Graphic Lasso: Possible Accuracy for Multi-Layer Model

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1 Discussion about Identifiability

Suppose we have a dataset with p variables and K categories. In multi-layer model, we assume the rank of decomposition r is known, and the precision matrices are of form

$$\Omega^k = \Theta_0 + \sum_{l=1}^r u_{lk} \Theta_l, \quad \text{for} \quad k = 1, ..., K.$$
 (1)

The identifiability problem for $\{\Theta_0, \Theta_1, ..., \Theta_r, \mathbf{u}_1, ..., \mathbf{u}_r\}$ is actually an identifiability problem for tensor decomposition.

Let $\mathcal{Y} \in \mathbb{R}^{p \times p \times K}$ denote the collection of K networks, where $\mathcal{Y}[,,k] = \Omega^k, k \in [K]$. Let $\mathcal{C} \in \mathbb{R}^{p \times p \times (r+1)}$ denote the collection of "core" networks, where $\mathcal{C}[,,1] = \sqrt{K}\Theta_0$, $\mathcal{C}[,,l] = \Theta_{l-1}, l = 2, ..., (r+1)$. Let $U \in \mathbb{R}^{K \times (r+1)} = (\mathbf{u}_0, \mathbf{u}_1, ..., \mathbf{u}_r)$ denote the factor matrix, where $\mathbf{u}_0 = \mathbf{1}_K/\sqrt{K}$. Rewrite the model (1) in tensor form.

$$\mathcal{Y} = \mathcal{C} \times_3 \mathbf{U}. \tag{2}$$

Therefore, the identifiability problem for $\{\Theta_l, \mathbf{u}_l\}$ becomes the identifiability problem for $\{\mathcal{C}, \mathbf{U}\}$. Before we discuss the identifiable condition case by case, we first assume \mathcal{C} is full rank on mode 3.

1. No sparsity constrain on U.

Proposition 1. The decomposition C and U are identifiable if U is an orthonormal matrix, i.e., $U^TU = I_{r+1}$.

Proof. Let Unfold(\cdot) denote the unfold representation of a tensor on mode 3. The model (2) is equal to

$$Unfold(\mathcal{Y}) = UUnfold(\mathcal{C}).$$

By matrix SVD, we have $\operatorname{Unfold}(\mathcal{Y}) = \tilde{U}\Sigma V^T$, where \tilde{U} is an orthonormal matrix. The SVD decomposition is unique up to orthogonal rotation (ignore row permutation).

Note that $\mathbf{u}_0 = \mathbf{1}_K/\sqrt{K}$. There always has a unique orthonormal matrix \mathbf{R} such that the first column of $\tilde{\mathbf{U}}\mathbf{R}$ is equal to $\mathbf{1}_K/\sqrt{K}$. Let $\mathbf{U} = \tilde{\mathbf{U}}\mathbf{R}$ and $\mathrm{Unfold}(\mathcal{C}) = \mathbf{R}^T \Sigma \mathbf{V}$. Then, \mathbf{U} and \mathcal{C} are identifiable.

2. Membership constrain on U. (Without intercept Θ_0)

If U is a membership matrix, we are clustering K categories into r groups. Then, the model (1) becomes

$$\Omega^k = \Theta_{i_k}, \quad \text{for} \quad k = 1, ..., K,$$

where $i_k \in [r]$ is the group for the k-th category. Then, let $C \in \mathbb{R}^{p \times p \times r}$, where $C[, l] = \Theta_l, l = 1, ..., r$, and $U \in \mathbb{R}^{K \times r} = (\mathbf{u}_1, ..., \mathbf{u}_r)$.

Proposition 2. The decomposition C and U are identifiable up to permutation if U is a membership matrix, i.e., in each row of U there is only 1 copy of 1 and massive 0.

Proof. If U is a membership matrix, the model (2) is a special case of tensor block model. By Proposition 1 in Wang, the matrix U is identifiable if C is irreducible on mode 3. In our case, we assume C is full rank on mode 3, and thus $\{U, C\}$ are identifiable.

Remark 1. The sparsity of Θ_l won't affect the identifiability in these two cases under the assumption that \mathcal{C} is full rank on mode 3. In no sparsity constrain case, we only need the full rankness of Unfold(\mathcal{C}), and the sparsity on the first and second mode of \mathcal{C} does not affect the rank of Unfold(\mathcal{C}). In membership constrain, we only need the mode 3 irreducibility of \mathcal{C} .

Remark 2. The two cases above are two extreme cases. Intermediate cases include the fuzzy clustering, where $\sum_{l=1}^{r} u_{lk} = 1, k \in [K]$, and the sparsity constrain for the column, where $|\mathbf{u}_l|_0 < a, l \in [r]$.

2 A simple extension

Let $Q^k(\Omega) = \operatorname{tr}(S^k\Omega) - \log |\Omega|$. Assume the rank of decomposition r is known. Consider the constrained optimization problem

$$\min_{\mathcal{C}} \sum_{k=1}^{K} \left[Q^{k}(\Omega^{k}) \right]$$
s.t. $\Omega^{k} = \Theta_{0} + \sum_{l=1}^{r} u_{lk} \Theta_{l}$, for $k = 1, ..., K$,
$$\|\Theta_{l}\|_{0} \leq b, \text{ for } l = 1, ..., r$$
,
$$\|\Theta_{0}\|_{0} \leq b_{0},$$
with more identifiability conditions,

where a, b, b_0 are fixed positive constants, $|\cdot|_0$ refers to the vector L_0 norm, and $||\cdot||_0$ refers to the matrix L_0 norm. For simplicity, let $\hat{\mathcal{C}} = \{\hat{\Theta}_0, \hat{\Theta}_1, ..., \hat{\Theta}_r, \hat{\mathbf{u}}_1, ..., \hat{\mathbf{u}}_r\}$ denote the estimation, and $\hat{\Omega}^k = \hat{\Theta}_0 + \sum_{l=1}^r \hat{u}_{lk} \hat{\Theta}_l$ for k = 1, ..., K.

For true precision matrices Ω^k , let $T^k = \{(j,j') | \omega_{j,j'}^k \neq 0\}$ and $q^k = |T^k|$. Assume $0 < \tau_1 < \phi_{\min}(\Omega^k) \leq \phi_{\max}(\Omega^k) < \tau_2, k = 1, ..., K$, for some positive constant τ_1, τ_2 . This condition can be transferred as some conditions for $\{\Theta_l, \mathbf{u}_l\}$. I will specify the conditions later.

Theorem 2.1. Suppose two assumptions hold. Let $\{\Omega^k\}$ denote the true precision matrices. For the estimation \hat{C} such that $\sum_{k=1}^K \left[Q^k(\hat{\Omega}^k)\right] \leq \sum_{k=1}^K \left[Q^k(\Omega^k)\right]$ and satisfies the constrains, the following accuracy bound holds with probability tending to 1.

$$\sum_{k=1}^{K} \left\| \hat{\Omega}^k - \Omega^k \right\|_F \le CK \left(C_1(b_0 + rb) \left(\frac{\log p}{n} \right)^{1/2} + C_2 \left(\frac{p \log p}{n} \right)^{1/2} \right),$$

where n is the sample size for each category, and C, C_1, C_2 are positive constants independent with p, n.

Proof. Let Ω^k denote the true precision matrices for k=1,...,K. Consider the estimation $\hat{\mathcal{C}}$ such that $\sum_{k=1}^K \left[Q^k(\hat{\Omega}^k)\right] \leq \sum_{k=1}^K \left[Q^k(\Omega^k)\right]$. Let $\Delta^k = \hat{\Omega}^k - \Omega^k$. For a matrix M, let M_T denote the matrix M with all elements outside the index set T replaced by 0, and $\tilde{M} = \text{vec}(M)$ be the vectorization of M. Define the function

$$G(\left\{\Delta^{k}\right\}) = \sum_{k=1}^{K} \operatorname{tr}(S(\Omega^{k} + \Delta^{k})) - \operatorname{tr}(\Omega^{k}) - \log|\Omega^{k} + \Delta^{k}| + \log|\Omega^{k}| = I_{1} + I_{2}, \tag{3}$$

where

$$I_{1} = \sum_{k=1}^{K} \operatorname{tr}((S^{k} - \Sigma^{k})\Delta^{k}), \quad I_{2} = \sum_{k=1}^{K} (\tilde{\Delta}^{k})^{T} \int_{0}^{1} (1 - v)(\Omega^{k} + v\Delta^{k})^{-1} \otimes (\Omega^{k} + v\Delta^{k})^{-1} dv \tilde{\Delta}^{k}.$$

With probability tending to 1, we have

$$|I_1| \leq C_1 \left(\frac{\log p}{n}\right)^{1/2} \sum_{k=1}^K \left(|\Delta_{T^k}^k|_1 + |\Delta_{T^{k,c}}^k|_1\right) + C_2 \left(\frac{p\log p}{n}\right)^{1/2} \sum_{k=1}^K \left\|\Delta^k\right\|_F, \quad I_2 \geq \frac{1}{4\tau_2^2} \sum_{k=1}^K \left\|\Delta^k\right\|_F^2.$$

Note that $|\Delta_{T^k}^k|_1 \leq \sqrt{q^k} \|\Delta^k\|_F$. Then, we only need to deal with $|\Delta_{T^{k,c}}^k|_1$. Rewrite the term, we have

$$|\Delta_{T^{k,c}}^{k}|_{1} = |\hat{\Theta}_{0,T^{k,c}} + \hat{u}_{1k}\hat{\Theta}_{1,T^{k,c}} + \dots + \hat{u}_{rk}\hat{\Theta}_{r,T^{k,c}}|_{1} \le (b_{0} + rb) \left\|\Delta^{k}\right\|_{\max} \le (b_{0} + rb) \left\|\Delta^{k}\right\|_{F}.$$

To let the equation (3) smaller than 0, we have

$$I_2 \le -I_1 \le |I_1|.$$
 (4)

Plugging the upper bound of $|I_1|$ and the lower bound of I_2 into the inequality (4), we have

$$\frac{1}{4\tau_2^2} \sum_{k=1}^K \left\| \Delta^k \right\|_F^2 \le C_1 \left(\frac{\log p}{n} \right)^{1/2} \sum_{k=1}^K \left(\sqrt{q^k} \left\| \Delta^k \right\|_F + (b_0 + rb) \left\| \Delta^k \right\|_F \right) + C_2 \left(\frac{p \log p}{n} \right)^{1/2} \sum_{k=1}^K \left\| \Delta^k \right\|_F.$$

By Cauchy Schwartz inequality, we know that $\sum_{k=1}^{K} \|\Delta^k\|_F^2 \ge \frac{1}{K} (\sum_{k=1}^{K} \|\Delta^k\|_F)^2$. Also, note that $q^k \le (b_0 + rb), k = 1, ...K$. Dividing by $\sum_{k=1}^{K} \|\Delta^k\|_F$ on both sides of the inequality, we obtain the accuracy rate

$$\sum_{k=1}^{K} \left\| \Delta^{k} \right\|_{F} = \sum_{k=1}^{K} \left\| \hat{\Omega}^{k} - \Omega^{k} \right\|_{F} \le 4\tau_{2}^{2} K \left(C_{1}(b_{0} + rb) \left(\frac{\log p}{n} \right)^{1/2} + C_{2} \left(\frac{p \log p}{n} \right)^{1/2} \right). \tag{5}$$

Remark 3. The accuracy (5) holds when q^k are fixed. Otherwise, the accuracy is of order $\mathcal{O}_p\left[q\left\{\frac{\log p}{n}\right\}^{1/2}\right]$.

Remark 4. This proof does not utilize the special structure of Ω^k . We can go through the proof with the constrain $|\Omega^k| < s$.

Remark 5. Both accuracy results of our constrained estimator and penalized estimator are of order $F(p,q) \left(\frac{\log p}{n}\right)^{1/2}$, where $F(p,q) = (p+q)^{1/2}$ for penalized estimator and $F(p,q) = (p+q^2)^{1/2}$ with $q = b_0 + rb$ in our estimator. In case of growing (p,n) and fixed q, the two estimators share the same accuracy rate.

3 Others

Can the factor K be improved?

First, consider the case r=0, K>1. Then, we have $\Theta_0=\Omega^k, k=1,...,K$. Let $\hat{\Theta}_0$ be the estimator of $\Omega^k, k=1,...,K$, and thus $\Delta^k=\hat{\Omega}^k-\Omega^k=\Delta, k=1,...,K$. Define the function

$$G(\Delta) = \frac{1}{K} \sum_{k=1}^{K} \operatorname{tr}(S^{k}(\Theta_{0} + \Delta)) - \operatorname{tr}(S^{k}\Theta_{0}) - \log|\Theta_{0} + \Delta| + \log|\Theta_{0}| = I_{1} + I_{2},$$

where

$$I_1 = \operatorname{tr}((\frac{1}{K} \sum_{k=1}^K S^k - \Sigma)\Delta), \quad I_2 = (\tilde{\Delta})^T \int_0^1 (1 - v)(\Theta_0 + v\Delta)^{-1} \otimes (\Theta_0 + v\Delta)^{-1} dv\tilde{\Delta}.$$

Note that $\frac{1}{K} \sum_{k=1}^{K} S^k$ can be considered as the sample covariance matrix with sample size nK. Then, the upper bound for $|I_1|$ is

$$|I_1| \le C_1 \left(\frac{\log p}{nK}\right)^{1/2} (|\Delta|_1) + C_2 \left(\frac{p \log p}{nK}\right)^{1/2} \|\Delta\|_F.$$

Since $I_2 \ge \frac{1}{4\tau_2^2} \|\Delta\|_F^2$, $|\Delta|_1 \le \sqrt{q} \|\Delta\|_F + (b_0 + rb) \|\Delta\|_F$, and we need $I_2 \le |I_1|$, we obtain the error bound

$$\|\Delta\|_F^2 \le \frac{4\tau_2^2}{K^{1/2}} F(p, q, n) \|\Delta\|_F$$

and thus $\|\Delta\|_F = \|\hat{\Theta}_0 - \Theta_0\|_F$ decreases in K of order $\mathcal{O}(K^{-1/2})$.

This result agrees with the intuition. As K growing, the sample size for estimating the Θ_0 becomes larger. Then, the error for the estimation goes smaller.

My thoughts.(Jan 11)

Consider the problem for scalar. Let $Y_{ij} \sim_{i.i.d.} N(\mu, \sigma^2), i = 1, ..., n, j = 1, ..., K$. Then, we have

$$\sum_{j=1}^{K} \sum_{i=1}^{n} (Y_{ij} - \bar{Y})^2 = \sum_{j=1}^{K} \sum_{i=1}^{n} (Y_{ij} - Y_{.j})^2 + \sum_{j=1}^{K} n(Y_{.j} - \bar{Y})^2,$$

where $\bar{Y} = \frac{1}{nK} \sum_{i,j} Y_{ij}$ and $Y_{.j} = \frac{1}{n} \sum_{i} Y_{ij}$. Note that $Y_{.j} \sim_{i.i.d.} N(\mu, \frac{\sigma^2}{n})$. We have

$$\frac{1}{K} \sum_{j=1}^{K} (Y_{.j} - \bar{Y})^2 \to_{a.s.} \frac{\sigma^2}{n},$$

as $K \to \infty$. For all $\epsilon > 0$, we have n, K large enough such that

$$\frac{1}{nK} \sum_{i=1}^{K} \sum_{j=1}^{n} (Y_{ij} - \bar{Y})^2 = \frac{1}{nK} \sum_{j=1}^{K} \sum_{i=1}^{n} (Y_{ij} - Y_{.j})^2 + \epsilon.$$

The term $\frac{1}{nK}\sum_{j=1}^K\sum_{i=1}^n(Y_{ij}-\bar{Y})^2$ is the sample variance with sample size nK, and $\frac{1}{nK}\sum_{j=1}^K\sum_{i=1}^n(Y_{ij}-Y_{ij})^2$ is the average of the sample variance for each group.

In multi-layer model, let S denote the sample covariance matrix with sample size nK and S^k be the sample covariance matrix for each group. Similarly as the scalar example, we may have S and $\frac{1}{K}\sum_k S^k$ close enough when n, K are large, and then we can go through the above proof.

For the log-determinant term,

$$\sum_{k=1}^{K} \log |\Omega^{k}| - \log |\Omega^{k} + \Delta^{k}| \text{ is replaced by } K \log |\Theta_{0}| - K \log |\Theta_{0} + \Delta|.$$

Consider the function $f(t) = \log |\Omega' + t\Delta'|$. By Taylor expansion for t = 1 around t = 0, we have

$$f(1) - f(0) = \log |\Omega'| - \log |\Omega' + \Delta'| = \operatorname{tr}(\Sigma'\Delta') + (\tilde{\Delta}')^T \int_0^1 (1 - v)(\Omega' + v\Delta')^{-1} \otimes (\Omega' + v\Delta')^{-1} dv \tilde{\Delta}'.$$

The Taylor expansion takes derivatives of t. It seems impossible to let $K \log |\Theta_0| - K \log |\Theta_0| + \Delta$ unrelated with K?

Thoughts (Jan 12)

Lemma 1. Let $Z_i \sim_{i.i.d.} \mathcal{N}(0, \Sigma)$ and $\phi_{max}(\Sigma) \leq \tau < \infty$. Let $\Sigma = [\![\Sigma_{ij}]\!]$, then

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

where c_1, c_2, δ depends on τ only.

Proof. See Lemma 1 of Rothman et.al.

Lemma 2. With the probability tending to 1, we have the upper bound

$$|I_1| = |tr((\frac{1}{K} \sum_{k=1}^K S^k - \Sigma)\Delta)| \le C_1 \left(\frac{\log p}{nK}\right)^{1/2} (|\Delta^-|_1) + C_2 \left(\frac{p \log p}{nK}\right)^{1/2} \|\Delta^+\|_F.$$

Proof. Let $\bar{S} = \frac{1}{K} \sum_{k=1}^{K} S^k$. Let $X_1^k, ..., X_n^k \sim_{i.i.d.} \mathcal{N}_p(0, \Sigma)$ denote the sample for k-th category. Consider the entry of \bar{S} .

$$\bar{S}_{jk} = \frac{1}{K} \sum_{m=1}^{K} \frac{1}{n} \sum_{i=1}^{n} (X_{ij}^{m} - X_{.j}^{m}) (X_{ik}^{m} - X_{.k}^{m})$$
$$= \frac{1}{nK} \sum_{i=1}^{n} \sum_{m=1}^{K} (X_{ij}^{m} X_{ik}^{m} - X_{.j}^{m} X_{.k}^{m}),$$

where $X_{ij}^{m} = \frac{1}{n} \sum_{i} X_{ij}^{m}$. By Lemma (1), we have

$$\left| \frac{1}{nK} \sum_{i=1}^{n} \sum_{m=1}^{K} X_{ij}^{m} X_{ik}^{m} - \Sigma_{jk} \right| \le C \sqrt{\frac{\log p}{nK}},$$

by letting n=nK and $\nu=\sqrt{\frac{\log p}{nK}}$, with probability tending to 1 as $p\to\infty$. Also, by SLLN, $X^m_{.j}\to_{a.s.}0$ as $n\to\infty$ for j=1,...,p, m=1,...,K. Then, we have

$$\max_{jk} |\bar{S}_{jk} - \Sigma_{jk}| \le C_1 \sqrt{\frac{\log p}{nK}},$$

with probability tending to 1 for some constant C_1 .

Back to $|I_1|$. We obtain the upper bound

$$|I_{1}| \leq |\sum_{i \neq j} (\bar{S}_{ij} - \Sigma_{ij}) \Delta_{ij}| + |\sum_{i=1}^{p} (\bar{S}_{ii} - \Sigma_{ii}) \Delta_{ii}|$$

$$\leq C_{1} \sqrt{\frac{\log p}{nK}} |\Delta^{-}|_{1} + \left[\sum_{i=1}^{p} (\bar{S}_{ii} - \Sigma_{ii})^{2} \right]^{1/2} ||\Delta^{+}||_{F}$$

$$\leq C_{1} \sqrt{\frac{\log p}{nK}} |\Delta^{-}|_{1} + C_{2} \sqrt{\frac{p \log p}{nK}} ||\Delta^{+}||_{F}$$

Comparison Table.

Penalized For $k \in [K]$, For $k \in [K]$. Ground $|\Omega^k|_0 < s$ Truth $|\Omega^k|_1 < c$. , where $|\cdot|_0$ denote the number of nonzero elements in the matrix, and s > 1 is a positive where norm $|\Omega|_1 = \sum_{(i,j)} |\omega_{ij}|$. Fitting The estimator is the solution to the optimiza-The estimator is the solution to the optimization problem techtion problem niques $\min_{\{\Omega^k\}} Q^k(\Omega^k) + \lambda \sum_{k=1}^K |\Omega^k|_0.$ $\min_{\{\Omega^k\}} Q^k(\Omega^k) + \lambda \sum_{i=1}^K |\Omega^k|_1.$ For $\lambda \geq \Lambda_1 \left(\frac{\log p}{n}\right)^{1/2}$, we have Accuracy For $\lambda \geq 0$, $\sum_{k} \|\Delta_{k}\|_{F}^{2} \leq 4\tau_{2}^{2} \left(F(p,q,n) \sum_{k} \|\Delta^{k}\|_{F} + K\lambda q \right) \sum_{k} \|\Delta_{k}\|_{F}^{2} \leq 4\tau_{2}^{2} \left(\lambda \sqrt{q} + F(p,q,n) \right) \sum_{k} \|\Delta^{k}\|_{F}^{2},$ where $F(p,q,n) = C_{1} p \left(\frac{\log p}{n} \right)^{1/2} + \text{ where } F(p,q,n) = C_{1} \left(\frac{q \log p}{n} \right)^{1/2} + C_{2} \left(\frac{p \log p}{n} \right)^{1/2}.$ Then, the error $C_{2} \left(\frac{p \log p}{n} \right)^{1/2}.$ Then, we have $\sum_{k} \left\| \Delta^{k} \right\|_{F} \leq 4\tau_{2}^{2} K \left(\lambda \sqrt{q} + F(p, q, n) \right).$ $\sum_{k} \|\Delta_k\|_F = \mathcal{O}(\frac{K\sqrt{\lambda}}{n^{1/4}}).$ If $\lambda \geq \Lambda_1 \left(\frac{\log p}{n}\right)^{1/2}$, the error becomes of or-

	Constrained	
	L_0	L_1
Ground	For $k \in [K]$,	For $k \in [K]$,
Truth	$ \Omega^k _0 < s$	$ \Omega^k _1 < c,$
	, where $ \cdot _0$ denote the number of nonzero elements in the matrix, and $s>1$ is a positive constant.	where norm $ \Omega _1 = \sum_{(i,j)} \omega_{ij} $.
Fitting tech-	The estimator is the solution to the optimization problem	The estimator is the solution to the optimization problem
niques	$\min_{\{\Omega^k\}}Q^k(\Omega^k)$	$\min_{\{\Omega^k\}}Q^k(\Omega^k)$
	$s.t. \Omega^k _0 < s, k \in [K]$	$s.t. \Omega^k _1 < c, k \in [K]$
Accuracy	We have	We have
	$\sum_{k} \ \Delta_k\ _F^2 \le 4\tau_2^2 F(p, s, n) \sum_{k} \ \Delta^k\ _F,$	$\sum_{k} \left\ \Delta_{k} \right\ _{F}^{2} \leq 4\tau_{2}^{2} F(p, q, n) \sum_{k} \left\ \Delta^{k} \right\ _{F},$
	where $F(p, s, n) = C_1 s \left(\frac{\log p}{n}\right)^{1/2} + C_2 \left(\frac{p \log p}{n}\right)^{1/2}$. Then	where $F(p,q,n) = C_1 p \left(\frac{\log p}{n}\right)^{1/2} + C_2 \left(\frac{p \log p}{n}\right)^{1/2}$. Then,
	$\sum_{k} \ \Delta_k\ _F \le 4\tau_2^2 KF(p, s, n).$	$\sum_{k} \ \Delta_k\ _F \le 4\tau_2^2 KF(p, q, n).$

4 Next

- Think about the identifiability of the intermediate cases (spare matrix factorization).
- Think about the proof which utilizes the special structure of the $\Omega^k.$