Variational Inference for Dirichlet Process Mixtures

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Motivation

- Non-parametric Bayesian models seem to be the right idea:
 - Do not fix the number of mixture components
- Dirichlet process is an elegant and principled way to "automatically" set the components
- Need to explore new methods that cope intractable nature of marginalization or conditional
- MCMC sampling methods widely used in this context, but there are other ideas

Motivation

- Variational inference have proved to be faster and more predictable (deterministic) than sampling
- The basic idea
 - Reformulate as an optimization problem
 - Relax the optimization problem
 - Optimize (find a bound of the original problem)

Background

- Dirichlet process mixture is a measure on measures
- Multiples representations and interpretations:
 - Ferguson Existent theorem
 - Blackwell-MacQueen urn scheme
 - Chinese restaurant process
 - Stick-breaking construction

Dirichlet process mixture model

$$G | \{ \alpha, G_0 \} \sim DP(\alpha, G_0)$$

$$\eta_n | G \sim G$$

$$X_n | \eta_n \sim p(x_n | \eta_n).$$

- G_0 Base distribution
- α Positive scaling parameter

 $\{\eta_1, \ldots, \eta_{n-1}\}$ exhibit a clustering effect

The DP mixture has a natural interpretation as a flexible mixture model in which the number of components is random and grows as new data are observed

Stick-breaking representation

 Two infinite collections of independent random variables

$$V_i \sim Beta(1,\alpha)$$

For i = {1,2,...}
 $\eta_i^* \sim G_0$
Stir-breaking representation of G

$$\pi_i(\mathbf{v}) = v_i \prod_{j=1}^{i-1} (1 - v_j)$$
$$G = \sum_{i=1}^{\infty} \pi_i(\mathbf{v}) \partial_{\eta_i^*}$$

G is discrete!

Sticking-breaking rep.

- The data can be described as arriving from
- 1) **Draw** $V_i \mid \alpha \sim Beta(1, \alpha), \quad i = \{1, 2, ...\}$
- 2) **Draw** $\eta_i^* \mid G_0 \sim G_0$ $i = \{1, 2, ...\}$
- 3) For the n-th data point
 - 1) Draw $Z_n | \{v_1, v_2, ...\} \sim Mult(\pi(\mathbf{v}))$

2) Draw
$$X_n \mid z_n \sim p(x_n \mid \eta_{z_n}^*)$$

DP mixture for exponential families

 Observable data drawn from exponential family, the base distribution is the conjugate



$$p(x_n \mid z_n, \eta_1^*, \eta_2^*, \ldots) = \prod_{i=1}^{\infty} \left(h(x_n) \exp\{\eta_i^{*T} x_n - a(\eta_i^*)\} \right)^{\mathbf{1}[z_n=i]}$$
$$p(\eta^* \mid \lambda) = h(\eta^*) \exp\{\lambda_1^T \eta^* + \lambda_2(-a(\eta^*)) - a(\lambda)\}$$

Variational inf. for DP mix.

- In DP, our goal $p(x \mid x_1, \dots, x_N, \alpha, G_0) = \int p(x \mid \eta) p(\eta \mid x_1, \dots, x_N, \alpha, G_0) d\eta$ = Put complex.
- But complex $p(\eta | x_1, \ldots, x_N, G_0, \alpha)$
- Variational inference uses a proposal distribution that breaks the dependency among latent variables

Variational inf. for DP mix.

In general, consider a model with hyperparameters θ , latent variables

 $\mathbf{W} = \{W_1, \dots, W_M\} \text{ and observations } \mathbf{x} = \{x_1, \dots, x_N\}$

The posterior distribution:



Variational inf. for DP mix

This is difficult

$$\log p(\mathbf{x} \mid \theta) = \log \int p(\mathbf{w}, \mathbf{x} \mid \theta) d\mathbf{w}$$

Because latent variables become dependent when conditioning on observed data

 We reformulate the problem using the mean-field method, which optimizes the KL divergence with respect to a variational distribution.

Variational inf. for DP mix

This is, we aim to minimize the KL divergence between $q_{\nu}(\mathbf{w})$ and $p(\mathbf{w} | \mathbf{x}, \theta)$

 $D(q_{\nu}(\mathbf{w})||p(\mathbf{w} | \mathbf{x}, \theta)) = E_q \left[\log q_{\nu}(\mathbf{W})\right] - E_q \left[\log p(\mathbf{W}, \mathbf{x} | \theta)\right] + \log p(\mathbf{x} | \theta)$

 Or equivalently, we try to maximize the lower bound

 $\log p(\mathbf{x} \mid \theta) \ge \mathbf{E}_q \left[\log p(\mathbf{W}, \mathbf{x} \mid \theta)\right] - \mathbf{E}_q \left[\log q_\nu(\mathbf{W})\right]$

Mean field of exponential fam.

For each latent variable, the conditional is a member of a exponential family:

 $p(w_i | \mathbf{w}_{-i}, \mathbf{x}, \theta) = h(w_i) \exp\{g_i(\mathbf{w}_{-i}, \mathbf{x}, \theta)^T w_i - a(g_i(\mathbf{w}_{-i}, \mathbf{x}, \theta))\}$

- Where g_i(w_{-i}, x, θ) is the natural parameter of w_i when conditioned on the remaining latent variables
- Here the family of distributions is

$$q_{\boldsymbol{\nu}}(\mathbf{w}) = \prod_{i=1}^{M} \exp\{\nu_i^T w_i - a(w_i)\}$$

 $\boldsymbol{\nu} = \{\nu_1, \nu_2, \dots, \nu_M\}$ Variational parameters

Mean-field of exponential family

The optimization of KL divergence

 $\nu_i = \mathbf{E}_q \left[g_i(\mathbf{W}_{-i}, \mathbf{x}, \theta) \right]$

after derivation (see Apendix)

- Notice:
 - Gibbs sampling, we draw w_i from $p(w_i|w_{-i}, x, \theta)$
 - Here, we update v_i to set it equal E[$g_i(w_{-i}, x, \theta)$]

DP mixtures

The latent variables are stick lengths, atoms, and cluster assignment

 $\mathbf{W} = \{\mathbf{V}, \boldsymbol{\eta}^*, \mathbf{Z}\}$

- The hyper parameters are the scaling and conjugate base distribution
- θ = {α, λ}
 And the bound now is

$$\log p(\mathbf{x} \mid \alpha, \lambda) \ge \mathbf{E}_q \left[\log p(\mathbf{V} \mid \alpha)\right] + \mathbf{E}_q \left[\log p(\boldsymbol{\eta}^* \mid \lambda)\right] \\ + \sum_{n=1}^N \left(\mathbf{E}_q \left[\log p(Z_n \mid \mathbf{V})\right] + \mathbf{E}_q \left[\log p(x_n \mid Z_n)\right] \\ - \mathbf{E}_q \left[\log q(\mathbf{V}, \boldsymbol{\eta}^*, \mathbf{Z})\right].$$

Relaxation of optimization

- To exploit this bound, with family q we need to approximate G
 - G is an *infinite-dimensional* random measure.
 - An approximation is to truncate the stickbreaking representation!

Relaxation of optimization

- Fix value T and $q(v_T = 1)=1$, then $\pi_t(\mathbf{v})$ are equal to zero for t>T
- (remember from $\pi_i(\mathbf{v}) = v_i \prod_{j=1}^{i-1} (1-v_j)$
- Propose, $q(\mathbf{v}, \boldsymbol{\eta}^*, \mathbf{z}) = \prod_{t=1}^{T-1} q_{\gamma_t}(v_t) \prod_{t=1}^{T} q_{\tau_t}(\eta_t^*) \prod_{n=1}^{N} q_{\phi_n}(z_n)$
- $q_{\gamma_t}(v_t)$ Beta distributions
- $q_{\tau_t}(\eta_t^*)$ Exponential family distributions
- $q_{\phi_n}(z_n)$ Multinomial distributions

$$\boldsymbol{\nu} = \{\gamma_1, \ldots, \gamma_{T-1}, \tau_1, \ldots, \tau_T, \phi_1, \ldots, \phi_N\}$$

Optimization

- The optimization is performed by coordinate ascent algorithm
- From,

$$\log p(\mathbf{x} \mid \alpha, \lambda) \geq \mathbf{E}_q \left[\log p(\mathbf{V} \mid \alpha)\right] + \mathbf{E}_q \left[\log p(\boldsymbol{\eta}^* \mid \lambda)\right] \\ + \sum_{n=1}^N \left(\mathbf{E}_q \left[\log p(Z_n \mid \mathbf{V})\right] + \mathbf{E}_q \left[\log p(x_n \mid Z_n)\right]\right) \\ - \mathbf{E}_q \left[\log q(\mathbf{V}, \boldsymbol{\eta}^*, \mathbf{Z})\right].$$
 Infinite!
$$\mathbf{E}_q \left[\log p(Z_n \mid \mathbf{V})\right] = \mathbf{E}_q \left[\log \left(\prod_{i=1}^{\infty} (1 - V_i)^{\mathbf{1}[Z_n > i]} V_i^{\mathbf{1}[Z_n = i]}\right)\right] \\ = \sum_{i=1}^{\infty} q(z_n > i) \mathbf{E}_q \left[\log(1 - V_i)\right] + q(z_n = i) \mathbf{E}_q \left[\log V_i\right]$$

Optimization

But, $E_q [log(1 - V_T)] = 0 \text{ and } q(z_n > T) = 0.$ Then

$$E_q \left[\log p(Z_n | \mathbf{V}) \right] = \sum_{i=1}^T q(z_n > i) E_q \left[\log(1 - V_i) \right] + q(z_n = i) E_q \left[\log V_i \right]$$

Where

$$q(z_n = i) = \phi_{n,i}$$

$$q(z_n > i) = \sum_{j=i+1}^T \phi_{n,j}$$

$$E_q [\log V_i] = \Psi(\gamma_{i,1}) - \Psi(\gamma_{i,1} + \gamma_{i,2})$$

$$E_q [\log(1 - V_i)] = \Psi(\gamma_{i,2}) - \Psi(\gamma_{i,1} + \gamma_{i,2}).$$

Optimization

Finally, the mean-field coordinate ascent algorithm boils down to updates:

$$\gamma_{t,1} = 1 + \sum_{n} \phi_{n,t}$$

$$\gamma_{t,2} = \alpha + \sum_{n} \sum_{j=t+1}^{T} \phi_{n,j}$$

$$\tau_{t,1} = \lambda_1 + \sum_{n} \phi_{n,t} x_n$$

$$\tau_{t,2} = \lambda_2 + \sum_{n} \phi_{n,t}.$$

$$\phi_{n,t} \propto \exp(S_t),$$

for $t \in \{1, \ldots, T\}$ and $n \in \{1, \ldots, N\}$

 $S_{t} = E_{q} \left[\log V_{t} \right] + \sum_{i=1}^{t-1} E_{q} \left[\log(1 - V_{i}) \right] + E_{q} \left[\eta_{t}^{*} \right]^{T} X_{n} - E_{q} \left[a(\eta_{t}^{*}) \right]$

Predictive distribution

$$p(x_{N+1} \mid \mathbf{x}, \alpha, \lambda) \approx \sum_{t=1}^{T} \mathbf{E}_q \left[\pi_t(\mathbf{V}) \right] \mathbf{E}_q \left[p(x_{N+1} \mid \eta_t^*) \right]$$

where q depends implicitly on \mathbf{x} , α , and λ

Empirical comparison



Figure 3: Mean convergence time and standard error across ten data sets per dimension for variational inference, TDP Gibbs sampling, and the collapsed Gibbs sampler.

Conclusion

- Faster than sampling for particular problems
- Unlikely, that one method will dominate another
 → both have their pros and cons
- This is the simplest variational method (mean-field). Other methods are worth exploring.
- Check www.videolectures.net