

# MATRIX ESTIMATION BASED ON SIMULTANEOUS CONFIDENCE INTERVALS

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**BIRS, January 20, 2011**

**Thanks for the invitation!**

We derive methods of learning population covariance and correlation matrices and their inverses based on simultaneous confidence intervals. The performance of these methods will be compared with the Lasso in selection consistency and estimation under the spectrum norm.

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## THE PROBLEM

- Data:  $\mathbf{x}_i$  iid from  $N(0, \boldsymbol{\Sigma}) \in \mathbb{R}^p$ ,  $i \leq n$
- Problem: estimation of the precision matrix  $\boldsymbol{\Theta} = \boldsymbol{\Sigma}^{-1}$
- Difficulty: For  $p > n$ ,  $\widehat{\boldsymbol{\Sigma}} = \mathbf{X}'\mathbf{X}/n$  is singular
- Sparsity: the sparsity of  $\boldsymbol{\Theta} = (\theta_{jk})_{p \times p}$ ;

$S = \{(j, k) : j \neq k, \theta_{jk} \neq 0\}$  is not too large

- Scale:  $\|\boldsymbol{\Sigma}\|_{2,2} + \|\boldsymbol{\Theta}\|_{2,2} = O(1)$
- Maximum note degree:  $d = \max_j \#\{k : \theta_{jk} \neq 0\} \ll n/\log p$
- Estimation error measure: spectrum norm  $\|\widehat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}\|_{2,2}$
- Graphical model selection:  $\widehat{S} = S$

## GLASSO: $\ell_1$ PENALIZED MLE OF $\boldsymbol{\Theta} = \boldsymbol{\Sigma}^{-1}$

- G-Lasso: With  $D = \{(j, k) : j = k\}$ ,

$$\widehat{\boldsymbol{\Theta}} = \arg \min_{\boldsymbol{\Theta}} \left\{ \text{trace}(\boldsymbol{\Theta} \widehat{\boldsymbol{\Sigma}}) - \log \det(\boldsymbol{\Theta}) + \lambda \|\boldsymbol{\Theta}_{D^c}\|_1^{(\text{vec})} \right\}$$

- $\ell_1$  penalized MLE
- Yuan and Lin (2007), Friedman, Hastie and Tibshirani (2008, GLasso), Rothman-Bickel-Levina-Zhu (2008, SPICE), Ravikumar et al (2008a,b), ... Lam-Fan (2007)

Rothman *et al* (2008), Ravikumar *et al* (2008b):

- Let  $\lambda = C\sqrt{(\log p)/n}$
- Error bound in the Frobenius norm

$$\|\widehat{\Theta} - \Theta\|_2^{(\text{vec})} = O_P(1)\sqrt{(|S| + p)(\log p)/n}$$

- A modification gives an error bound in the  $\ell_2$  operator norm

$$\|\widehat{\Theta} - \Theta\|_{2,2} = O_P(1)\sqrt{|S|(\log p)/n}$$

- The result for  $\|\cdot\|_2^{(\text{vec})}$  is of sharp order, but not  $\|\cdot\|_{2,2}$
- $\lambda = C\sqrt{(\log p)/n}$ ;  $C = ?$

## CONNECTIONS TO LINEAR REGRESSION

Let  $(X_1, \dots, X_p) \sim N(0, \Sigma)$  and  $\Theta = \Sigma^{-1}$ .

- Partial correlation:

$$\text{Corr}(X_j, X_k | X_\ell, \ell \neq j, \ell \neq k) = -\theta_{jk}/\{\theta_{jj}\theta_{kk}\}^{1/2}$$

- Linear model:

$$X_j | (X_k, k \neq j) \sim N\left(\sum_{k \neq j} \beta_{jk} X_k, \sigma_j^2\right),$$

$$\beta_{jk} = -\theta_{jk}/\theta_{jj}, \quad \sigma_j^2 = 1/\theta_{jj}$$

- One may piece together estimates in the  $p$  linear regression models to produce an estimate of  $\Theta$
- Need to estimate both  $\sigma_j$  and  $\beta_{-j} = (\beta_{jk}, k \neq j)'$

## COLUMN-BY-COLUMN P-LINEAR REGRESSIONS:

- Städler, Bühlmann and van de Geer (2010): PMLE

$$\{\hat{\boldsymbol{\beta}}_{-j}, \hat{\sigma}_j\} = \arg \min_{\boldsymbol{\beta}, \sigma} \left\{ \frac{\|\mathbf{x}_j - \mathbf{X}_{-j}\boldsymbol{\beta}_{-j}\|^2}{2\sigma_j^2 n} - \log \sigma_j + \lambda_0 \frac{\|\boldsymbol{\beta}_{-j}\|_1}{\sigma_j} \right\}.$$

This is a convex minimization problem in  $\{\boldsymbol{\beta}_{-j}/\sigma_j, 1/\sigma_j\}$

- Since  $\theta_{jk} = -\beta_{jk}/\sigma_j^2$  and  $\theta_{jj} = 1/\sigma_j^2$ ,

$$(\hat{\theta}_{jk}, k \neq j)' = -\hat{\boldsymbol{\beta}}_{-j}/\hat{\sigma}_j^2, \quad \hat{\theta}_{jj} = 1/\hat{\sigma}_j^2$$

- $\|\hat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}\|_{2,2} \leq \|\hat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}\|_{\infty, \infty} = \|\hat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}\|_{1,1} = \max_j \|\hat{\boldsymbol{\theta}}_j - \boldsymbol{\theta}_j\|_1$

## COLUMN-BY-COLUMN P-LINEAR REGRESSIONS:

- Analysis: For  $\lambda_0 = 2\sqrt{(\log p)/n}$ ,

$$\|\widehat{\boldsymbol{\beta}}_{-j}/\widehat{\sigma}_j - \boldsymbol{\beta}_{-j}/\sigma_j\|_1 \lesssim \|\boldsymbol{\beta}_{-j}\|_0 \lambda_0, \quad |\widehat{\sigma}_j/\sigma_j - 1| \asymp \lambda_0 \|\boldsymbol{\beta}_{-j}/\sigma_j\|_1$$

- Since  $\widehat{\theta}_{jk} = -\widehat{\beta}_{jk}/\widehat{\sigma}_j^2$  and  $\widehat{\theta}_{jj} = 1/\widehat{\sigma}_j^2$ ,

$$\|\widehat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}\|_{2,2} \leq \max_j \|\widehat{\boldsymbol{\theta}}_j - \boldsymbol{\theta}_j\|_1 \lesssim \lambda_0(d + \|\boldsymbol{\Theta}\|_{\infty,\infty}^2)$$

- Is  $d\lambda_0$  optimal under the assumption  $\|\boldsymbol{\Theta}\|_{\infty,\infty} = O(1)$ ?
- Is  $\|\widehat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}\|_{2,2} \lesssim \sqrt{d(\log p)/n}$  possible?

## COLUMN-BY-COLUMN P-LINEAR REGRESSIONS:

- Alternative analysis:  $\|\hat{\beta}_{-j} - \beta_{-j}\|_q \leq (1 + 1/\sqrt{2})\hat{\sigma}_j\lambda_0/CIF_q$ ,

$$CIF_q = \inf_{cone} \frac{\|\mathbf{X}'_{-j} \mathbf{X}_{-j} \mathbf{u}\|_\infty |S_{-j}|^{1/q}}{n \|\mathbf{u}\|_q}$$

with  $S_{-j} = \{k : k \neq j, \theta_{jk} \neq 0\}$

- $\max_j(1/CIF_\infty) \approx \|\Theta\|_{\infty,\infty} = O(1)$
- $\|\hat{\beta}_{-j} - \beta_{-j}\|_\infty \lesssim \sqrt{(\log p)/n}$
- Compatibility/restricted eigenvalues: van der Geer (2007), Bickel et al (2009), ...

Cai, Liu and Luo (2010, CLIME):

$$\min \|\boldsymbol{\theta}\|_1 \text{ subj to } \|\widehat{\boldsymbol{\Sigma}}\boldsymbol{\theta}_j - \mathbf{e}_j\|_\infty \leq \lambda$$

If  $\max_j \|(\widehat{\boldsymbol{\Sigma}} - \boldsymbol{\Sigma})\boldsymbol{\theta}_j\|_\infty \leq \lambda$ , then

$$\max_j \|\widehat{\boldsymbol{\theta}}_j - \boldsymbol{\theta}_j\|_1 = O(\|\boldsymbol{\Theta}\|_{\infty,\infty})\lambda d$$

- $\lambda = C\sqrt{(\log p)/n}$ ;  $C \propto \|\boldsymbol{\Theta}\|_{\infty,\infty}$

## GMACS (GRAPHICAL MAXIMUM ABSOLUTE CONTROL SELECTOR)

- Given symmetric data matrix  $\widehat{\mathbf{M}}$ ,

$$\min \|\boldsymbol{\Theta}\|_{\infty,\infty} \text{ subject to } \|\boldsymbol{\Theta}\widehat{\mathbf{M}} - \mathbf{I}\|_{\infty}^{(\text{vec})} \leq \lambda(\boldsymbol{\Theta})$$

- Convex minimization for fixed  $\lambda$ ; General  $\lambda(\boldsymbol{\Theta})$ ?
- Simple uniform bound:

$$\widehat{\boldsymbol{\Theta}} - \boldsymbol{\Theta} = \widehat{\boldsymbol{\Theta}}(\mathbf{I} - \widehat{\mathbf{M}}\boldsymbol{\Theta}) + (\widehat{\boldsymbol{\Theta}}\widehat{\mathbf{M}} - \mathbf{I})\boldsymbol{\Theta}$$

In the event  $\|\boldsymbol{\Theta}\widehat{\mathbf{M}} - \mathbf{I}\|_{\infty}^{(\text{vec})} \leq \lambda(\boldsymbol{\Theta})$  (feasibility of  $\boldsymbol{\Theta}$ ),

$$\|\widehat{\boldsymbol{\Theta}}\|_{\infty,\infty} \leq \|\boldsymbol{\Theta}\|_{\infty,\infty}$$

$$\|\widehat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}\|_{\infty}^{(\text{vec})} \leq \lambda(\boldsymbol{\Theta})\|\widehat{\boldsymbol{\Theta}}\|_{\infty,\infty} + \lambda(\widehat{\boldsymbol{\Theta}})\|\boldsymbol{\Theta}\|_{\infty,\infty}$$

- $\lambda(\widehat{\boldsymbol{\Theta}}) \leq \lambda(\boldsymbol{\Theta})?$

- Let  $\boldsymbol{\Theta} = \boldsymbol{\Sigma}^{-1}$ ,  $\widehat{\mathbf{M}} = \widehat{\boldsymbol{\Sigma}}$  and  $\kappa_\alpha$  satisfy  
 $\sqrt{2}\kappa_\alpha + \log(1 + \sqrt{2}\kappa_\alpha) = (n/2)\log(p(p+1)/\alpha)$  and  
 $\lambda_\alpha(\boldsymbol{\Theta}) = \kappa_\alpha \sqrt{2 + 2 \max_i \sum_{jj} \max_j \theta_{jj}}$ . Then,

$$\|\boldsymbol{\Theta}\widehat{\mathbf{M}} - \mathbf{I}\|_\infty^{(vec)} \leq \lambda_\alpha(\boldsymbol{\Theta})$$

with at least probability  $1 - \alpha$ . In the same event

$$\|\widehat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}\|_\infty^{(vec)} \leq \lambda(\boldsymbol{\Theta})\|\widehat{\boldsymbol{\Theta}}\|_{\infty,\infty} + \lambda(\widehat{\boldsymbol{\Theta}})\|\boldsymbol{\Theta}\|_{\infty,\infty} = \tau^*$$

- If we threshold  $\widehat{\boldsymbol{\Theta}}$  are level  $\tau^*$ , then for “most” norms  $\|\cdot\|$

$$\|\widehat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}\| \leq 2\tau^* \|\mathbf{1}_{D \cup S}\|$$

- $\tau^* \leq C \sqrt{(\log p)/n}$ ?  $C = ?$

## GMACS: ESTIMATION OF $\boldsymbol{\Sigma}^{-1}$

- If  $\tau^* \leq C\sqrt{(\log p)/n}$  with a known  $C$ , then

$$\|\widehat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}\|_{2,2} \lesssim \|\mathbf{1}_{D \cup S}\|_{2,2} \sqrt{(\log p)/n}$$

- This will give a better rate

$$\sqrt{d} \leq \|\mathbf{1}_{D \cup S}\|_{2,2} = \max_{\|\mathbf{u}\|=1} \sum_{(j,k) \in S \cup D} u_j u_k \leq d$$

## ESTIMATION OF A SPARSE COVARIANCE MATRIX $\Sigma$

- Let  $h_\lambda$  be the hard threshold function. If  $\lambda$  is sufficiently large,

$$\|h_\lambda(\widehat{\Sigma}) - \Sigma\|_{2,2} \leq \lambda \max_{\|\mathbf{u}\|=1} \sum_{\sigma_{jk} \neq 0} u_j u_k$$

where  $\sigma_{jk}$  are elements of  $\Sigma$

- Bickel-Levina (2008b); number of closed walks of length  $m$  on the graph, El Karoui (2008), ...

GMACS:  $\lambda(\Theta) = \xi \|\Theta\|_{\infty,\infty}$

- Given symmetric data matrix  $\widehat{\mathbf{M}}$ ,

$$\min \|\Theta\|_{\infty,\infty} \text{ subject to } \|\Theta \widehat{\mathbf{M}} - \mathbf{I}\|_{\infty}^{(vec)} \leq \lambda = \xi \|\Theta\|_{\infty,\infty}$$

- Linear program:

$$\min \left\{ t : \|\Theta \widehat{\mathbf{M}} - \mathbf{I}\|_{\infty}^{(vec)} / \xi = t, \|\Theta\|_{\infty,\infty} = t \right\}$$

- Simple uniform bound: In the event  $\|\widehat{\mathbf{M}} - \mathbf{M}\|_{\infty}^{(vec)} \leq \xi$ ,

$$\|\Theta \widehat{\mathbf{M}} - \mathbf{I}\|_{\infty}^{(vec)} = \|\Theta(\widehat{\mathbf{M}} - \mathbf{M})\|_{\infty}^{(vec)} \leq \xi \|\Theta\|_{\infty,\infty}$$

$$\|\widehat{\Theta}\|_{\infty,\infty} \leq \|\Theta\|_{\infty,\infty}$$

$$\|\widehat{\Theta} - \Theta\|_{\infty}^{(vec)} \leq \xi \|\widehat{\Theta}\|_{\infty,\infty} \|\Theta\|_{\infty,\infty}$$

- $\|\widehat{\mathbf{M}} - \mathbf{M}\|_{\infty}^{(vec)} \leq \xi; \xi = ?$

SCI for covariances  $\sigma_{jk}$

- Let  $\widehat{\sigma}_{jk}$  be elements of  $\widehat{\Sigma}$
- Let  $\kappa_\alpha$  satisfy (Bonferroni adjustment)

$$2 \binom{p}{2} \exp \left( -\frac{n}{2} \left\{ \sqrt{2}\kappa_\alpha - \log(1 + \sqrt{2}\kappa_\alpha) \right\} \right) \\ + p P \left\{ \left| \chi_n^2/n - 1 \right| > \kappa_\alpha \right\} \leq \alpha,$$

- With  $\widehat{V}_{jj} = (1 - \kappa_\alpha)^{-2} \min \left\{ 2\widehat{\sigma}_{jj}\widehat{\sigma}_{kk}, \widehat{\sigma}_{jj}\widehat{\sigma}_{kk}/(1 - \kappa_\alpha)^2 + \widehat{\sigma}_{jk}^2 \right\}$ ,
- $P \left\{ \left| \widehat{\sigma}_{jk} - \sigma_{jk} \right| \leq \kappa_\alpha \widehat{V}_{jk}^{1/2} \forall jk \right\} \geq 1 - \alpha$
- $\|\widehat{\Sigma} - \Sigma\|_{\infty}^{(\text{vec})} \leq \xi = \kappa_\alpha \max_{jk} V_{jk}^{1/2} \asymp \sqrt{n^{-1} \log(p/\alpha)}$ ,  
w.p.  $1 - \alpha$

## SIMULTANEOUS CONFIDENCE INTERVALS

SCI for correlations  $\rho_{jk} = \sigma_{jk}/\sqrt{\sigma_{jj}\sigma_{kk}}$  and

- Let  $\hat{\rho}_{jk} = \hat{\sigma}_{jk}/\sqrt{\hat{\sigma}_{jj}\hat{\sigma}_{kk}}$  and  $\kappa_\alpha$  satisfy

$$p(p-1)P\left\{|N(0, 1/n)| > \kappa_\alpha\right\} + p P\left\{\chi_n^2/n \leq 1 - \kappa_\alpha\right\} \leq \alpha$$

- SCI:

$$P\left\{|\hat{\rho}_{ij} - \rho_{ij}| \leq \kappa_\alpha \forall ij\right\} \geq 1 - \alpha$$

- $\|\hat{\rho} - \rho\|_\infty^{(\text{vec})} \leq \xi = \kappa_\alpha \approx \sqrt{(4/n)\log(p/\alpha)}$  w.p.  $1 - \alpha$

- GMACS based on SCI

$$\min \|\Theta\|_{\infty,\infty} \text{ subject to } \|\Theta \widehat{\mathbf{M}} - \mathbf{I}\|_{\infty}^{(\text{vec})} \leq \xi \|\Theta\|_{\infty,\infty}$$

- For  $\widehat{\mathbf{M}} = \widehat{\boldsymbol{\Sigma}}$  or  $\widehat{\mathbf{M}} = \widehat{\rho}$ ,

$$\begin{aligned} \|\widehat{\Theta} - \Theta\|_{\infty}^{(\text{vec})} &\leq 2\xi \|\widehat{\Theta}\|_{\infty,\infty} \|\Theta\|_{\infty,\infty} = 2\widehat{\lambda}_{\alpha} \|\Theta\|_{\infty,\infty} \\ \|\widehat{\Theta}\|_{\infty,\infty} &\leq \|\Theta\|_{\infty,\infty} \\ \widehat{\lambda}_{\alpha} &\asymp \sqrt{n^{-1} \log(p/\alpha)} \end{aligned}$$

- Since  $\|\Theta\|_{\infty,\infty} \leq d \|\Theta\|_{\infty}^{(\text{vec})}$ ,

$$\|\widehat{\Theta} - \Theta\|_{\infty}^{(\text{vec})} \leq 2\widehat{\lambda}_{\alpha} \|\widehat{\Theta}\|_{\infty,\infty} / (1 - 2\widehat{\lambda}_{\alpha} d)$$

- Thresholding at level  $4\hat{\lambda}_\alpha \|\hat{\Theta}\|_{\infty,\infty}$ :

$$\widehat{\hat{\Theta}} = \left( \hat{\theta}_{jk} I\{|\hat{\theta}_{jk}| \geq 4\lambda_\alpha \|\hat{\Theta}\|_{\infty,\infty}\} \right)_{p \times p}$$

- Suppose  $\|\Sigma\|_{2,2} + \|\Theta\|_{\infty,\infty} = O(1)$  and  $d\sqrt{\log(p/\alpha)}/\sqrt{n} \leq a_0$  for a certain fixed  $a_0 \in (0, 1)$ . Then,

$$\|\widehat{\hat{\Theta}} - \Theta\|_{2,2} \lesssim \|\mathbf{1}_{D \cup S}\|_{2,2} \sqrt{\log(p/\alpha)}/\sqrt{n}$$

- Removing the condition  $\|\Theta\|_{\infty,\infty} = \max_j \sum_k |\theta_{jk}| = O(1)$
- Removing the condition  $d\sqrt{\log(p/\alpha)}/\sqrt{n} \leq a_0$

- Multiple testing with FWER  $\leq \alpha$ :

$$\text{Rej } H_{0k} \text{ iff } \inf_{\Theta \in H_{0k}} \frac{\|\widehat{\Theta} - \Theta\|_{\infty}^{(\text{vec})}}{2\widehat{\lambda}_{\alpha}\|\Theta\|_{\infty,\infty}} > 1$$

- Testing a single model:

Rej model  $S$  iff

$$\max_{(i,j) \notin S \cup D} |\widehat{\theta}_{ij}| > \max_i \sum_j \frac{2\widehat{\lambda}_{\alpha}|\widehat{\theta}_{ij}|I_{\{(i,j) \in S \cup D\}}}{1 - 2\widehat{\lambda}_{\alpha}(|S_i| + 1)}$$

where  $S_j = \#\{i : (i,j) \in S\}$

- Candidate models:

$$\widehat{S}_\tau = \left\{ (i, j) \notin D : |\widehat{\theta}_{ij}| > 2\widehat{\lambda}_\alpha \tau \right\}$$

- Statistical selection:

$$\widehat{S}_{\widehat{\tau}}, \quad \widehat{\tau} = \max \left\{ \tau : \widehat{S}_\tau \text{ not rejected} \right\}$$

- All proper submodel of  $\widehat{S}_{\widehat{\tau}}$  are rejected with FWER  $\leq \alpha$
- If  $\min_{(i,j) \in S} |\theta_{ij}| \geq 4\lambda_\alpha^* \|\Theta\|_{\infty,\infty} / (1 - 2\lambda_\alpha^* d)$ , then

$$P\{\widehat{S}_{\widehat{\tau}} = S\} \geq 1 - \alpha - P\{\widehat{\lambda}_\alpha > \lambda_\alpha^*\}$$

- $\ell_\infty$  incoherence condition is not needed
- Ravikumar et al (2008a) on G-Lasso

**THANKS!**