Regularized Estimation of Sparse Spectral Precision Matrices

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Navonil Deb
(Joint work with Amy Kuceyeski and Sumanta Basu)

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Department of Statistics and Data Science
Cornell University

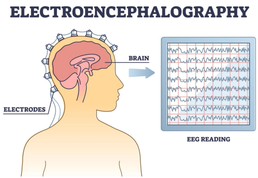
Outline

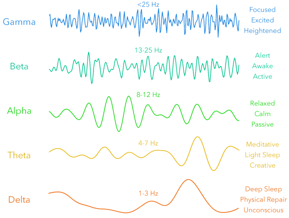
- Frequency-specific graphical model.
- Penalized whittle likelihood estimator of spectral precision matrix.
- Develop a fast, pathwise coordinate descent based estimation procedure.
    1. Complex lasso (CLASSO).
    2. Complex graphical lasso (CGLASSO).
- CGLASSO with adaptive penalization.

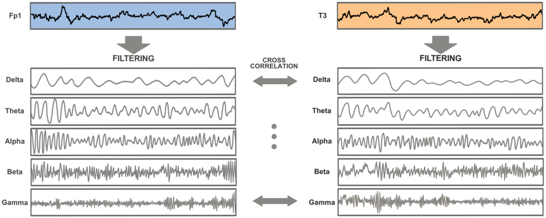
Frequency Domain Graphical Models

Motivation: Construct functional connectivity (FC) network among brain regions.

- Can we learn the *correlation structure* among frequency-*specific* physiological activities?







Reference: Ombao and Pinto (2022).

Frequency-Domain Graphical Models

Stationary, zero-mean $X_t \in \mathbb{R}^p$, autocovariance $\Gamma(h) = \mathbb{E}[X_{t+h}X_t^\top]$.
Spectral density: $f(\omega) = (2\pi)^{-1} \sum_{h=-\infty}^{\infty} \Gamma(h) e^{-ih\omega}$.

Structure	**Classical Domain**	**Spectral Domain**
Second-order structure	Σ	$f(\omega)$
Conditional dependence	Σ^{-1}	$\Theta(\omega) = f(\omega)^{-1}$
Marginal association	Correlation	Coherence
Conditional association	Partial correlation	Partial coherence

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- **Applications:** Neuroscience, economics, finance.
  - **Motivation:** Rich description of dependence.
  - Captures contemporaneous and lead-lag associations.
- **Graphical interpretation:** Edge $r \leftrightarrow s$ exists if $[\Theta(\omega)]_{r,s} \neq 0$ for some ω.

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- **Graphical interpretation:** Edge $r \leftrightarrow s$ exists if $[\Theta(\omega)]_{r,s} \neq 0$ for some ω.
- **Goal:** Estimate full $\Theta(\omega)$ at given ω, rather than single entry across all ω.
  – **Challenges**: Heteroskedasticity, high-dimensionality, temporal dependence.

References: Dahlhaus (2000), Böhm and von Sachs (2009)

Bridging the Gap: Our Contributions

Limitations of existing approaches.

1. Off-the-shelf solvers e.g. ADMM do not exploit the problem structure, not adaptive. (Baek et al., 2021)
2. Real imaginary separation $\implies$ dimension $\times 4$. (Fiecas et al., 2019, SIPE based on CLIME).
3. Separate treatment of real and imaginary parts in nodewise regression ignores joint likelihood. (Krampe and Paparoditis, 2022)

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   (Krampe and Paparoditis, 2022)

Our contributions.

- **Algorithmic**: CGLASSO — fast, pathwise coordinate descent-based algorithm.
  – Leverages high-dimensional tricks viz. warm starts and active set screening.
- **Optimization Insight**: Ring isomorphism-based realification.
  – Generalizes to broader complex-valued problems.

– **Methodological**: Adaptive CGLASSO introduces entry-wise penalization.
  – Improved structural recovery in heterogeneous variability.

– **Theoretical**: Non-asymptotic error bounds for both standard and adaptive CGLASSO.

Averaged Periodogram

- Data: n observations from a p-dim stationary series $\{X_1, X_2, \ldots, X_n\}$.
- Fourier frequencies: $\omega_j = 2\pi j/n$, $j \in F_n = \{-[(n-1)/2], \ldots, [n/2]\}$.
- DFT: $d_j = n^{-1/2} \sum_{t=1}^{n} X_t e^{-it\omega_j}$.

$$X = \begin{bmatrix} X_{11} & \cdots & X_{np} \\ \vdots & \ddots & \vdots \\ X_{n1} & \cdots & X_{np} \end{bmatrix} \xrightarrow{\text{FFT}} \begin{bmatrix} d_{j-m,1} & \cdots & d_{j-m,p} \\ \vdots & \ddots & \vdots \\ \color{red}{d_{j,1}} & \color{red}{\cdots} & \color{red}{d_{j,p}} \\ \vdots & \ddots & \vdots \\ d_{j+m,1} & \cdots & d_{j+m,p} \end{bmatrix} = \mathcal{Z}$$

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- Under regularity conditions, $\mathrm{Cov}(d_{j,r}, d_{j,s}) \approx 2\pi[f(\omega_j)]_{r,s}$ and d_j are asymptotically independent across j.
- Averaged periodogram for bandwidth m: $\hat{f}(\omega_j) = \frac{1}{2\pi(2m+1)} \mathcal{Z}^\top \overline{\mathcal{Z}}$.

Penalized Whittle log-Likelihood

- For Gaussian time series, $d_j \sim \mathcal{N}_{\mathbb{C}}(0, 2\pi\Theta^{-1}(\omega_j))$, asymp. independent across j.
- Approximated Whittle (negative log) likelihood takes the form

$$\frac{1}{2} \sum_{j \in F_n} \log\det \Theta(\omega_j) - \sum_{j \in F_n} d_j^* \, \Theta(\omega_j) \, d_j$$

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- Approximated and penalized problem:

$$\boxed{\hat{\Theta}_j \equiv \hat{\Theta}(\omega_j) = \underset{\Theta\in\mathcal{H}^p_{++}}{\text{argmin}} \; -\log\det\Theta + \text{trace}(\hat{f}(\omega_j)\Theta) + \lambda\|\Theta\|_{1,\text{off}},}$$

where $\|\Theta\|_{1,\text{off}} = \sum_{r\neq s}|\Theta_{rs}|$.

– We call this problem **CGLASSO** $\equiv$ complex graphical lasso.

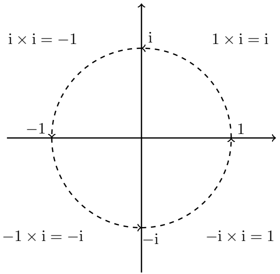
The Isomorphism Trick

We consider the map $\varphi(z) : \mathbb{C} \to \mathbb{R}^{2\times 2}$ s.t.

$$\varphi(z) = \begin{bmatrix} \mathbf{Re}(z) & -\mathbf{Im}(z) \\ \mathbf{Im}(z) & \mathbf{Re}(z) \end{bmatrix}.$$

- Properties of $\varphi(z) = (\varphi_1(z), \varphi_2(z))$:

1. $\langle \varphi_1(z), \varphi_2(z) \rangle = 0$.
2. $\|\varphi_1(z)\|^2 = \|\varphi_2(z)\|^2 = |z|^2$.
3. $\varphi(z^\dagger) = [\varphi(z)]^\top$.
4. φ is a field isomorphism.



$$1 \equiv \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathrm{i} \equiv \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

1 and $\mathrm{i} \equiv 2 \times 2$ orthogonal matrices!

The Isomorphism Trick

φ: extendable to $\mathbb{C}^p$ and $\mathbb{C}^{n\times p}$ with a k-dim permutation matrix Π_k.

'Tilde' notation:

$$\begin{aligned} \tilde{z} &= \Pi_n^\top \varphi(z) e_1 = \begin{pmatrix} \mathbf{Re}(z) \\ \mathbf{Im}(z) \end{pmatrix}, \\ \tilde{\tilde{Z}} &= \Pi_m^\top \varphi(Z) \Pi_n = \begin{pmatrix} \mathbf{Re}(z) & -\mathbf{Im}(Z) \\ \mathbf{Im}(Z) & \mathbf{Re}(Z) \end{pmatrix}. \end{aligned}$$

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Context	Complex Loss Function	Realified Loss Function
OLS (X, y, β)	$\frac{1}{2n}\lVert y - X\beta\rVert^2$	$\frac{1}{4n}\lVert \tilde{y} - \tilde{\tilde{X}}\tilde{\beta}\rVert^2$
log-det program $Z_i \sim \mathcal{N}(0, \Theta^{-1})$ $P = \frac{1}{n}\sum_i Z_i Z_i^\dagger$	$-\log\det\Theta + \mathrm{trace}(P\Theta)$	$\frac{1}{2}\left[-\log\det\tilde{\tilde{\Theta}} + \mathrm{trace}(\tilde{\tilde{P}}\tilde{\tilde{\Theta}})\right]$

CLASSO $\equiv$ Group Lasso

Complex Lasso (CLASSO):

$$\underset{\beta \in \mathbb{C}^p}{\operatorname{argmin}} \frac{1}{2n} \|Y - X\beta\|_2^2 + \lambda \|\beta\|_1.$$

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$$\Updownarrow$$

$$\boxed{\underset{\tilde{\beta}_1, \ldots, \tilde{\beta}_p \in \mathbb{R}^2}{\operatorname{argmin}} \frac{1}{2n} \Big\| \tilde{Y} - \sum_{j=1}^{p} \tilde{\tilde{X}}_j \tilde{\beta}_j \Big\|_2^2 + \lambda \sum_{j=1}^{p} \|\tilde{\beta}_j\|_2.}$$

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- CLASSO $\equiv$ Group Lasso over reals Maleki et al. (2013)
  - Orthogonal predictors within a group.
  - Closed form updates of (blockwise) coordinate descent.

CGLASSO Algorithm Sketch

$\hat{f} \equiv \hat{f}(\omega_j)$ for a fixed ω_j.

$$\hat{\Theta}_j = \underset{\Theta \in \mathcal{H}^p_{++}}{\operatorname{argmin}} \; -\log\det\Theta + \operatorname{trace}(\hat{f}\Theta) + \lambda\|\Theta\|_{1,\text{off}}.$$

Along Friedman et al. (2008):

- **KKT condition**: $\boxed{\hat{f} - \Theta^{-1} + \lambda\Psi = 0}$, $\Psi_{r,s} = \operatorname{sign}(\Theta_{r,s})$.

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- W: Working version of Θ^{-1}.
- Partition Θ as $\begin{bmatrix} \Theta_{11} & \boldsymbol{\theta}_{12} \\ \boldsymbol{\theta}^{\dagger}_{12} & \theta_{22} \end{bmatrix}$, same for W and $\hat{f}$.
- KKT + $[\Theta W = I_p] \implies$ Last column iteration :

$$W_{11}\beta - \hat{f}_{12} + \lambda \operatorname{sign}(\beta) = 0, \;\; \beta = -\boldsymbol{\theta}_{12}/\theta_{22}.$$

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- KKT condition of CLASSO(X, y, β):

$$\left(\frac{1}{n}X^{\dagger}X\right)\beta - \left(\frac{1}{n}X^{\dagger}y\right) + \lambda\,\operatorname{sign}(\beta) = 0.$$

Pathwise performance enhancement

Regularization grid: $\{\lambda_t\}$.

Warm start (CGLASSO)
$\hat{\Theta}(\lambda_{t-1}) \rightarrow \hat{\Theta}(\lambda_t)$

+

Warmer start (CLASSO)
$\hat{\beta}^{(\text{ cycle}=k-1)} \rightarrow \hat{\beta}^{(\text{ cycle}=k})$

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- Sequential strong *active set screening* (Tibshirani et al., 2012).
- **Convergence safeguard**: *Early stopping rule* implementation based on the underlying selection criterion (e.g. estimation error, BIC etc).
  – Prevents unstable updates at small λ.

Adaptive CGLASSO

- **CGLASSO-1**: Coherency scaling-

$$\hat{D}^2 = \mathrm{diag}(\hat{f}_{1,1}, \ldots, \hat{f}_{p,p}).$$

$$\hat{\Theta}_D \leftarrow \hat{D}^{-1} \cdot \text{CGLASSO}(\hat{D}^{-1}\hat{f}\hat{D}^{-1}, \lambda) \cdot \hat{D}^{-1}.$$

  – Similar to Janková and van de Geer (2018).

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- **CGLASSO-2**: CLASSO level normalization-

$$(p-1)\text{-dim diagonal matrix } \hat{D}_{11} \text{ with } (\hat{D}^2_{11})_{r,r} = (\hat{f}_{11})_{r,r}.$$

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- **CGLASSO-3**: NWR partial variance scaling-

$$\hat{\tau}_k^2 : \text{Estimated MSE from CLASSO}(\mathcal{Z}_{-k}, \mathcal{Z}_k, \lambda_k).$$

$$\hat{D}^2 = \text{diag}(\hat{\tau}_1^2, \ldots, \hat{\tau}_p^2).$$

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Method	CGLASSO-1	CGLASSO-2	CGLASSO-3
Scales	$\mathrm{diag}(\hat{f})$	$\mathrm{diag}(\hat{f}_{11})$	$\{\hat{\tau}_k^2\}_{k\in[p]}$

Simulation studies

- Results reported for $\omega_j = 0$ and 50 Monte Carlo trials.
- λ selected with BIC.
- $m \asymp \sqrt{n}$ (Böhm and von Sachs, 2009).

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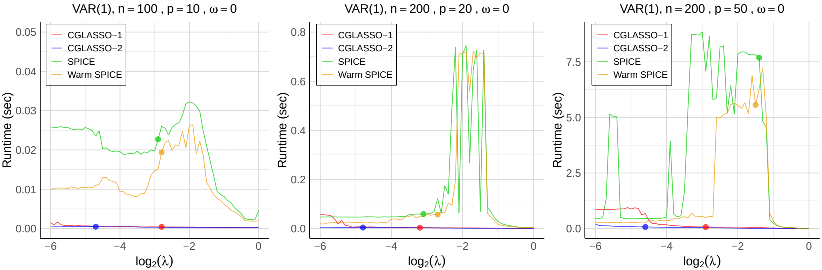
Benchmarks:

- **Speed**: *ADMM* vs *coordinate descent*.
- **Estimation accuracy**: SIPE (CLIME) (Fiecas et al., 2019) with *separate penalty* vs CGLASSO with *joint penalty*.
- **Model selection**: *Nodewise regression* of DFTs (Krampe and Paparoditis, 2022) vs *Whittle likelihood* maximization.
- **Scaling**: *Vanilla CGLASSO* vs *adaptive CGLASSO* variants.

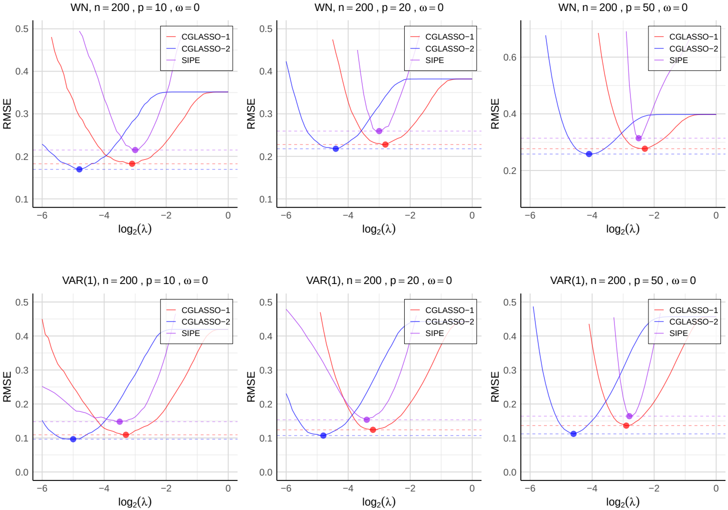
Coordinate descent improves runtime over ADMM

- **SPICE**: Sparse inverse covariance estimator (Scheinberg et al., 2010; Baek et al., 2021), implements ALM algorithm, a variant of ADMM.
- **Warm SPICE**: Pathwise SPICE equipped with warm start.



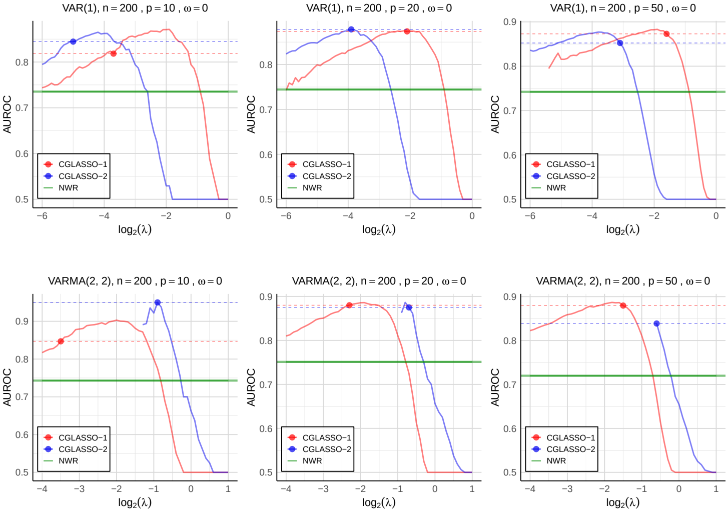
Joint penalty improves estimation accuracy

Benchmark: Sparse inverse periodogram estimator (Fiecas et al., 2019, SIPE), uses CLIME (Cai et al., 2011).



Joint penalty improves model selection

Benchmark: Nodewise regression (Meinshausen and Bühlmann, 2006, NWR) of DFTs (Krampe and Paparoditis, 2022).



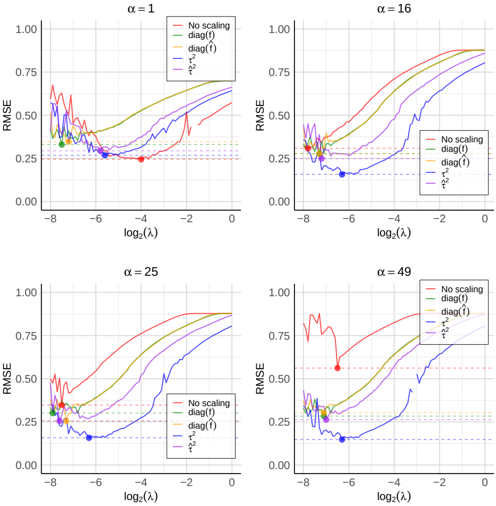
Adaptive penalization improves estimation accuracy

- **DGP**: WN(Σ), Σ^{-1} has two Toeplitz blocks A and B with

$$A_{i,j} = (0.2)^{|i-j|},$$
$$B_{i,j} = (0.8)^{|i-j|}.$$

- α: Signal contrast between the blocks.

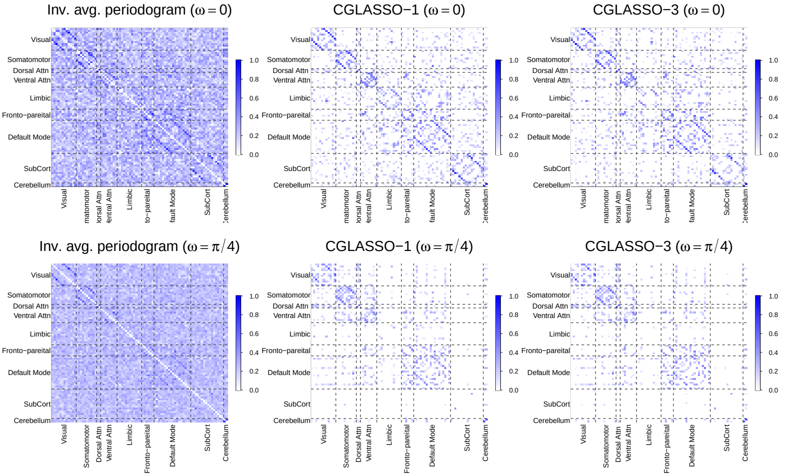
$$\Sigma^{-1} = \frac{1}{15}\begin{bmatrix} A & 0 \\ 0 & \alpha B \end{bmatrix}.$$



fMRI data analysis

CGLASSO applied on resting state fMRI data set with 86 brain region parcellation, from HCP-Young Adult S1200.

Yeo Parcellation Heatmaps (sq-root transformed)



Theoretical guarantees

Bound on estimation error $\|\hat{\Theta}(\omega_j) - \Theta^*(\omega_j)\|_\infty$.

1. *Entry-wise max norm guarantees* for vanilla CGLASSO under stronger condition.
2. *Matrix ℓ_1-norm guarantees* for CGLASSO-1 and CGLASSO-3 under weaker condition.

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Key technical pieces:

- Single deviation bound on $\|\hat{f}(\omega_j) - f(\omega_j)\|_\infty$ (Sun et al., 2018).
- **Vanilla CGLASSO**: α-incoherence condition on Hessian of the Whittle log-likelihood (Ravikumar et al., 2011).
- **CGLASSO-3**: consistency of $\hat{\tau}_k^2$ (van de Geer et al., 2014).

CGLASSO consistency

- $\alpha \in (0, 1]$: incoherence parameter, $C_\alpha = 1 + 8/\alpha$.
- Stability parameter: $|||f||| = \operatorname{ess\,sup}_{\omega \in [-\pi, \pi]} \|f(\omega)\|_2$.
- Model parameters: $\kappa_f, \kappa_{\Theta^*}$, temporal dependence parameters: L_n, Ω_n.
- s: Number of edges, d: max-row degree.
- Threshold: $\Delta = |||f||| \sqrt{C \log p/m} + \frac{m}{n}\Omega_n + L_n$.

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Theorem (Simplified)

Let X_t be a p-dim linear Gaussian time series satisfying α-incoherence condition. Under certain regularity condition with $n/\Omega_n \gtrsim m \gtrsim \Omega_n |||f|||^2 \log p$, $\lambda = (8/\alpha)\Delta$, and $\Delta d \le 1/(6\kappa^2_{\Theta^*}\kappa^3_f C_\alpha)$, with high probability,

$$\left\|\hat{\Theta} - \Theta^*\right\|_\infty \le 2\kappa_{\Theta^*} C_\alpha \Delta,$$

$$\{|\Theta^*_{k,\ell}| > 2\kappa_{\Theta^*} C_\alpha \Delta\} \subset E(\hat{\Theta}) \subset E(\Theta^*).$$

CGLASSO consistency

- $\alpha \in (0, 1]$: incoherence parameter, $C_\alpha = 1 + 8/\alpha$.
- Stability parameter: $|||f||| = \operatorname{ess\,sup}_{\omega \in [-\pi, \pi]} \|f(\omega)\|_2$.
- Model parameters: $\kappa_f, \kappa_{\Theta^*}$, temporal dependence parameters: L_n, Ω_n.
- s: Number of edges, d: max-row degree.
- Threshold: $\Delta = |||f||| \sqrt{C \log p/m} + \frac{m}{n}\Omega_n + L_n$.

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Remark. If $m \asymp n^\xi$ for $\xi > 0$, and $\|\Gamma(h)\| \leq \sigma\rho^{|h|}$, $\Delta \asymp \sqrt{\log p/m}$ and $m \gtrsim d^2 \log p$.

Consistency of the adaptive variant

- **Assume bounded spectrum**: $\max\{|||f|||, |||\Theta|||\} \leq M$.
- Nodewise regression penalty for CGLASSO-3: $\lambda_j \asymp M\sqrt{\log p/m}$.

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Theorem (Simplified)

Let X_t be a p-dim linear Gaussian time series with bounded spectrum. Under certain regularity condition with $n/\Omega_n \gtrsim m \gtrsim M^6 d\log p$, $s\lambda \lesssim 1/M^5$, with high probability,

CGLASSO-1: *For* $\lambda \asymp M^4\sqrt{\log p/m}$, $\left|\left|\left|\hat{\Theta}_D - \Theta^*\right|\right|\right|_1 \leq C_M s\lambda$,

CGLASSO-3: *For* $\lambda \asymp M^4\sqrt{d\log p/m}$, $\left|\left|\left|\hat{\Theta}_D - \Theta^*\right|\right|\right|_1 \leq C'_M(p+s)\lambda$.

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$$\text{CGLASSO-1:} \quad \textit{For } \lambda \asymp M^4\sqrt{\log p/m}, \quad \left|\left|\left|\hat{\Theta}_D - \Theta^*\right|\right|\right|_1 \le C_M s\lambda,$$

$$\text{CGLASSO-3:} \quad \textit{For } \lambda \asymp M^4\sqrt{d\log p/m}, \quad \left|\left|\left|\hat{\Theta}_D - \Theta^*\right|\right|\right|_1 \le C'_M (p+s)\lambda.$$

Remark. $s\lambda \lesssim 1/M^5$: stronger condition on the sparsity.

$$\text{CGLASSO-1} : m \gtrsim s^2 \log p, \quad \text{CGLASSO-3} : m \gtrsim s^2 d\log p.$$

Main takeaways

Our contribution:

- Fast pathwise coordinate descent algorithm for complex variable lasso.
- Frequency-domain graphical lasso using CLASSO.
- Adaptive CGLASSO.

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- Bandwidth selection.
- Aggregation across frequencies + recovery of the true graph for stationary time series.
- Non-stationary GGMs (Basu and Subba Rao, 2023).

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Paper: `https://arxiv.org/abs/2401.11128`
R Package `cxreg`: `https://github.com/navonildeb/cxreg`

Thank you!

Navonil Deb

E-mail: nd329@cornell.edu

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