

Course project

”Optimization approaches to community detection”

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3.1 Semidefinite relaxations

3.2 Natural conjugate gradients method

It is assumed, that latent group labels Z has a multinomial distribution with parameter π and each element of A has a Bernoulli distribution with parameter θ_{ij} :

$$Z_i \sim \text{Poly}(\pi), \quad \pi^T = (\pi_1, \dots, \pi_k), \\ a_{ij} \sim \text{Bernoulli}(P_{Z(i)Z(j)}), \quad i, j = \overline{1, n},$$

A Bayesian approach is used to estimate the most probable configuration of Z given an adjacency matrix A

$$Z^* = \arg \max_Z p(Z|A) = \arg \max_Z \iint p(Z, \pi, P|A) d\pi dP \quad (3.2.1)$$

It treats parameters π and θ_{ij} as random variables with following prior distributions

$$\pi \sim \text{Dirichlet}(\alpha) \\ P_{ii} \sim \text{Beta}(\beta), \quad i = \overline{1, k},$$

where α and β are predefined hyperparameters and P_{ij} , $i \neq j$ are set to equal to a small constant ε . Furthermore, to tackle the intractable integration in 3.2.1 a restriction on the family of factorized distributions is considered

$$\mathcal{Q} = \{q : q(Z, \pi, P) = q(\pi)q(P) \prod_i q(Z_i)\},$$

where

$$q(Z_i) : Z_i \sim \text{Poly}(\tilde{\pi}) \\ q(\pi) : \pi \sim \text{Dirichlet}(\tilde{\alpha}) \\ q(P) : P_{ii} \sim \text{Beta}(\tilde{\beta}_i)$$

The optimal distribution $q^* \in \mathcal{Q}$, that approximates the true posterior $p(Z, \pi, P|A)$ minimizes the Kullback-Leibler divergence

$$q^* = \arg \min_{q \in \mathcal{Q}} \text{KL}(q \| p(Z, \pi, P|X)) \quad (3.2.2)$$

Define

$$\mathcal{L}(q) = \sum_Z \iint q(Z, \pi, P) \log \frac{p(A, Z, \pi, P)}{q(Z, \pi, P)} d\pi dP \quad (3.2.3)$$

Since

$$\mathcal{L}(q) + \text{KL}(q \| p(Z, \pi, P|X)) = \log p(A)$$

the minimization problem 3.2.2 can be equivalently solved by maximizing $\mathcal{L}(q)$

$$q^* = \arg \max_{q \in \mathcal{Q}} \mathcal{L}(q) \quad (3.2.4)$$

Denote $\tilde{\Pi} = \|\tilde{\pi}_{ij}\|$, $i = \overline{1, n}$, $j = \overline{1, k}$. Given $\tilde{\Pi}$ values of parameters, that maximize $\mathcal{L}(q)$ can be found according to formulas

$$\begin{aligned} \tilde{\alpha} &= \alpha + \tilde{\Pi}^T \mathbf{1} \\ \tilde{\beta}_i &= \beta + \frac{1}{2} \left(\tilde{\Pi}_i^T A \tilde{\Pi}_i, \tilde{\Pi}_i^T \bar{A} \tilde{\Pi}_i \right)^T, \quad i = \overline{1, k}, \end{aligned} \quad (3.2.5)$$

where $\mathbf{1}$ denotes an all-ones vector, $\bar{A} = \mathbf{1}\mathbf{1}^T - I - A$, and $\tilde{\Pi}_i$ stands for the i -th column of the matrix $\tilde{\Pi}$. A corresponding value of log-likelihood is equal to

$$\mathcal{L}(\tilde{\Pi}) = \sum_{i < j} \tilde{\Pi}_i^T A \tilde{\Pi}_j \log \varepsilon + \tilde{\Pi}_i^T \bar{A} \tilde{\Pi}_j \log(1 - \varepsilon) - \sum_{i,j} \tilde{\pi}_{ij} \log \tilde{\pi}_{ij} + \log \frac{\mathcal{B}(\tilde{\alpha})}{\mathcal{B}(\alpha)} + \sum_i \log \frac{\mathcal{B}(\tilde{\beta})}{\mathcal{B}(\beta)}, \quad (3.2.6)$$

where $\tilde{\alpha} = \tilde{\alpha}(\tilde{\Pi})$ and $\tilde{\beta} = \tilde{\beta}(\tilde{\Pi})$ can be found from 3.2.5, $\mathcal{B}(\alpha) \triangleq \frac{\Gamma(\sum_i \alpha_i)}{\prod_i \Gamma(\alpha_i)}$ and Γ is gamma-function. Now the maximization problem 3.2.4 can be reformulated as follows

$$\begin{cases} \mathcal{L}(\tilde{\Pi}) \longrightarrow \max \\ \sum_j \tilde{\pi}_{ij} = 1, \quad i = \overline{1, n} \end{cases} \quad (3.2.7)$$

One can use reparametrization

$$\begin{aligned} \tilde{\pi}_{ij} &= e^{\theta_{ij} - \mathcal{A}_i}, \quad i = \overline{1, n}, j = \overline{1, k-1}, \\ \tilde{\pi}_{ik} &= e^{-\mathcal{A}_i}, \quad i = \overline{1, n}, \\ \mathcal{A}_i &= \log \left(1 + \sum_{j=1}^{k-1} e^{\theta_{ij}} \right), \quad i = \overline{1, n} \end{aligned} \quad (3.2.8)$$

and obtain a problem of unconstrained maximization

$$\mathcal{L}(\theta) \longrightarrow \max \quad (3.2.9)$$

The problem 3.2.9 can be solved via natural conjugate gradient method. Namely, given an initial value $\theta^{(0)}$, one iteratively finds optimal value of θ as follows

$$\theta^{(t+1)} = \theta^{(t)} + \lambda^{(t)} d^{(t)}, \quad t = 0, 1, 2, \dots$$

Here $d^{(t)}$ is so called natural conjugate gradient. $d^{(t)}$ can be found according to formulas

$$d^{(t)} = \begin{cases} g^{(t)}, & t = 0 \\ g^{(t)} + \frac{\|g^{(t)}\|_\theta^2}{\|g^{(t-1)}\|_\theta^2} d^{(t-1)}, & t > 0, \end{cases} \quad (3.2.10)$$

where $g^{(t)}$ is a natural gradient of $\mathcal{L}(\theta)$. $\|\cdot\|_\theta$ stands for the norm with respect to Riemannian metrics

$$G(\theta) = \text{diag}(\mathcal{I}(\theta_1), \dots, \mathcal{I}(\theta_N)),$$

where $\theta_i = (\theta_{i1}, \dots, \theta_{ik})^T$, $i = \overline{1, n}$ and (θ_i) is a Fischer information. This method is nothing else but a conjugate gradient method in a Riemannian space with metrics $G(\theta)$. Given θ , g and $\|g\|_\theta$ can be found as follows

$$\begin{aligned} g = \nabla_{\tilde{\Pi}} \mathcal{L}(\tilde{\Pi}) &= \begin{pmatrix} (I, -1) \nabla_{\tilde{\pi}_1} \mathcal{L}(\tilde{\Pi}) \\ \vdots \\ (I, -1) \nabla_{\tilde{\pi}_n} \mathcal{L}(\tilde{\Pi}) \end{pmatrix} \\ \|g\|_\theta^2 &= \sum_{i=1}^n \left(\nabla_{\tilde{\pi}_1} \mathcal{L}(\tilde{\Pi}) \right)^T \left(\text{diag}(\tilde{\pi}_i) - \tilde{\pi}_i^T \tilde{\pi}_i \right) \left(\nabla_{\tilde{\pi}_1} \mathcal{L}(\tilde{\Pi}) \right), \end{aligned} \quad (3.2.11)$$

where $\tilde{\Pi} = \tilde{\Pi}(\theta)$ and

$$\begin{aligned} \frac{\partial \mathcal{L}(\tilde{\Pi})}{\partial \pi_{ij}} &= \sum_{l \neq j} \left(A_{i \cdot \tilde{\Pi} \cdot l} \log \varepsilon + \bar{A}_{i \cdot \tilde{\Pi} \cdot j} \log(1 - \varepsilon) \right) + \\ &\quad \left(A_{i \cdot \tilde{\Pi} \cdot j}, \bar{A}_{i \cdot \tilde{\Pi} \cdot j} \right) \nabla \log \mathcal{B}(\tilde{\beta}_j) + \psi(\tilde{\alpha}_j) - \log \tilde{\pi}_{ij} - 1, \end{aligned} \quad (3.2.12)$$

where $\psi(\cdot)$ is digamma function.

The final algorithm is given in 1.

Algorithm 1: Natural Conjugate Gradient

Input: adjacency matrix A , maximum number of clusters k , tolerance η , maximum number of iterations t_{\max}

Output: array of predicted labels Z

Initialize θ ;

$\mathcal{L}_{old} \leftarrow -\infty$;

$\lambda \leftarrow 1$;

for t *in range* (t_{\max}) **do**

 Calculate $\tilde{\Pi}$ using 3.2.8;

 Calculate $\tilde{\alpha}, \tilde{\beta}$ using 3.2.5;

 Calculate \mathcal{L} using 3.2.6;

if $0 \leq \frac{\mathcal{L} - \mathcal{L}_{old}}{|\mathcal{L}|} < \eta$ **then**

break

if $\eta \geq 0$ **then**

 Update d using 3.2.10, 3.2.11, 3.2.12;

$\theta_{old} \leftarrow \theta$

$\theta \leftarrow \theta_{old} + \lambda d$;

$\mathcal{L}_{old} \leftarrow \mathcal{L}$;

else

$\lambda \leftarrow \frac{\lambda}{2}$

$\theta \leftarrow \theta_{old} + \lambda|\eta|d$

end

end

$Z = \left(\arg \max_{1 \leq j \leq k} \tilde{\pi}_{1j}, \dots, \arg \max_{1 \leq j \leq k} \tilde{\pi}_{nj} \right)$

return Z

Initial value of θ was generated from a standart normal distribution $\mathcal{N}(0, 1)$. Probability of occurence an inter-cluster edge ε was set to 10^{-10} . The maximal number of iterations and relative tolerance were taken equal to 100 and 10^{-6} respectively. Examples of performance of the natural conjugate gradient method can be found, for example, in [1].

3.3 Modularity-based methods

3.4 Spectral method

4 Data

5 Experimental results

6 Work split

7 References

References

- [1] A fast inference algorithm for stochastic blockmodel, Zhiqiang Xu, Yiping Ke, Yi Wang, 2014.