lambda_{z_j, 1} + \lambda_{z_j, 2})) - \log(\zeta_i) \right] \end{split}$$

Taking the expectation with respect to $Q(z_i)$ gives the stated bound.

2.5 x_i term

$$\mathbb{E}_{\mathbf{z}, \boldsymbol{\mu}, \boldsymbol{\tau} \sim Q} \left[\log P(x_i | \mu_{z_i}, \tau_{z_i}) \right] = \sum_{k=1}^{T} \zeta_{i,k} \left(-\frac{D}{2} \left(\log(2\pi) - \Psi(a_k) + \log(b_k) \right) - \frac{a}{2b} \left(||x_i - \nu_k||^2 + \frac{\Gamma(1.5)}{(2\pi)^{\frac{D}{2}} 0.5^{1.5}} \right) \right)$$

For convenience later, we define:

$$\eta_{x_{i,k}} = -\frac{D}{2} \left(\log(2\pi) - \Psi(a_k) + \log(b_k) \right) - \frac{a}{2b} \left(||x_i - \nu_k||^2 + \frac{\Gamma(1.5)}{(2\pi)^{\frac{D}{2}} 0.5^{1.5}} \right)$$

2.5.1 Derivation

First taking the expectation with respect to $Q(z_i)$:

$$\mathbb{E}_{\boldsymbol{z},\boldsymbol{\mu},\boldsymbol{\tau}\sim Q} \left[\log P(x_i|\mu_{z_i}, \tau_{z_i}) \right] \\
= \sum_{k=1}^{T} \zeta_{i,k} \mathbb{E}_{\tau_k \sim Q} \left[\mathbb{E}_{\mu_k \sim Q} [\log P(x_i|\mu_k, \tau_k)] \right] \\
= \sum_{k=1}^{T} \zeta_{i,k} \mathbb{E}_{\tau_k \sim Q} \left[\mathbb{E}_{\mu_k \sim Q} [\log N(x_i; \mu_k, \frac{1}{\tau_k} \mathbf{I})] \right] \\
= \sum_{k=1}^{T} \zeta_{i,k} \mathbb{E}_{\tau_k \sim Q} \left[\int_{\mu_k} N(\mu_k; \nu_k, \mathbf{I}) \log N(x_i; \mu_k, \frac{1}{\tau_k} \mathbf{I}) d\mu_k \right] \tag{1}$$

First looking at the integral inside the expectation:

$$\begin{split} & \int_{\mu_k} N(\mu_k; \nu_k, \mathbf{I}) \log N(x_i; \mu_k, \frac{1}{\tau_k} \mathbf{I}) d\mu_k \\ & = \int_{\mu_k} (2\pi)^{-\frac{D}{2}} \exp(-\frac{1}{2} ||\mu_k - \nu_k||^2) \Big(-\frac{D}{2} \log \Big(\frac{2\pi}{\tau_k} \Big) - \frac{\tau_k}{2} ||x_i - \mu_k||^2 \Big) d\mu_k \\ & = -\frac{D}{2} \log \Big(\frac{2\pi}{\tau_k} \Big) + \int_{\mu_k} (2\pi)^{-\frac{D}{2}} \exp(-\frac{1}{2} ||\mu_k - \nu_k||^2) \Big(-\frac{\tau_k}{2} (x_i^2 - 2\mu_k x_i + \mu_k^2) \Big) d\mu_k \end{split}$$

To compute this integral, we use a change of variables $m=\mu_k-\nu_k$ and the equation $\int_0^\infty m^n e^{-am^2} dm = \frac{\Gamma(\frac{n+1}{2})}{2a^{\frac{n+1}{2}}}$:

$$\begin{split} & \int_{\mu_k} (2\pi)^{-\frac{D}{2}} \exp(-\frac{1}{2}||\mu_k - \nu_k||^2) \Big(-\frac{\tau_k}{2} \big(x_i^2 - 2\mu_k x_i + \mu_k^2\big) \Big) d\mu_k \\ & = \int_m (2\pi)^{-\frac{D}{2}} \exp(-\frac{1}{2}m^2) \Big(-\frac{\tau_k}{2} \big(||x_i - \nu_k||^2 + (2\nu_k - 2x_i)m + m^2\big) \Big) dm \\ & = -\frac{\tau_k}{2} \Big(||x_i - \nu_k||^2 + \frac{\Gamma(1.5)}{(2\pi)^{\frac{D}{2}} 0.5^{1.5}} \Big) \end{split}$$

The term linear in m equals 0 because it is an odd function. Overall,

$$\int_{\mu_k} N(\mu_k; \nu_k, \mathbf{I}) \log N(x_i; \mu_k, \frac{1}{\tau_k} \mathbf{I}) d\mu_k
= -\frac{D}{2} \log(\frac{2\pi}{\tau_k}) - \frac{\tau_k}{2} \left(||x_i - \nu_k||^2 + \frac{\Gamma(1.5)}{(2\pi)^{\frac{D}{2}} 0.5^{1.5}} \right)$$
(2)

Now, substituting (2) into (1) and taking the expectation with respect to $Q(\tau_k)$:

$$\begin{split} &\sum_{k=1}^{T} \zeta_{i,k} \mathop{\mathbb{E}}_{\tau_{k} \sim Q} \left[\mathop{\mathbb{E}}_{\mu_{k} \sim Q} [\log P(x_{i} | \mu_{k}, \tau_{k})] \right] \\ &= \sum_{k=1}^{T} \zeta_{i,k} \mathop{\mathbb{E}}_{\tau_{k} \sim Q} \left[-\frac{D}{2} \log(\frac{2\pi}{\tau_{k}}) - \frac{\tau_{k}}{2} \left(||x_{i} - \nu_{k}||^{2} + \frac{\Gamma(1.5)}{(2\pi)^{\frac{D}{2}} 0.5^{1.5}} \right) \right] \\ &= \sum_{k=1}^{T} \zeta_{i,k} \left(-\frac{D}{2} (\log(2\pi) - \mathop{\mathbb{E}}_{\tau_{k} \sim Q} [\log(\tau_{k})]) - \frac{\mathbb{E}_{\tau_{k} \sim Q} [\tau_{k}]}{2} \left(||x_{i} - \nu_{k}||^{2} + \frac{\Gamma(1.5)}{(2\pi)^{\frac{D}{2}} 0.5^{1.5}} \right) \right) \end{split}$$

For $G \sim Gamma(g_1, g_2)$ with a rate parametrization, $\mathbb{E}[G] = \frac{g_1}{g_2}$ and $\mathbb{E}[\log(G)] = \Psi(g_1) - \log(g_2)$. Using these gives the stated bound.

3 Variational updates

3.1 λ updates

Blei and Jordan present the updates for the cluster probabilities in equations (18) and (19).

$$\lambda_{k,1} = 1 + \sum_{i} \zeta_{i,k}$$

$$\lambda_{k,2} = \alpha + \sum_{i} \sum_{j>k} \zeta_{i,j}$$

3.2 ν update

$$\nu_k = \frac{\sum_{i=1}^{N} \frac{\zeta_{i,k} a_k}{b_k} x_i}{1 + \sum_{i=1}^{N} \frac{\zeta_{i,k} a_k}{b_k}}$$

3.2.1 Derivation

Taking the derivative of the evidence lower bound with respect to ν_k gives:

$$\frac{\delta L}{\delta \nu_k} = -\nu_k + \sum_{i=1}^{N} \frac{\zeta_i a_k}{b_k} (x_i - \nu_k)$$

Setting this to zero and solving for ν_k gives the update.

3.3 a and b updates

$$a_k = 1 + \frac{D}{2} \sum_{i=1}^{N} \zeta_{i,k}$$

$$b_k = 1 + \frac{1}{2} \sum_{i=1}^{N} \zeta_{i,k} \left(||x_i - \nu_k||^2 + \frac{\Gamma(1.5)}{(2\pi)^{\frac{D}{2}} 0.5^{1.5}} \right)$$

3.3.1 Derivation

Rather than maximising the ELBO with respect to a and b directly (which does not yield a closed-form derivative), we instead maximise the ELBO directly with respect to Q_{τ} and show that the result takes the functional form of a Gamma distribution for some particular a and b.

Using the calculus of variations, the optimal Q_{τ} can be shown to be

$$Q(\tau_{k^*}) \propto \exp\left(\mathbb{E}_{\phi,\mathbf{z},\boldsymbol{\mu},\boldsymbol{\tau}_{-k^*}\sim Q}P(\boldsymbol{\phi},\mathbf{z},\boldsymbol{\mu},\boldsymbol{\tau},X)\right)$$

Collecting all constant factors with respect to τ_{k^*} , we get:

$$\begin{split} \log Q(\tau_{k^*}) &= \underset{\mathbf{z}, \mu, \tau_{-k^*} \sim Q}{\mathbb{E}} [\log(P(\tau_{k^*}) + \log(P(X|z, \mu, \tau_{-k^*}, \tau_{k^*})] + \text{Const.} \\ &= \underset{\mathbf{z}, \mu, \tau_{-k^*} \sim Q}{\mathbb{E}} [\log Gamma(\tau_{k^*}; 1, 1) + \sum_{i=1}^{N} \log(N(x_i; \mu_{z_i}, \frac{1}{\tau_{z_i}}\mathbf{I}))] + \text{Const.} \\ &= \log Gamma(\tau_{k^*}; 1, 1) + \sum_{i=1}^{N} \sum_{k=1}^{T} \zeta_{i, k} \underset{\mu, \tau_{-k^*} \sim Q}{\mathbb{E}} [\log N(x_i; \mu_{z_i}, \frac{1}{\tau_{z_i}}\mathbf{I}] + \text{Const.} \\ &= \log Gamma(\tau_{k^*}; 1, 1) + \sum_{i=1}^{N} \zeta_{i, k^*} \underset{\mu \sim Q}{\mathbb{E}} [\log N(x_i; \mu_{k^*}, \frac{1}{\tau_{k^*}}\mathbf{I}] + \text{Const.} \end{split}$$

Substituting in equation (2):

$$\log Q(\tau_{k^*}) = \log Gamma(\tau_{k^*}; 1, 1)$$

$$+ \sum_{i=1}^{N} \zeta_{i,k^*} \left(-\frac{D}{2} \log \left(\frac{2\pi}{\tau_{k^*}} \right) - \frac{\tau_{k^*}}{2} \left(||x_i - \nu_{k^*}||^2 + \frac{\Gamma(1.5)}{(2\pi)^{\frac{D}{2}} 0.5^{1.5}} \right) \right)$$
+ Const.
$$= -\tau_{k^*} - \tau_{k^*} \sum_{i=1}^{N} \frac{\zeta_{i,k^*}}{2} \left(||x_i - \nu_{k^*}||^2 - \frac{\Gamma(1.5)}{(2\pi)^{\frac{D}{2}} (0.5)^{1.5}} \right)$$
+
$$\log(\tau_{k^*}) \sum_{i=1}^{N} \frac{\zeta_{i,k^*} D}{2} + \text{Const.}$$

Gathering up the terms containing τ_k and $\log(\tau_k)$, one can show that this is the expression for the log of a Gamma distribution with shape parameter a and rate parameter b equal to the updates above.

3.4 ζ update

Using the η terms defined in the sections on the z and x terms of the ELBO, which are constant with respect to ζ :

$$\zeta_{i,k} = \frac{\exp(\eta_{z_{i,k}} + \eta_{x_{i,k}} - 1)}{\sum_{j=1}^{T} \exp(\eta_{z_{i,j}} + \eta_{x_{i,j}} - 1)}$$

3.4.1 Derivation

To maximize the ELBO with respect to ζ_i subject to $\sum_k \zeta_{i,k} = 1$, we use Lagrange multipliers. (The λ below is not the variational parameter.)

$$\mathcal{L}(\zeta_{\mathbf{i}}, \lambda) = \left(\sum_{j=1}^{T} \zeta_{i,j} \left[-\log(\zeta_{i,j}) + \eta_{z_{i,j}} \right] + \sum_{j=1}^{T} \zeta_{i,j} \eta_{x_{i,j}} \right) - \lambda \left(\sum_{k} \zeta_{i,k} - 1\right)$$

$$\frac{\delta \mathcal{L}(\zeta_{\mathbf{i}}, \lambda)}{\delta \zeta_{i,k}} = \left(-1 - \log(\zeta_{i,k}) + \eta_{z_{i,k}} + \eta_{x_{i,k}} \right) - \lambda$$

$$\frac{\delta \mathcal{L}(\zeta_{\mathbf{i}}, \lambda)}{\delta \lambda} = 1 - \sum_{j=1}^{T} \zeta_{i,j}$$

Setting these partial derivatives to 0 and solving for $\zeta_{i,k}$ gives the stated update.