Three Siblings: EM, Variational Inference, and Gibbs Sampling

Harrison H. Zhang Department of Statistics and Data Science Yale University

1



Anderson Y. Zhang

<u>Outline</u>

- Stochastic Block Model
- EM, Variational Inference, and Gibbs Sampling
- Computational and Statistical Guarantees
- Questions and Extensions

Stochastic Block Model

Model: Two Communities

Partition

$$z: \{1, 2, ..., n\} \to \{0, 1\}^n.$$

Observation: Adjacency matrix A

 $A_{ij} \sim \text{Bernoulli}(P_{ij}), \text{ for } i > j,$ where $P_{ij} = p$ when $z_i = z_j$, and $P_{ij} = q$ when $z_i \neq z_j$.

Goal: Recover z from A.



Bayesian Inference

Prior: $z_i \sim \text{Ber}(1/2), \forall i \in [n]$ and $p, q \sim \text{Beta}(1, 1)$ independently.

Challenge: The posterior is computationally intractable:

$$\mathbf{p}(z, p, q | A) = \frac{\mathbf{p}(z, p, q, A)}{\sum_{z \in \{0,1\}^n} \int_{p,q} \mathbf{p}(z, p, q, A)}$$



Three Siblings: EM, Variational Inference, and Gibbs Sampling

Mean Field Variational Inference

Main Idea: Approximate by a product measure $\mathbf{q}(z, p, q) = \prod_i \mathbf{q}_i(z_i)\mathbf{q}(p)\mathbf{q}(q)$ where $z_i \sim \text{Ber}(\pi_i), \forall i \in [n], p \sim \text{Beta}(\alpha_p, \beta_p), q \sim \text{Beta}(\alpha_q, \beta_q)$ and the Kullback-Leibler divergence is minimized:

$$\hat{\mathbf{q}} = \operatorname*{arg\,min}_{\mathbf{q}\in\mathbf{Q}} \mathrm{KL}\Big[\mathbf{q}(z,p,q) \,\Big\| \mathbf{p}(z,p,q|A)\Big].$$

Iterative Algorithm: Approach $\hat{\mathbf{q}}$ by an iterative algorithm:

$$\{\pi^{(s)}, \alpha_p^{(s)}, \beta_p^{(s)}, \alpha_q^{(s)}, \beta_q^{(s)}\}_{s \ge 0}.$$



Mean Field Variational Inference

General Setting

- approximate $\mathbf{p}(\theta|\mathbf{x})$ by some product measure $\mathbf{q}(\theta) = \prod \mathbf{q}_i(\theta_i)$
- minimize the Kullback-Leibler divergence

$$\mathbf{\hat{q}}^{\mathrm{MF}} = \operatorname*{arg\,min}_{q \in \mathcal{Q}} \mathrm{KL} \Big[\mathbf{q}(\theta) \Big\| \mathbf{p}(\theta | \mathbf{x}) \Big]$$

• Iterative Algorithm:

$$\hat{\mathbf{q}}_{i} = \operatorname*{arg\,min}_{\mathbf{q}_{i}} \operatorname{KL} \left[\mathbf{q}_{i}(\theta_{i}) \times \prod_{j \neq i} \mathbf{q}_{j}(\theta_{j}) \left\| p(\theta | \mathbf{x}) \right], \forall i \in [n]$$

$$\iff \quad \hat{\mathbf{q}}_{i}(\theta_{i}) \propto \exp\{\mathbb{E}_{\mathbf{q}_{-i}}[\log \mathbf{p}(\theta_{i} | \theta_{-i}, \mathbf{x})]\}, \forall i \in [n].$$

Iterative Algorithm

• Updates on $\alpha_p^{(s+1)}, \beta_p^{(s+1)}, \alpha_q^{(s+1)}, \beta_q^{(s+1)}$:

$$\alpha_p^{(s+1)} = 1 + \sum_{a=1}^k \sum_{i < j} A_{i,j} \pi_{i,a}^{(s)} \pi_{j,a}^{(s)}, \quad \beta_p^{(s+1)} = 1 + \sum_{a=1}^k \sum_{i < j} (1 - A_{i,j}) \pi_{i,a}^{(s)} \pi_{j,a}^{(s)},$$
$$\alpha_q^{(s+1)} = 1 + \sum_{a \neq b} \sum_{i < j} A_{i,j} \pi_{i,a}^{(s)} \pi_{j,b}^{(s)}, \quad \beta_q^{(s+1)} = 1 + \sum_{a \neq b} \sum_{i < j} (1 - A_{i,j}) \pi_{i,a}^{(s)} \pi_{j,b}^{(s)}.$$

• Updates on $\{\pi_i^{(s+1)}\}$:

$$\pi_{i}^{(s+1)} = \frac{\exp\left(2t^{(s)}\sum_{j\neq i}\pi_{j}^{(s)}(A_{i,j}-\lambda^{(s)})\right)}{\exp\left(2t^{(s)}\sum_{j\neq i}\pi_{j}^{(s)}(A_{i,j}-\lambda^{(s)})\right) + \exp\left(2t^{(s)}\sum_{j\neq i}(1-\pi_{j}^{(s)})(A_{i,j}-\lambda^{(s)})\right)},$$

where $t^{(s)}, \lambda^{(s)}$ are functions of $\alpha_{p}^{(s)}, \beta_{p}^{(s)}, \alpha_{q}^{(s)}, \beta_{q}^{(s)}.$

Three Siblings

Similarity: Coordinate updates with $\mathbf{p}(\theta_i | \theta_{-i}, \mathbf{x})$.

Mean Field Variational Inference	Gibbs Sampling
For all $i \in [n]$, $\exp\{\mathbb{E}_{\mathbf{q}-i}[\log \mathbf{p}(\theta_i \theta_{-i}, \mathbf{x})]\}$	$\forall i \in [n], \text{ sample}$ from $\mathbf{p}(\theta_i \theta_{-i}, \mathbf{x})$
	Mean Field Variational Inference For all $i \in [n]$, $\exp\{\mathbb{E}_{\mathbf{q}-i}[\log \mathbf{p}(\theta_i \theta_{-i}, \mathbf{x})]\}$

Statistical and Computational Guarantees

Loss Function

- Let z^*, p^*, q^* be the underlying ground truth from which A is generated.
- We consider the distance between z^* and $\pi^{(s)}$.

Loss Function

$$\ell(\pi, z^*) = \frac{1}{n} \min \left\{ \|\pi - z^*\|_1, \|\pi - (1_n - z^*)\|_1 \right\}$$
$$= \frac{1}{n} \min \left\{ \sum_{i=1}^n |\pi_i - z^*_i|, \sum_{i=1}^n |\pi_i - (1 - z^*_i)| \right\}$$

Theoretical Guarantees for Mean Field

Theorem (Zhang & Z. 2017). Let $I = (\sqrt{p^*} - \sqrt{q^*})^2$ [signal-to-noise ratio]. Assume the initializer $\pi^{(0)}$ satisfies $\ell(\pi^{(0)}, z^*) \leq c$ for some small constant c with high probability. Further we assume the following equation holds

 $nI \to \infty$.

Then in each iteration of the iterative algorithm for mean field, with high probability

$$\ell(\pi^{(s+1)}, z^*) \le \exp\left(-(1 - o(1))nI/2\right) + \frac{1}{\sqrt{nI}}\ell(\pi^{(s)}, z^*).$$

Corollary 1 (Zhang & Z. 2017). For $s \ge \log n$, we have with high probability $\ell(\hat{\pi}^{(s)}, z^*) \le \exp(-(1 - o(1))nI/2)) + o(n^{-D}), k = 2$ for every D > 1.

Remark: Rate-optimal. Matches with the minimax rate in Zhang and Z. (2016, AoS).

Theoretical Guarantees for Gibbs Sampling

Theorem (Zhang & Z. 2017). Let $I = (\sqrt{p^*} - \sqrt{q^*})^2$ [signal-to-noise ratio]. Assume the initializer $z^{(0)}$ satisfies $\ell(z^{(0)}, z^*) \leq c$ for some small constant c with high probability. Further we assume the following equation holds

 $nI \to \infty$.

Then in each iteration of the batched Gibbs sampling, with high probability

 $\mathbb{E}\left[\ell(z^{(s)}, z^*)|A, z^{(0)}\right] \le \exp\left(-(1 - o(1))nI/2\right) + \left[\frac{1}{\sqrt{nI}}\right]^s \ell(z^{(0)}, z^*) + sb_n,$

where $b_n = o(\exp(-n^{3/2}I)).$

Questions and Extensions

Questions

• Initializer: What is the sharp condition for initializer?(c.f., analysis on Lloyd's Algorithm in Lu & Z. 2016 to have c = 1/2 - o(1))

• **Parameter Estimation:** Can we prove that $\{p^{(s)}\}_{s\geq 1}$ and $\{q^{(s)}\}_{s\geq 1}$ converge to the optimal rates?

Extensions

• Models: Computational and statistical guarantees of variational inference for a general class of latent variable models.

• Algorithms: A unified framework to understand iterative algorithm.