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Topic 16: Graphical Network Inference

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Key points:

Disclaimer: *The note is built on Prof. Jinchi Lv's lectures of the course at USC, DSO 607, High-Dimensional Statistics and Big Data Problems.*

16.1 Motivation

Consider a classic question: For n observations of dimension p, how can we capture the statistical relationships between the variables of interest? Consider the example of the multivariate Gaussian distribution:

Example 16.1.1: Multivariate Gaussian Distribution

Suppose we have n observations of dimension p, $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. let $\mathbf{S}$ be the empirical covariance matrix. Then the probability density

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{p/2}\det(\boldsymbol{\Sigma})^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})'\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

define the **inverse covariance matrix** or **precision matrix** as $\boldsymbol{\Omega} = \boldsymbol{\Sigma}^{-1}$, then we have

$$f_{\mu,\boldsymbol{\Omega}} = \exp\left\{\boldsymbol{\mu}'\boldsymbol{\Omega}\boldsymbol{x} - \left\langle \boldsymbol{\Omega}, \frac{1}{2}\mathbf{x}\mathbf{x}' \right\rangle - \frac{p}{2}\log(2\pi) + \frac{1}{2}\log\det(\boldsymbol{\Omega}) - \frac{1}{2}\boldsymbol{\mu}'\boldsymbol{\Omega}\boldsymbol{\mu}\right\}$$

where $\langle \mathbf{A}, \mathbf{B} \rangle = \operatorname{tr}(\mathbf{A}\mathbf{B})$.

In this example, we know that **every** multivariate Gaussian distribution can be represented by a pairwise **Gaussian Markov Random Field (GMRF)**, which an **undirected graph** $G = (V, E)$

- representing the collection of variables $\mathbf{x}$ by a vertex set $\mathcal{V} = \{1, \cdots, p\}$
- encoding correlations between variables by a set of edges $\mathcal{E} = \{(i,j) \in \mathcal{V} \mid i =\neq j, \Omega_{ij} \neq 0\}$

For simplicity, we normalize $\boldsymbol{\mu} = \mathbf{0}$. If we draw n i.i.d. samples $\mathbf{x}_1, \cdots, \mathbf{x}_n \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$, then the log-likelihood is

$$\begin{aligned}\mathcal{L}(\boldsymbol{\Omega}) &= \frac{1}{n}\sum_{i=1}^{n}\log f(\mathbf{x}_i) = \frac{1}{2}\log\det(\boldsymbol{\Omega}) - \frac{1}{2n}\sum_{i=1}^{n}\mathbf{x}_1'\boldsymbol{\Theta}\mathbf{x}_i \\ &= \frac{1}{2}\log\det(\boldsymbol{\Omega}) - \frac{1}{2}\left\langle \Omega, \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i'\mathbf{x}_i' \right\rangle\end{aligned}$$

What's the goal? We want to estimate a **sparse** graph structure given $n \ll p$ i.i.d. observations. But what does sparsity means in this context? A sparse graph is **equivalent** to a sparse precision matrix: the precision

matrix should have many 0s.

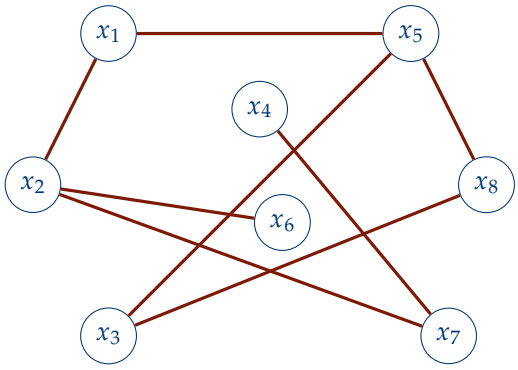
Sparse precision matrix for the Gaussian vector mentioned above $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$, we have $\forall u, v$

$$x_u \perp x_v \mid \mathbf{x}_{\mathcal{V}\setminus\{u,v\}} \Leftrightarrow \Omega_{u,v} = 0$$

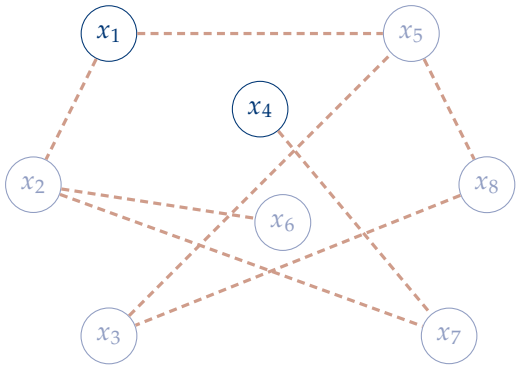
that is, sparsity of the precision matrix is equivalent to **conditional independence**[1]. Consider a graph, where x_1 and x_4 are only connected through other nodes, that is x_1 and x_4 are conditional independent, then we can have the precision matrix be something like:

$$\mathbf{\Theta} = \begin{bmatrix} * & * & 0 & 0 & * & 0 & 0 & 0 \\ * & * & 0 & 0 & 0 & * & * & 0 \\ 0 & 0 & * & 0 & * & 0 & 0 & * \\ 0 & 0 & 0 & * & 0 & 0 & * & 0 \\ * & 0 & * & 0 & * & 0 & 0 & * \\ 0 & * & 0 & 0 & 0 & * & 0 & 0 \\ 0 & * & 0 & * & 0 & 0 & * & 0 \\ 0 & 0 & * & 0 & * & 0 & 0 & * \end{bmatrix}$$

where 0 captures precisely the conditional independence.



x_1 **and** x_4 **are** ***connected***



x_1 **and** x_4 **are** ***NOT connected*****, conditionally**

Intuitively, a sparse graph is much simpler, which is why conditional independence is desired. So how to achieve sparsity? We can again use a L-1 regularization when maximizing the log-likelihood $\mathcal{L}(\mathbf{\Omega})$. Denote the sample covariance matrix as $\mathbf{S} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i'$, then the problem becomes the so-called **Graphical Lasso**

$$\max_{\mathbf{\Omega} \succeq \mathbf{0}} \log\det(\mathbf{\Omega}) - \operatorname{tr}(\mathbf{S\Omega}) - \rho \|\mathbf{\Omega}\|_1$$

which is equivalent to

$$\min_{\mathbf{\Omega} \succeq \mathbf{0}} -\log\det(\mathbf{\Omega}) + \operatorname{tr}(\mathbf{S\Omega}) + \rho \|\mathbf{\Omega}\|_1$$

16.2 Graphical Lasso

The graphical lasso method is developed by (Friedman et al., 2008). For the optimization problem

$$\min_{\mathbf{\Omega} \succeq \mathbf{0}} -\log\det(\mathbf{\Omega}) + \operatorname{tr}(\mathbf{S\Omega}) + \rho \|\mathbf{\Omega}\|_1 \tag{16.1}$$

[1] Meanwhile, for independence: $\Sigma_{u,v} = 0 \Leftrightarrow x_u \perp x_v$

The first-order optimality condition gives

$$\mathbf{0} \in \boldsymbol{\Omega}^{-1} - \mathbf{S} - \lambda \boldsymbol{\Gamma}$$

where $\boldsymbol{\Gamma}$ is a matrix of component-wise signs of $\boldsymbol{\Omega}$

$$\boldsymbol{\Gamma} = \partial \|\boldsymbol{\Omega}\|_1 \Rightarrow \gamma_{jk} \begin{cases} = \text{sign}(\omega_{jk}), & \omega_{jk} \neq 0 \\ \in [-1, 1], & \omega_{jk} = 0 \end{cases}$$

since in a graph, we always have that, following the global stationarity conditions, $\omega_{jj} > 0$, which implies that

$$w_{ii} = s_{ii} + \lambda \qquad\qquad i = 1, \cdots, p \tag{16.2}$$

where we denote a working version of $\boldsymbol{\Omega}^{-1}$ as $\mathbf{W}$.

The idea is to repeatedly cycle through all columns-rows and in each step optimize only a single column-row. Consider the following partition where all matrices are partitioned into one column/row versus the rest

$$\boldsymbol{\Omega} = \begin{pmatrix} \boldsymbol{\Omega}_{11} & \boldsymbol{\omega}_{12} \\ \boldsymbol{\omega}_{12}' & \omega_{22} \end{pmatrix} \qquad \mathbf{S} = \begin{pmatrix} \mathbf{S}_{11} & \mathbf{s}_{12} \\ \mathbf{s}_{12}' & s_{22} \end{pmatrix} \qquad \mathbf{W} = \begin{pmatrix} \mathbf{W}_{11} & \mathbf{w}_{12} \\ \mathbf{w}_{12}' & w_{22} \end{pmatrix} \qquad \boldsymbol{\Gamma} = \begin{pmatrix} \boldsymbol{\Gamma}_{11} & \boldsymbol{\gamma}_{12} \\ \boldsymbol{\gamma}_{12}' & \gamma_{22} \end{pmatrix}$$

apply this partition to the optimality condition, get

$$\boldsymbol{\Omega}^{-1} = \mathbf{S} - \lambda \boldsymbol{\Gamma}$$
$$\begin{pmatrix} \mathbf{W}_{11} & \mathbf{w}_{12} \\ \mathbf{w}_{12}' & w_{22} \end{pmatrix} = \begin{pmatrix} \mathbf{S}_{11} & \mathbf{s}_{12} \\ \mathbf{s}_{12}' & s_{22} \end{pmatrix} + \lambda \begin{pmatrix} \boldsymbol{\Gamma}_{11} & \boldsymbol{\gamma}_{12} \\ \boldsymbol{\gamma}_{12}' & \gamma_{22} \end{pmatrix}$$

where $\boldsymbol{\Omega}_{11}$ is $(p-1) \times (p-1)$, $\boldsymbol{\omega}_{12}$ is $(p-1) \times 1$, ω_{22} is a scalar.

Consider a **blockwise** step: suppose we fix all but the last row/column, then using properties of inverses of block-partitioned matrices, we have

$$\begin{aligned} \begin{pmatrix} \mathbf{W}_{11} & \mathbf{w}_{12} \\ \mathbf{w}_{12}' & w_{22} \end{pmatrix} &= \begin{pmatrix} \left(\boldsymbol{\Omega}_{11} - \frac{\boldsymbol{\omega}_{12}\boldsymbol{\omega}_{12}'}{\omega_{22}}\right)^{-1} & -\mathbf{W}_{11}\frac{\boldsymbol{\omega}_{12}}{\omega_{22}} \\ & \frac{1}{\omega_{22}} - \frac{\boldsymbol{\omega}_{12}'\mathbf{W}_{11}\boldsymbol{\omega}_{12}}{\omega_{22}^2} \end{pmatrix} \\ &= \begin{pmatrix} \boldsymbol{\Omega}_{11}^{-1} + \frac{\boldsymbol{\Omega}_{11}^{-1}\boldsymbol{\omega}_{12}\boldsymbol{\omega}_{12}'\boldsymbol{\Omega}_{11}^{-1}}{\omega_{22} - \boldsymbol{\omega}_{12}'\boldsymbol{\Omega}_{11}^{-1}\boldsymbol{\omega}_{12}} & -\frac{\boldsymbol{\Omega}_{11}^{-1}\boldsymbol{\omega}_{12}}{\omega_{22} - \boldsymbol{\omega}_{12}'\boldsymbol{\Omega}_{11}^{-1}\boldsymbol{\omega}_{12}} \\ & \frac{1}{\omega_{22} - \boldsymbol{\omega}_{12}'\boldsymbol{\Omega}_{11}^{-1}\boldsymbol{\omega}_{12}} \end{pmatrix} \end{aligned}$$

then, by the partitioned optimality condition, we have[2]:

$$\mathbf{0} = -\mathbf{w}_{12} + \mathbf{s}_{12} + \lambda \boldsymbol{\gamma}_{12} = \mathbf{W}_{11}\frac{\boldsymbol{\omega}_{12}}{\omega_{22}} + \mathbf{s}_{12} + \lambda \boldsymbol{\gamma}_{12} \tag{16.3}$$

$$\mathbf{0} = \frac{\boldsymbol{\Omega}_{11}^{-1}\boldsymbol{\omega}_{12}}{\omega_{22} - \boldsymbol{\omega}_{12}'\boldsymbol{\Omega}_{11}^{-1}\boldsymbol{\omega}_{12}} + \mathbf{s}_{12} + \lambda \boldsymbol{\gamma}_{12} = w_{22}\boldsymbol{\Omega}_{11}^{-1}\boldsymbol{\omega}_{12} + \mathbf{s}_{12} + \lambda \boldsymbol{\gamma}_{12} \tag{16.4}$$

The graphic Lasso algorithm them solves Eq.16.3 for $\boldsymbol{\beta} = \boldsymbol{\omega}_{12}/\omega_{12}$, that is

$$\mathbf{W}_{11}\boldsymbol{\beta} + \mathbf{s}_{12} + \lambda \boldsymbol{\gamma}_{12} = \mathbf{0}$$

[2]For Eq.16.4, by Eq.16.2, we know that $w_{22} = s_{22} + \lambda$, which is fixed.

where $\gamma_{12} \in \text{sign}(\beta)$ since $\omega_{22} > 0$, which is essentially solving:

$$\min_{\beta \in \mathbb{R}^{p-1}} \left\{ \frac{1}{2} \beta' \mathbf{W}_{11} \beta + \beta' \mathbf{s}_{12} + \lambda \left\| \beta \right\|_1 \right\}$$

and $\mathbf{W}_{11} > 0$ is assumed to be fixed.

This problem is analogous to a lasso regression problem of the **last variable** on **the rest**, but the cross-product matrix $\mathbf{S}_{11}$ is replaced by its **current estimation** $\mathbf{W}_{11}$. It is relatively easier to solve using elementwise coordinate descent, then

$$\begin{aligned}
&\mathbf{w}_{12} = -\mathbf{W}_{11} \frac{\boldsymbol{\omega}_{12}}{\omega_{22}} && \Rightarrow \hat{\mathbf{w}}_{12} = -\mathbf{W}_{11} \hat{\boldsymbol{\beta}} && \text{Step 1} \\
&w_{22} = \frac{1}{\omega_{22}} - \frac{\boldsymbol{\omega}_{12}' \mathbf{W}_{11} \boldsymbol{\omega}_{12}}{\omega_{22}^2} && \Rightarrow \frac{1}{\hat{\omega}_{22}} = w_{22} - \hat{\boldsymbol{\beta}}' \hat{\mathbf{w}}_{12} && \text{Step 2} \\
&\boldsymbol{\omega}_{12} = -\mathbf{W}_{11}^{-1} \mathbf{w}_{12} \omega_{22} && \Rightarrow \hat{\boldsymbol{\omega}}_{12} = -\mathbf{W}_{11}^{-1} \hat{\mathbf{w}}_{12} \hat{\omega}_{22} && \text{Step 3}
\end{aligned}$$

notice that after solving for $\boldsymbol{\beta}$ and updating $\mathbf{w}_{12}$ in Step 1, the graphic Lasso procedure can move onto the next block, that is, only Step 1 is used in the loop, Step 2 and 3 can be done at the end. The algorithm can be summarized as:

Algorithm 16.2.1: Graphical Lasso algorithm

1 Initialize $\mathbf{W} = \mathbf{S} + \lambda \mathbf{I}$

- Cycle around the columns repeatedly, performing the following steps till convergence:
  - a rearrange the rows/columns so that the target column is **the last** (implicitly)
  - b solve the lasso problem, starting the solution from the previous round for this column
  - c update the row/column (***off-diagonal***) of the covariance using $\hat{\mathbf{w}}_{12}$
  - d save $\hat{\boldsymbol{\beta}}$ for this column in the matrix $\mathbf{B}$

3 after convergence, for every row/column, compute the diagonal entries $\hat{\omega}_{jj}$, and covert the $\mathbf{B}$ matrix to $\boldsymbol{\Omega}$

16.3 What Is GLasso Solving?

Again, consider the optimization problem

$$\min_{\boldsymbol{\Omega} \geq \mathbf{0}} -\log\det(\boldsymbol{\Omega}) + \text{tr}(\mathbf{S}\boldsymbol{\Omega}) + \rho \left\| \boldsymbol{\Omega} \right\|_1$$

and its stationarity condition

$$\mathbf{0} = \boldsymbol{\Omega}^{-1} - \mathbf{S} - \lambda \boldsymbol{\Gamma}$$

rewrite the stationarity condition

$$\mathbf{0} = \boldsymbol{\Omega}^{-1} - \mathbf{S} - \lambda \boldsymbol{\Gamma} = \boldsymbol{\Omega} - (\mathbf{S} + \lambda \boldsymbol{\Gamma})^{-1}$$

since $\boldsymbol{\Gamma} = \text{sign}(\boldsymbol{\Omega})$, write $\tilde{\boldsymbol{\Gamma}} = \lambda \boldsymbol{\Gamma}$, we have $\left\| \tilde{\boldsymbol{\Gamma}} \right\|_\infty \leq \lambda$. Denote the element-wise absolute value matrix of $\boldsymbol{\Omega}$ as $\text{abs}(\boldsymbol{\Omega})$, then let $\tilde{\boldsymbol{\Gamma}} = \lambda \boldsymbol{\Gamma}$, $\mathbf{P} = \text{abs}(\boldsymbol{\Omega})$, we have

$$\begin{aligned}
\mathbf{0} &= \boldsymbol{\Omega} - (\mathbf{S} + \lambda \boldsymbol{\Gamma})^{-1} \\
&= \mathbf{P} \circ \text{sign}(\tilde{\boldsymbol{\Gamma}}) - (\mathbf{S} + \tilde{\boldsymbol{\Gamma}})^{-1}
\end{aligned}$$

and mechanically, we also have

$$\mathbf{P} \circ \left(\text{abs}(\tilde{\mathbf{\Gamma}}) - \lambda \mathbf{1}_p \mathbf{1}_p' \right) = \mathbf{0}$$
$$\left\| \tilde{\mathbf{\Gamma}} \right\|_\infty \leq \lambda$$

together, these are just hte KKT optimality condition for the following box-constrained SDP

$$\max_{\tilde{\mathbf{\Gamma}}: \left\| \tilde{\mathbf{\Gamma}} \right\|_\infty \leq \lambda} g(\tilde{\mathbf{\Gamma}}) \coloneqq \log\det(\mathbf{S} + \tilde{\mathbf{\Gamma}}) + p \tag{16.5}$$

with the transformation $\mathbf{S} + \tilde{\mathbf{\Gamma}} = \mathbf{\Omega}^{-1}$. Essentially, this is the dual problem of the initial optimization problem, both of them are solved by the GLasso algorithm.

Issues of GLasso method :

- the non-monotonic behavior of Glasso in minimizing $f(\mathbf{\Omega})$
  - $\boldsymbol{\theta}_{12}$ is entangled in $\mathbf{W}_{11}$, which is ***incorrectly*** treated as a constant
  - after updating $\boldsymbol{\theta}_{12}$, the entire (working) covariance matrix $\mathbf{W}$ changes, but Glasso algorithm only updates $\mathbf{w}_{12}$ and $\mathbf{w}_{12}'$
- high dimesnionality problems
  - not computationally efficient when p is ultra-large
  - $\mathbf{\Sigma}^{-1}$ doesn't exist when $p > n$
  - method is not scalable

Next, we address these issues by introducing some modifications.

16.4 Graphical Lasso: Modifications

16.4.1 Primal GLasso

Consider the optimality condition in Eq.16.4:

$$\mathbf{0} = \frac{\mathbf{\Omega}_{11}^{-1} \boldsymbol{\omega}_{12}}{\omega_{22} - \boldsymbol{\omega}_{12}' \mathbf{\Omega}_{11}^{-1} \boldsymbol{\omega}_{12}} + \mathbf{s}_{12} + \lambda \boldsymbol{\gamma}_{12} = w_{22} \mathbf{\Omega}_{11}^{-1} \boldsymbol{\omega}_{12} + \mathbf{s}_{12} + \lambda \boldsymbol{\gamma}_{12}$$

Here, the dependence of the covariance submatrix $\mathbf{W}_{11}$ on $\mathbf{\Omega}_{12}$ is **explicit**. Let $\boldsymbol{\alpha} = \boldsymbol{\omega}_{12} w_{22}$ with fixed $w_{22} \geq 0$[3], then this optimality condition is essentially solving

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^{p-1}} \left\{ \frac{1}{2} \boldsymbol{\alpha}' \mathbf{\Omega}_{11}^{-1} \boldsymbol{\alpha} + \boldsymbol{\alpha}' \mathbf{s}_{12} + \lambda \left\| \boldsymbol{\alpha} \right\|_1 \right\}$$

the minimizer of this problem $\hat{\boldsymbol{\alpha}}$ can then be used to derive the estimation for $\boldsymbol{\omega}_{12}$:

$$\hat{\boldsymbol{\omega}}_{12} = \frac{\hat{\boldsymbol{\alpha}}}{w_{22}}$$

, then we can update ω_{22} as before via

$$\hat{\omega}_{22} = \frac{1}{w_{22}} + \hat{\boldsymbol{\omega}}_{12}' \mathbf{\Theta}_{11}^{-1} \hat{\boldsymbol{\omega}}_{12}$$

[3] $w_{22} = 1/(\omega_2 2 - \boldsymbol{\omega}_{12}' \mathbf{\Omega}_{11}^{-1} \boldsymbol{\omega}_{12})$

with $w_{22} = s_{22} + \lambda$. Another problem is how to obtain $\mathbf{\Omega}_{11}^{-1}$: as the iterations proceed, maintain $\mathbf{W} = \mathbf{\Omega}^{-1}$, and $\mathbf{\Omega}_{11}^{-1}$ can be derived from

$$\mathbf{\Omega}_{11}^{-1} = \mathbf{W}_{11} - \frac{\mathbf{w}_{12}\mathbf{w}_{12}'}{w_{22}}$$

once $\boldsymbol{\omega}_{12}$ is updated, the ***entire*** working covariance matrix $\mathbf{W}$ is updated using $\mathbf{\Omega}_{11}^{-1}$. This procedure, the so-called primal graphical lasso, can be represented in the following algorithm:

Algorithm 16.4.1: P-GLasso Algorithm

1 Initialize $\mathbf{W} = \text{diag}(\mathbf{S}) + \lambda\mathbf{I}$ and $\mathbf{\Omega} = \mathbf{W}^{-1}$
2 Cycle around the columns repeatedly, performing the following steps till convergence:
   a rearrange the rows/columns so that the target column is the last (implicitly)
   b compute $\mathbf{\Omega}_{11}^{-1}$ using $\mathbf{\Omega}_{11}^{-1} = \mathbf{W}_{11} - \frac{\mathbf{w}_{12}\mathbf{w}_{12}'}{w_{22}}$
   c solve $\min_{\boldsymbol{\alpha}\in\mathbb{R}^{p-1}} \left\{\frac{1}{2}\boldsymbol{\alpha}'\mathbf{\Omega}_{11}^{-1}\boldsymbol{\alpha} + \boldsymbol{\alpha}'\mathbf{s}_{12} + \lambda\|\boldsymbol{\alpha}\|_1\right\}$ for $\boldsymbol{\alpha}$, using as warm starts the solution from the previous round of row/column updates. Then update $\hat{\boldsymbol{\omega}}_{12} = \hat{\boldsymbol{\alpha}}/w_{22}$ and $\hat{\omega}_{22}$
   d update $\mathbf{\Omega}$ and $\mathbf{W}$, ensuring that $\mathbf{\Omega}\mathbf{W} = \mathbf{I}_p$
3 output the solution: precision matrix $\mathbf{\Omega}$ and its exact inverse, covariance matrix $\mathbf{W}$

16.4.2 Innovated Scalable Efficient Estimation

Now, we try to tackle the high-dimesnionality issues: $\mathbf{\Sigma}^{-1}$ does **not** exist when $p > n$. Again,

$$\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$$

consider a linear transformation where $\tilde{\mathbf{x}} = \mathbf{\Omega}\mathbf{x}$ ($\mathbf{\Omega}$ is still the precision matrix $\mathbf{\Sigma}^{-1}$), and

$$\text{cov}(\tilde{\mathbf{x}}) = \mathbf{\Omega}\text{cov}(\mathbf{x})\mathbf{\Omega} = \mathbf{\Omega}\mathbf{\Sigma}\mathbf{\Omega} = \mathbf{\Omega}$$

But $\mathbf{\Omega}$ is unknown and to be estimated. To get around this, we **break** the long vector $\tilde{\mathbf{x}}$ into small sub-vectors and then estimate each one.

Notation for subsets $A, B \subset \{1, \cdots, p\}$, let $\mathbf{x}_A$ denote a sub-vector of $\mathbf{x}$ formed by its components with indices in A, and the sub-(precision)-matrix is $\mathbf{\Omega}_{A,B} = (\omega_{jk})_{j\in A, k\in B}$, $\mathbf{\Omega}_A := \mathbf{\Omega}_{A,A}$ for simplicity. Then define

$$\tilde{\mathbf{x}}_A = \mathbf{\Omega}_A\boldsymbol{\eta}_A$$

where $\boldsymbol{\eta}_A = \mathbf{x}_A + \mathbf{\Omega}_A^{-1}\mathbf{\Omega}_{A,A^C}\mathbf{x}_{A^C}$, and $A^C := \{1, \cdots, p\} \setminus A$. With this definition, we have the following proposition:

Proposition 16.4.2: Conditional Distribution of Sub-vectors

Conditional distribution $\mathbf{x}_A \mid \mathbf{x}_B \sim \mathcal{N}\left(\boldsymbol{\mu}_{A|B}, \mathbf{\Sigma}_{A|B}\right)$, where

$$\boldsymbol{\mu}_{A|B} = \boldsymbol{\mu}_A + \mathbf{\Sigma}_{A,B}\mathbf{\Sigma}_B^{-1}\left(\mathbf{x}_B - \boldsymbol{\mu}_B\right)$$
$$\mathbf{\Sigma}_{A|B} = \mathbf{\Sigma}_A - \mathbf{\Sigma}_{A,B}\mathbf{\Sigma}_B^{-1}\mathbf{\Sigma}_{B,A}$$

and when $\mathbf{x}_B = \mathbf{x}_{A^C}$, we have

$$\mathbf{x}_A \mid \mathbf{x}_{A^C} \sim \mathcal{N}\left(-\boldsymbol{\Omega}_A^{-1}\boldsymbol{\Omega}_{A,A^C}\mathbf{x}_{A^C}, \boldsymbol{\Omega}_A^{-1}\right)$$

Prop.16.4.2 gives a multivariate linear regression model:

$$\mathbf{x}_A = \mathbf{C}_A'\mathbf{x}_{A^C} + \boldsymbol{\eta}_A$$

where $\mathbf{C}_A = -\boldsymbol{\Omega}_{A^C,A}\boldsymbol{\Omega}_A^{-1}$ is the coefficient matrix, and $\boldsymbol{\eta}_A$ is model errors with Gaussian distribution $\mathcal{N}(\mathbf{0}, \boldsymbol{\Omega}_A^{-1})$. Then we can have the following algorithm to solve this problem:

Algorithm 16.4.3: ISEE Algorithm

1 Let $(A_l)_{l=1}^L$ be a partition of index set $\{1, \cdots, p\}$, s.t. $\bigcup_{l=1}^L A_l = \{1, \cdots, p\}$
2 estimate $\boldsymbol{\eta}_{A_l}$ and then obtain estimated $\tilde{\mathbf{x}}_{A_l}$
3 stack all estimated sub-vectors $\tilde{\mathbf{x}}_{A_l}$ together to obtain $\tilde{\mathbf{x}}$

ISEE algorithm breaks large-scale precision estimation into **small-scale linear regression problems**, each of which is computationally efficient and effective.

Estimation for the $n \times p$ data matrix $\mathbf{X} = (\mathbf{x}_1, \cdots, \mathbf{x}_n)'$, we construct the linear transformation

$$\tilde{\mathbf{X}} = (\tilde{\mathbf{x}}_1, \cdots, \tilde{\mathbf{x}}_n) = \mathbf{X}\boldsymbol{\Omega}$$

then the multivariate linear regression model by matrix notation is

$$\mathbf{X}_A = \mathbf{X}_{A^C}\mathbf{C}_A + \mathbf{E}_A$$

and the corresponding sub-matrix $\tilde{\mathbf{X}}_A$ can be written as

$$\tilde{\mathbf{X}}_A = (\mathbf{X}\boldsymbol{\Omega})_A = \mathbf{X}_A\boldsymbol{\Omega}_A + \mathbf{X}_{A^C}\boldsymbol{\Omega}_{A^C,A} = \left(\mathbf{X}_A + \mathbf{X}_{A^C}\boldsymbol{\Omega}_{A^C,A}\boldsymbol{\Omega}_A^{-1}\right)\boldsymbol{\Omega}_A = \mathbf{E}_A\boldsymbol{\Omega}_A$$

Sparsity is achieved bia scaled Lasso: for each node j in index set A,

$$\mathbf{X}_j = \mathbf{A}^{\mathbf{C}}\boldsymbol{\beta}_j + \mathbf{E}_j$$

where $\boldsymbol{\beta}_j$ is the column of $\mathbf{C}_A$ corresponds to node j. The estimation is then done in the following steps:

- run the PLS

$$\left(\hat{\boldsymbol{\beta}}_j, \hat{\theta}_j^{1/2}\right) = \arg\min_{\boldsymbol{\beta}\in\mathbf{R}^{p-|A|}, \sigma\geq 0}\left\{\frac{\left\|\mathbf{X}_j - \mathbf{X}_{A^C}\boldsymbol{\beta}\right\|_2^2}{2n\sigma} + \frac{\sigma}{2} + \lambda\left\|\boldsymbol{\beta}_*\right\|_1\right\}$$

  where $\boldsymbol{\beta}_*$ is component-wise product of $\boldsymbol{\beta}$ and $\left(\frac{1}{\sqrt{n}}\left\|\mathbf{X}_k\right\|_2\right)_{k\in A^C}$, and the penalizing factor is $\lambda = C\left(\frac{2\log p}{n}\right)$.
- after obtaining $\hat{\boldsymbol{\beta}}_j$, get the estimation of the (partitioned) precision matrix $\hat{\boldsymbol{\Omega}}_A$

$$\hat{\Omega}_A = \left(\frac{1}{n}\hat{\mathbf{E}}_A'\hat{\mathbf{E}}_A\right)^{-1}$$

  where $\hat{\mathbf{E}}_j = \mathbf{X}_j - \mathbf{X}_{A^C}\hat{\boldsymbol{\beta}}_j$, $\hat{\mathbf{E}}_A = \left(\hat{\mathbf{E}}_j\right)_{j\in A}$

- for the whole partition $(A_l)_{l=1}^L$, we have $\hat{\mathbf{X}} = (\hat{\mathbf{X}}_{A_l})_{1\le l\le L}$ where $\hat{\mathbf{X}}_{A_l} = \hat{\mathbf{E}}_{A_l}\hat{\mathbf{\Omega}}_{A_l}$, then the initital estiation of the whole precision matrix is $\hat{\Omega}_{ISEE,ini} = \frac{1}{n}\hat{\mathbf{X}}'\hat{\mathbf{X}}$
- next, introduce a threshold $\tau \ge 0$, define

$$\hat{\mathbf{\Omega}}_{ISEE,g} = T_\tau\left(\hat{\mathbf{\Omega}}_{ISEE,ini}\right)$$

where $T_\tau(\mathbf{B}) = \left(b_{jk}\mathbf{1}_{|b_{jk}|\ge\tau}\right)$ for matrix $\mathbf{B} = \left(b_{jk}\right)$, then estimate the structure $\mathbf{E}$ as $\hat{\mathbf{E}}_{ISEE} = \text{supp}\left(\hat{\mathbf{\Omega}}_{ISEE,g}\right)$. One can then use the cross validation method to choose the optimal threshold:

- randomly split sample of n rows into 2 samples of n_1 and n_2, repeat N_1 times. Denote $\hat{\Omega}^{1,v}_{ISEE,ini}, \hat{\Omega}^{2,v}_{ISEE,ini}$ the corresponding covariance matrices
- choose τ by minimizing

$$\mathcal{R}(\tau) = \frac{1}{N_1}\sum_{v=1}^{N_1}\left\|T_\tau\left(\hat{\Omega}^{1,v}_{ISEE,ini}\right) - \hat{\Omega}^{1,v}_{ISEE,ini}\right\|^2$$

16.5 Heterogeneous Graphical Networks

Next, we introduce heterogeneity into this problem: the samples are now drawn from k different subpopulations

$$\mathbf{X}^{(t)} = \left(\mathbf{X}_1^{(t)}, \cdots, \mathbf{X}_p^{(t)}\right) \sim \mathcal{N}\left(\mathbf{0}, \left(\mathbf{\Omega}^{(t)}\right)^{-1}\right) \qquad t = 1, \cdots, k$$

Some simple observations on this problem are

- For each node $1 \le j \le p$ in graph $1 \le t \le k$

$$\mathbf{X}_j^{(t)} \mid \mathbf{X}_{-j}^{(t)} \sim \mathcal{N}\left(\mathbf{X}_{-j}^{(t)\prime}\mathbf{C}_j^{(t)}, \frac{1}{\omega_{j,j}^{(t)}}\right)$$

with $\mathbf{C}_j^{(t)} = -\frac{\mathbf{\Omega}_{-j,j}^{(t)}}{\omega_{j,j}^{(t)}}$ and $\mathbf{\Omega}^{(t)} = \left(\omega_{a,b}^{(t)}\right)_{p\times p}$

- For each pair of nodes (a, b),

$$\text{Cov}\left(\boldsymbol{\epsilon}_a^{(t)}, \boldsymbol{\epsilon}_b^{(t)}\right) = \frac{\omega_{a,b}^{(t)}}{\omega_{a,a}^{(t)}\omega_{b,b}^{(t)}}$$

with $\boldsymbol{\epsilon}^{(t)} = \mathbf{X}_j^{(t)} - \mathbf{X}_{-j}^{(t)\prime}\mathbf{C}_j^{(t)} \sim \mathcal{N}\left(\mathbf{0}, \frac{1}{\omega_{j,j}^{(t)}}\right)$ **independent** across t

here the number of subpopulations k, like the dimensionality p, could also be large. Again, we apply the same idea of ISEE,

References

Jerome Friedman, Trevor Hastie, and Robert Tibshirani. Sparse inverse covariance estimation with the graphical lasso. *Biostatistics*, 9(3):432–441, 2008.