Estimating partial correlations and recovering network hubs with PCGLASSO

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# Outline

#### Introduction and Motivation

- Graphical LASSO (GLASSO)
- Partial Correlation LASSO (PCGLASSO)
  - Algorithm
  - Convexity issues
  - Asymptotic distribution
  - Irrepresentability condition
  - Identifying the hub structure

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 $\Omega = \Sigma^{-1}$  - precision matrix

# Motivation: Global Minimum Variance Portfolio

 $R = [R_1 \ \cdots \ R_K]'$  - a random vector of returns

$$\mu = [\mathbb{E}[R_1] \cdots \mathbb{E}[R_K]]'$$

$$\Sigma = \mathbb{E}\left[(R - \mu)(R - \mu)'\right].$$

$$w \in R^K \quad \text{- portfolio weights}$$

$$Var(w'R) = w'\Sigma w$$

$$w^* = \underset{w \in \mathbb{R}^K}{\operatorname{arg min}} w'\Sigma w \text{ subject to } w'\mathbf{1}_K = 1,$$

$$w^* = \frac{\Sigma^{-1}\mathbf{1}_K}{\mathbf{1}'_K \Sigma^{-1}\mathbf{1}_K}$$

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# **Graphical Model**

 $X = (X_1, \ldots, X_p)$  - a random vector



# Graphical Model

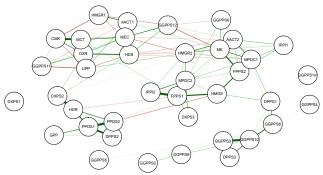
$$\begin{split} &X = (X_1, \dots, X_p) \text{ - a random vector} \\ &\text{Graph: } G = (V, E) \\ &\text{Vertices (V): indices (names) of components of } X: V = \{1, \dots, p\} \\ &\text{Edges (E): } (u, v) \notin V \Longleftrightarrow X_u \perp X_v | X_{V \setminus \{u, v\}} \end{split}$$

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Glasso



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$$X=(X_1,\ldots,X_p)\sim {\sf N}(0,\Sigma), \;\; \Omega=\Sigma^{-1} \;\;$$
 - precision matrix

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 $Var(X_1) = Var(\varepsilon_j) = 2$ 

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for  $i \neq j$ ,  $Cov(X_i, X_j) = Var(X_1) = 2$ 

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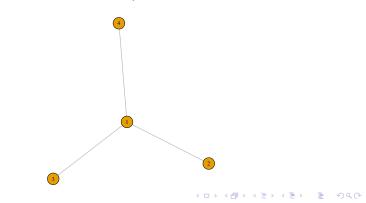
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Example: for j = 2, ..., p  $X_j = X_1 + \varepsilon_j$ , where  $Var(X_1) = Var(\varepsilon_j) = 2$ for  $i \neq j$ ,  $Cov(X_i, X_j) = Var(X_1) = 2$ for  $j \ge 2$ ,  $Var(X_j) = 4$  Hub

$$\Sigma = \begin{bmatrix} 2 & 2 & 2 & 2 \\ 2 & 4 & 2 & 2 \\ 2 & 2 & 4 & 2 \\ 2 & 2 & 2 & 4 \end{bmatrix}, \Omega = \begin{bmatrix} 2 & -0.5 & -0.5 & -0.5 \\ -0.5 & 0.5 & 0 & 0 \\ -0.5 & 0 & 0.5 & 0 \\ -0.5 & 0 & 0 & 0.5 \end{bmatrix}$$

Example 1



 $X_{n \times p}$  - *n* independent realizations of the p-dimensional random vector  $S = \frac{1}{n} X^T X$  - sample covariance matrix

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Gaussian cross-entropy function:  $L(\Omega, X)C + \frac{n}{2}\log \det \Omega - \frac{n}{2}tr(S\Omega)$ .

When S is invertible, 
$$\hat{\Omega}_{MLE} = S^{-1}$$



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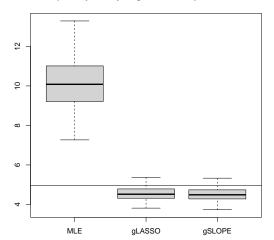
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 $\hat{\Omega}_{MLE}$  is dense (inverse Wishart distribution) For large  $p, MSE = E ||\hat{\Omega} - \Omega||_{E}^{2}$  is large

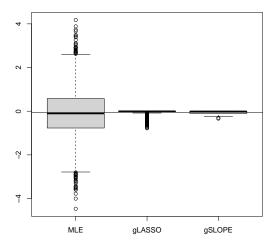
# Simulation example (1)



Compund symmetry diagonal, n=200, p=100, rho=0.8

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# Simulation example (2)



Compound symmetry, off-diagonals

$$L(\Omega, X) = C + \frac{n}{2} \log \det \Omega - \frac{n}{2} tr(S\Omega).$$

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$$\begin{split} L(\Omega, X) &= C + \frac{n}{2} \log \det \Omega - \frac{n}{2} tr(S\Omega). \\ \text{gLASSO:} \widehat{\Omega}_L &= \arg \max_{\Omega \in Sym^p_+} \left[ \log \det \Omega - tr(S\Omega) - \lambda ||\Omega||_1 \right] \ , \\ &||\Omega||_1 = \sum_{i < j} |\omega_{ij}| \ . \end{split}$$

Example: n = 50, p = 30,  $\Sigma$  - block diagonal with 3 blocks of dimension  $10 \times 10$ , correlation within blocks  $\rho = 0.8$ 

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$$\lambda_{\alpha}^{Banerjee} = \frac{t_{n-2} \left(1 - \frac{\alpha}{2p^2}\right)}{\sqrt{n-2 + t_{n-2}^2 \left(1 - \frac{\alpha}{2p^2}\right)}} \quad , \tag{1}$$

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Perfect graph discovery,  $||\Omega - \hat{\Omega}_{gLASSO}||_F = 468$ 

Precision matrix depends on scaling factors:  $Cov(aX_i, X_j) = aCov(X_i, X_j)$ 

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More reasonable solution - penalize the partial correlation matrix instead of the precision

## Dependence of scaling

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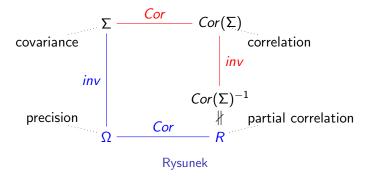
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Partial correlation :  $ho_{i,j} = -\frac{\Omega_{i,j}}{\sqrt{\Omega_{i,i}\Omega_{j,j}}} = -R_{i,j}$ 

## Precision vs Partial correlation



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### Partial correlation vs inverse of the correlation

Typically, partial correlation R has a different ordering of off-diagonal entries than the precision of the standardised data  $Cor(\Sigma)^{-1}$ .

$$\Sigma = \begin{bmatrix} 2 & -1 & -2 & 2 \\ -1 & 1 & 1 & -1 \\ -2 & 1 & 3 & -3 \\ 2 & -1 & -3 & 3.5 \end{bmatrix} \quad Cor(\Sigma)^{-1} = \begin{bmatrix} 4 & 1.414 & 2.449 & 0 \\ 1.414 & 2 & 0 & 0 \\ 2.449 & 0 & 9 & 6.48 \\ 0 & 0 & 6.48 & 7 \end{bmatrix}$$
$$\Omega = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 1 & 2 & 0 & 0 \\ 1 & 0 & 3 & 2 \\ 0 & 0 & 2 & 2 \end{bmatrix} \qquad \qquad R = \begin{bmatrix} 1 & 0.5 & 0.408 & 0 \\ 0.5 & 1 & 0 & 0 \\ 0.408 & 0 & 1 & 0.816 \\ 0 & 0 & 0.816 & 1 \end{bmatrix}$$

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### Partial correlation LASSO

A. Chojecki, I. Hejny, B. Kołodziejek, J. Wallin, MB J.S.Carter, D. Rossell, J. Q. Smith, SJS, 2023 We represent  $\Omega = DRD$ , where  $D^2 = diag(\Omega)$ , and define its estimator as

$$\hat{\Omega}_{
m pcg} = \hat{D}\hat{R}\hat{D},$$

where

$$(\hat{R}, \hat{D}) \in Argmax_{R,D} \{ \log \det(DRD) - SDRD - \lambda \|R\|_{1, \text{off}} - 2\alpha \log \det(DRD) - (2) \}$$

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and  $\lambda \geq {\rm 0}$  and  $\alpha < {\rm 1}$  are tuning parameters.

## Convexity issues

The objective function is non-concave and there might exist more than one global maxima

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Let  $\hat{C}$  denote the sample correlation matrix.

Theorem

- (i) If  $\|\hat{C} I_p\|_{\infty} \le (2(1-\alpha)p^3)^{-1/2}$ , then for any  $\lambda \ge 0$ , *PCGLASSO* admits a unique local maximum.
- (ii) There exist λ<sub>0</sub> > 0 and α<sub>0</sub> > 0 such that, for every Ĉ, λ ∈ (0, λ<sub>0</sub>) and α ∈ (-∞, α<sub>0</sub>), PGLASSO admits a unique local maximum.

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The function is biconcave, i.e. for fixed D it is concave as a function of R and vice versa



## Algorithm

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We iteratively optimize with respect to D and R

## Algorithm

- The function is biconcave, i.e. for fixed D it is concave as a function of R and vice versa
- We iteratively optimize with respect to D and R
- For fixed D we optimize R using an adaptation of the block coordinate descent method for GLASSO

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## Algorithm

- The function is biconcave, i.e. for fixed D it is concave as a function of R and vice versa
- We iteratively optimize with respect to D and R
- For fixed D we optimize R using an adaptation of the block coordinate descent method for GLASSO
- For fixed R we optimize D using a modified Newton-Raphson method with backtracking line search.

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### Asymptotic distribution

We minimize

$$-logdet(\Omega) + tr(\Omega S) + n^{-1/2}Pen(\Omega)$$

We want to compare penalization of the precision matrix  $\boldsymbol{\Omega}$  and of the partial correlation matrix

$$R = g(\Omega) = Cor(\Omega) = d(\Omega)^{-1/2} \Omega d(\Omega)^{-1/2}$$
:

 $Pen(\Omega) = \begin{cases} f(\Omega) + h(\Omega) \dots \text{ precision penalization} \\ f(g(\Omega)) + h(\Omega) \dots \text{ partial correlation penalization} \end{cases}$ 

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where  $h(\Omega) = \alpha log(det(d(\Omega)))$  is a separate penalty on the diagonal of  $\Omega$ .

### Low dimensional asymptotics

#### Theorem

Assume x follows a centered elliptical distribution with  $Cov(x) = \Sigma = \Omega_0^{-1}$ . Then  $\sqrt{n}(\widehat{\Omega}_n - \Omega_0)$  converges weakly and in pattern to the minimizer of  $V : \mathbb{R}^{p^2} \to \mathbb{R}$ ;

$$\frac{1}{2}\operatorname{vec}(U)^{\mathsf{T}}\operatorname{Cvec}(U) - \operatorname{vec}(U)^{\mathsf{T}}W + \operatorname{Pen}'(\Omega_0; U), \qquad (3)$$

where  $W \sim \mathcal{N}(0, \mathcal{C}_{ riangle})$ ,

$$C = \frac{1}{2} (\Omega_0^{-1} \otimes \Omega_0^{-1}),$$
  
$$C_{\triangle} = Cov(vec(x^T x))/4$$

and  $Pen'(\theta_0; u)$  denotes the directional derivative of the penalty Pen at  $\theta_0$  in direction u.

### Pattern recovery

### Theorem Let $\Omega_0 = DRD$ . The irrepresentability condition is

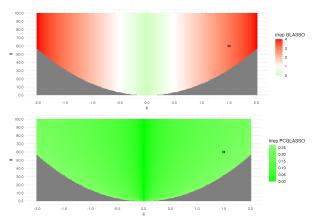
$$||\tilde{\Gamma}_{\mathcal{S}^{c}\mathcal{S}}(\tilde{\Gamma}_{\mathcal{S}\mathcal{S}})^{+} \textit{vec}(\textit{sign}(\textit{od}(R)))||_{\infty} < 1$$

where  $\tilde{\Gamma} := M_R^+(R^{-1} \otimes R^{-1})$ ,  $M_R = I - (1/2)P_d(I \otimes R + R \otimes I)$ ,  $P_d$  a projection satisfying  $P_d \operatorname{vec}(U) = \operatorname{vec}(d(U))$  and  $M_R^+$  the Moore-Penrose inverse. If the above condition is satisfied, then PCGLasso is model consistent in the sense

$$\lim_{n\to\infty}\mathbb{P}(sign(\hat{\Omega}_n)=sign(\Omega_0))>1-e^{c\gamma},$$

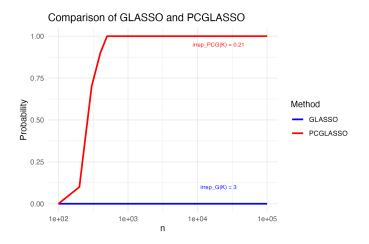
for some c > 0 and arbitrary  $\gamma \ge 0$ , where  $\hat{\Omega}_n$  minimizes  $-\log det(\Omega) + tr(\Omega S) + n^{-1/2} \gamma Pen(\Omega)$ .

# Irrepresentability condition (1)

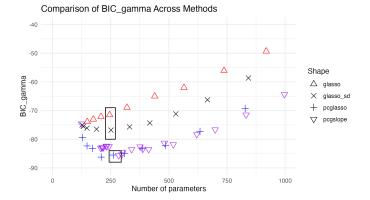


**Rysunek**: Heatmap representing the value of the IRR formula for the hub graphs such that K[1,1] = a; K[i,i] = 1; K[i,1] = K[1,i] = c and K[i,j] = 0; size p = 15. Green area marks the region where IR is satisfied, grey area marks the region where K is not positive semidefinite (namely,  $a \le (p-1)c^2$ ).

## Irrepresentability condition (2)

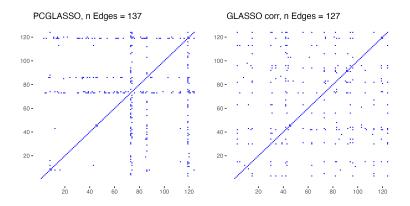


## Analysis of gene expression data



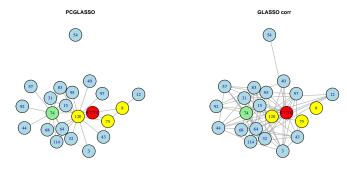
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## Analysis of gene expression data (2)



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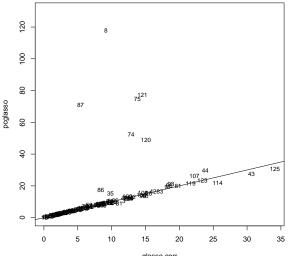
# Analysis of gene expression data (3)



A D > A P > A D > A D >

# Analysis of gene expression data(4)

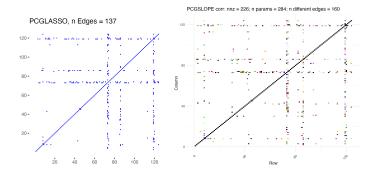
**Diagonal entries** 



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# Analysis of gene expression data (5)



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