Functional Sparse Estimation of Time Varying Graphical Model

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Overview

- Introduction
- Sparse Gaussian Graphical Model Estimation
 - Neighborhood Selection Approach
 - Penalized Likelihood Estimation Approach
 - ullet Constrained ℓ_1 Minimization Approach
- 3 Heterogeneous Data And Joint Estimation Of Multiple Graphs
- 4 Time Varying Graphical Model
 - Varying Coefficient Model
 - Functional Coefficient Model
- Simulation Study



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- Classification and discriminant analysis.
- Applications: portfolio optimization, speech recognition and genomics.
- Graphical Model: recovering the structure of undirected Gaussian graph is equivalent to the support of the precision matrix.

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 - $e_{jl} \in E$ if and only if $\rho^{jl} \neq 0$
 - $e_{jl} \in E$ if and only if $\omega_{jl} \neq 0$
- Estimation of ${\cal G}$ is equivalent to recover the non-zero entry of the precision matrix $\Omega.$

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- When n < p, the estimation of Ω becomes much more challenging due to singularity of $\hat{\Sigma}_n$.

Connection between linear regression and prediction matrix $\pmb{\Omega}$: For each $j \in \{1, \cdots, n\}$

$$\mathbf{X}_{j} = \mathbf{X}_{-j}\beta_{j} + \varepsilon_{j} = \sum_{l \neq j} \mathbf{X}_{l}\beta_{jl} + \varepsilon_{j}$$
 (1)

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- Select the non-zero entry for jth row of Ω is equivalent to the multivariate regression problem (1).

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- Graph structures can be recovered consistently in a high dimension settings. (Meinshausen and Bühlmann, 2006; Peng et al, 2012)

Another nature way is to estimate Ω is the penalized likelihood approach.

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- 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.

Constrained ℓ_1 Minimization Approach

• Cai et al. (2011) performed a constrained I1 minimization approach to estimate sparse precision matrix (CLIME).

$$\begin{split} \hat{\Omega}_1 &= \arg\min \|\Omega\|_1, \text{subject to:} \\ |\Sigma_n^* \Omega - \mathbf{I}|_{\infty} &\leq \tau_n \end{split} \tag{3}$$

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• Problem 3 can be decomposed to *p* vector-minimization problem:

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 Cai et al. (2016) proposed adaptive constrained I1 minimization estimator (ACLIME), which achieved the optimal minimax rate of convergence.

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- Data are heterogeneous with *p* variables and *G* groups.
 - $\mathbf{X}_{i}^{(g)} = (X_{i,1}^{(g)}, X_{i,2}^{(g)}, \cdots, X_{i,p}^{(g)}) \sim \mathcal{N}(0, \Sigma^{(g)}), i = 1, \dots, n_g; g = 1, \dots, G.$

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 - $\{\Omega\} = \{\Omega^{(g)} = (\Sigma^{(g)})^{-1} | g = 1 \cdots G\}$

Joint penalized likelihood of multiple precision matrices

$$\left\{\hat{\Omega}\right\} = \underset{\left\{\Omega\right\}}{\operatorname{arg\,min}} \sum_{g=1}^{G} n_g \left[\operatorname{tr}(\Omega^{(g)} \hat{\Sigma}^g) - \log |\Omega^{(g)}| \right] + P(\left\{\Omega\right\}) \tag{4}$$

• Guo et al. (2011) employs a non-convex penalty called hierarchical group penalty: $P(\{\Omega\}) = \lambda \sum_{j \neq l} \left(\sum_{g=1}^{G} |\omega_{jl}^{(g)}| \right)^{1/2}$

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- Honorio and Samaras (2012) adopts a convex penalty, $P(\{\Omega\}) = \lambda \sum_{j \neq l} |\omega_{jl}^{(1)}, \cdots, \omega_{jl}^{(G)}|_q$.
- Danaher et al. (2014) considered a fused lasso penalty, $P(\{\Omega\}) = \lambda_1 \sum_{j \neq l} \sum_{g=1}^G |\omega_{jl}^{(g)}| + \lambda_2 \sum_{g < g'} \sum_{jl} |\omega_{jl}^{(g)} \omega_{jl}^{(g')}|.$



• Lee and Liu (2015) decomposed $\{\Omega\}$ into the common structure $M=\frac{1}{G}\sum_{g}\Omega^{(g)}$ and the individual structure $R^{(g)}=\Omega^{(g)}-M$, and applied constrained ℓ_1 minimization to estimate the parameters.

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Time Varying Graphical Model

It is not unusual that the index of groups of samples have a order. A common situation is that the data are collected by time order.

- $X(t) \sim (0, \Sigma(t)), t = t_1, \ldots, t_n$.
 - Denote $\mathbf{X}^i = \mathbf{X}(t_i), i = 1, \cdots, n$.
- Dynamic graph: G(t) = (V, E(t))
 - $V = \{1, \cdots, p\}.$
 - $E(t) = \{(j, l) \in V^2 : \text{Cov}[X_j(t), X_l(t)|X_k(t), k \neq j, l] \neq 0, j \neq l\}.$

Time Varying Graphical Model: Penalized likelihood estimation

Zhou (2010) developed a nonparametric framework for estimating time varying graphical model by kernel smoothing and ℓ_1 penalty.

$$\hat{\Omega}(\tau) = \arg\min_{\Omega} \left\{ \operatorname{tr}(\Omega \hat{\Sigma}(\tau)) - \log |\Omega| + \lambda \|\Sigma^{-}\|_{1} \right\}$$
where
$$\hat{\Omega}(\tau) = \sum_{i} \omega_{i}^{\tau} \mathbf{X}^{i} (\mathbf{X}^{i})', \text{ and } \omega_{i}^{\tau} = \frac{K_{h}(t_{i} - \tau)}{\sum_{i'} K_{h}(t_{i'} - \tau)}$$
(5)

Time Varying Graphical Model And Varying Coefficient Model

- ullet Dynamic partial correlation coefficient $ho_{jl}(t) = -\omega_{jl}(t)/\sqrt{\omega_{jj}(t)\omega_{ll}(t)}$
- Dynamic neighborhood selection:

$$X_{j}(t) = \mathbf{X}'_{-j}(t)\beta_{j}(t) + \varepsilon_{j}(t) = \sum_{l \neq j} X_{l}(t)\beta_{jl}(t) + \varepsilon_{j}(t).$$
 (6)

- Varying coefficient model (Hastie and Tibshirani, 1993)
- Kolar et al. (2009, 2010); Kolar and Xing (2011) proposed a local linear regression approach with kernel ℓ_1 penalty to estimate the smoothly varying graph,

$$\hat{\beta}_{j}(\tau) = \underset{\beta \in \mathbb{R}^{p-1}}{\min} \sum_{i} (X_{j}^{i} - \sum_{l \neq i} X_{l}^{i} \beta_{l})^{2} \omega_{i}^{\tau} + \lambda |\beta|_{1}$$
 (7)

Time Varying Graphical Model And Varying Coefficient Model

• Kolar et al. (2009, 2010); Kolar and Xing (2011, 2012) proposed a combination of ℓ_1 and fused lasso penalty to estimate graph with jump.

$$\left\{\hat{\beta}_{j}(t_{1}), \cdots, \hat{\beta}_{j}(t_{n})\right\} = \arg\min_{\beta(t_{i}), i \leq n} \sum_{i} (X_{j}^{i} - \sum_{l \neq j} X_{l}^{i} \beta_{l}(t_{i}))^{2} + \lambda_{1} \sum_{i} |\beta(t_{i})|_{1} + \lambda_{2} \sum_{i=2}^{n} |\beta(t_{i}) - \beta(t_{i-1})|_{1}$$
(8)

Time Varying Graphical Model And Functional Coefficient Model: Motivation

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 Apply local linear regression on the model (7) can only get the estimation on input time point.

Use basis expansion to estimate $\beta_j(t)$ directly.

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Limitation of aforementioned method:

- Apply local linear regression on the model (7) can only get the estimation on input time point.
- The assumption in the model (8) of the coefficient is piecewise constant is usually not realistic.

Use basis expansion to estimate $\beta_i(t)$ directly.

• Assuming data are collected at t_1, \dots, t_n , and at each time point t, we have n_t replicates (Huang et al, 2004).

$$X_{j}^{r}(t) = \mathbf{X}_{-j}^{r}(t)'\beta_{j}(t) + \varepsilon_{j}^{r}(t)$$

$$= \sum_{l \neq j} X_{l}^{r}(t)\beta_{jl}(t) + \varepsilon_{j}^{r}(t), \qquad (9)$$

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- $\bullet \ \ t=t_1,\cdots,t_n, j=1,\cdots,p.$
- ullet For each t, let $\mathbf{X}_j(t) = (X_j^1(t), \cdots, X_j^{n_t}(t))^T \in \mathbb{R}^{n_t imes 1}$, then

$$\mathbf{X}_{j}(t) = \mathbf{X}_{-j}(t)'\beta_{j}(t) + \varepsilon_{j}(t)$$

$$= \sum_{l \neq i} \mathbf{X}_{l}(t)\beta_{jl}(t) + \varepsilon_{j}(t), \qquad (10)$$

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

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

- $\beta_j(t) = \mathbf{B}(t)\gamma_j + \mathbf{e}_j(t) = (\beta_{jl}|j \neq l) \in \mathbb{R}^{p-1}$
 - $\mathbf{B}(t) = \operatorname{diag}\left\{\mathbf{B}_{jl}(t)\right\} \in \mathbb{R}^{(p-1) \times \sum_{l \neq j} k_{jl}}$
 - $\gamma_i = (\gamma_{il})_{l \neq i} \in \mathbb{R}^{\sum_{l \neq j} k_{jl} \times 1}$
 - $\mathbf{e}(t) = (\mathbf{e}_{jl}|j \neq l) \in \mathbb{R}^{p-1}$

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$$\begin{aligned} \mathbf{X}_{j}(t) &= \mathbf{X}_{-j}(t)\mathbf{B}_{j}(t)\gamma_{j} + \tilde{\varepsilon}(t) \\ &= \mathbf{U}(t)\gamma_{j} + \tilde{\varepsilon}(t), \\ \text{where } \mathbf{U}(t) &= \mathbf{X}_{-j}(t)\mathbf{B}_{j}(t) \in \mathbb{R}^{\sum_{t=1}^{n} n_{t} \times \sum_{j \neq i} k_{jl}}, \\ \tilde{\varepsilon}(t) &= \mathbf{X}_{-j}(t)\mathbf{e}_{j}(t) + \varepsilon(t) \\ &= \sum_{l \neq j} \mathbf{X}_{l}(t)e_{jl}(t) + \varepsilon(t), \\ t &= t_{1}, \cdots, t_{n}, j = 1, \cdots, p. \end{aligned}$$

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$$(11)$$

As seen in Equation (11), our model is quite flexible since the basis of each functional coefficient can be different.

Combing the data from t_1, \dots, t_n , we can get

$$\mathbf{X}_{j} = \mathbf{U}_{j}\gamma_{j} + \tilde{\varepsilon}_{j}, j = 1, \cdots, p.$$
where
$$\mathbf{X}_{j} = (X_{j}(t_{1})', \cdots, X_{j}(t_{n})')' \in \mathbb{R}^{\sum_{t=1}^{n} n_{t} \times 1}$$

$$\mathbf{U}_{j} = (\mathbf{U}_{j}(t_{1})', \cdots, \mathbf{U}_{j}(t_{n})')' \in \mathbb{R}^{\sum_{t=1}^{n} n_{t} \times \sum_{j \neq i} k_{jl}}$$

$$\tilde{\varepsilon}_{j} = (\tilde{\varepsilon}_{j}(t_{1}), \cdots, \tilde{\varepsilon}_{j}(t_{n}))^{T} \in \mathbb{R}^{\sum_{t=1}^{n} n_{t} \times 1}$$

$$(12)$$

For each j, least square of γ_j in the model 12 is

$$I(\gamma_j) = (\mathbf{X}_j - \mathbf{U}_j \gamma_j)' \mathbf{W} (\mathbf{X}_j - \mathbf{U}_j \gamma_j)$$

$$= \sum_{i=1}^n (\mathbf{X}_j(t_i) - \mathbf{U}_j(t_i) \gamma_j)^2 w_i$$

$$= \sum_{i=1}^n (\mathbf{X}_j(t_i) - \mathbf{X}_{-j}(t_i) \beta_j(t_i))^2 w_i$$

In Model (12), we want to estimate a sparse graph and interpretable coefficient functions.

• For each j and $l \neq j$, put ℓ_1 penalty on $\beta_{jl}^{(m)} = \frac{\mathrm{d}^{\mathrm{m}}}{\mathrm{d}t^m}\beta_{jl}(t) \approx \frac{\mathrm{d}^{\mathrm{m}}}{\mathrm{d}t^m}\mathbf{B}_{jl}(t)\gamma_{jl}$ for some m.

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- 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 $\mathbf{A}^{(m)}(t) = \frac{\mathrm{d}^{\mathrm{m}}}{\mathrm{d}t^{m}} \mathbf{B}(t) \in \mathbb{R}^{(p-1) \times \sum_{l \neq j} k_{jl}}$ and $\mathbf{A}^{(m)} = (\mathbf{A}^{(m)}(t_1)', \cdots, \mathbf{A}^{(m)}(t_n)')' \in \mathbb{R}^{n(p-1) \times \sum_{l \neq j} k_{jl}}$

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The penalty for Model (12) is

$$p(\gamma_j) = \lambda_0 |\mathbf{A}^{(0)} \gamma_j|_1 + \lambda_m |\mathbf{A}^{(m)} \gamma_j|_1$$

= $\sum_{i=1}^n \lambda_0 |\beta_j^{(0)}(t_i)|_1 + \sum_{i=1}^n \lambda_2 |\beta_j^{(m)}(t_i)|_1$

Functional Coefficient Model: Optimization Problem

The optimization problem for Model (12) with sparse coefficient derivatives:

$$\mathcal{J}(\gamma_{j}) = I(\gamma_{j}) + p(\gamma_{j})$$

$$= (\mathbf{X}_{j} - \mathbf{U}_{j}\gamma_{j})'\mathbf{W}(\mathbf{X}_{j} - \mathbf{U}_{j}\gamma_{j}) + \lambda_{0}|\mathbf{A}^{(0)}\gamma_{j}|_{1} + \lambda_{m}|\mathbf{A}^{(m)}\gamma_{j}|_{1}$$

$$= \sum_{i=1}^{n} (\mathbf{X}_{j}(t_{i}) - \mathbf{X}_{-j}(t_{i})\beta_{j}(t_{i}))^{2}w_{i} +$$

$$\sum_{i=1}^{n} \lambda_{0}|\beta_{j}^{(0)}(t_{i})|_{1} + \sum_{i=1}^{n} \lambda_{m}|\beta_{j}^{(m)}(t_{i})|_{1}$$
(13)

This is a generalized lasso optimization problem (Tibshirani, 2011).

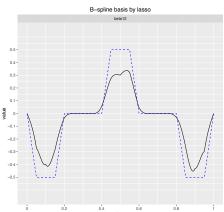
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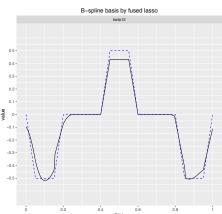
Simulation





Simulation





Simulation



