Functional Sparse Estimation of Time Varying Graphical Model

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1 Introduction

Graphical models are quite useful in many domains to uncover the dependence structure among observed variables. Typically, we consider a p-dimensional multivariate normal distributed random variable

$$\mathbf{X} = (X_1, \cdots, X_p) \sim \mathbb{N}(\mathbf{0}, \mathbf{\Sigma}),$$

where p is the number of features. Then a useful graph of these p features can be constructed based on there conditional dependence structure. More precisely, we can construct a Gaussian graphical model

$$\begin{aligned}&\mathcal{G} = (V, E), \text{ where } V = \{1, \cdots, p\} \text{ is the set of nodes,}\\ &\text{and } E = \left\{(j,l) | X_j \text{ is conditionally dependent with } X_l, \text{given } X_{V/\{j,l\}}\right\}.\end{aligned}$$

Let $\mathbf{\Omega} = \mathbf{\Sigma}^{-1} = (\omega_{j,l})_{1 \le j,l \le p}$ be the precision matrix. Then X_j and X_l are conditionally dependent given other features if and only if $\omega_{jl} = 0$. Therefore, estimating the covariance matrix and precision matrix of X is equivalent to estimate the structure of Gaussian graphical model $\mathcal{G}$. More discussion can be found in (Lauritzen, 1996).

1.1 Estimation Sparse Precision Matrix $\mathbf{\Omega}$

Given a random sample $\mathbf{X}^{(1)}, \cdots, \mathbf{X}^{(n)}$ of $\mathbf{X}$, we aim to estimate $\mathbf{\Omega}$ and recover its support, i.e. the corresponding undirected Gaussian graph. When $n > p$, a nature estimator of $\mathbf{\Omega}$ can be $\hat{\mathbf{\Omega}}_n = \hat{\mathbf{\Sigma}}_n^{-1}$, where $\hat{\mathbf{\Sigma}}_n = \sum_{k=1}^n (\mathbf{X}^{(k)} - \bar{\mathbf{X}}_n)(\mathbf{X}^{(k)} - \bar{\mathbf{X}}_n)'$ is the sample covariance matrix. In the case $n < p$, which is quite common in the many applications, the estimation of $\mathbf{\Omega}$ is much more challenging since $\hat{\mathbf{\Sigma}}_n$ is no longer invertible.

There are lots of literatures discussing about the estimation of sparse precision matrix $\mathbf{\Omega}$ in high dimension low sample size settings, i.e. $p > n$. Generally speaking, there are three main approaches.

1. **Covariance selection approach.** There is a connection between linear regression and prediction matrix $\mathbf{\Omega}$:

$$\mathbf{X}_j = \mathbf{X}_{-j}\boldsymbol{\beta}_j + \boldsymbol{\varepsilon}_j = \sum_{l \neq j} \mathbf{X}_l \beta_{jl} + \boldsymbol{\varepsilon}_j \tag{1}$$

   It could be shown that $\beta_{jl} = \omega_{jl}/\omega_{jj}$. Thus estimating $\boldsymbol{\beta}_j$ can identify the support of ith row of $\mathbf{\Omega}$. Meinshausen and Bühlmann (2006) applied LASSO penalty (Tibshirani, 1996) on multivariate regression 1 to estimate the support of $\mathbf{\Omega}$ row by row. Peng et al. (2012) considered a joint sparse regression to estimate the support of $\mathbf{\Omega}$ together through an active-shooting algorithm. Yuan (2010) applied Danzig selector (Candes and Tao, 2007) to the problem 1 to estimate each column of $\mathbf{\Omega}$.

2. **Penalized likelihood approach.** Another nature way is to estimate $\mathbf{\Omega}$ is the penalized likelihood approach. The log-likelihood of the parameters in $\mathbf{\Omega}$ is as following:

$$l(\mathbf{X}^(i), 1 \leq i \leq n | \mathbf{\Omega}) = -\mathrm{tr}(\mathbf{\Omega}\hat{\mathbf{\Sigma}}_n) + \log|\mathbf{\Omega}| \tag{2}$$

   In order to have a sparse estimation of $\mathbf{\Omega}$, different penalized likelihood estimator are considered. Yuan and Lin (2007) proposed the *max-det problem* to solve the LASSO-type estimator.

$$\hat{\mathbf{\Omega}}_L = \arg\min \mathrm{tr}(\mathbf{\Omega}\hat{\mathbf{\Sigma}}_n) - \log|\mathbf{\Omega}| + \lambda\|\mathbf{\Omega}\|_1 \tag{3}$$

   and the non-negative garrote-type estimator.

$$\begin{aligned} \hat{\mathbf{\Omega}}_G &= \arg\min \mathrm{tr}(\mathbf{\Omega}\hat{\mathbf{\Sigma}}_n) - \log|\mathbf{\Omega}| + \lambda \sum_{j \neq i} \frac{\omega_{jl}}{\tilde{\omega}_{jl}} \\ \text{subject to } & \frac{\omega_{jl}}{\tilde{\omega_{jl}}} \geq 0, \mathbf{\Omega} \text{ p.d.} \end{aligned} \tag{4}$$

   Banerjee et al. (2008) used a block coordinate descent algorithm to solve (3). And then Friedman et al. (2008) proposed the *graphical lasso* algorithm for (3) based on least square lasso type estimator, which is simple and fast. Rothman et al. (2008) proposed the sparse permutation invariant covariance estimator (SPICE) which could extend to the ℓ_q-type penalized likelihood estimator. Fan et al. (2009), Lam et al. (2009) studied the penalized likelihood estimator with the smoothly clipped absolute deviation (SCAD) penalty and the adaptive LASSO penalty.

3. ℓ_1 **constrained minimization approach.** Cai et al. (2011) performed a constrained ℓ_1 minimization approach to estimate sparse precision matrix (CLIME).

$$\begin{aligned} \hat{\mathbf{\Omega}}_C &= \arg\min \|\mathbf{\Omega}\|_1 \\ \text{subject to } &\|\mathbf{\Omega}\hat{\mathbf{\Sigma}} - \mathbf{I}\|_\infty \leq \lambda_n \end{aligned} \tag{5}$$

Cai et al. (2016) proposed adaptive constrained ℓ_1 minimization estimator (ACLIME), which achieved the optimal minimax rate of convergence.

1.2 Heterogeneous Data And Time Varying Graphical Model

The methods aforementioned focus on estimating a single Gaussian graph by assuming samples are identically distributed. However, in many applications it is more realistic to assume that data are heterogeneous due to batch effects or latent factors. Guo et al. (2011) reparameterized the off-diagonal entry $\omega_{jl} = \theta_{jl}\gamma_{jl}^k$ and estimated them through a penalized likelihood with the hierarchical penalty on common structures θ_{jl} and individual structureγ_{jl}^k. Danaher et al. (2014) propose the *joint graphical lasso*, to estimate multiple graphical models corresponding to distinct but related conditions. The *joint graphical lasso* utilized fussed lasso and group lasso on log-likelihood to force similarity among graphs. Lee and Liu (2015) proposed a method to estimate the common structure and unique structure through the constrained ℓ_1 minimization.

In many cases the sample indexes have orders, e.g. time, and the corresponding graphs evolve through the order. In such cases it could be quite interesting to estimate a time varying graphical model.

$$\mathbf{X}(t) \sim \mathbb{N}(\mathbf{0}, \mathbf{\Sigma}(t)) \tag{6}$$

Zhou et al. (2010) developed a nonparametric framework for estimating time varying graphical model by kernel smoothing and ℓ_1 panelty. Zhou's model assumed that the observations X^t are independent and changed smoothly.

$$\begin{aligned} \hat{\mathbf{\Omega}}(\tau) &= \arg\min_{\mathbf{\Omega}} \left\{ \text{tr}(\mathbf{\Omega}\hat{\mathbf{\Omega}}(\tau)) - \log|\mathbf{\Omega}| + \lambda\|\mathbf{\Sigma}^-\|_1 \right\} \\ \text{where } \hat{\mathbf{\Omega}}(\tau) &= \sum_i \omega_i^\tau \mathbf{X}^i (\mathbf{X}^i)', \text{and } \omega_i^\tau = \frac{K_h(t_i - \tau)}{\sum_{i'} K_h(t_{i'} - \tau)} \end{aligned} \tag{7}$$

Lu et al. (2015) proposed a dynamic nonparanormal graphical model, which is more robust, by estimating a weighted Kendall's tau correlation matrix. These approaches generated estimation of similar graphs by weighting the samples among different times.

1.3 Varying Coefficient Model And Sparse Derivatives

If we are interested in estimating a dynamic graph which is smoothing over a time region, a functional model which consider each feature as functional data over time is very attractive. Since the structure of Gaussian graph can be recovered though regression approach, we can consider dynamic graphical model under the context of varying coefficient model (Hastie and Tibshirani, 1993; Fan and Zhang, 2008). Typically, we are interested in the basis expansion approach to estimate the varying coefficient models (Huang et al., 2002, 2004).

$$Y(t) = X(t)^T \boldsymbol{\beta}(t) + \varepsilon(t)$$

Then we are looking at the following model

$$X_j(t) = \mathbf{X}'_{-j}(t)\boldsymbol{\beta}_j(t) + \varepsilon_j(t) = \sum_{l \neq j} X_l(t)\beta_{jl}(t) + \varepsilon_j(t). \tag{8}$$

Assume that we collect sample at $t_1, \cdots, t_n$, denote $X_j^i = X_j(t_i)$. Kolar et al. (2009, 2010); Kolar and Xing (2011, 2012) proposed a local linear regression approach with "kernel ℓ_1" penalty to estimate the smoothly varying graph,

$$\hat{\boldsymbol{\beta}}_j(\tau) = \arg\min_{\boldsymbol{\beta} \in \mathbb{R}^{p-1}} \sum_i (X_j^i - \sum_{l \neq j} X_l^i \beta_l)^2 \omega_i^\tau + \lambda |\boldsymbol{\beta}|_1 \tag{9}$$

and total variation penalty to estimate graph with jumps.

$$\left\{\hat{\boldsymbol{\beta}}_j(t_1), \cdots, \hat{\boldsymbol{\beta}}_j(t_n)\right\} = \arg\min_{\boldsymbol{\beta}(t_i), i \leq n} \sum_i (X_j^i - \sum_{l \neq j} X_l^i \beta_l(t_i))^2 + \lambda_1 \sum_i |\boldsymbol{\beta}(t_i)|_1 + \lambda_2 \sum_{i=2}^n |\boldsymbol{\beta}(t_i) - \boldsymbol{\beta}(t_{i-1})|_1 \tag{10}$$

Moreover, in order to estimate a sparse graph, we need to gain sparse functional coefficient $\boldsymbol{\beta}(t)$. Based on the idea of FLiRTI in James, Wang and Zhu's paper James et al. (2009), we put penalty on the derivative matrices of $\boldsymbol{\beta}(t)$. Kim et al. (2009) also put the l_1 penalty on derivative of coefficient function in the trend filtering problem. Tibshirani et al. (2014) applied the generalized lasso (Tibshirani and Taylor, 2011) to solve the optimization problem in the trendfilter. We will apply similar algorithm to solve our optimization problem.

2 Methodology

2.1 Functional Undirected Graph

Consider p smooth functional continuous variables $\{X_1(t), X_2(t) \cdots, X_p(t)\}$ on the 'time' domain $\mathcal{T}$. On each t, we assume

$$(X_1(t), X_2(t) \cdots, X_p(t)) \sim \mathbb{N}(\mathbf{0}, \boldsymbol{\Sigma}(t)).$$

Define the undirected graph

$$\begin{aligned} G(t) &= \{V, E(t)\}, \text{ where } V = \{1, \cdots, p\}, \\ \text{and } E(t) &= \left\{(j,l) \in V^2 : \text{Cov}\left[X_j(t), X_l(t) | X_k(t), k \neq j, l\right] \neq 0, j \neq l\right\}. \end{aligned} \tag{11}$$

Namely, $G(t)$ is the Gaussian graphical model at each t. This model is quite flexible, which allows $G(t)$ evolve over time and includes the time dependence. Assume that data are observed at $t_1, \cdots, t_n$ and at each time point t we have n_t samples.

2.2 Functional Nearest Neighborhood Selection

Consider the following functional linear model

$$\begin{aligned} X_j^r(t) &= \mathbf{X}_{-j}^r(t)^T \boldsymbol{\beta}_j(t) + \varepsilon_j^r(t) = \sum_{l \neq j} X_l^r(t)\beta_{jl}(t) + \varepsilon_j^r(t), \\ \text{where } \mathbf{X}_{-j}^r(t) &= (X_l^r(t))_{l \neq j} \in \mathbb{R}^{(p-1)\times 1}, r = 1, \cdots, n_t, t = t_1, \cdots, t_n, j = 1, \cdots, p. \end{aligned} \tag{12}$$

For each functional coefficient $\beta_{jl}(t)$, we consider the basis $\mathbf{B}_{jl}(t) = (B_{jl1}(t), \cdots, B_{jlk_{jl}}(t))$ and then

$$\beta_{jl}(t) = \sum_{s=1}^{k_{jl}} B_{jls}(t)\gamma_{jls} + e_{jl}(t) = \mathbf{B}_{jl}(t)\boldsymbol{\gamma}_{jl}$$

Thus Equation (12) can be represented as

$$\begin{aligned} X_j^r(t) &= \sum_{l \neq j} \sum_{s=1}^{k_{jl}} X_l^r(t) B_{jls}(t)\gamma_{jls} + \tilde{\varepsilon}^r(t), \\ \text{where } \tilde{\varepsilon}^r(t) &= \sum_{l \neq j} X_l^r(t) e_{jl}^r(t) + \varepsilon^r(t), r = 1, \cdots, n_t, t = t_1, \cdots, t_n, j = 1, \cdots, p. \end{aligned} \tag{13}$$

As seen in Equation (13), our model is quite flexible since the basis of each functional coefficient can be different.

To get the matrix form of Equation (13), denote

$$\begin{aligned}
&\mathbf{B}(t) = \text{diag}\{\mathbf{B}_{jl}(t)\} \in \mathbb{R}^{(p-1)\times\sum_{l\neq j} k_{jl}},\\
&\mathbf{U}_j^r(t) = \mathbf{B}(t)^T X_{-j}^r(t) \in \mathbb{R}^{\sum_{l\neq j} k_{jl}\times 1},\\
&\mathbf{U}_j(t) = (\mathbf{U}_j^1(t), \cdots, \mathbf{U}_j^{n_t}(t))^T \in \mathbb{R}^{n_t\times\sum_{l\neq j} k_{jl}},\\
&\mathbf{U}_j = (\mathbf{U}_j(t_1), \cdots, \mathbf{U}_j(t_n))^T \in \mathbb{R}^{\sum_{t=1}^n n_t\times\sum_{j\neq i} k_{jl}},\\
&\mathbf{X}_j(t) = (X_j^1(t), \cdots, X_j^{n_t}(t))^T \in \mathbb{R}^{n_t\times 1},\\
&\mathbf{X}_j = (X_j(t_1), \cdots, X_j(t_n))^T \in \mathbb{R}^{\sum_{t=1}^n n_t\times 1},\\
&\boldsymbol{\varepsilon}_j(t) = (\varepsilon_j^1(t), \cdots, \varepsilon_j^{n_t}(t))^T \in \mathbb{R}^{n_t\times 1},\\
&\boldsymbol{\varepsilon}_j = (\varepsilon_j(t_1), \cdots, \varepsilon_j(t_n))^T \in \mathbb{R}^{\sum_{t=1}^n n_t\times 1},\\
&\boldsymbol{\gamma}_j = (\boldsymbol{\gamma}_{jl})_{l\neq j} \in \mathbb{R}^{\sum_{l\neq j} k_{jl}\times 1}.
\end{aligned}$$

Then the Equation (13) can be expressed as

$$\mathbf{X}_j = \mathbf{U}_j\boldsymbol{\gamma}_j + \boldsymbol{\varepsilon}_j, j = 1, \cdots, p. \tag{14}$$

2.3 Control The Sparsity Of Derivatives

In Model (14), we want to estimate a sparse graph and interpretable coefficient functions. For each i and $l \neq j$, we want to control the sparsity of $\beta_{jl}^{(m)} = \frac{\mathrm{d}^\mathrm{m}}{\mathrm{d}t^m}\beta_{jl}(t) \approx \frac{\mathrm{d}^\mathrm{m}}{\mathrm{d}t^m}\mathbf{B}_{jl}(t)^T\boldsymbol{\gamma}_{jl}$ for some m. Say assume $\beta_{jl}^{(0)}(t) = 0$ and $\beta_{jl}^{(2)}(t) = 0$ in large area, then $\beta_{jl}(t)$ is zero in many region and linear in the left regions.

Let

$$\mathbf{A}_{jl} = \begin{bmatrix} D^m\mathbf{B}_{jl}(t_1) & \cdots & D^m\mathbf{B}_{jl}(t_n)\end{bmatrix}^T \in \mathbb{R}^{n\times k_{jl}}, \tag{15}$$

where D^m is the mth finite difference operator, i.e., $D\mathbf{B}_{jl}(t_k) = [\mathbf{B}_{jl}(t_k) - \mathbf{B}_{jl}(t_{k-1})]/[t_k - t_{k-1}]$, $D^2\mathbf{B}_{jl}(t_k) = [D\mathbf{B}_{jl}(t_k) - D\mathbf{B}_{jl}(t_{k-1})]/[t_k - t_{k-1}]$, etc.

Next, set

$$\boldsymbol{\eta}_{jl} = \mathbf{A}_{jl}\boldsymbol{\gamma}_{jl} \in \mathbb{R}^{n\times 1} \tag{16}$$

Then $\boldsymbol{\eta}_{jl} \approx (\beta_{jl}^{(m)}(t_k))_{1\leq k\leq n}$. Moreover, we denote

$$\begin{aligned}
\boldsymbol{\eta}_j = (\boldsymbol{\eta}_{jl})_{l\neq j} = \mathbf{A}_j\boldsymbol{\gamma}_j \in \mathbb{R}^{n(p-1)},\\
\text{where } \mathbf{A}_j = \text{diag}(\mathbf{A}_{jl})_{l\neq j} \in \mathbb{R}^{n(p-1)\times\sum_{l\neq j} k_{jl}}.
\end{aligned} \tag{17}$$

We want to put the sparsity penalty on the $\boldsymbol{\eta}_j$. Then Model 14 can be expressed as the following optimization problem, which is a generalized lasso problem.

$$\begin{aligned}
\hat{\boldsymbol{\gamma}}_{j,L} &= \arg\min_{\boldsymbol{\gamma}_j} \frac{1}{2}\|\mathbf{X}_j - \mathbf{U}_j\boldsymbol{\gamma}_j\|_2^2\\
\text{subject to } \|\boldsymbol{\eta}_j\|_1 &= \|\mathbf{A}_j\boldsymbol{\gamma}_j\|_1 \leq t\\
\text{i.e. } \hat{\boldsymbol{\gamma}}_{j,L} &= \arg\min_{\boldsymbol{\gamma}_j} \frac{1}{2}\|\mathbf{X}_j - \mathbf{U}_j\boldsymbol{\gamma}_j\|_2^2 + \lambda\|\mathbf{A}_j\boldsymbol{\gamma}_j\|_1
\end{aligned} \tag{18}$$

Moreover, if we want to control the sparsity of multiple derivatives of $\boldsymbol{\beta}_{jl}(t)$, say we want both $\boldsymbol{\beta}_{jl}^{(0)}(t) = 0$ and $\boldsymbol{\beta}_{jl}^{(2)}(t) = 0$ in large area.

There is a connection between Model 18 and fused lasso.

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