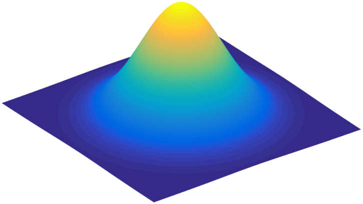
Gaussian Graphical Models and Graphical Lasso

Yuxin Chen

Princeton University, Spring 2017

Multivariate Gaussians

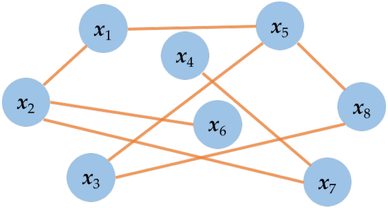


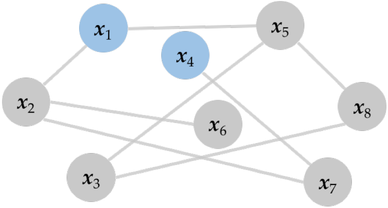
Consider a random vector $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Sigma})$ with pdf

$$\begin{aligned} f(\boldsymbol{x}) &= \frac{1}{(2\pi)^{p/2} \det(\boldsymbol{\Sigma})^{1/2}} \exp\left\{-\frac{1}{2}\boldsymbol{x}^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{x}\right\} \\ &\propto \det(\boldsymbol{\Theta})^{1/2} \exp\left\{-\frac{1}{2}\boldsymbol{x}^\top \boldsymbol{\Theta} \boldsymbol{x}\right\} \end{aligned}$$

where $\boldsymbol{\Sigma} = \mathbb{E}[\boldsymbol{x}\boldsymbol{x}^\top] \succ \boldsymbol{0}$ is covariance matrix, and $\boldsymbol{\Theta} = \boldsymbol{\Sigma}^{-1}$ is inverse covariance matrix / precision matrix

Undirected graphical models





$$x_1 \perp\!\!\!\perp x_4 \mid \{x_2, x_3, x_5, x_6, x_7, x_8\}$$

- Represent a collection of variables $\boldsymbol{x} = [x_1, \cdots, x_p]^\top$ by a vertex set $\mathcal{V} = \{1, \cdots, p\}$
- Encode conditional independence by a set $\mathcal{E}$ of edges
  - For any pair of vertices u and v,

$$(u, v) \notin \mathcal{E} \quad \Longleftrightarrow \quad x_u \perp\!\!\!\perp x_v \mid \boldsymbol{x}_{\mathcal{V} \setminus \{u,v\}}$$

Gaussian graphical models

Fact 5.1

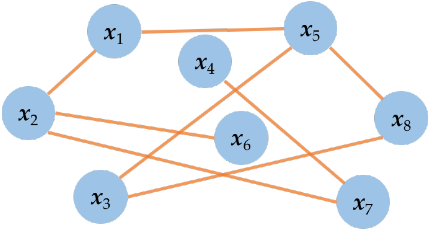
(Homework) Consider a Gaussian vector $\boldsymbol{x} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$*. For any* u *and* v*,*

$$x_u \perp\!\!\!\perp x_v \mid \boldsymbol{x}_{\mathcal{V}\backslash\{u,v\}}$$

iff $\Theta_{u,v} = 0$*, where* $\boldsymbol{\Theta} = \boldsymbol{\Sigma}^{-1}$*.*

$$\text{conditional independence} \quad \Longleftrightarrow \quad \text{sparsity}$$

Gaussian graphical models



$$\underbrace{\begin{bmatrix} * & * & 0 & 0 & * & 0 & 0 & 0 \\ * & * & 0 & 0 & 0 & * & * & 0 \\ 0 & 0 & * & 0 & * & 0 & 0 & * \\ 0 & 0 & 0 & * & 0 & 0 & * & 0 \\ * & 0 & * & 0 & * & 0 & 0 & * \\ 0 & * & 0 & 0 & 0 & * & 0 & 0 \\ 0 & * & 0 & * & 0 & 0 & * & 0 \\ 0 & 0 & * & 0 & * & 0 & 0 & * \end{bmatrix}}_{\boldsymbol{\Theta}}$$

Likelihoods for Gaussian models

Draw n i.i.d. samples $\boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(n)} \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$, then log-likelihood (up to additive constant) is

$$\begin{aligned} \ell(\mathbf{\Theta}) &= \frac{1}{n}\sum_{i=1}^{n} \log f(\boldsymbol{x}^{(i)}) = \frac{1}{2}\log\det(\mathbf{\Theta}) - \frac{1}{2n}\sum_{i=1}^{n} \boldsymbol{x}^{(i)\top}\mathbf{\Theta}\boldsymbol{x}^{(i)} \\ &= \frac{1}{2}\log\det(\mathbf{\Theta}) - \frac{1}{2}\langle \boldsymbol{S}, \mathbf{\Theta}\rangle, \end{aligned}$$

where $\boldsymbol{S} := \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{x}^{(i)}\boldsymbol{x}^{(i)\top}$ is sample covariance; $\langle \boldsymbol{S}, \mathbf{\Theta}\rangle = \mathrm{tr}(\boldsymbol{S}\mathbf{\Theta})$

Maximum likelihood estimation

$$\text{maximize}_{\mathbf{\Theta}\succeq \mathbf{0}} \quad \log\det(\mathbf{\Theta}) - \langle \boldsymbol{S}, \mathbf{\Theta}\rangle$$

Challenge in high-dimensional regime

Classical theory says MLE coverges to the truth as sample size $n \to \infty$

Practically, we are often in the regime where sample size n is small $(n < p)$

- In this regime, $\boldsymbol{S}$ is rank-deficient, and MLE does not even exist

Graphical lasso (Friedman, Hastie, &Tibshirani '08)

Many pairs of variables are conditionally independent

$\Longleftrightarrow$ many missing links in the graphical model (sparsity)

Key idea: apply lasso by treating each node as a response variable

$$\text{maximize}_{\boldsymbol{\Theta}\succeq \mathbf{0}} \quad \log\det(\boldsymbol{\Theta}) - \langle \boldsymbol{S}, \boldsymbol{\Theta}\rangle - \underbrace{\lambda\|\boldsymbol{\Theta}\|_1}_{\text{lasso penalty}}$$

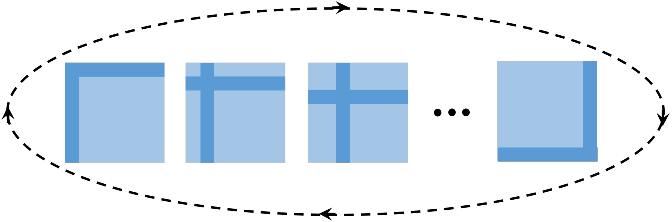
- It is a convex program! (homework)
- First-order optimality condition

$$\boldsymbol{\Theta}^{-1} - \boldsymbol{S} - \lambda \underbrace{\partial\|\boldsymbol{\Theta}\|_1}_{\text{subgradient}} = \mathbf{0} \tag{5.1}$$

$$\Longrightarrow \quad (\boldsymbol{\Theta}^{-1})_{i,i} = S_{i,i} + \lambda, \quad 1 \le i \le p$$

Blockwise coordinate descent

Idea: repeatedly cycle through all columns/rows and, in each step, optimize only a single column/row



Notation: use $\boldsymbol{W}$ to denote working version of $\boldsymbol{\Theta}^{-1}$. Partition all matrices into 1 column/row vs. the rest

$$\boldsymbol{\Theta} = \begin{bmatrix} \boldsymbol{\Theta}_{11} & \boldsymbol{\theta}_{12} \\ \boldsymbol{\theta}_{12}^\top & \theta_{22} \end{bmatrix} \quad \boldsymbol{S} = \begin{bmatrix} \boldsymbol{S}_{11} & \boldsymbol{s}_{12} \\ \boldsymbol{s}_{12}^\top & s_{22} \end{bmatrix} \quad \boldsymbol{W} = \begin{bmatrix} \boldsymbol{W}_{11} & \boldsymbol{w}_{12} \\ \boldsymbol{w}_{12}^\top & w_{22} \end{bmatrix}$$

Blockwise coordinate descent

Blockwise step: suppose we fix all but the last row / column. It follows from (5.1) that

$$\mathbf{0} \in \boldsymbol{W}_{11}\boldsymbol{\beta} - \boldsymbol{s}_{12} - \lambda\partial\|\boldsymbol{\theta}_{12}\|_1 = \boldsymbol{W}_{11}\boldsymbol{\beta} - \boldsymbol{s}_{12} + \lambda\partial\|\boldsymbol{\beta}\|_1 \tag{5.2}$$

where $\boldsymbol{\beta} = -\boldsymbol{\theta}_{12}/\tilde{\theta}_{22}$ (since $\underbrace{\begin{bmatrix} \boldsymbol{\Theta}_{11} & \boldsymbol{\theta}_{12} \\ \boldsymbol{\theta}_{12}^\top & \theta_{22} \end{bmatrix}^{-1} = \begin{bmatrix} * & -\frac{1}{\tilde{\theta}_{22}}\boldsymbol{\Theta}_{11}^{-1}\boldsymbol{\theta}_{12} \\ * & * \end{bmatrix}}_{\text{matrix inverse formula}}$) with

$\tilde{\theta}_{22} = \theta_{22} - \boldsymbol{\theta}_{12}^\top\boldsymbol{\Theta}_{11}^{-1}\boldsymbol{\theta}_{12} > 0$

This coincides with the optimality condition for

$$\text{minimize}_{\boldsymbol{\beta}} \quad \frac{1}{2}\|\boldsymbol{W}_{11}^{1/2}\boldsymbol{\beta} - \boldsymbol{W}_{11}^{-1/2}\boldsymbol{s}_{12}\|_2^2 + \lambda\|\boldsymbol{\beta}\|_1 \tag{5.3}$$

Blockwise coordinate descent

Algorithm 5.1 Block coordinate descent for graphical lasso

Initialize $\boldsymbol{W} = \boldsymbol{S} + \lambda \boldsymbol{I}$ and fix its diagonals $\{w_{i,i}\}$.

Repeat until covergence:

for $t = 1, \cdots p$**:**

(i) Partition $\boldsymbol{W}$ (resp. $\boldsymbol{S}$) into 4 parts, where the upper-left part consists of all but the jth row / column

(ii) Solve

$$\text{minimize}_{\boldsymbol{\beta}} \quad \frac{1}{2} \|\boldsymbol{W}_{11}^{1/2} \boldsymbol{\beta} - \boldsymbol{W}_{11}^{-1/2} \boldsymbol{s}_{12}\|^2 + \lambda \|\boldsymbol{\beta}\|_1$$

(iii) Update $\boldsymbol{w}_{12} = \boldsymbol{W}_{11} \boldsymbol{\beta}$

Set $\hat{\boldsymbol{\theta}}_{12} = -\hat{\theta}_{22} \boldsymbol{\beta}$ with $\hat{\theta}_{22} = 1/(w_{22} - \boldsymbol{w}_{12}^\top \boldsymbol{\beta})$

Blockwise coordinate descent

The only remaining thing is to ensure $\boldsymbol{W} \succeq \mathbf{0}$. This is automatically satisfied:

Lemma 5.2 (Mazumder & Hastie, '12)

If we start with $\boldsymbol{W} \succ \mathbf{0}$ satisfying $\|\boldsymbol{W} - \boldsymbol{S}\|_\infty \le \lambda$, then every row/column update maintains positive definiteness of $\boldsymbol{W}$.

- If we start with $\boldsymbol{W}^{(0)} = \boldsymbol{S} + \lambda \boldsymbol{I}$, then $\boldsymbol{W}^{(t)}$ will always be positive definite

Proof of Lemma 5.2

A key observation for the proof of Lemma 5.2

Fact 5.3 (Lemma 2, Mazumder & Hastie, '12)

Solving (5.3) is equivalent to solving

$$\text{minimize}_{\boldsymbol{\gamma}} \ (\boldsymbol{s}_{12} + \boldsymbol{\gamma})^\top \boldsymbol{W}_{11}^{-1} (\boldsymbol{s}_{12} + \boldsymbol{\gamma}) \quad \text{s.t. } \|\boldsymbol{\gamma}\|_\infty \le \lambda \qquad (5.4)$$

where solutions to 2 problems are related by $\hat{\boldsymbol{\beta}} = \boldsymbol{W}_{11}^{-1}(\boldsymbol{s}_{12} + \hat{\boldsymbol{\gamma}})$

- Check that optimality condition of (5.3) and that of (5.4) match

Proof of Lemma 5.2

Suppose in t^{th} iteration one has $\|\boldsymbol{W}^{(t)} - \boldsymbol{S}\|_\infty \le \lambda$ and

$$\boldsymbol{W}^{(t)} \succ \boldsymbol{0}$$

$$\iff \quad \boldsymbol{W}_{11}^{(t)} \succ \boldsymbol{0}; \quad w_{22} - \boldsymbol{w}_{12}^{(t)\top} \left(\boldsymbol{W}_{11}^{(t)}\right)^{-1} \boldsymbol{w}_{12}^{(t)} > 0 \quad \text{(Schur complement)}$$

We only update $\boldsymbol{w}_{12}$, so it suffices to show

$$w_{22} - \boldsymbol{w}_{12}^{(t+1)\top} \left(\boldsymbol{W}_{11}^{(t)}\right)^{-1} \boldsymbol{w}_{12}^{(t+1)} > 0 \tag{5.5}$$

Recall that $\boldsymbol{w}_{12}^{(t+1)} = \boldsymbol{W}_{11}^{t} \boldsymbol{\beta}^{t+1}$. It follows from Fact 5.3 that and

$$\begin{aligned} &\|\boldsymbol{w}_{12}^{(t+1)} - \boldsymbol{s}_{12}\|_\infty \le \lambda; \\ &\boldsymbol{w}_{12}^{(t+1)\top} (\boldsymbol{W}_{11}^{(t)})^{-1} \boldsymbol{w}_{12}^{(t+1)} \le \boldsymbol{w}_{12}^{(t)\top} (\boldsymbol{W}_{11}^{(t)})^{-1} \boldsymbol{w}_{12}^{(t)}. \end{aligned}$$

Since $w_{22} = s_{22} + \lambda$ remains unchanged, we establish (5.5).

Reference

[1] "*Sparse inverse covariance estimation with the graphical lasso*," J. Friedman, T. Hastie, and R. Tibshirani, *Biostatistics*, 2008.

[2] "*The graphical lasso: new insights and alternatives*," R. Mazumder and T. Hastie, *Electronic journal of statistics*, 2012.

[3] "*Statistical learning with sparsity: the Lasso and generalizations*," T. Hastie, R. Tibshirani, and M. Wainwright, 2015.