Approximate Inference

Jinhwan Suk

Department of Mathematical Science, KAIST

July 30, 2020

Contents

Contents

Motivation

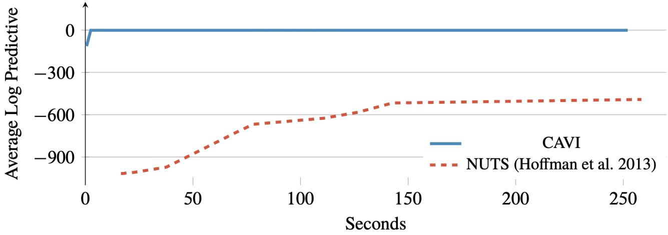
- In general model, it is difficult to compute posterior due to $p(x)$
- **Variational inference** is widely used to approximate posterior for Bayesian models
- Compared to **MCMC**, variational inference tends to be faster and easier to scale to large data.
- Rather than using sampling, variational inference uses optimization

$$q^*(z) = \underset{q \in \mathscr{F}}{\arg\min} \mathscr{D}_{KL}(q(z)||p(z|x))$$

- $q^*(z)$ serves as a proxy for $p(z|x)$

When MCMC, When Variational Inference?

- MCMC is computationally intensive, but provides guarantees
- Variational inference doesn't provide such guarantees, but suited to large data.
- Multi-modal?



Contents

Goal : solve the following optimization problem,

$$q^*(z) = \underset{q \in \mathscr{F}}{\arg\min} \mathscr{D}_{KL}(q(z)||p(z|x))$$

Recall that

$$\begin{aligned} \mathscr{D}_{KL}(q(z)||p(z|x)) &= \mathbb{E}_{z \sim q}\left[\log q(z) - \log p(z|x)\right] \\ &= \mathbb{E}_{z \sim q}\left[\log q(z) - \log p(x,z)\right] + \log p(x) \end{aligned}$$

Thus, we cannot compute $\mathscr{D}_{KL}$. We optimize an alternative objective that is equivalent to $\mathscr{D}_{KL}$,

$$ELBO(q) = \mathbb{E}_{z \sim q}\left[\log p(x,z) - \log q(z)\right]$$

- $ELBO(q)$ lower-bounds the evidence, $\log p(x) \geq ELBO(q)$

$$\log p(x) = \mathscr{D}_{KL}(q(z)||p(z|x)) + ELBO(q)$$

- $ELBO(q)$ also can be used as a good approximation of $\log p(x)$.
- Variational Inference vs. EM algorithm
    - Put $q(z) = p(z|x;\theta_0)$
    - E step : compute $Q(\theta; x, \theta_0) = \mathbb{E}_{z \sim p(z|x;\theta_0)} \log p(x, z; \theta)$
    - M step : $\theta' = \arg\max_\theta Q(\theta; x, \theta_0)$
    - *Variational EM*

- The complexity of a variational family $\mathscr{F}$ determines the complexity of the optimization
- A generic member of the **mean-field variational family** is

$$q(z) = \prod_j q_j(z_j)$$

- It cannot capture correlation between them.

  $\rightarrow$ Structured variational inference

Contents

- **Binary sparse coding model :** $q_i(z_i = 1) = \hat{z}_i$

$$p(z_i = 1) = \sigma(b_i), \quad p(x|z) = \mathcal{N}(Wz; \beta^{-1} I)$$

- Make a mean field approximation

$$q(z) = \prod_{i=1}^{m} q_i(z_i)$$

- Solve the fixed-point equation,

$$\frac{\partial}{\partial \hat{z}_i} ELBO(\hat{z}_1, \cdots, \hat{z_m}) = 0$$

Discrete Latent Variable

$$
\begin{aligned}
ELBO &= \mathbb{E}_{z\sim q}\left[\log p(z) + \log p(x|z) - \log q(z)\right] \\
&= \mathbb{E}_{z\sim q}\left[\sum_{i=1}^{m} \log p(z_i) + \sum_{i=1}^{n} \log p(x_i|z) - \sum_{i=1}^{m} \log q_i(z_i)\right] \\
&= \sum_{i=1}^{m} \mathbb{E}_{z_i\sim q_i}\left[\log p(z_i) - \log q_i(z_i)\right] + \mathbb{E}_{z\sim q}\left[\sum_{i=1}^{n} \log p(x_i|z)\right] \\
&= \sum_{i=1}^{m}\left[\hat{z}_i(\log\sigma(b_i) - \log\hat{z}_i) + (1-\hat{z}_i)(\log\sigma(-b_i) - \log(1-\hat{h}_i))\right] \\
&\quad + \frac{1}{2}\sum_{i=1}^{n}\left[\log\frac{\beta_i}{2\pi} - \beta_i\left(x_i^2 - 2x_i W_{i,:}\hat{z} + \sum_{j}\left[W_{ij}^2\hat{z}_j + \sum_{k\neq j} W_{ij}W_{ik}\hat{z}_j\hat{z}_k\right]\right)\right]
\end{aligned}
$$

Discrete Latent Variable

$$
\begin{aligned}
&\frac{\partial}{\partial \hat{z}_i} ELBO \\
&= b_i - \log \hat{z}_i + \log(1 - \hat{z}_i) + x^T \beta W_{:,i} - \frac{1}{2} W_{:,i}^T \beta W_{:,i} - \sum_{j \neq i} W_{:,j}^T \beta W_{:,i} \hat{z}_j \\
&= 0
\end{aligned}
$$

We solve for the $\hat{z}_i$:

$$
\hat{z}_i = \sigma \left(b_i + x^T \beta W_{:,i} - \frac{1}{2} W_{:,i}^T \beta W_{:,i} - \sum_{j \neq i} W_{:,j}^T \beta W_{:,i} \hat{z}_j \right)
$$

Repeat the cycle until we satisfy a converge criterion

Contents

Continuous Latent Variable

Coordinate ascent mean-field variational inference (Bishop, 2006)

- Same assumption : Mean-field family
- **CAVI**(coordinate ascent variational inference) is one of the most commonly used algorithms for solving the optimization problem.
- Fix the other variational factors $q_\ell(z_\ell)$, $\ell \neq j$

$$q_j^*(z_j) \propto \exp\left(\mathbb{E}_{-j}[\log p(z_j|z_{-j}, x)]\right)$$

Algorithm 1: Coordinate Ascent Variational Inference(CAVI)

Input: A model $p(x,z)$, a data set x
Output: A variational density $q(z) = \prod_{j=1}^{m} q_j(z_j)$
Initialize: Variational factors $q_j(z_j)$;
while *the $ELBO$ has not converged* **do**
  Set $q_j(z_j) \propto \exp\left(\mathbb{E}_{-j}[\log p(z_j|z_{-j},x)]\right)$
  Compute $ELBO(q) = \mathbb{E}_{z\sim q}\left[\log p(x,z) - \log q(z)\right]$
end

- *Gibbs sampler* maintains a realization of the latent variables
- *CAVI* takes the expected log

Derivation :

$$\begin{aligned} ELBO(q;q_{-j}) &= \mathbb{E}_{z\sim q}\left[\log p(x,z) - \log q(z)\right] \\ &= \mathbb{E}_{z_j\sim q_j}\mathbb{E}_{z_{-j}\sim q_{-j}}\left[\log p(x,z) - \log q(z)\right] \\ &= \mathbb{E}_j[\mathbb{E}_{-j}\left[\log p(x,z)\right] - \log q_j(z_j)] - \mathbb{E}_{-j}[\log q_{-j}(z_{-j})] \\ &= -\mathscr{D}_{KL}(q_j \| \frac{q_j^*}{Z}) + Const. \end{aligned}$$

So, $ELBO_j$ is minimized when $q_j = \frac{q_j^*}{Z}$ (Calculus of Variation)

Contents

- Suppose each **complete conditional** is in the exponential family :

$$p(z_j|z_{-j},x) = h(z_j)\exp(\eta_j^T z_j - \alpha(\eta_j)), \quad \eta_j = \eta_j(z_{-j},x)$$

  (e.g) Gaussian Mixture Model
- CAVI is simplified by

$$\begin{aligned} q(z_j)^* &\propto \exp\left(\mathbb{E}_{-j}[\log p(z_j|z_{-j},x)]\right) \\ &= \exp\left[\log h(z_j) + \mathbb{E}_{-j}[\eta_j]^T z_j - \mathbb{E}_{-j}\alpha(\eta_j)\right] \\ &\propto h(z_j)\exp(\mathbb{E}_{-j}[\eta_j]^T z_j) \\ &(\nu_j = \mathbb{E}_{-j}[\eta_j]^T) \end{aligned}$$

  ν_j is the variational parameter for local latent variable z_j

Variational Inference with Exponential Family

Conditional conjugacy and Bayesian models

- Let β be a vector of *global latent variables*
- Let z be a vector of *local latent variables*
- Then, the joint density is

$$p(\beta, z, x) = p(\beta) \prod_{i=1}^{n} p(z_i, x_i | \beta)$$

- Assume that $p(z_i, x_i | \beta)$ has an exponential family form.

$$p(z_i, x_i | \beta) = h(z_i, x_i) \exp(\beta^T t(z_i, x_i) - a(\beta))$$

- Take the prior

$$p(\beta) = h(\beta) \exp(\alpha^T [\beta, -a(\beta)] - a(\alpha))$$
$$\alpha = [\alpha_1, \alpha_2]^T$$

- With the conjugate prior,

$$p(\beta \mid z, x) = h(\beta) \exp(\hat{\alpha}^T [\beta, -a(\beta)] - a(\hat{\alpha}))$$

$$\hat{\alpha} = [\alpha_1 + \sum_{i=1}^{n} t(z_i, x_i),\ \alpha_2 + n]^T$$

- Assume that

$$p(z_i | x_i, \beta, z_{-i}, x_{-i}) = p(z_i | x_i, \beta)$$

- Then, local variational update is

$$\nu_i \leftarrow \mathbb{E}_{-i} \eta_i(\beta, z_{-i}, x) = \mathbb{E}_{-i} \eta_i(\beta, x_i)$$

- $q(\beta|\lambda)$: variational posterior approximation on β
- $q(z_i|\phi_i)$: variational posterior approximation on z_i
- Then, local variational update is

$$\nu_i \leftarrow \mathbb{E}_{\lambda,\phi_{-i}} \eta_i(\beta, z_{-i}, x) = \mathbb{E}_{\lambda} \eta_i(\beta, x_i)$$

- global variational update is

$$\lambda \leftarrow [\alpha_1 + \sum_{i=1}^{n} \mathbb{E}_{\phi_i} t(z_i, x_i),\ \alpha_2 + n]^T$$

- When updating global variational parameter, the algorithm requires iterating through the **entire data set**.

Contents

- Most posterior inference algorithms do not easily scale(MCMC)
- CAVI is no exception

$$q_j^*(z_j) \propto \exp\left(\mathbb{E}_{-j}[\log p(z_j|z_{-j}, \mathbf{x})]\right)$$

- An alternative to CAVI is gradient-based optimization.

$$\nabla_\lambda ELBO = a''(\lambda)(\mathbb{E}_\phi[\hat{\alpha}] - \lambda), \quad g(\lambda) = \mathbb{E}_\phi[\hat{\alpha}] - \lambda$$

(e.g.) Neural Net

- global variational update is

$$\lambda_t = \lambda_{t-1} + \varepsilon_t g(\lambda_{t-1}) = (1-\varepsilon_t)\lambda_{t-1} + \varepsilon_t \mathbb{E}_\phi[\hat{\alpha}]$$

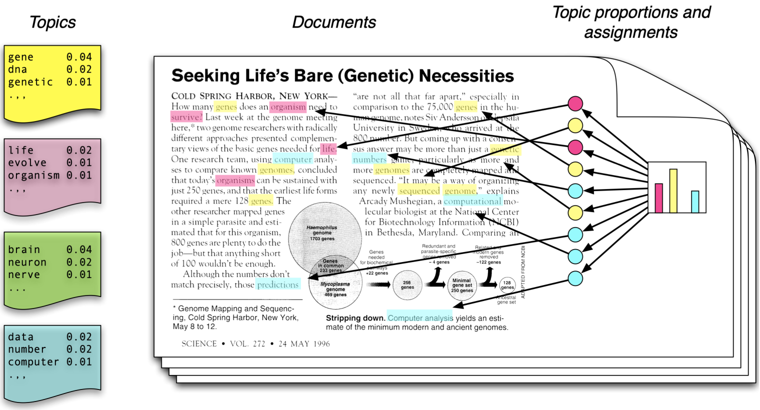
- The noisy unbiased estimator for $g(\lambda)$ is

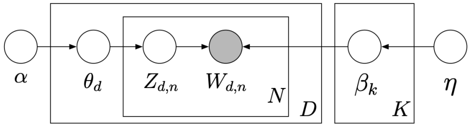
$$j \sim \text{Unif}(1, 2, ..., n)$$
$$\hat{g}(\lambda) = \alpha + n\left[\mathbb{E}_{\phi_j} t(z_j, x_j), 1\right]^T - \lambda$$

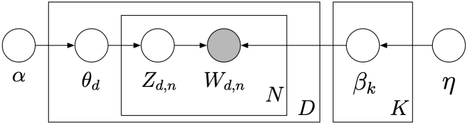
Contents

Variational Inference with Exponential Family

Application : Probabilistic Topic Models







1. For each topic in $k = 1, 2, ..., K$,
    1. draw a distribution over words $\beta_k \sim Dir_V(\eta)$
2. For each document in $d = 1, 2, ..., D$,
    1. draw a vector of topic proportions $\theta_d \sim Dir_K(\alpha)$
    2. For each word in $n = 1, 2, ..., N_d$
        1. draw a topic assignment $z_{dn} \sim Mult(\theta_d)$
        2. draw a word $w_{dn} \sim Mult(\beta_{z_{dn}})$

- Posit a mean-field variational family

$$q(\beta,\theta,z) = \prod_{k=1}^{K} q(\beta_k;\lambda_k) \prod_{d=1}^{D} \left(q(\theta_d\,;\gamma_d) \prod_{n=1}^{N_d} q(z_{dn};\phi_{dn}) \right)$$

- $p(\theta_d\,|z_d) = Dir_K(\alpha + \sum_{n=1}^{N_d} z_{dn}) \leftarrow q(\theta_d;\gamma_d)$
- $p(\beta_k|z,w) = Dir_V(\eta + \sum_{d,n} z_{dn}^{k} w_{dn}) \leftarrow q(\beta_k;\lambda_k)$

- CAVI update rule :

$$\phi_{dn}^k \propto \exp\left(\Psi(\gamma_{dk}) + \Gamma(\lambda_{k,w_{dn}}) - \Gamma(\sum_v \lambda_{kv})\right)$$

$$\gamma_d = \alpha + \sum_{n=1}^{N_d} \phi_{dn}$$

$$\lambda_k = \eta + \sum_{d,n} \phi_{dn}^k w_{dn}$$

- (Hoffman, 2013) Stochastic variational inference

- (You et al. 2014) Variational posterior for Bayesian linear model.
- (Hall et al. 2011) Poisson mixed-effects model
- (Westling and McCormick, 2015)

  Consistency of VI throuch a connection to M-estimation
- (Wang and Titterington, 2006) VI for mixtures of Gaussians
  - CAVI converges to a local optimum
  - VI estimate and MLE approach each other at a rate of $\mathcal{O}(1/n)$

Conclusion

Theory

- $\mathscr{D}_{KL}(q(z)||p(z|x))$
  - (Minka, 2001) $\mathscr{D}_{KL}(p(z|x)||q(z))$
  - (Barber and de van Laar, 1999) Tighter lower bounds than ELBO
- Mean-field approximation
  - help with scalable optimization, but limit the expressibility
  - Structured variational inference
- Interface between MCMC and variational inference
  - (Freitas et al., 2001) proposal distribution
  - (Salimans et al., 2015) variational approximation + MCMC chain
- **(Reference) Variational Inference : A Review for Statisticians**