Adaptation to unknown number of clusters

Chanwoo Lee
April 19, 2021

1 Estimation for the number of clusters

When the generating model is from α-smooth probability tensor, we do not have the true number of group k. In this case, we can easily pick $k = \lfloor n^{\frac{m}{m+2\alpha}} \rfloor$ which guarantees the convergence rate $\mathcal{O}(n^{\frac{-2m\alpha}{m+2\alpha}} + \log n/n)$. If we take nonparametric histogram perspective and consider k as bandwidth, we do not need to estimate k but set optimal $k = \lfloor n^{\frac{m}{m+2\alpha}} \rfloor$.

However, when we believe that the probability tensor has block structure, there is true k so we need to set k for the estimation. Under the stochastic block model assumption, we take a variation of a 2-folded cross validation approach. To be specific, we split the observed entries into two half with probability 1/2 and use one for the training data set and the other for the test dataset. Let Ω_1 be the training set and Ω_2 be the test set from Bernoulli(1/2) sampling. Define the training tensor $\mathcal{A}^{(1)}$ and $\mathcal{A}^{(2)}$ such that,

$$\mathcal{A}^{(1)}_\omega = \begin{cases} \mathcal{A}_\omega & \text{if } \omega \in \Omega_1, \\ 0 & \text{if } \omega \in \Omega_2. \end{cases} \quad \text{and} \quad \mathcal{A}^{(2)}_\omega = \begin{cases} 0 & \text{if } \omega \in \Omega_1, \\ \mathcal{A}_\omega & \text{if } \omega \in \Omega_2. \end{cases}$$

For many different $k \in [n]$, we calculate

$$\hat{\Theta}^{(i)}_k = \operatorname*{arg\,min}_{\Theta \in \text{cut}(\mathcal{P}_k)} \|\mathcal{A}^{(i)} - \Theta\|_F^2,$$

for $i = 1, 2$. We select the parameter which minimizes the MSE error on the test dataset

$$k_i = \operatorname*{arg\,min}_{k \in [n]} \sum_{\omega \in \Omega_i^c} |\mathcal{A}_\omega - (\hat{\Theta}^{(i)}_k)_\omega|^2, \text{ for } i = 1, 2. \tag{1}$$

The final estimation is given by

$$\hat{\Theta}_{\hat{k}} = \begin{cases} (\hat{\Theta}^{(2)}_{k_2})_\omega & \text{if } \omega \in \Omega_1, \\ (\hat{\Theta}^{(1)}_{k_1})_\omega & \text{if } \omega \in \Omega_2. \end{cases} \tag{2}$$

Remark 1. The above adaptation is based on Gao et al. [2016] and different from regular cross validation approach. My previous thought was to use

$$\hat{\Theta}_{\hat{k}} = \operatorname*{arg\,min}_{\Theta \in \text{cut}(\mathcal{P}_k)} \|\mathcal{A} - \Theta\|_F^2, \tag{3}$$

—> hat k

where hat k is obtained by (1) with objective replaced by sum_{i=1,2}\sum_{omega…}….

which is regular hyperparameter setting based on cross validation.

We can show that the convergence rate of the estimator (2) is the same as $\hat{\Theta}_k$ where k is the true number of group.

Theorem 1.1 (Stochastic block model with adaptation of the number of group k)**.** Let $\hat{\Theta}_{\hat{k}}$ be the estimator from (2). Suppose true probability tensor $\Theta \in \text{cut}(\mathcal{P}_k)$ for fixed block size k Then, there exists two constants $C_1, C_2, C_3 > 0$, such that

$$\frac{1}{n^m}\|\hat{\Theta}_{\hat{k}} - \Theta^{\text{true}}\|_F^2 \leq \frac{C_1}{\rho}\left(\left(\frac{k}{n}\right)^m + \frac{\log k}{n^{m-1}} + \left(\frac{\log n}{\rho}\right)^2\right),$$

with probability at least $1 - \exp\left(-C_2(n \log k + k^m)\right) - (n^m)^{-C_3}$.

Proof. From theorem with known k case, we have

$$\frac{1}{n^m}\|\hat{\Theta}_k - \Theta^{\text{true}}\|_F^2 \le \frac{C_1}{\rho}\left(\left(\frac{k}{n}\right)^m + \frac{\log k}{n^{m-1}}\right), \tag{4}$$

with probability at least $1 - \exp\left(-C_2(n \log k + k^m)\right)$. By triangular inequality,

split into Omega 1 and Omega 2

$$\|\hat{\Theta}_{\hat{k}} - \Theta^{\text{true}}\|_F^2 \le \cancel{2\underbrace{\|\hat{\Theta}_{\hat{k}} - \hat{\Theta}_k\|_F^2}_{\text{(i)}} + 2\underbrace{\|\hat{\Theta}_k - \Theta^{\text{true}}\|_F^2}_{\text{(ii)}}}. \tag{5}$$

estimation error within Omega 1: reproduce the same proof as in (4). Same within Omega 2

Since we have the error bound (ii) as in (4), we find the upper bound of the error (i). Based on definition of $\hat{\Theta}_{\hat{k}}$, we have the following inequality,

$$\|\hat{\Theta}_{\hat{k}} - \hat{\Theta}_k\|_{\Omega_2}^2 \le 2\left\langle \hat{\Theta}^{(1)}_{k_1} - \hat{\Theta}_k, \frac{\mathcal{A} - \rho\hat{\Theta}_k}{\rho}\right\rangle_{\Omega_2}$$

the red inequality does not hold. Holds if yellow term is replaced by ground truth (no randomness)

replace all yellow terms by Theta_true

$$= 2\left(\left\langle \hat{\Theta}^{(1)}_{k_1} - \hat{\Theta}_k, \frac{\mathcal{A} - \rho\Theta^{\text{true}}}{\rho}\right\rangle_{\Omega_2} + \cancel{\langle \hat{\Theta}^{(1)}_{k_1} - \hat{\Theta}_k, \Theta^{\text{true}} - \hat{\Theta}_k\rangle_{\Omega_2}}\right)$$

$$\le 2\|\hat{\Theta}^{(1)}_{k_1} - \hat{\Theta}_k\|_{\Omega_2}\left(\left\langle \frac{\hat{\Theta}^{(1)}_{k_1} - \hat{\Theta}_k}{\|\hat{\Theta}^{(1)}_{k_1} - \hat{\Theta}_k\|_{\Omega_2}}, \frac{\mathcal{A} - \rho\Theta^{\text{true}}}{\rho}\right\rangle_{\Omega_2} \cancel{+ \|\Theta^{\text{true}} - \hat{\Theta}_k\|_{\Omega_2}}\right).$$

Left term in the inner product: randomness comes from Omega 1 Right term: randomness comes from Omega 2

It suffices to bound the inner product term because of (4). I haven't figure out how to derive this inner product part.

$$\max_{k_1 \in [n]}\left\langle \frac{\hat{\Theta}^{(1)}_{k_1} - \hat{\Theta}_k}{\|\hat{\Theta}^{(1)}_{k_1} - \hat{\Theta}_k\|_{\Omega_2}}, \frac{\mathcal{A} - \rho\Theta^{\text{true}}}{\rho}\right\rangle_{\Omega_2} \le C\frac{\log n}{\rho},$$

inner product of <x,y>, where x and y are mutually independent random variables.

with probability at least $1 - (n^m)^{-C'}$ for some universal constants $C, C' > 0$. Assuming we proved this bound, we have

$$\|\hat{\Theta}_{\hat{k}} - \hat{\Theta}_k\|_{\Omega_2}^2 \le C_1\left(\|\Theta^{\text{true}} - \hat{\Theta}_k\|_{\Omega_2}^2 + \left(\frac{\log n}{\rho}\right)^2\right),$$

for some constant $C_1 > 0$. A symmetric argument leads to,

$$\|\hat{\Theta}_{\hat{k}} - \hat{\Theta}_k\|_{\Omega_1}^2 \le C_2\left(\|\Theta^{\text{true}} - \hat{\Theta}_k\|_{\Omega_1}^2 + \left(\frac{\log n}{\rho}\right)^2\right),$$

for some constant $C_2 > 0$.

Summing up the above two inequalities, we have

$$\text{(i)} \le C\left(\|\Theta^{\text{true}} - \hat{\Theta}_k\|_{\text{F}}^2 + \left(\frac{\log n}{\rho}\right)^2\right).$$

Plugging the above inequality in (5) completes the proof. □

2 Simulation results

Gao et al. [2016] does not estimate the number of clusters in unknown k but suggested new estimation method. Instead, I estimated k in the simulation by following procedure. First, I calculate $\mathcal{A}^{\text{test}}$ as

$$\mathcal{A}_\omega^{\text{test}} = \begin{cases} \mathcal{A}_\omega & \text{if } \omega \in \Omega_1, \\ 0 & \text{if } \omega \in \Omega_2. \end{cases}$$

For many different $k \in [n]$, we calculate

missing superscript “test”?

$$\hat{\Theta}_k = \underset{\Theta \in \text{cut}(\mathcal{P}_k)}{\arg\min} \|\mathcal{A}^{\text{test}} - \Theta\|_F^2,$$

Based on a series of $\hat{\Theta}_k$, I estimate $\hat{k} = k_1$ such that

$$\hat{k} = \underset{k \in [n]}{\arg\min} \sum_{\omega \in \Omega_2} |\mathcal{A}_\omega - (\hat{\Theta}_k^{\text{test}})_\omega|^2.$$

Gao et al has a simulation in table 1, page 13.

Remark 2. This procedure is to calculate k_1 in (1). I have not calculated the adaptive estimation of Gao et al. [2016]'s paper. I will compare (2) and (3) later and update the note.

Ground truth of the model is smooth symmetric Θ with $k \in \{5, 10, 15, 20\}$ and $n \in \{50, 100, 150, 200\}$. Table 1 summarizes the estimated number of clusters for different true k and the number of nodes. It seems that the estimated number of cluster quite close to true one when $n > 50$. Figure 1 shows the MSE according to the number of clusters as an input of the algorithm across different ground truth settings.

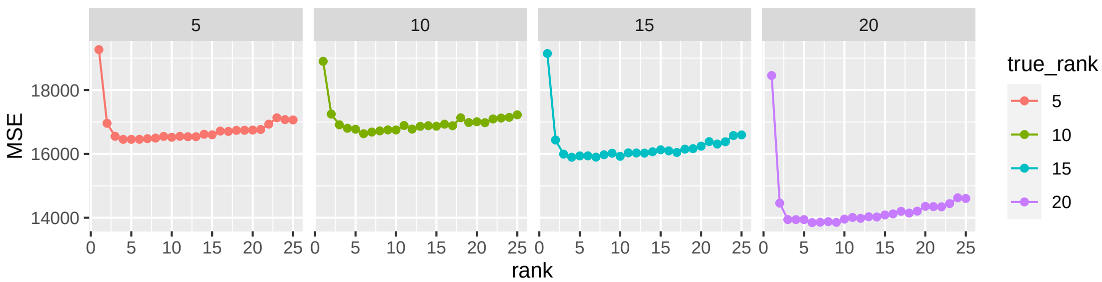
True # of clusters	5	10	15	20
node 50	4	6	4	6
node 100	5	10	14	9
node 150	5	9	12	16
node 200	5	9	9	15

Table 1: Estimation for the number of clusters according to the number of nodes and true clusters.

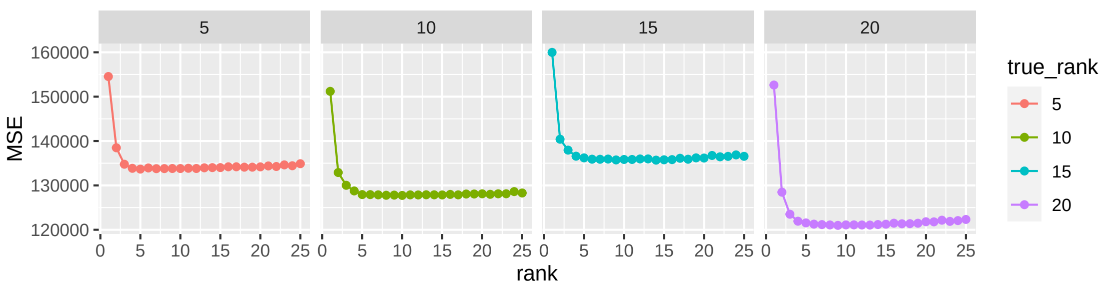
References

Chao Gao, Yu Lu, Zongming Ma, and Harrison H Zhou. Optimal estimation and completion of matrices with biclustering structures. *The Journal of Machine Learning Research*, 17(1):5602–5630, 2016.

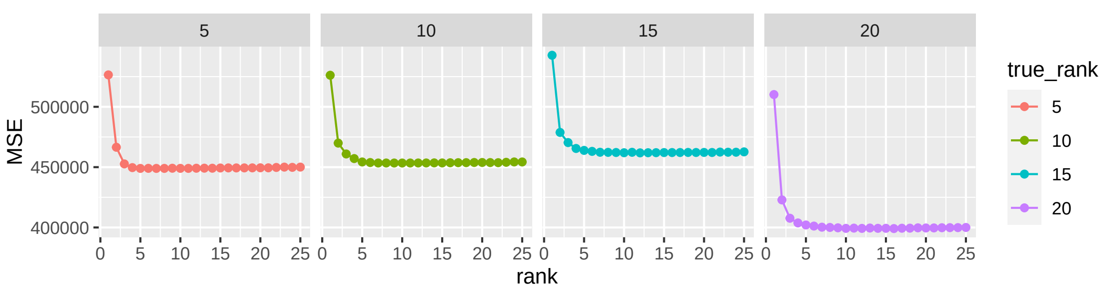
Is the MSE in y-axis testing error or estimation error?



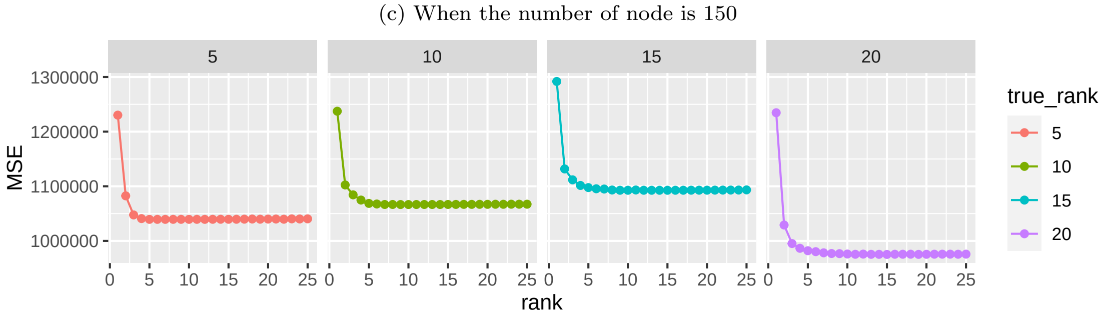
(a) When the number of node is 50



(b) When the number of node is 100.



(c) When the number of node is 150



(d) When the number of node is 200

Figure 1: MSE errors on the test set with different input for the number of clusters given the number of node and true clusters.