Precision matrix estimation in Gaussian graphical models

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Overview

Graphical models

- Each vertex represents a random variable.
- Useful for either unsupervised or supervised learning.
- Directed or undirected.
- Represents joint distribution.

Undirected graphical models

The absence of an edge between two vertices has a special meaning: the corresponding random variables are conditionally independent, given the other variables.

Example 1/2

Figures/Senators.png

Example 2/2

Figures/Genes.png

Factorization

Any multivariate normal distribution $\mathcal{N}(\mu, \mathbf{\Sigma})$ can reparametrized into canonical parameters of the form

$$\gamma = \mathbf{\Sigma}^{-1}\mu \quad \text{and} \quad \mathbf{\Theta} = \mathbf{\Sigma}^{-1}.$$

Factorization

Any multivariate normal distribution $\mathcal{N}(\mu, \mathbf{\Sigma})$ can reparametrized into canonical parameters of the form

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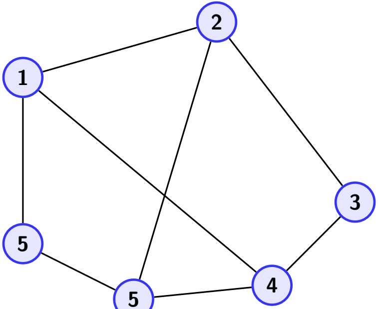
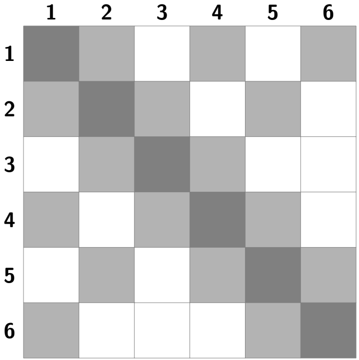
If $X \sim \mathcal{N}(\mu, \mathbf{\Sigma})$ factorizes according to some graph G, $\theta_{st} = 0$ for any pair $(s, t) \notin E$, which sets up correspondence between the zero pattern of the matrix $\mathbf{\Theta}$ and pattern of the underlying graph. In particular, if the $\theta_{st} = 0$, then variables s and t are conditionally independent, given the other variables.

Graph and matrix correspondence



(a) The undirected graph G on six vertices.



(b) The associated sparsity pattern of the precision matrix $\mathbf{\Theta}$. White squares correspond to zero entries.

Maximum likelihood estimator...

MLE

$$\widehat{\mathbf{\Theta}}_{ML} \in \underset{\Theta \in S_{+}^{p}}{\arg\max} \left\{ \log \det \mathbf{\Theta} - \operatorname{tr}\left(\mathbf{S}\,\mathbf{\Theta}\right) \right\}$$

Maximum likelihood estimator...

MLE

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When the maximum is attained the solution is given by

$$\mathbf{S}^{-1} = \widehat{\mathbf{\Theta}},$$

or its truncated version

...and its problems

In case when the number of nodes p is comparable to, or larger than, the sample size N, the sample covariance $\mathbf{S}$ is singular (so $\mathbf{S}^{-1}$ does not exist), so the MLE. Moreover, sometimes we are looking for *sparse* solutions.

Regularization

We can control the number of edges, which can be measured by ℓ_0-based quantity

$$\rho_0(\mathbf{\Theta}) = \sum_{s \neq t} \mathbb{I}[\theta_{st} \neq 0].$$

Note that $\rho_0(\mathbf{\Theta}) = 2|E(G)|$ for a given graph G.

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ℓ_0-based problem

$$\widehat{\Theta} \in \arg\max_{\substack{\Theta \in S_+^p \\ \rho_0(\mathbf{\Theta}) \leq k}} \{\log\det \mathbf{\Theta} - \operatorname{tr}(\mathbf{S}\,\mathbf{\Theta})\}$$

Unfortunately, the ℓ_0-based constrained defines a highly nonconvex constraint set.

Graphical Lasso

Convex relaxation of ℓ_0-based constrain leads to

$$\mathbb{L}_\lambda(\mathbf{\Theta}, \mathbf{X}) = \log\det \mathbf{\Theta} - \operatorname{tr}(\mathbf{S}\,\mathbf{\Theta}) - \lambda \| \mathbf{\Theta} \|_1.$$

where $\| \cdot \|_1$ states for entrywise off-diagonal ℓ_1-norm $\|A\|_1 = \sum_{i \neq j} |a_{ij}|$.

Graphical Lasso

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Graphical Lasso problem

$$\widehat{\mathbf{\Theta}} \in \underset{\Theta\in S^p_+}{\arg\max}\left\{\log\det\mathbf{\Theta} - \operatorname{tr}(\mathbf{S}\,\mathbf{\Theta}) - \lambda\|\,\mathbf{\Theta}\,\|_1\right\}.$$

Graphical Lasso parameter choice

Banerjee lambda for Graphical Lasso

$$\lambda^{\text{Banerjee}}(\alpha) = \max_{i<j}(s_{ii}, s_{jj}) \frac{\mathrm{qt}_{n-2}(1 - \frac{\alpha}{2p^2})}{\sqrt{n - 2 + \mathrm{qt}^2_{n-2}(1 - \frac{\alpha}{2p^2})}} \quad (1)$$

The following theorem was formulated by Banerjee et al.

Theorem

Using (1) *as the penalty parameter in Graphical Lasso problem, for any fixed level* α *we obtain*

$$\mathbb{P}(\text{False Discovery}) \leq \alpha,$$

where **False Discovery** *means there is a nonzero coefficient of the estimated precision matrix, which is zero in the real precision matrix.*

Graphical SLOPE

Instead of ordinary ℓ_1 norm we want to use OL1 norm

OL1

$$\mathrm{J}_\lambda(\boldsymbol{\Theta}) = \sum_i \lambda_i |\theta|_{(i)}$$

Graphical SLOPE

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Thus, we maximize

$$\mathbb{L}_\lambda(\mathbf{\Theta}, \mathbf{X}) = \log\det\mathbf{\Theta} - \mathrm{tr}\left(\mathbf{S}\,\mathbf{\Theta}\right) - \mathrm{J}_\lambda(\mathbf{\Theta}).$$

Graphical SLOPE problem

$$\widehat{\mathbf{\Theta}} \in \underset{\Theta \in S_+^p}{\arg\max} \left\{\log\det\mathbf{\Theta} - \mathrm{tr}\left(\mathbf{S}\,\mathbf{\Theta}\right) - \mathrm{J}_\lambda(\mathbf{\Theta})\right\},$$

Graphical SLOPE parameter choice (1/2)

Holm lambda for Graphical SLOPE

$$m = \frac{p(p-1)}{2},$$

$$\lambda_k^{\text{Holm}} = \frac{\text{qt}_{n-2}(1 - \frac{\alpha k}{m})}{\sqrt{n - 2 + \text{qt}^2_{n-2}(1 - \frac{\alpha k}{m})}},$$

$$\lambda^{\text{Holm}} = \{\lambda_1^{\text{Holm}}, \lambda_2^{\text{Holm}}, ..., \lambda_m^{\text{Holm}}\}.$$

It is based on Holm method for multiple testing.

Graphical SLOPE parameter choice (2/2)

BH lambda for Graphical SLOPE

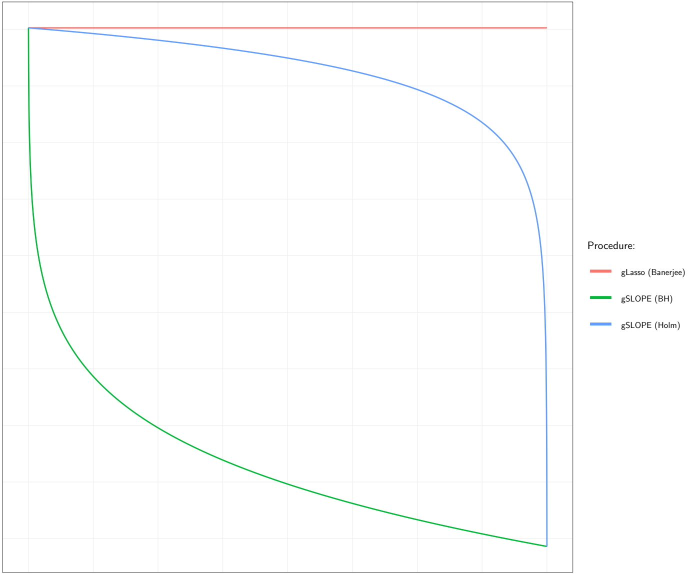
$$m = \frac{p(p-1)}{2},$$

$$\lambda_k^{\mathrm{BH}} = \frac{\mathrm{qt}_{n-2}(1 - \frac{\alpha}{m+1-k})}{\sqrt{n - 2 + \mathrm{qt}_{n-2}^2(1 - \frac{\alpha}{m+1-k})}},$$

$$\lambda^{\mathrm{BH}} = \{\lambda_1^{\mathrm{BH}}, \lambda_2^{\mathrm{BH}}, ..., \lambda_m^{\mathrm{BH}}\}.$$

It is based on Benjamini-Hochberg procedure for multiple testing.

Lambda comparison



Algorithms

For solving the Graphical SLOPE problem we used the *Alternating direction method of multipliers*, it can solve convex problems of the form

$$\begin{aligned} \text{minimize} \quad & f(x) + g(y) \\ \text{subject to} \quad & Ax + By = c. \end{aligned}$$

Algorithms

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$$\begin{aligned} \text{minimize} \quad & f(x) + g(y) \\ \text{subject to} \quad & Ax + By = c. \end{aligned}$$

For solving the Graphical Lasso problem we used an algorithm proposed by Friedman et al. in theirs first work about this method. Although we derived an ADMM-based algorithm, it was orders of magnitude slower than original one.

Overview

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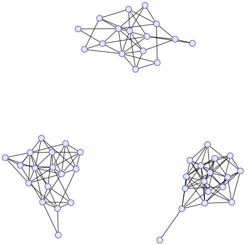
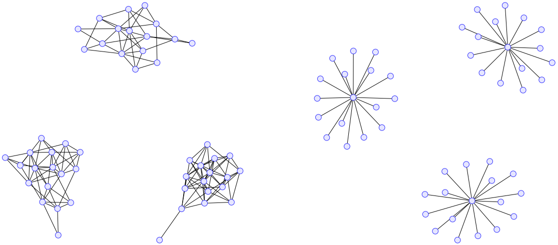
- Various types of graphs structure: cluster



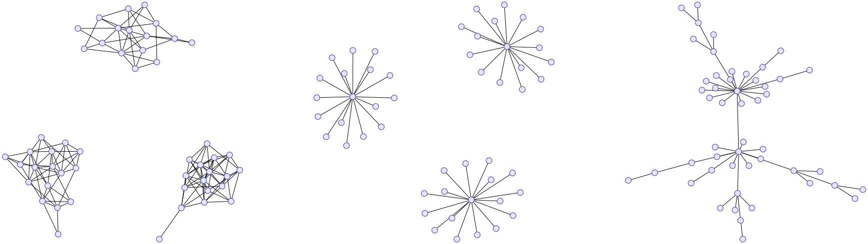
Overview

- Implementation with R, **huge** package for simulation.
- Various types of graphs structure: cluster, hub



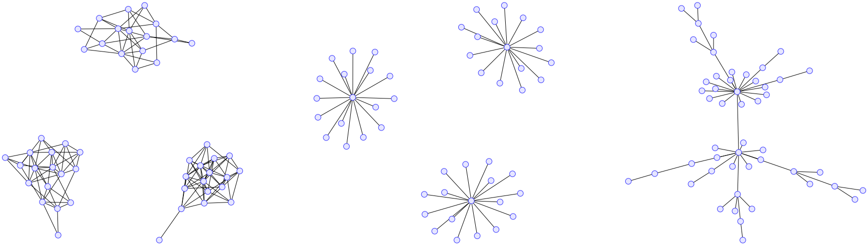
Overview

- Implementation with R, **huge** package for simulation.
- Various types of graphs structure: cluster, hub, and scale-free.



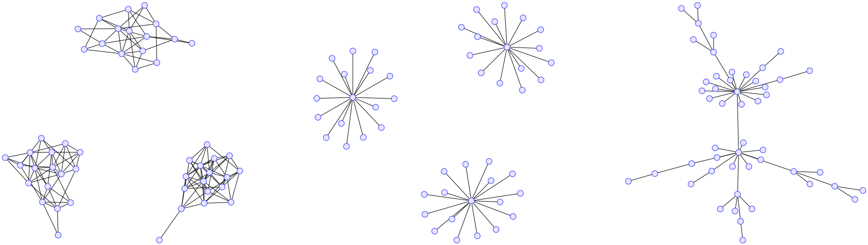
Overview

- Implementation with R, **huge** package for simulation.
- Various types of graphs structure: cluster, hub, and scale-free.
- Data: $p = 100$, $n \in \{50, 100, 200, 400\}$; different magnitude ratio; different sparsity and size of component.



Overview

- Implementation with R, **huge** package for simulation.
- Various types of graphs structure: cluster, hub, and scale-free.
- Data: $p = 100$, $n \in \{50, 100, 200, 400\}$; different magnitude ratio; different sparsity and size of component.
- Two levels of desirable FDR control: 0.05 and 0.2 .

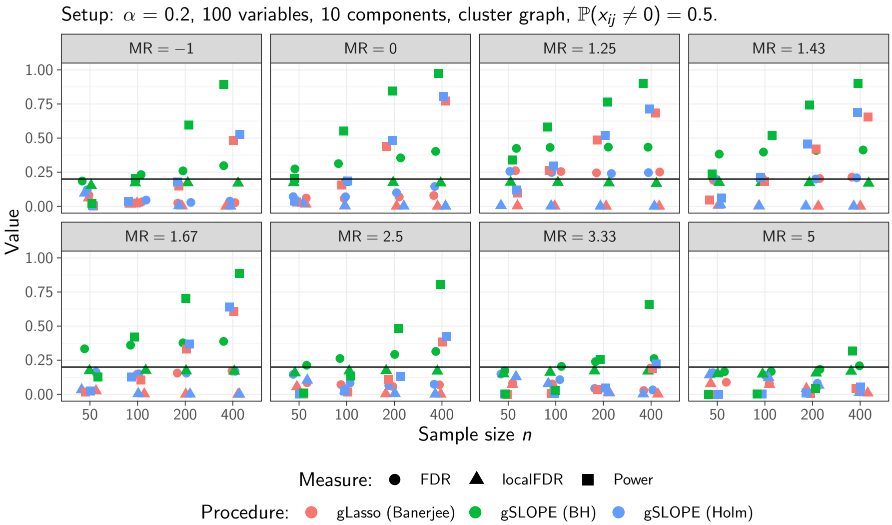


Measures

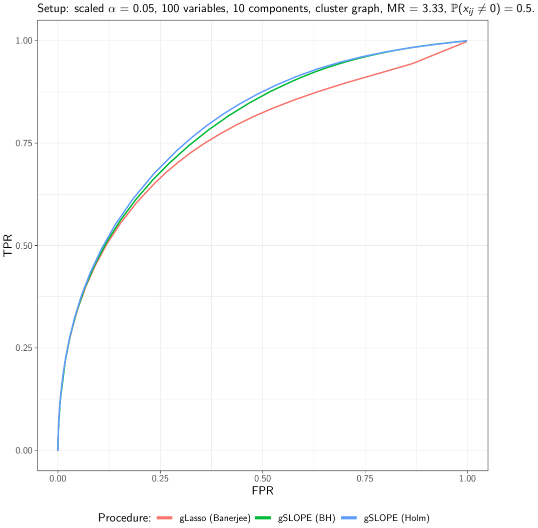
$$\mathrm{FDR} = \mathbb{E}\left[\frac{\#[\text{False positive}]}{\#[\text{False positive}] + \#[\text{True positive}]}\right]$$

$$\mathrm{localFDR} = \mathbb{E}\left[\frac{\#[\text{False positive outside the component}]}{\#[\text{False positive}] + \#[\text{True positive}]}\right]$$

Cluster results

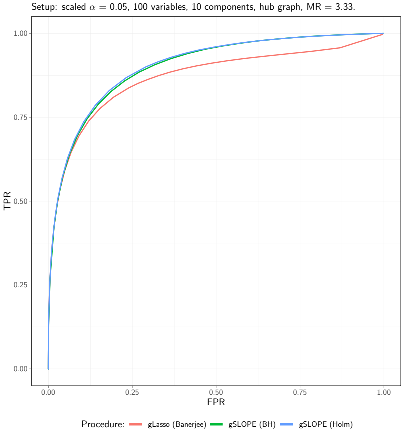


Cluster ROC



Setup: scaled $\alpha = 0.05$, 100 variables, 10 components, cluster graph, MR = 3.33, $\mathbb{P}(x_{ij} \neq 0) = 0.5$.
1.00
0.75
0.50
0.25
0.00
TPR
0.00
0.25
0.50
0.75
1.00
FPR
Procedure:
gLasso (Banerjee)
gSLOPE (BH)
gSLOPE (Holm)

Hub ROC



Setup: scaled $\alpha = 0.05$, 100 variables, 10 components, hub graph, MR = 3.33.
TPR
FPR
0.00
0.25
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1.00
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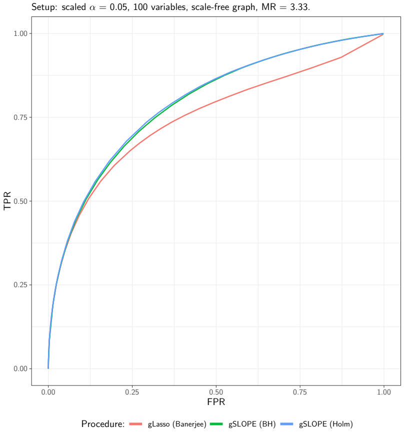

Setup: scaled $\alpha = 0.05$, 100 variables, scale-free graph, MR = 3.33.
TPR
FPR
0.00
0.25
0.50
0.75
1.00
Procedure: gLasso (Banerjee) gSLOPE (BH) gSLOPE (Holm)

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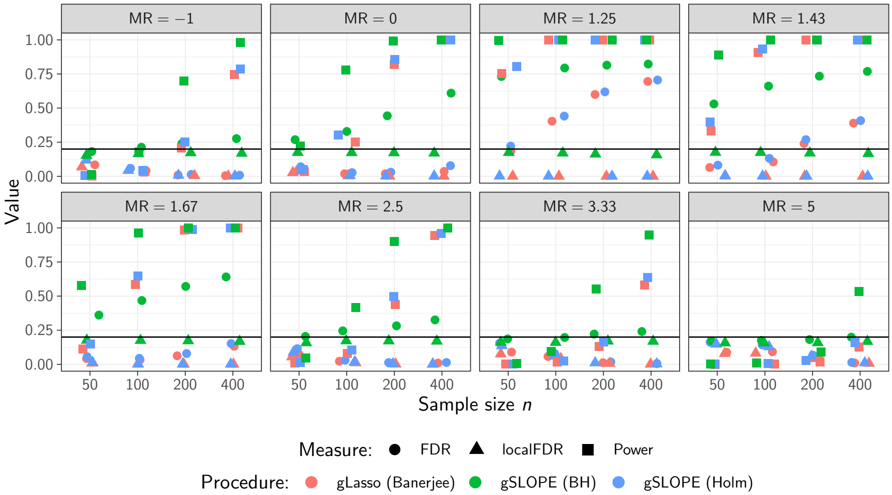
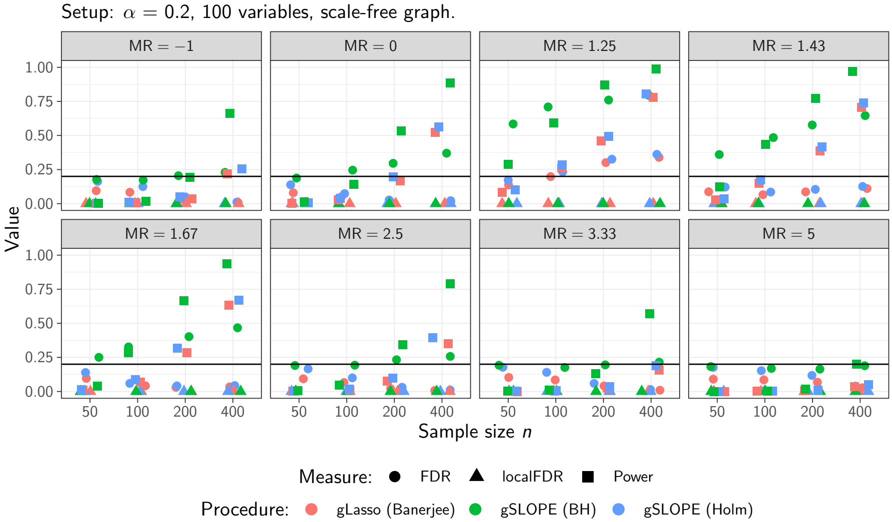
Thank you!

Hub results

Setup: $\alpha = 0.2$, 100 variables, 10 components, hub graph.



Scale-free results



Factorization theorem

Compatibility function

Let $G = (V, E)$ be a graph with a vertex set $V = 1, 2, \ldots, p$ and $\mathfrak{C}$ be its clique set. Let $\mathbb{X} = (X_1, \ldots, X_p)$ be a random vector defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, indexed by the graph nodes.

Definition (Compatibility function)

Let $C \in \mathfrak{C}$ be a clique of the graph G and let $\mathbb{X}_C$ be a subvector of the vector $\mathbb{X}$ indexed by the elements of the clique C, that is $\mathbb{X}_C = (X_s, s \in C)$. A real-valued function ψ_C of the vector $\mathbb{X}_C$ taking positive real values is called a *compatibility function*.

Factorization property

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Given a collection of compatibility functions, we say that probability distribution $\mathbb{P}$ *factorizes over G* if it has decomposition

$$\mathbb{P}(x_1, \ldots, x_n) = \frac{1}{Z} \prod_{C \in \mathfrak{C}} \psi_C(x_C), \tag{2}$$

where Z is the normalizing constant, known as the *partition function*. It is given by

$$Z = \sum_{x} \prod_{C \in \mathfrak{C}} \psi_C(x_C), \tag{3}$$

where the sum goes over all possible realizations of $\mathbb{X}$.

Markov property

Consider a cut set S of the given graph and let introduce a symbol $\perp\!\!\!\perp$ to denote the relation *is conditionally independent of*. With this notation, we say that the random vector $\mathbb{X}$ is Markov with respect to G if

$$\mathbb{X}_A \perp\!\!\!\perp \mathbb{X}_B \mid \mathbb{X}_S \qquad \text{for all cut sets } S \subset V, \tag{4}$$

where $\mathbb{X}_A$ denotes the subvector indexed by the subgraph A.

Canonical formulation

Canonical formulation

Any nondegenerated multivariate normal distribution $\mathcal{N}(\mu, \mathbf{\Sigma})$ can reparametrized into canonical parameters of the form

$$\gamma = \mathbf{\Sigma}^{-1}\mu \quad \text{and} \quad \mathbf{\Theta} = \mathbf{\Sigma}^{-1}.$$

Then density function is given by

$$\mathbb{P}_{\gamma,\mathbf{\Theta}}(x) = \exp\left\{ \sum_{s=1}^{p} \gamma_s x_s - \frac{1}{2} \sum_{s,t=1}^{p} \theta_{st} x_s x_t - A(\gamma, \mathbf{\Theta}) \right\},$$

where $A(\gamma, \mathbf{\Theta}) = -\frac{1}{2}\left(\det[(2\pi)^{-1}\,\mathbf{\Theta}] + \gamma^T\,\mathbf{\Theta}^{-1}\,\gamma\right)$.

Canonical formula derivation

$$\mathbb{P}_{\mu,\boldsymbol{\Sigma}}(x) = \left(\sqrt{\det[2\pi\boldsymbol{\Sigma}]}\right)^{-1} \exp\left\{(-\frac{1}{2}(x-\mu)^T\boldsymbol{\Sigma}^{-1}(x-\mu)\right\}$$

Canonical formula derivation

$$
\begin{aligned}
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&= \left(\sqrt{\det[(2\pi\mathbf{\Sigma})^{-1}]}\right) \exp\left\{-\frac{1}{2}x^T\mathbf{\Sigma}^{-1}x + x^T\mathbf{\Sigma}^{-1}\mu - \frac{1}{2}\mu^T\mathbf{\Sigma}^{-1}\mu\right\}
\end{aligned}
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&= \left(\sqrt{\det[(2\pi)^{-1}\,\boldsymbol{\Theta}]}\right)^{-1} \exp\left\{-\frac{1}{2}x^T\,\boldsymbol{\Theta}\,x + x^T\gamma - \frac{1}{2}\gamma^T\,\boldsymbol{\Theta}^{-1}\,\gamma\right\}
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&= \exp\left\{-\frac{1}{2}x^T\,\boldsymbol{\Theta}\,x + x^T\gamma - \frac{1}{2}\left(\det[(2\pi)^{-1}\,\boldsymbol{\Theta}] + \gamma^T\,\boldsymbol{\Theta}^{-1}\,\gamma\right)\right\}
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&= \exp\left\{-\frac{1}{2}x^T\,\boldsymbol{\Theta}\,x + x^T\gamma - A(\gamma,\boldsymbol{\Theta})\right\} \\
&= \mathbb{P}_{\gamma,\boldsymbol{\Theta}}(x)
\end{aligned}
$$

Log-likelihood derivation

Log-likelihood derivation (1/2)

$$\mathbb{L}(\mathbf{\Theta}, \mathbf{X}) = \frac{1}{N} \sum_{i=1}^{N} \log \mathbb{P}_{\mathbf{\Theta}}(x_i)$$

Log-likelihood derivation (1/2)

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&= \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} \log \det[(2\pi)^{-1} \, \mathbf{\Theta}] - \frac{1}{2} x_i^T \, \mathbf{\Theta} \, x_i
\end{aligned}
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Log-likelihood derivation (1/2)

$$
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\mathbb{L}(\mathbf{\Theta}, \mathbf{X}) &= \frac{1}{N} \sum_{i=1}^{N} \log \mathbb{P}_{\mathbf{\Theta}}(x_i) \\
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&= \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} \log \det[(2\pi)^{-1} \, \mathbf{\Theta}] - \frac{1}{2} x_i^T \, \mathbf{\Theta} \, x_i \\
&= \frac{1}{2N} \sum_{i=1}^{N} \log \left((2\pi)^{-N} \det[\mathbf{\Theta}] \right) - x_i^T \, \mathbf{\Theta} \, x_i
\end{aligned}
$$

Log-likelihood derivation (1/2)

$$
\begin{aligned}
\mathbb{L}(\boldsymbol{\Theta}, \mathbf{X}) &= \frac{1}{N} \sum_{i=1}^{N} \log \mathbb{P}_{\boldsymbol{\Theta}}(x_i) \\
&= \frac{1}{N} \sum_{i=1}^{N} -\frac{1}{2} x_i^T \, \boldsymbol{\Theta} \, x_i - A(\boldsymbol{\Theta}) \\
&= \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} \log \det[(2\pi)^{-1} \, \boldsymbol{\Theta}] - \frac{1}{2} x_i^T \, \boldsymbol{\Theta} \, x_i \\
&= \frac{1}{2N} \sum_{i=1}^{N} \log \left((2\pi)^{-N} \det[\boldsymbol{\Theta}] \right) - x_i^T \, \boldsymbol{\Theta} \, x_i \\
&= \frac{1}{2N} \sum_{i=1}^{N} \log \det \boldsymbol{\Theta} - N \log 2\pi - x_i^T \, \boldsymbol{\Theta} \, x_i = \ldots
\end{aligned}
$$

Log-likelihood derivation (2/2)

$$\ldots = \frac{1}{2N} \sum_{i=1}^{N} \log\det \boldsymbol{\Theta} - N \log 2\pi - x_i^T \, \boldsymbol{\Theta} \, x_i$$

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&= \frac{1}{2} \log\det \boldsymbol{\Theta} - \frac{N}{2} \log 2\pi - \frac{1}{2} \mathrm{tr}\left(\mathbf{S} \, \boldsymbol{\Theta} \right),
\end{aligned}$$

where $\mathbf{S}$ is an empirical covariance matrix given by $\frac{1}{N} \sum_{i=1}^{N} x_i x_i^T$.

ADMM for Graphical SLOPE

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Graphical SLOPE problem - ADMM formulation

$$\begin{aligned} \text{minimize} \quad & -\log\det X + \operatorname{tr}(XS) + \mathbb{I}[X \succeq 0] + \mathrm{J}_\lambda(Y) \\ \text{subject to} \quad & X = Y. \end{aligned}$$

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Graphical SLOPE problem - Augmented Lagrangian

$$\begin{aligned} \mathcal{L}_\rho(X, Y, N) = & -\log\det X + \operatorname{tr}(XS) + \mathbb{I}[X \succeq 0] \\ & + \lambda\|Y\|_1 + \rho\langle N, X - Y\rangle_F + \frac{\rho}{2}\|X - Y\|_F^2 \end{aligned}$$

X-update (1/3)

We have

$$X_k = \arg\min_{X} \mathcal{L}_\rho(X, Y_{k-1}, N_{k-1}) = \arg\min_{X \succeq 0} \left\{ -\log\det X + \frac{\rho}{2} \left\| X - \tilde{S}_{k-1} \right\|_F^2 \right\},$$

where

$$\tilde{S}_{k-1} = -N_{k-1} + Y_{k-1} - \frac{1}{\rho} S,$$

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The X-gradient of the augmented Lagrangian is given by

$$\nabla_X \mathcal{L}_\rho(X, Y_{k-1}, N_{k-1}) = -X^{-1} + \rho X - \rho \tilde{S}_{k-1}.$$

As the augmented Lagrangian is convex, it is clear that for some $X^* \succeq 0$

$$\nabla_X \mathcal{L}_\rho(X^*, Y_{k-1}, N_{k-1}) = -(X^*)^{-1} + \rho X^* - \rho \tilde{S}_{k-1} = 0.$$

X-update (2/3)

Rewriting equation as

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we can find a matrix that meets this condition.

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Then by multiplying right and left side by Q and Q^T respectively, we obtain

$$-(\tilde{X}^*)^{-1} + \rho \tilde{X}^* = \rho \Lambda,$$

where $\tilde{X}^* = Q^T X^* Q$.

X-update (3/3)

We have to find positive numbers $\tilde{x}_{ii}^*$ that satisfy

$$(\tilde{x}_{ii}^*)^2 - l_{ii}\tilde{x}_{ii}^* - \frac{1}{\rho} = 0.$$

It is obvious that

$$\tilde{x}_{ii} = \frac{l_i + \sqrt{l_i^2 + 4/\rho}}{2}.$$

Thus X^* is given by $X^* = Q^T \tilde{X}^* Q$. All diagonals are positive since $\rho > 0$.
Define $\mathcal{F}_\rho(\Lambda)$ as

$$\mathcal{F}_\rho(\Lambda) = \frac{1}{2}\,\mathrm{diag}\left\{ l_i + \sqrt{l_i^2 + 4/\rho} \right\}.$$

Since that

$$X^* = Q^T \tilde{X}^* Q = Q^T \mathcal{F}_\rho(\Lambda) Q = \mathcal{F}_\rho(\tilde{S}_{k-1}) = \mathcal{F}_\rho\left(-N_{k-1} + Y_{k-1} - \frac{1}{\rho} S \right),$$

we obtain a formula for updating X_k in each step.

Y-update

A formula for Y_k is different. We have

$$
\begin{aligned}
Y_k &= \arg\min_Y \mathcal{L}_\rho(X_k, Y, N_{k-1}) \\
&= \arg\min_Y \left\{ \mathrm{J}_\lambda(Y) + \frac{\rho}{2} \| Y - (X_k + N_{k-1}) \|_F^2 \right\}
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$$\begin{aligned} Y_k &= \arg\min_Y \mathcal{L}_\rho(X_k, Y, N_{k-1}) \\ &= \arg\min_Y \left\{ \mathrm{J}_\lambda(Y) + \frac{\rho}{2} \| Y - (X_k + N_{k-1}) \|_F^2 \right\} \end{aligned}$$

The last line of Y-update can be represented as a **proximity operator** which has closed form formula for SLOPE

$$\arg\min_Y \left\{ \mathrm{J}_\lambda(Y) + \frac{\rho}{2} \| Y - (X_k + N_{k-1}) \|_F^2 \right\} = \mathbf{prox}_{\mathrm{J}_\lambda, \rho} (X_k + N_{k-1}) . \quad (5)$$

ADMM for Graphical SLOPE

Figures/ADMMgSLOPE.png

FWER

FWER definition

Definition (Familywise error rate)

A *family-wise error rate* (FWER) is the probability of making one or more false discoveries, that is,

$$\text{FWER} = \mathbb{P}(\text{type I error}).$$