Mixed Membership Stochastic Blockmodels


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as interpreted by Ted Westling

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Overview

1. Review

2. Variational Bayes: General Theory

3. Variational Bayes for the MMSB

4. Conclusion and next steps

5. Issues
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Individuals $p, q \in \{1, \ldots, N\}$. We observe relations/interactions $R(p, q)$ on pairs of individuals. Here we assume $R(p, q) \in \{0, 1\}$, $R(p, p) = 0$, but do not assume $R(p, q) = R(q, p)$ (we deal with directed networks).
Network theory: data representations

<table>
<thead>
<tr>
<th></th>
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<th>( R(p,q) )</th>
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<tr>
<td>1</td>
<td>2</td>
<td>1</td>
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<td>2</td>
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Table

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Adjacency matrix, black=1, white=0
```

```
(0 1 0)
(0 0 1)
(0 1 0)
```

Adjacency matrix, black=1, white=0
We believe the relations are a function of unobserved groupings among the individuals.

We want to recover the groups so we can a) predict new relations or b) interpret the existing network structure.

Example: Monk network.
The Problem: Pictures

Figure: Two visualizations of the same binary adjacency matrix. Each filled-in square represents a directed edge. Left: ordered randomly. Right: ordered by group membership.
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Brief blockmodel history

- 1975: CONCOR developed by Harrison White and colleagues
- 2004: Kemp, Griffiths & Tenenbaum allow unknown and unlimited number of blocks in the Infinite Relational Model.
Infinite Relational Model

- Observe binary relations $R(p, q)$ between nodes $p, q \in \{1, \ldots, N\}$.
- Each node $p$ is a member of exactly one block of $K$ total blocks, $K \leq N$ unknown. Let $z_p$ be an indicator vector of block membership for node $p$, i.e. $z_p = (0, 1, 0)$.
- $B$ is a $K \times K$ matrix of block relationships. If $p$ is in block $g$ and $q$ is in block $h$ then the probability of observing an interaction from node $p$ to node $q$ is $B_{gh}$.
- $R(p, q) \sim \text{Bernoulli}(z_p^T B z_q)$.
- For example, if $p$ is in block 3 and $q$ is in block 2 then $P(R(p, q) = 1) = B_{32}$. 
Block structure

\[
\begin{pmatrix}
0.8 & 0.3 & 0 & 0 \\
0.1 & 0.2 & 0.9 & 0 \\
0 & 0.5 & 0.6 & 0 \\
0.1 & 0 & 0.4 & 0.8 \\
\end{pmatrix}
\]
The Mixed Membership Stochastic Blockmodel

- Previous models assume each node is assumed to belong to exactly one latent block - e.g. \( z_p = (0, 1, 0, 0) \).
- Instead, in the MMB we assume each node has a distribution \( \pi_p \) over the latent blocks.
- For each interaction from \( p \) to \( q \), both \( p \) and \( q \) draw a particular block to be a part of for the interaction: \( z_{p\rightarrow q} \sim \text{Discrete}(\pi_p) \), \( z_{p\leftarrow q} \sim \text{Discrete}(\pi_q) \).
- Then \( R(p, q) \sim \text{Bernoulli}(z_{p\rightarrow q}^T B z_{p\leftarrow q}) \).
- \( K \) chosen by BIC.
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Estimation Basics

- Strategy: treat \( \{\pi, Z_\rightarrow, Z_\leftarrow\} \equiv \theta \) as random latent variables and obtain posterior distribution. Treat \( \{\alpha, B\} \equiv \beta \) as fixed parameters to estimate via Empirical Bayes.

- The typical approach in this setting is to use the EM algorithm, which involves calculating the posterior distribution \( p(\theta|Y, \beta) \).
Great! Write down the form of the posterior $p(\theta|Y, \beta)$:

$$\frac{p(Y|\theta, \beta)p(\theta|\beta)}{p(Y|\beta)}.$$ 

The denominator requires calculating the integral

$$\int \prod_{\pi} \sum_{p,q} \prod_{\Omega} [P(Y(p, q)|z_{p\rightarrow q}, z_{p\leftarrow q}, B)p(z_{p\rightarrow q}|\pi_p)p(z_{p\leftarrow q}|\pi_q)]$$

$$\prod_{p} p(\pi_p|\alpha) d\pi_1:N$$

No closed form solution
Variational Bayes

- Main idea: write down a simple parametric form \( q(\theta|\Delta) \) for the posterior distribution that depends on free variational parameters \( \Delta \).
- At each E-step, minimize the KL divergence between \( q \) and the true posterior in terms of the free variational parameters.

\[
K(q, p) = \mathbb{E}_q \left[ \log \frac{q(\theta|\Delta)}{p(\theta|Y, \beta)} \right] \\
= \mathbb{E}_q [\log q(\theta|\Delta)] - \mathbb{E}_q [\log p(\theta|Y, \beta)] \\
= \mathbb{E}_q [\log q(\theta|\Delta)] - \mathbb{E}_q \left[ \log \frac{p(\theta, Y|\beta)}{p(Y|\beta)} \right] \\
= \mathbb{E}_q [\log q(\theta|\Delta)] - \mathbb{E}_q [\log p(\theta, Y|\beta)] + \log p(Y|\beta).
\]

This is equivalent to maximizing the evidence lower bound or ELBO

\[
\mathcal{L}(\Delta|Y, \beta) = \mathbb{E}_q [\log p(\theta, Y|\beta)] - \mathbb{E}_q [\log q(\theta|\Delta)].
\]
Suppose we have a complicated posterior distribution $p$ (the one below is a mix of lognormal and t - yuck). We use a variational posterior $\text{Gamma}(\alpha, \beta)$. We minimize the KL divergence between the true and variational posteriors in terms of $\alpha$ and $\beta$ to get an approximate posterior.
Suppose we have a complicated posterior distribution $p$ (the one below is a mix of lognormal and t - yuck). We use a variational posterior $\text{Gamma}(\alpha, \beta)$. We minimize the KL divergence between the true and variational posteriors in terms of $\alpha$ and $\beta$ to get an approximate posterior.
How do we know what sort of variational posterior $q$ is easy to work with?

Most popular strategy is called the mean field approximation: assume $q$ factorizes into a term for each latent variable:

$$q(\theta_1, \ldots, \theta_r | \Delta) = \prod_{i=1}^{r} q_i(\theta_i | \Delta_i).$$

The optimal form for $q_i$ can be derived from the calculations of variations (hence the name variational inference).

To minimize the KL divergence (maximize the ELBO) between $p$ and $q$, we use coordinate descent over the $\Delta_i$. 
Variational EM algorithm

1. Initialize $\beta^{(0)}$, $\Delta^{(0)}$.

2. E-step: Find the $\Delta_{1:r}^{(j)}$ that maximizes $L(\Delta, \beta^{(j-1)})$ via coordinate ascent:
   (i) For $i = 1, \ldots, r$, maximize $L(\Delta^{(jk)}, \beta^{(j-1)})$ with respect to $\Delta_i$.
   (ii) If $\|\Delta^{(jk)} - \Delta^{(j(k+1))}\| > \epsilon$ has not converged, return to (i)

3. M-step: Find the $\beta^{(j)}$ that maximizes $L(\Delta^{(j)}, \beta)$.

4. If $\|\Delta^{(j)} - \Delta^{(j-1)}\| > \epsilon$ or $\|\beta^{(j)} - \beta^{(j-1)}\| > \epsilon$, return to 2.
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Mean-field approximation

- Recall $\theta = \{\pi_{1:N}, Z_{\rightarrow}, Z_{\leftarrow}\}$
- Recall the model distribution for $\theta$:
  - $\pi_p \sim \text{Dirichlet}(\alpha)$
  - $z_{p\rightarrow q} \sim \text{Discrete}(\pi_p)$
  - $z_{p\leftarrow q} \sim \text{Discrete}(\pi_q)$
- Assume the posterior factors as:
  - $\pi_p \sim \text{Dirichlet}(\gamma_p)$
  - $z_{p\rightarrow q} \sim \text{Discrete}(\phi_{p\rightarrow q})$
  - $z_{p\leftarrow q} \sim \text{Discrete}(\phi_{p\leftarrow q})$
- Variation parameters $\Delta = \{\gamma_{1:N}, \Phi_{\rightarrow}, \Phi_{\leftarrow}\}$
- Full approximate posterior:

$$q(\pi_{1:N}, Z_{\rightarrow}, Z_{\leftarrow} | \gamma_p, \Phi_{\rightarrow}, \Phi_{\leftarrow}) = \prod_p q_1(\pi_p | \gamma_p) \prod_{p,q} q_2(z_{p\rightarrow q} | \phi_{p\rightarrow q}) q_2(z_{p\leftarrow q} | \phi_{p\leftarrow q}).$$
Parameter updates

- Now we have to calculate the ELBO

\[ \mathcal{L}(\Delta|Y, \beta) = \mathbb{E}_q[\log p(\theta, Y|\beta)] - \mathbb{E}_q[\log q(\theta|\Delta)] \]

\[ = \mathbb{E}_q[\log p(\pi_{1:N}, Z_{\rightarrow}, Z_{\leftarrow}, Y|\alpha, B)] \]

\[ - \mathbb{E}_q[\log q(\pi_{1:N}, Z_{\rightarrow}, Z_{\leftarrow}|\gamma_{1:N}, \Phi_{\rightarrow}, \Phi_{\leftarrow})] \]

\[ = \ldots \]

\[ = \mathcal{L}(\gamma_{1:N}, \Phi_{\rightarrow}, \Phi_{\leftarrow}|Y, \alpha, B) \]

(appendix calculations)

- Then differentiate with respect to \( \gamma_i, \phi_{p\rightarrow q}, \phi_{p\leftarrow q}, \alpha_i, B(g, h) \), set to 0, and solve.
Get closed form updates:

$$
\hat{\phi}_{p \rightarrow q, g} \propto e^{\psi(\gamma_{p, g}) - \psi(\sum_j \gamma_{p,j})} \prod_h \left( B(g, h)^{Y(p, q)} (1 - B(g, h))^{1 - Y(p, q)} \right)^{\phi_{p \leftarrow q}} \\
\hat{\phi}_{p \leftarrow q, h} \propto e^{\psi(\gamma_{q, h}) - \psi(\sum_j \gamma_{q,j})} \prod_g \left( B(g, h)^{Y(p, q)} (1 - B(g, h))^{1 - Y(p, q)} \right)^{\phi_{p \rightarrow q}} \\
\hat{\gamma}_{p, k} = \alpha_k + \sum_q \phi_{p \rightarrow q, k} + \sum_q \phi_{q \leftarrow p, k} \\
\hat{B}(g, h) = \frac{\sum_{p, q} \phi_{p \rightarrow q, g} \phi_{p \leftarrow q, h} Y(p, q)}{\sum_{p, q} \phi_{p \rightarrow q, g} \phi_{p \leftarrow q, h}}
$$
No closed form solution for $\alpha$, so we use a Newton-Raphson algorithm to find maximum:

$$\alpha^{(t+1)} = \alpha^{(t)} - (H_\alpha(L(\alpha^{(t)})))^{-1}\nabla_\alpha L(\alpha^{(t)})$$

where $\nabla_\alpha L(\alpha^{(t)})$ is the gradient (vector of first derivatives) of the ELBO $L$ with respect to $\alpha$ and $H_\alpha(L(\alpha^{(t)}))$ is the hessian (matrix of second derivatives) of the $L$ with respect to $\alpha$:

$$\frac{\partial}{\partial \alpha_k} L = N \left[ \psi(\sum_j \alpha_j) - \psi(\alpha_k) \right] + \sum_p \left[ \psi(\gamma_{p,k}) - \psi(\sum_j \gamma_{p,j}) \right]$$

$$\frac{\partial^2}{\partial \alpha_k \partial \alpha_l} L = N \left[ \psi'(\sum_j \alpha_j) - \psi'(\alpha_k) 1_{k=l} \right]$$
“Naive” algorithm for the MMSB

1. Initialize $B^{(0)}, \alpha^{(0)}, \gamma_{1:N}^{(0)}, \Phi_{\rightarrow}, \Phi_{\leftarrow}$.

2. E-step: Find the $\gamma_{1:N}^{(j)}, \Phi_{\rightarrow}^{(j)}, \Phi_{\leftarrow}^{(j)}$ that maximizes $L(\cdot, \alpha^{(j-1)}, B^{(j-1)})$ via coordinate ascent:
   
   (i) Update $\gamma_i^{(j)}$ for $i = 1, \ldots, N$
   
   (ii) Update $\phi_{p\rightarrow q}, \phi_{p\leftarrow q}$ for all $p, q$
   
   (iii) Until convergence

3. M-step: Update $B^{(j)}, \alpha^{(j)}$.

4. Until convergence.
“Nested” algorithm for the MMSB

1. Initialize $B^{(0)}$, $\alpha^{(0)}$, $\gamma^{(0)}_{1:N}$, $\Phi^{(0)}_\rightarrow$, $\Phi^{(0)}_\leftarrow$.
2. E-step:
   (a) for each $p, q$:
      (i) Update $\phi_{p \rightarrow q}$, $\phi_{p \leftarrow q}$ for all $p, q$
      (ii) Update $\gamma_p$, $\gamma_q$
      (iii) Update $B$.
   (b) Until convergence
3. M-step: Update $\alpha^{(j)}$.
4. Until convergence.
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Conclusion and next steps

- Variational inference: approximate the posterior with an easier closed-form posterior; make the approximation as good as possible
- Pros: scales very well, get an exact posterior rather than samples. Cons: Posterior is approximate, and we don’t know how good (or bad) the approximation is.
- Next steps: apply to data, simulations
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The authors introduce a sparsity parameter $\rho$

Instead of $Y(p, q) \sim z^T_{p \rightarrow q} B z_{p \leftarrow q}$, set $Y(p, q) \sim z^T_{p \rightarrow q} (1 - \rho) B z_{p \leftarrow q}$.

Identifiability?