Graphic Lasso: Self-Consistency

Jiaxin Hu

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1 Noiseless case

Consider the noiseless case

$$\mathcal{Y} = f(\Theta)$$
.

where $\Theta = \mathcal{C} \times_1 M_1 \times_2 \cdots \times_K M_K$, and $f(\cdot)$ is an entry-wise link function. Suppose we have the following optimization problem.

$$\max_{\Theta = \mathcal{C} \times_1 \mathbf{M}_1 \times_2 \dots \times_K \mathbf{M}_K} \mathcal{L}_{\mathcal{Y}}(\Theta) = \langle \mathcal{Y}, \Theta \rangle - \sum_{i_1, \dots, i_K} g(\Theta_{i_1, \dots, i_K}). \tag{1}$$

Lemma 1 (Noiseless estimation). Let $\{C, M_k\}$ denote the true parameters and $\{\hat{C}, \hat{M}_k\}$ are the estimation which maximizes the loss function. Suppose $g(\cdot)$ is a convex function with bounded second derivative $\sup_x g''(x) \leq a$, and $\max_{r_1,\ldots,r_K} |(g')^{-1}(f(c_{r_1,\ldots,r_K}))| \leq C$, where C is a positive constant depends on C. Assume the minimal gap between blocks is strictly larger than 0, i.e., $\delta > 0$. Then, for any $\epsilon > 0$, we have

$$\mathbb{P}(MCR(\hat{\boldsymbol{M}}_k, \boldsymbol{M}_k) \ge \epsilon) = 0.$$

Proof. We prove the accuracy in following steps.

1. With given membership matrix \hat{M}_k , the estimate \hat{C} is

$$\hat{c}_{r_1,...,r_K}(\hat{M}_k) = (g')^{-1} \left(\frac{1}{\prod_k d_k \prod_k \hat{p}_{r_k}^{(k)}} [f(\mathcal{C}) \times_1 \mathbf{M}_1 \hat{\mathbf{M}}_1^T \times_2 \cdots \times_K \mathbf{M}_K \mathbf{M}_K^T]_{r_1,...,r_K} \right).$$

Note that the estimation $\hat{\mathcal{C}}$ depends on \hat{M}_k . Therefore, we denote the estimation as $\hat{\mathcal{C}}(\hat{M}_k) = [\hat{c}_{r_1,...,r_K}(\hat{M}_k)]$.

2. We define some useful functions. First, we define

$$F(\hat{\pmb{M}}_k) = \mathcal{L}_{\mathcal{Y}}(\hat{\mathcal{C}}(\hat{\pmb{M}}_k), \hat{\pmb{M}}_k) = \sum_{r_1, \dots, r_K} \prod_k d_k \prod_k \hat{p}_{r_k}^{(k)} h(g'(\hat{c}_{r_1, \dots, r_K}(\hat{\pmb{M}}_k))),$$

where
$$h(x) = x(g')^{-1}(x) - g((g')^{-1}(x))$$
.

Note that $\hat{\mathcal{C}}(\hat{M}_k)$ does not include the randomness. Thus, we have $g'(\hat{c}_{r_1,\dots,r_K}(\hat{M}_k)) = \mathbb{E}\left[g'(\hat{c}_{r_1,\dots,r_K}(\hat{M}_k))\right]$, and

$$G(\hat{\boldsymbol{M}}_k) = \sum_{r_1,\dots,r_K} \prod_k d_k \prod_k \hat{p}_{r_k}^{(k)} h(\mathbb{E}\left[g'(\hat{c}_{r_1,\dots,r_K}(\hat{\boldsymbol{M}}_k))\right]) = F(\hat{\boldsymbol{M}}_k),$$

which implies that there does not exist the estimation error.

Note that for true membership, we have

$$F(\mathbf{M}_k) = G(\mathbf{M}_k) = \mathcal{L}_{\mathcal{Y}}(\hat{\mathcal{C}}(\mathbf{M}_k), \mathbf{M}_k),$$

where $\hat{\mathcal{C}}(M_k) = (g')^{-1}(f(\mathcal{C}))$ is not equal to the true core tensor \mathcal{C} .

3. We only need to consider the classification error. Under the assumptions of the positive minimal gap and the boundedness of the second derivative of g, when $MCR(\hat{M}_k, M_k) \geq \epsilon$ for any $\epsilon > 0$, we have

$$G(\hat{M}_k) - G(M_k) \le -\frac{\epsilon}{4a} \tau^{K-1} \delta.$$

4. Since $\{\hat{\mathcal{C}}\hat{M}_k, \hat{M}_k\}$ is the maximizer of the loss function, we have

$$0 \le F(\hat{\mathbf{M}}_k) - F(\mathbf{M}_k) = G(\hat{\mathbf{M}}_k) - G(\mathbf{M}_k).$$

Therefore, we obtain that

$$\mathbb{P}(MCR(\hat{\boldsymbol{M}}_k, \boldsymbol{M}_k) \ge \epsilon) = \mathbb{P}(G(\hat{\boldsymbol{M}}_k) - G(\boldsymbol{M}_k) \le -\frac{\epsilon}{4a}\tau^{K-1}\delta) = 0.$$

Remark 1. The lemma 1 implies that the true membership M_k is the maximizer of the function $G(M_k')$. Due to the noiselessness, $G(M_k') = \mathcal{L}_{\mathcal{Y}}(\hat{\mathcal{C}}(M_k'), M_k')$, and $\{\hat{\mathcal{C}}(M_k), M_k\}$ is the maximizer of the noiseless loss function. However, the true parameter $\{\mathcal{C}, M_k\}$ is not the maximizer of the noiseless loss function, since $\hat{\mathcal{C}}(M_k) \neq \mathcal{C}$. Therefore, we conclude that the loss function (1) is self-consistent to $\{\hat{\mathcal{C}}(M_k), M_k\}$ but not self-consistent to Θ .

Remark 2. Define

$$\hat{\Theta} = \hat{\mathcal{C}}(\mathbf{M}_k) \times_1 \mathbf{M}_1 \times_1 \cdots \times_K \mathbf{M}_K.$$

Then, $\hat{\Theta}$ is an unbiased estimate of Θ if and only if g' = f.

Remark 3. Which assumption in the noisy case corresponds to the self-consistency of M_k ?

Note that in the noisy case, we have

$$\begin{split} G_{noise}(\hat{\boldsymbol{M}}_{k}) &= \sum_{r_{1}, \dots, r_{K}} \prod_{k} d_{k} \prod_{k} \hat{p}_{r_{k}}^{(k)} h(\mathbb{E}\left[g'(\hat{c}_{r_{1}, \dots, r_{K}}(\hat{\boldsymbol{M}}_{k}))\right]) \\ &= \langle f(\mathcal{C}) \times_{1} \boldsymbol{M}_{1} \hat{\boldsymbol{M}}_{1}^{T} \times_{2} \dots \times_{K} \boldsymbol{M}_{K} \boldsymbol{M}_{K}^{T}, (g')^{-1} \left[f(\mathcal{C}) \times_{1} \boldsymbol{M}_{1} \hat{\boldsymbol{M}}_{1}^{T} \times_{2} \dots \times_{K} \boldsymbol{M}_{K} \boldsymbol{M}_{K}^{T}\right] \rangle \\ &- \sum_{i_{1}, \dots, i_{K}} g\left((g')^{-1} \left[f(\mathcal{C}) \times_{1} \boldsymbol{M}_{1} \hat{\boldsymbol{M}}_{1}^{T} \times_{2} \dots \times_{K} \boldsymbol{M}_{K} \boldsymbol{M}_{K}^{T}\right] \times_{1} \boldsymbol{M}_{1} \times_{2} \dots \times_{K} \boldsymbol{M}_{K}\right)_{i_{1}, \dots, i_{K}} \end{split}$$

$$= F_{noiseless}(\hat{M}_k).$$

Therefore, we use the self-consistency when we derive the misclassification error. Note that the result that when $MCR(\hat{M}_k, M_k) \geq \epsilon$,

$$G_{noise}(\hat{\mathbf{M}}_k) - G_{noise}(\mathbf{M}_k) \le -\frac{\epsilon}{4a} \tau^{K-1} \delta$$
 (2)

implies the self-consistency of M_k . To obtain the result (2), we require

- 1. the convexity of g and $\sup_x g''(x) \ge a$;
- 2. minimal gap strictly larger than 0, i.e., $\delta > 0$.

2 General loss function

Consider the model

$$\mathbb{E}[\mathcal{Y}] = f(\Theta), \text{ where } \Theta = \mathcal{C} \times_1 \mathbf{M}_1 \times_2 \cdots \times_K \mathbf{M}_K.$$

Theorem 2.1 (General property for loss function to guarantee the clustering accuracy). Let $\{C, M_k\}$ denote the true parameters, and $\mathcal{L}_{\mathcal{Y}}(C', M_k')$ denote the sample-based loss function. Define the sample-based loss function with respect to M_k' as

$$F(\mathbf{M}_k') = \mathcal{L}_{\mathcal{Y}}(\hat{\mathcal{C}}(\mathbf{M}_k'), \mathbf{M}_k'),$$

where

$$\hat{\mathcal{C}}(M'_k) = \underset{\mathcal{C}}{\operatorname{arg max}} \mathcal{L}_{\mathcal{Y}}(\mathcal{C}, M'_k).$$

Correspondingly, define the population-based loss function with respect to M'_k as

$$G(\mathbf{M}'_k) = l(\tilde{\mathcal{C}}(\mathbf{M}'_k), \mathbf{M}'_k),$$

where

$$l(\mathcal{C}, \mathbf{M}_k) = \mathbb{E}_{\mathcal{Y}}[\mathcal{L}_{\mathcal{Y}}(\mathcal{C}, \mathbf{M}_k)], \quad and \quad \tilde{\mathcal{C}}(\mathbf{M}_k') = \operatorname*{arg\,max}_{\mathcal{C}} l(\mathcal{C}, \mathbf{M}_k').$$

Suppose the loss function satisfies the following properties

1. (Self-consistency to M_k) Suppose $MCR(M'_k, M_k) \ge \epsilon$ for $\epsilon > 0$. We have

$$G(\mathbf{M}_k') - G(\mathbf{M}_k) \le -C(\epsilon),\tag{3}$$

where $C(\cdot)$ takes positive values.

2. (Bounded difference between sample- and population-based loss) The difference between sample-based and population-based loss function is bounded in probability, i.e.,

$$p(t) = \mathbb{P}(|F(\mathbf{M}_k') - G(\mathbf{M}_k')| \ge t) \to 0, \quad as \quad t \to \infty.$$
(4)

Let $\{\hat{M}_k\}$ be the maximizer of $F(M_k)$. Then, we have the following clustering accuracy, for any $\epsilon > 0$,

$$\mathbb{P}(MCR(\hat{\boldsymbol{M}}_k, \boldsymbol{M}_k) \ge \epsilon) \le p\left(\frac{C(\epsilon)}{2}\right).$$

Proof. Since $\{\hat{\mathcal{C}}, \hat{M}_k\}$ is the maximizer of the population-based objective function $\mathcal{L}_{\mathcal{Y}}$, we have

$$0 \le F(\hat{\mathbf{M}}_k) - F(\mathbf{M}_k)$$

= $F(\hat{\mathbf{M}}_k) - G(\hat{\mathbf{M}}_k) + G(\hat{\mathbf{M}}_k) - G(\mathbf{M}_k) + G(\mathbf{M}_k) - F(\mathbf{M}_k)$.

Suppose $MCR(\hat{M}_k, M_k) \geq \epsilon$. By the property (3), we have

$$0 \le 2r - C(\epsilon),$$

where $r = \sup_{M'_k} |F(M'_k) - G(M'_k)|$. Therefore, we have

$$\mathbb{P}(MCR(\hat{\boldsymbol{M}}_k, \boldsymbol{M}_k) \ge \epsilon) = \mathbb{P}(G(\boldsymbol{M}_k') - G(\boldsymbol{M}_k) \le -C(\epsilon))$$

$$\le \mathbb{P}(C(\epsilon) \le 2r)$$

$$= p\left(\frac{C(\epsilon)}{2}\right),$$

where the last equation follows the second property (4).

Remark 4. For the model in Tensor Block model, we have

$$C(\epsilon) = \frac{\epsilon}{4a} \tau^{K-1} \delta,$$

where a is the upper bound of g''(x), τ is minimal proportion of the cluster, and δ is the minimal gap between blocks. By the sub-Gaussianity of \mathcal{Y} and Hoeffding's inequality, we have

$$\begin{aligned} p(t) &\leq \mathbb{P}(C_1 \left\| g'(\hat{c}_{r_1,\dots,r_K}) - \mathbb{E}[g'(\hat{c}_{r_1,\dots,r_K})] \right\|_{\max} \geq t) \\ &\leq \mathbb{P}\left(\sup_{I_{r_1,\dots,r_K}} \frac{\left| \sum_{(i_1,\dots,i_K) \in I_{r_1,\dots,r_K}} \mathcal{Y}_{i_1,\dots,i_K} - \mathbb{E}[\mathcal{Y}_{i_1,\dots,i_K}] \right|}{|I_{r_1,\dots,r_K}|} \geq \frac{t}{C_1} \right) \\ &\leq 2^{1+\sum_k d_k} \exp\left(-\frac{t^2 L}{C_1^2} \right), \end{aligned}$$

where C_1 is a positive constant related to the true core tensor \mathcal{C} , I_{r_1,\dots,r_K} is the index set of the block (r_1,\dots,r_K) based on the estimate membership \hat{M}_k , and $L=\inf|I_{r_1,\dots,r_K}|\geq \tau^K\prod_k d_k$.

Remark 5. When $\tilde{\mathcal{C}}(M_k) = \mathcal{C}$, i.e., g' = f in the tensor block model, the self-consistency to M_k implies the self-consistency to $\{\mathcal{C}, M_k\}$ or $\Theta = \mathcal{C} \times_1 M_1 \times_2 \cdots \times_K M_K$.

3 Precision matrix model

The precision model is stated as

$$\mathbb{E}[S^k] = \Omega^k = \sum_{l=1}^r u_{kl} \Theta^l, \quad k \in [K].$$

Without the sparsity penalty, we consider the optimization problem

$$\max_{\boldsymbol{U},\Theta^l} \mathcal{L}_S(\boldsymbol{U},\Theta^l) = -\sum_{k=1}^K \operatorname{tr}(S^k \Omega^k) + \log \det(\Omega^k),$$

where U is a membership matrix, and $\{\Theta^l\}$ are irreducible and invertible.

Proposition 1. The loss function \mathcal{L}_S satisfies the conditions for Theorem 2.1, and thus the clustering accuracy for precision matrix model is guaranteed.

Proof. First, we define the functions $F(\cdot)$ and $G(\cdot)$ in the Theorem 2.1 under the precision matrix context.

Given the membership matrix U', we want to find the estimate $\hat{\Theta}^l(U') = \arg \max_{\Theta^l} \mathcal{L}_S(U', \Theta^l)$. Note that the $\mathcal{L}_S(U', \Theta^l)$ is concave respect to Θ^l . Then, by the first order condition, we have

$$\hat{\Theta}^l = \left(\frac{\sum_{k \in I_l'} S^k}{|I_l'|}\right)^{-1},$$

where $I'_l = \{k : u_{kl} = 1\}, l \in [r]$. Thus, we obtain the function $F(U') = \mathcal{L}_S(U', \hat{\Theta}^l(U'))$, which is

$$F(\mathbf{U}') = -\sum_{l=1}^{r} |I'_l|p + |I'_l| \log \det \left(\frac{\sum_{k \in I'_l} S^k}{|I'_l|}\right)^{-1}.$$

Note that

$$l(\boldsymbol{U}', \Theta^l) = \mathbb{E}_S[\mathcal{L}_S(\boldsymbol{U}', \Theta^l)] = -\sum_{k=1}^K \operatorname{tr}(\Sigma^k \Omega^k) + \log \det(\Omega^k).$$

Therefore, we have

$$\tilde{\Theta}^l(U') = \left(\frac{\sum_{k \in I'_l} \Sigma^k}{|I'_l|}\right)^{-1},$$

and

$$G(U') = l(U', \tilde{\Theta}^l(U')) = -\sum_{l=1}^r |I'_l| p + |I'_l| \log \det \left(\frac{\sum_{a=1}^r D_{al} \sum^a}{|I'_l|}\right)^{-1},$$

where D_{al} is the elements of the confusion matrix.

Next, we verify the functions $F(\cdot)$ and $G(\cdot)$ satisfy the conditions in the Theorem 2.1. Let $\{U, \Theta^l\}$ denote the true membership and precision matrices, and \hat{U} denote the estimated U which maximizes F(U).

1. (Self-consistency to U)

Consider the subtraction

$$G(\hat{\boldsymbol{U}}) - G(\boldsymbol{U}) = -\sum_{l=1}^{r} \log \det \left(\frac{\sum_{a=1}^{r} D_{al} \Sigma^{a}}{|\hat{I}_{l}|} \right) + \sum_{l=1}^{r} \left(\frac{\sum_{a=1}^{r} D_{al} \log \det(\Sigma^{a})}{|\hat{I}_{l}|} \right).$$

Since $MCR(\hat{\boldsymbol{U}}, \boldsymbol{U}) \geq \epsilon$, there exist $l, k \neq k' \in [r]$ such that $\min\{D_{kl}, D_{k'l}\} \geq \epsilon$. Let $\tilde{\Sigma} = \frac{\sum_{a=1}^r D_{al} \Sigma^a}{|\hat{I}_l|}$. Consider the function $f(t) = \log \det(\tilde{\Sigma} + t\Delta)$, where $\Delta = \Sigma - \tilde{\Sigma}$. By Taylor Expansion, we have

$$\log \det(\Sigma) - \log \det(\tilde{\Sigma}) = f(1) - f(0) = f'(0) + \frac{f''(\xi)}{2}, \quad \text{for some} \quad \xi \in [0, 1],$$

where

$$f'(0) = \langle (\tilde{\Sigma})^{-1}, \Delta \rangle, \quad \text{and} \quad f''(\xi) = -\text{vec}(\Delta)^T (\tilde{\Sigma} + \xi \Delta)^{-1} \otimes (\tilde{\Sigma} + \xi \Delta)^{-1} \text{vec}(\Delta) \le -s \|\Delta\|_F^2,$$
(5)

where s is a positive constant which $s \leq \varphi_{\max}^{-2}(\tilde{\Sigma} + \xi \Delta)$.

Let $\Delta^l = \Sigma^l - \tilde{\Sigma}, l \in [r]$. With the Taylor Expansion (5), we have

$$\left(\frac{\sum_{a=1}^{r} D_{al} \log \det(\Sigma^{a})}{|\hat{I}_{l}|}\right) - \log \det\left(\tilde{\Sigma}\right) = \sum_{a=1}^{l} \frac{D_{al}}{|\hat{I}_{l}|} \left[\log \det(\Sigma^{a}) - \log \det(\tilde{\Sigma})\right]
\leq \sum_{a=1}^{r} \frac{D_{al}}{|\hat{I}_{l}|} \left(\langle(\tilde{\Sigma})^{-1}, \Delta^{a}\rangle - \frac{1}{2}s \|\Delta^{a}\|_{F}^{2}\right)
\leq -\frac{D_{kl}}{2|\hat{I}_{l}|}s \|\Delta^{k}\|_{F}^{2} - \frac{D_{k'l}}{2|\hat{I}_{l}|}s \|\Delta^{k'}\|_{F}^{2},$$

where the last inequality follows by the fact that $\sum_{a=1}^r \frac{D_{al}}{|\hat{I}_l|} \langle \tilde{\Sigma}, \Delta^a \rangle = 0$. By the inequality $\frac{1}{2} \|A + B\|_F^2 \leq \|A\|_F^2 + \|B\|_F^2$, we obtain that

$$\left(\frac{\sum_{a=1}^{r} D_{al} \log \det(\Sigma^{a})}{|\hat{I}_{l}|}\right) - \log \det\left(\tilde{\Sigma}\right) \leq -\frac{\min\{D_{kl}, D_{k'l}\}s}{|\hat{I}_{l}|} \left\|\Sigma^{k} - \Sigma^{k'}\right\|_{F}^{2} \leq -\frac{\epsilon}{4s|I_{l}|}\delta.$$

For other $l' \in [r]/l$, since $-\log \det(\cdot)$ is a convex function, by Jensen's inequality, we have

$$\left(\frac{\sum_{a=1}^r D_{al'} \log \det(\Sigma^a)}{|\hat{I}_{l'}|}\right) - \log \det \left(\frac{\sum_{a=1}^r D_{al'} \Sigma^a}{|\hat{I}_{l'}|}\right) \le 0.$$

Then, we have

$$G(\hat{\boldsymbol{U}}) - G(\boldsymbol{U}) \le -\frac{\epsilon}{4s}\delta,$$

which implies the self-consistency holds.

2. (Bounded difference between sample- and population-based loss)

For arbitrary U, consider the absolute subtraction

$$|F(\boldsymbol{U}) - G(\boldsymbol{U})| \le \sum_{l=1}^{r} |I_l| \left| \log \det \left(\frac{\sum_{k \in I_l} S^k}{|I_l|} \right) - \log \det \left(\mathbb{E} \left[\frac{\sum_{k \in I_l} S^k}{|I_l|} \right] \right) \right|.$$

Consider the function $f(t) = -\log \det \left(\frac{\sum_{k \in I_l} S^k}{|I_l|} + t\Delta\right)$, where $\Delta = \mathbb{E}\left[\frac{\sum_{k \in I_l} S^k}{|I_l|}\right] - \frac{\sum_{k \in I_l} S^k}{|I_l|}$.

By the previous calculation (5), we know that f(t) is a convex function. Then, the function is locally Lipschitz with $L = \sup_t |f'(t)|$. Therefore, we have

$$|F(\boldsymbol{U}) - G(\boldsymbol{U})| \leq \sum_{l=1}^{r} |I_l||f(1) - f(0)|$$

$$\leq \sum_{l=1}^{r} |I_l||f'(1)|$$

$$\leq K \sup \left| \left\langle \left(\mathbb{E} \left[\frac{\sum_{k \in I_l} S^k}{|I_l|} \right] \right)^{-1}, \frac{\sum_{k \in I_l} S^k}{|I_l|} - \mathbb{E} \left[\frac{\sum_{k \in I_l} S^k}{|I_l|} \right] \right\rangle \right|$$

$$\leq K p^2 \max_{l \in [r]} \left\| \Theta^l \right\|_{\max_{k,(i,j)}} |S_{(i,j)}^k - \mathbb{E}[S_{(i,j)}^k]|.$$

Therefore, by Lemma 2, we have

$$\begin{aligned} p(t) &= \mathbb{P}(|F(\boldsymbol{U}) - G(\boldsymbol{U})| \ge t) \\ &\leq \mathbb{P}\left(Kp^2 \max_{l \in [r]} \left\|\Theta^l\right\|_{\max k, (i, j)} |S_{(i, j)}^k - \mathbb{E}[S_{(i, j)}^k]| \ge t\right) \\ &\leq C_1 \exp\left(-C_2 \frac{\min_{k \in [K]} n_k t^2}{K^2 p^4 \max_{l \in [r]} \left\|\Theta^l\right\|_{\max}^2}\right), \end{aligned}$$

where C_1, C_2 are two constants.

Remark 6. The above proof does not consider the sparsity constrains. Recall the general tensor block model. The convexity of g and boundedness of g'' (as well as irreducibility of C) ensures the self-consistency of M_k . In precision matrix model, if we add a convex sparsity penalty $R(\Theta^l)$ (e.g. L_1, L_0 norm) to the objective function, the nonlinear term $\log \det(\Omega^k) + R(\Theta^l)$ still keeps convex, which can be considered as the function "g" in the precision matrix context. Therefore, my conjecture is that the sparsity penalty to the objective function won't affect the self-consistency to U. Meanwhile, the difference between sample- and population-based is independent with the penalty. Thus, the loss function with sparsity penalty guarantees the clustering accuracy.

Lemma 2. Let $Z_i \sim_{i.i.d.} \mathcal{N}(0, \Sigma)$ and $\varphi_{max}(\Sigma) \leq \tau < \infty$. Let $\Sigma = [\![\Sigma_{ij}]\!]$, then

$$P\left(\left|\sum_{i=1}^{n} Z_{ij} Z_{ik} - n \Sigma_{jk}\right| \ge n\nu\right) \le c_1 e^{-c_2 n\nu^2}, \quad \text{for} \quad |\nu| \le \delta,$$

where c_1, c_2, δ depends on τ only.

Proof. See Lemma 1 of Rothman et.al.