Gaussian graphical model

DSA5103 Lecture 10

Yangjing Zhang

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NUS

Today's content

1. Basics of graphical models
2. Gaussian graphical models and graphical Lasso
3. Neighbourhood selection
4. Applications

Basics of graphical models

Joint distribution

Toy example Given a coin (possibly biased). Toss the coin twice.

- x_1: H(head)/T(tail). x_2: H/T. x_3: F(fair coin)/B(biased coin)
- Joint distribution $p(x_1, x_2, x_3)$
- Conditional distribution $p(x_1, x_2 \mid x_3 = B)$

Table 1: Joint distribution

x_1	x_2	x_3	Probability
H	H	F	0.125
H	T	F	0.125
T	H	F	0.125
T	T	F	0.125
H	H	B	0.32
H	T	B	0.08
T	H	B	0.08
T	T	B	0.02

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Table 2: Conditioning on $x_3 = B$

x_1	x_2	x_3	Probability
H	H	B	0.64
H	T	B	0.16
T	H	B	0.16
T	T	B	0.04

Conditional independence

Toy example

- Marginalization

Table 3: Conditioning on $x_3 = B$

x_1	x_2	x_3	Probability
H	H	B	0.64
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T	H	B	0.16
T	T	B	0.04

Table 4: Marginalization

x_1	x_3	Probability
H	B	0.8
T	B	0.2

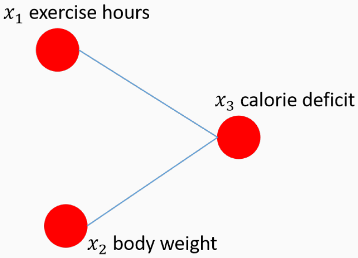
x_2	x_3	Probability
H	B	0.8
T	B	0.2

- x_1 and x_2 are conditionally independent given x_3 if
  $p(x_1, x_2 \mid x_3) = p(x_1 \mid x_3)p(x_2 \mid x_3)$

Conditional independence

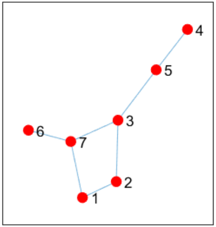
Toy example

- x_1: the number of hours a person spends exercising in a week
- x_2: the person's body weight
- x_3: the person's calorie deficit in a week
  — calorie deficit = calorie received (eating) − calorie spent (breathing, walking, exercising, etc)
- they are correlated
- given x_3, x_1 and x_2 are conditionally independent



Undirected graph

- A **undirected graph** $G = (V, E)$ consists of a vertex set $V = \{1, 2, \ldots, p\}$, and an edge set $E \subset V \times V$
- "Undirected": the edge $(s, t) \in E =$ the edge $(t, s) \in E$.
- Assume no self-loop



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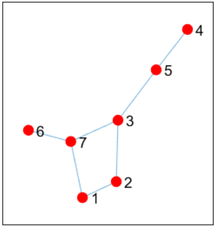

Connected

Vertex set $V = \{1, 2, 3, 4, 5, 6, 7\}$

Edge set $E =$

$\{(6, 7), (7, 3), (7, 1), (1, 2), (2, 3), (3, 5), (5, 4)\}$

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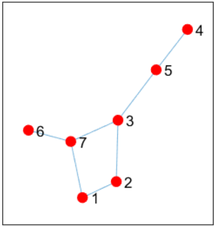

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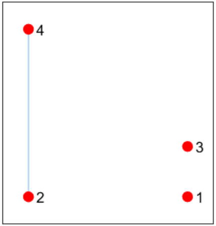


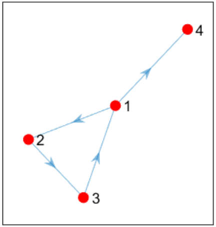
Disconnected

Vertex set $V = \{1, 2, 3, 4\}$

Edge set $E = \{(2, 4)\}$

Directed graphs

- In directed graphs, the edges have directionality. Directed graphs are more difficult to handle
- In our context, we only consider undirected graphs without self-loop



Vertex set $V = \{1, 2, 3, 4\}$

Edge set $E = \{(2,3), (3,1), (1,2), (1,4)\}$

The edge $(2,3)$ is from node 2 to node 3, different from the edge $(3,2)$

Markov property

- Consider a cut set S that separates the graph into disconnected components A and B
- Use $\perp\!\!\!\perp$ to denote the relation "is conditionally independent of"
- We say that the random variable x is Markov with respect to $G = (V, E)$ if

$$x_A \perp\!\!\!\perp x_B \mid x_S \quad \text{for all cut sets } S \subset V$$

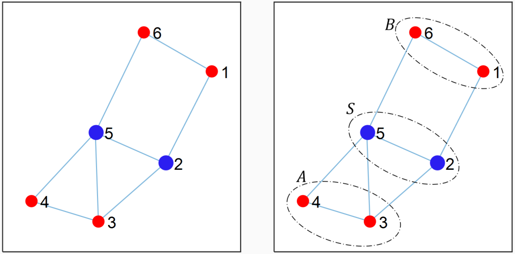
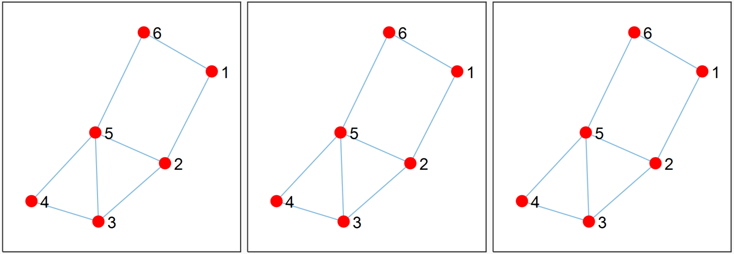


Figure 1: When the vertices in the cut set S are removed, the graph is broken into two sub-components A and B.

Illustration of Markov property



(a) **(b)** **(c)**

For example, we have the conditional independence

(a) $x_6 \perp\!\!\!\perp x_2, x_3, x_4 \mid x_1, x_5$

(b) $x_6, x_1, x_2 \perp\!\!\!\perp x_4 \mid x_3, x_5$

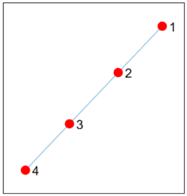
(c) $x_1 \perp\!\!\!\perp x_5 \mid x_2, x_3, x_5, x_6$

Illustration of Markov property

- Consider a chain-structured graph with edge set

$$E = \{(1,2), (2,3), \ldots, (p-1, p)\}$$

- Any single vertex $s \in \{2, 3, \ldots, p-1\}$ forms a cut set



- The cut set $\{s\}$ separates the graph into two sub-components

$$\text{past } P = \{1, \ldots, s-1\}$$
$$\text{furture } F = \{s+1, \ldots, p\}$$

- Markov property: for a Markov chain, the future x_F is conditionally independent of the past x_P given the present x_s.

Multivariate Gaussians

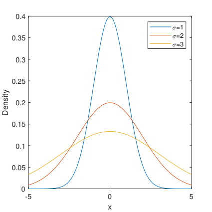
The probability density function of a multivariate Gaussian distribution with mean vector $\mu \in \mathbb{R}^p$ and covariance matrix $\Sigma \in \mathbb{S}^p_{++}$ is

$$f(x) = \frac{1}{(2\pi)^{p/2} \det(\Sigma)^{1/2}} \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right)$$

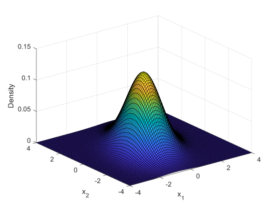
- $x \sim N(\mu, \Sigma)$ in $\mathbb{R}^p$
- $\det(\Sigma)$ denotes the determinant of the covariance matrix
  - ▷ $\det(\Sigma) = \prod_{j=1}^{p} \lambda_j(\Sigma)$, where $\lambda_j(\Sigma)$ is the j-the eigenvalue of $\Sigma \in \mathbb{S}^p$
- $\Theta = \Sigma^{-1}$ denotes the inverse covariance matrix or precision matrix
  - ▷ $\det(\Theta) = \dfrac{1}{\det(\Sigma)}$
- For simplicity, assume $\mu = 0$

Multivariate Gaussians

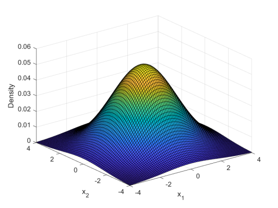
$$f(x) = \frac{1}{(2\pi)^{p/2}\det(\Sigma)^{1/2}} \exp\left(-\frac{1}{2}x^T\Sigma^{-1}x\right)$$



(d)



(e)



(f)

(d) $p = 1$. Let $\Sigma = \sigma^2$, the probability density function reduces to

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma^2}\right), \qquad x \sim N(0, \sigma^2)$$

(e) $p = 2$, $\Sigma = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 2 \end{bmatrix}$ (f) $p = 2$, $\Sigma = \begin{bmatrix} 3 & 0 \\ 0 & 3 \end{bmatrix}$

Gaussian graphical models

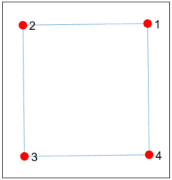
Gaussian graphical models

The essential idea of Gaussian graphical models are

- to represent a collection of Gaussian random variables $x = (x_1, \ldots, x_p)^T$ by the vertex set $V = \{1, \ldots, p\}$
- to represent the "relationships" (conditional independence) of variables by the edge set E
  - ▷ For any pair of vertices s and t,

$$(s,t) \notin E \iff x_s \perp\!\!\!\perp x_t \mid x_{V \setminus \{s,t\}}$$

where $V \setminus \{s,t\} = \{k \mid 1 \le k \le p,\ k \ne s,\ k \ne t\}$



If random variable $x = (x_1, x_2, x_3, x_4)^T$ is Markov w.r.t. the left graph, then

$x_1 \perp\!\!\!\perp x_3 \mid x_2, x_4$

$x_2 \perp\!\!\!\perp x_4 \mid x_1, x_3$

Gaussian graphical models

Fact [4] Consider a Gaussian vector $x \sim N(0, \Sigma)$. For any s and t,

$$x_s \perp\!\!\!\perp x_t \mid x_{V \setminus \{s,t\}}$$

if and only if

$$\Theta_{st} = 0, \quad \Theta = \Sigma^{-1}.$$

That is, we can characterize the conditional independence of Gaussian random variables by the graph with edge set $E = \{(s,t) \mid \Theta_{st} \neq 0, s < t\}$

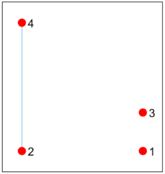
	conditional independence	$x_s \perp\!\!\!\perp x_t \mid x_{V \setminus \{s,t\}}$
$\iff$	zero in precision	$\Theta_{st} = 0$
$\iff$	no edge in graph	$(s,t) \notin E$

Example

Example. Represent by a graph the conditional independence of a Gaussian vector $(x_1, x_2, x_3, x_4) \sim N(0, \Sigma)$, $\Sigma = \begin{bmatrix} 1 & & & \\ & 4/3 & & -2/3 \\ & & 1 & \\ & -2/3 & & 4/3 \end{bmatrix}$.

Solution.

1. Compute the precision matrix $\Theta = \Sigma^{-1} = \begin{bmatrix} 1 & & & \\ & 1 & & 0.5 \\ & & 1 & \\ & 0.5 & & 1 \end{bmatrix}$
2. Edge set $E = \{(2,4)\}$ since $\Theta_{24} \neq 0$. Vertex set $V = \{1,2,3,4\}$
3. Plot



Example

Example. Represent by a graph the conditional independence of a Gaussian vector $x \sim N(0, I)$, $x \in \mathbb{R}^p$.

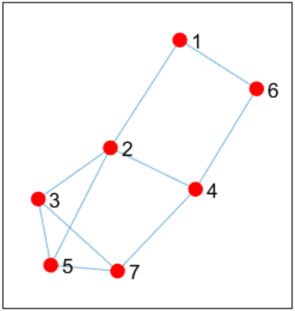
Solution.

1. Compute the precision matrix $\Theta = \Sigma^{-1} = I$
2. Edge set $E = \{(s,t) \mid \Theta_{st} \neq 0, s < t\} = \emptyset$ since all off-diagonal entries are zero. Vertex set $V = \{1, 2, \ldots, p\}$
3. The graph has p nodes and no edge.

- The graph interprets that $x_s \perp\!\!\!\perp x_t \mid \{1, \ldots, p\} \backslash \{s, t\}$
- In fact, $x \sim N(0, I) \iff x_i \sim N(0, 1) \, \forall \, i = 1, \ldots, p$. The random variable x_s and x_t are independent for $s \neq t$.

Gaussian graphical models

Correspondence between the zero pattern of Θ and the edge structure E of the graph



$$\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 \end{bmatrix}$$

Zero pattern of the precision matrix Θ. Here 1 correspond to $\Theta_{st} \neq 0$, $s \neq t$. Diagonals are 0.

Maximum likelihood estimation

- Given n samples $x^{(1)}, \ldots, x^{(n)} \sim N(0, \Sigma)$ independently
- Suppose the true covariance matrix Σ is unknown
- Aim to learn the covariance matrix Σ or the precision matrix $\Theta = \Sigma^{-1}$
- This problem is called covariance selection, precision estimation, or inverse covariance estimation

$$x \sim N(0, \Sigma), \quad f(x) = \frac{1}{(2\pi)^{p/2} \det(\Sigma)^{1/2}} \exp\left(-\frac{1}{2} x^T \Sigma^{-1} x\right)$$

Maximum likelihood estimation (MLE)

$$\max \quad \frac{1}{n} \sum_{i=1}^{n} \log f(x^{(i)})$$

It is equivalent to maximize the likelihood $\prod_{i=1}^{n} f(x^{(i)})$

Likelihoods

$$x \sim N(0, \Sigma), \quad f(x) = \frac{1}{(2\pi)^{p/2} \det(\Sigma)^{1/2}} \exp\left(-\frac{1}{2} x^T \Sigma^{-1} x\right)$$

Likelihoods

$$x \sim N(0, \Sigma), \quad f(x) = \frac{1}{(2\pi)^{p/2} \det(\Sigma)^{1/2}} \exp\left(-\frac{1}{2} x^T \Sigma^{-1} x\right)$$

$$\begin{aligned}\log f(x) &= \underbrace{-\log\left((2\pi)^{p/2}\right)}_{\text{constant}} - \frac{1}{2}\log\det(\Sigma) - \frac{1}{2}\langle \Sigma^{-1}, xx^T \rangle \\ &= \frac{1}{2}\log\det(\Theta) - \frac{1}{2}\langle \Theta, xx^T \rangle + \text{constant}\end{aligned}$$

The log-likelihood (up to additive constant) is

$$\frac{1}{n}\sum_{i=1}^{n} \log f(x^{(i)}) = \frac{1}{2}\log\det(\Theta) - \frac{1}{2n}\sum_{i=1}^{n}\langle \Theta, x^{(i)}(x^{(i)})^T \rangle$$

$$= \frac{1}{2}\log\det(\Theta) - \frac{1}{2}\langle S, \Theta \rangle$$

- $S = \frac{1}{n}\sum_{i=1}^{n} x^{(i)}(x^{(i)})^T$ is the sample covariance matrix
- $\Theta = \Sigma^{-1} \Rightarrow \det(\Theta) = \frac{1}{\det(\Sigma)} \Rightarrow \log\det(\Theta) = -\log\det(\Sigma)$

Maximum likelihood estimation

Maximum likelihood estimation (MLE)

$$
\begin{aligned}
&\max_{\Theta \in \mathbb{S}^p_{++}} \quad \log\det(\Theta) - \langle S, \Theta \rangle \\
\iff &\min_{\Theta \in \mathbb{S}^p_{++}} \quad -\log\det(\Theta) + \langle S, \Theta \rangle
\end{aligned}
\tag{MLE}
$$

- The log-determinant function

$$
h(\Theta) = -\log\det(\Theta) = \begin{cases} -\sum_{j=1}^{p} \log(\lambda_j(\Theta)), & \text{if } \Theta \in \mathbb{S}^p_{++} \\ +\infty, & \text{otherwise.} \end{cases}
$$

  Here $\lambda_j(\Theta)$ is the j-th eigenvalue of Θ
- $h(\Theta) = -\log\det(\Theta)$ is convex on $\mathbb{S}^p_{++}$
- $\nabla h(\Theta) = -\Theta^{-1}$ for any $\Theta \in \mathbb{S}^p_{++}$
- If the solution $\widehat{\Theta}$ to (MLE) exists, then $\widehat{\Theta} = S^{-1}$

Understand log-determinant function

It is nontrivial to prove

- $h(\Theta) = -\log\det(\Theta)$ is convex on $\mathbb{S}^p_{++}$
- $\nabla h(\Theta) = -\Theta^{-1}$ for any $\Theta \in \mathbb{S}^p_{++}$

Let's understand them on a diagonal $\Theta = \mathrm{Diag}(\Theta_{jj})$, $\Theta_{jj} > 0$

- $h(\Theta) = -\log\det(\Theta) = -\sum_{j=1}^p \log(\Theta_{jj})$ is convex since $-\log(\cdot)$ is convex
- $\nabla h(\Theta) = \begin{bmatrix} \frac{\partial}{\partial \Theta_{11}} h & & \\ & \ddots & \\ & & \frac{\partial}{\partial \Theta_{pp}} h \end{bmatrix} = \begin{bmatrix} -\frac{1}{\Theta_{11}} & & \\ & \ddots & \\ & & -\frac{1}{\Theta_{pp}} \end{bmatrix} = -\Theta^{-1}$

Challenge in high-dimensional regime

- MLE coverges to the truth as sample size $n \to +\infty$
- Practically, we are often in the regime where $n < p$
- In this regime, S is rank-deficient, and the solution to (MLE) does not even exist
- Consider regularization
  - ▷ Guarantee that a solution exists
  - ▷ The estimated precision matrix tends to be sparse and easy to interpret

Consider the following MLE with regularization (often reffered to as graphical Lasso)

$$\min_{\Theta \in \mathbb{S}^p_{++}} \quad -\log\det(\Theta) + \langle S, \Theta \rangle + \lambda \|\Theta\|_{1,\text{off}}$$

$\|\Theta\|_{1,\text{off}} = \sum_{s \neq t} |\Theta_{ij}|$ the ℓ_1-norm of the off-diagonal entries

Algorithm: ADMM

Apply ADMM for solving the graphical Lasso problem

$$\min_{\Theta \in \mathbb{S}^p_{++}} \quad -\log\det(\Theta) + \langle S, \Theta \rangle + \lambda \|\Theta\|_{1,\text{off}}$$

- Transform it into the form that ADMM can handle

$$\begin{aligned} \min_{\Theta, Y} \quad & -\log\det(\Theta) + \langle S, \Theta \rangle + \delta_{\mathbb{S}^p_{++}}(\Theta) + \lambda \|Y\|_{1,\text{off}} \\ \text{s.t.} \quad & \Theta - Y = 0 \end{aligned}$$

- The augmented Lagrangian

$$\begin{aligned} L_\sigma(\Theta, Y, Z) = & -\log\det(\Theta) + \langle S, \Theta \rangle + \delta_{\mathbb{S}^p_{++}}(\Theta) + \lambda \|Y\|_{1,\text{off}} \\ & + \langle Z, \Theta - Y \rangle + \frac{\sigma}{2} \|\Theta - Y\|_F^2 \end{aligned}$$

- ADMM iterations $\begin{cases} \Theta \leftarrow \arg\min_{\Theta} L_\sigma(\Theta, Y, Z) \\ Y \leftarrow \arg\min_{Y} L_\sigma(\Theta, Y, Z) \\ Z \leftarrow Z + \tau\sigma(\Theta - Y) \end{cases}$

Subproblem-Θ

$$L_\sigma(\Theta, Y, Z) = -\log\det(\Theta) + \langle S, \Theta\rangle + \delta_{\mathbb{S}^p_{++}}(\Theta) + \lambda\|Y\|_{1,\text{off}}$$
$$+ \langle Z, \Theta - Y\rangle + \frac{\sigma}{2}\|\Theta - Y\|_F^2$$

Consider minimizing w.r.t. Θ

$$\begin{aligned}
&\arg\min_{\Theta\in\mathbb{S}^p_{++}} -\log\det(\Theta) + \langle S+Z, \Theta\rangle + \frac{\sigma}{2}\|\Theta - Y\|_F^2 \\
&= \arg\min_{\Theta\in\mathbb{S}^p_{++}} -\log\det(\Theta) + \frac{\sigma}{2}\|\Theta - Y + \sigma^{-1}(S+Z)\|_F^2 \\
&= P_{\frac{1}{\sigma}h}\left(Y - \sigma^{-1}(S+Z)\right)
\end{aligned}$$

where $h(\Theta) = -\log\det(\Theta) = \begin{cases} -\sum_{j=1}^p \log(\lambda_j(\Theta)), & \text{if } \Theta \in \mathbb{S}^p_{++} \\ +\infty, & \text{otherwise.} \end{cases}$

Proximal mapping of log-determinant function

Theorem The proximal mapping

$$P_{\frac{1}{\sigma}h}(Y) = \operatorname*{arg\,min}_{\Theta \in \mathbb{S}^p_{++}} \left\{ -\log\det(\Theta) + \frac{\sigma}{2}\|\Theta - Y\|_F^2 \right\}$$

is obtained by

$$\begin{aligned} Y &= Q\mathrm{Diag}(\rho)Q^T \\ \gamma_j &= \tfrac{1}{2}\left(\rho_j + \sqrt{\rho_j^2 + 4/\sigma}\right) \\ P_{\frac{1}{\sigma}h}(Y) &= Q\mathrm{Diag}(\gamma)Q^T \end{aligned}$$

Proof The proof is based on

1. The log-determinant function and Frobenius norms are orthogonally invariant: $\det(U\Sigma V^T) = \det(\Sigma)$, $\|U\Sigma V^T\|_F = \|\Sigma\|_F$ for any Σ and orthogonal U, V
2. Therefore, we can work with diagonal matrices Θ and Y

Proximal mapping of log-determinant function

Proof For $\Theta = \mathrm{Diag}(\gamma)$, $Y = \mathrm{Diag}(\sigma)$ (we need $\gamma > 0$, but no constraints for ρ), solve the problem

$$\min_{\Theta \in \mathbb{S}^p_{++}} \left\{ -\log\det(\Theta) + \frac{\sigma}{2}\|\Theta - Y\|_F^2 \right\}$$

Compute the gradient

$$0 = -\Theta^{-1} + \sigma(\Theta - Y) = -\begin{bmatrix} \frac{1}{\gamma_1} & & \\ & \ddots & \\ & & \frac{1}{\gamma_p} \end{bmatrix} + \sigma \begin{bmatrix} \gamma_1 - \rho_1 & & \\ & \ddots & \\ & & \gamma_p - \rho_p \end{bmatrix}$$

$$\Rightarrow -\frac{1}{\gamma_j} + \sigma(\gamma_j - \rho_j) = 0 \Rightarrow \gamma_j = \frac{1}{2}\left(\rho_j + \sqrt{\rho_j^2 + 4/\sigma}\right) > 0$$

Subproblem-Y

$$
\begin{aligned}
L_\sigma(\Theta, Y, Z) = & -\log\det(\Theta) + \langle S, \Theta\rangle + \delta_{\mathbb{S}^p_{++}}(\Theta) + \lambda\|Y\|_{1,\text{off}} \\
& + \langle Z, \Theta - Y\rangle + \frac{\sigma}{2}\|\Theta - Y\|_F^2
\end{aligned}
$$

Consider minimizing w.r.t. Y

$$
\begin{aligned}
& \arg\min_Y \lambda\|Y\|_{1,\text{off}} - \langle Z, Y\rangle + \frac{\sigma}{2}\|Y - \Theta\|_F^2 \\
= & \arg\min_Y \lambda\|Y\|_{1,\text{off}} + \frac{\sigma}{2}\|Y - \Theta - \sigma^{-1}Z\|_F^2 \\
= & P_{\frac{\lambda}{\sigma}\|\cdot\|_{1,\text{off}}}\left(Y - \sigma^{-1}(S + Z)\right) \\
= & S^{\text{off}}_{\frac{\lambda}{\sigma}}\left(Y - \sigma^{-1}(S + Z)\right)
\end{aligned}
$$

$S^{\text{off}}_{\frac{\lambda}{\sigma}}$ only thresholds the off-diagonal entries:

$$
\begin{cases}
Y_{ii} - \sigma^{-1}(S_{ii} + Z_{ii}) & \text{if } i = j \\
S_{\frac{\lambda}{\sigma}}\left(Y_{ij} - \sigma^{-1}(S_{ij} + Z_{ij})\right) & \text{if } i \neq j
\end{cases}
$$

ADMM framework

Algorithm (ADMM for graphical Lasso)

Choose $\sigma > 0$, $0 < \tau < \frac{1+\sqrt{5}}{2}$, $Y^{(0)} = (S + \lambda I)^{-1}$, $Z^{(0)} = I$. $k \leftarrow 0$

repeat until convergence

$T^{(k)} \leftarrow Y^{(k)} - \sigma^{-1}\left(S + Z^{(k)}\right)$

$T^{(k)} = Q^{(k)}\mathrm{Diag}(d^{(k)})(Q^{(k)})^T$ (eigen. decomp. of $T^{(k)}$)

for $j = 1, \ldots, p$ $\quad \gamma_j^{(k)} \leftarrow \dfrac{1}{2}\left(d_j^{(k)} + \sqrt{(d_j^{(k)})^2 + 4/\sigma}\right)$ **end(for)**

$\Theta^{(k+1)} \leftarrow Q^{(k)}\mathrm{Diag}(\gamma^{(k)})(Q^{(k)})^T$

$Y^{(k+1)} \leftarrow S^{\mathrm{off}}_{\frac{\lambda}{\sigma}}\left(Y^{(k)} - \sigma^{-1}(S + Z^{(k)})\right)$

$Z^{(k+1)} \leftarrow Z^{(k)} + \tau\sigma(\Theta^{(k+1)} - Y^{(k+1)})$

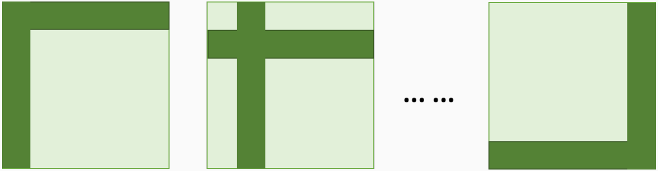
end(repeat)

return $\Theta^{(k)}, Y^{(k)}, Z^{(k)}$

Existing methods

In addition to ADMM, existing first order methods in the literature includes:

- [1] BCD, in each step, optimize a single column/row



- [5] APG

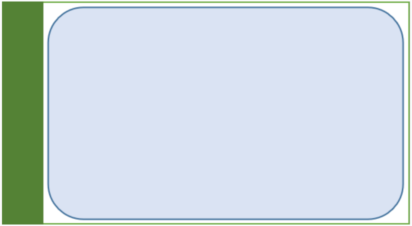
Neighbourhood selection

Neighbourhood selection

Recall we aim to learn the precision matrix $\Theta = \Sigma^{-1}$ given n samples $x^{(1)}, \ldots, x^{(n)} \sim N(0, \Sigma)$ independently, where the true covariance matrix Σ is unknown

- Data matrix $X = [x^{(1)}, \ldots, x^{(n)}]^T \in \mathbb{R}^{n \times p}$

Neighbourhood selection



- $X_{\cdot j}$: j-th column, $X_{\cdot -j}$: delete j-th column
- Sparse linear regression for each vertex

$$X_{\cdot j} \approx X_{\cdot -j} \beta^j$$

- Via solving Lasso

$$\beta^j = \underset{\beta \in \mathbb{R}^{p-1}}{\arg\min} \frac{1}{2} \|X_{\cdot -j}\beta - X_{\cdot j}\|^2 + \lambda \|\beta\|_1$$

- Determine the neighbourhood $\mathcal{N}(j)$ of vertex j

- Form a graph via the AND or OR rule
  - ▷ AND rule: edge (s, t) exists if $s \in \mathcal{N}(t)$ and $t \in \mathcal{N}(s)$
  - ▷ OR rule: edge (s, t) exists if $s \in \mathcal{N}(t)$ or $t \in \mathcal{N}(s)$

Example. Given the neighbourhood of four variables:

$$\mathcal{N}(1) = \{3, 4\}, \quad \mathcal{N}(2) = \{3\}, \quad \mathcal{N}(3) = \{1\}, \quad \mathcal{N}(4) = \{1, 2\}$$

Form a graph via the AND rule (and OR rule).

Solution.

AND rule gives $E = \{(1, 3), (1, 4)\}$

OR rule gives $E = \{(1, 3), (1, 4), (2, 4), (2, 3)\}$

Neighbourhood selection framework

Algorithm (Neighbourhood selection)

for $j = 1, \dots, p$

$$\beta^j \leftarrow \arg\min_{\beta \in \mathbb{R}^{p-1}} \frac{1}{2} \|X_{\cdot -j}\beta - X_{\cdot j}\|^2 + \lambda \|\beta\|_1$$

$$\mathcal{N}(j) = \{t \mid \beta^j_t \neq 0\}$$

end(for)

Form a graph $G = (V, E)$ from $\mathcal{N}(j), j = 1, \dots, p$ via AND/OR rule

return graph G

Neighbourhood selection

Example

$n = 3$, $p = 4$. Observe 4 Gaussian samples

$$x^{(1)} = (0.54, 0.95, -0.25, 2.39)^T \quad x^{(2)} = (1.85, 0.12, 0.40, -1.60)^T$$
$$x^{(3)} = (-2.28, -1.24, 3.61, 2.21)^T$$

Data matrix $X \in \mathbb{R}^{3\times 4}$

$$\begin{bmatrix} 0.54 & 0.95 & -0.25 & 2.39 \\ 1.85 & 0.12 & 0.40 & -1.60 \\ -2.28 & -1.24 & 3.61 & 2.21 \end{bmatrix}$$

```
X = [0.54  0.95  -0.25  2.39;
     1.85  0.12   0.40 -1.60;
    -2.28 -1.24   3.61  2.21]; % data matrix
% lasso for vertex 1
beta = lasso(X(:,2:4),X(:,1),'Lambda',0.5)
beta =
         0
   -0.5271
   -0.2449
```

For vertex 1, the neighbourhood is $\mathcal{N}(1) = \{3, 4\}$

```
X = [0.54  0.95  -0.25  2.39;
      1.85  0.12   0.40 -1.60;
     -2.28 -1.24   3.61  2.21]; % data matrix
% lasso for vertex 1
beta = lasso(X(:,2:4),X(:,1),'Lambda',0.5)
beta =
         0
   -0.5271
   -0.2449
```

For vertex 1, the neighbourhood is $\mathcal{N}(1) = \{3, 4\}$

```
X = [0.54  0.95  -0.25  2.39;
      1.85  0.12   0.40 -1.60;
     -2.28 -1.24   3.61  2.21]; % data matrix
% lasso for vertex 2
beta = lasso(X(:,[1,3,4]),X(:,2),'Lambda',0.5)
beta =
         0
   -0.2250
         0
```

For vertex 2, the neighbourhood is $\mathcal{N}(2) = \{3\}$

```
X = [0.54  0.95  -0.25  2.39;
      1.85  0.12   0.40 -1.60;
     -2.28 -1.24   3.61  2.21]; % data matrix
% lasso for vertex 3
beta = lasso(X(:,[1,2,4]),X(:,3),'Lambda',0.5)
beta =
   -0.1774
   -1.0086
         0
```

For vertex 3, the neighbourhood is $\mathcal{N}(3) = \{1, 2\}$

```
X = [0.54  0.95  -0.25  2.39;
      1.85  0.12   0.40 -1.60;
     -2.28 -1.24   3.61  2.21]; % data matrix
% lasso for vertex 4
beta = lasso(X(:,1:3),X(:,4),'Lambda',0.5)
beta =
   -0.4752
         0
         0
```

For vertex 4, the neighbourhood is $\mathcal{N}(4) = \{1\}$

Neighbourhood selection

Example Neighbourhood

$$\mathcal{N}(1) = \{3, 4\}, \quad \mathcal{N}(2) = \{3\}, \quad \mathcal{N}(3) = \{1, 2\}, \quad \mathcal{N}(4) = \{1\}$$

AND rule gives $E = \{(1, 3), (2, 3), (1, 4)\}$. OR rule gives the same graph.

Neighbourhood selection

Example Neighbourhood

$$\mathcal{N}(1) = \{3, 4\}, \quad \mathcal{N}(2) = \{3\}, \quad \mathcal{N}(3) = \{1, 2\}, \quad \mathcal{N}(4) = \{1\}$$

AND rule gives $E = \{(1,3), (2,3), (1,4)\}$. OR rule gives the same graph.

Remarks

- Neighbourhood selection is fast since
- many efficient solvers for lasso are available
- the p Lasso problems for each vertex can be solved in parallel

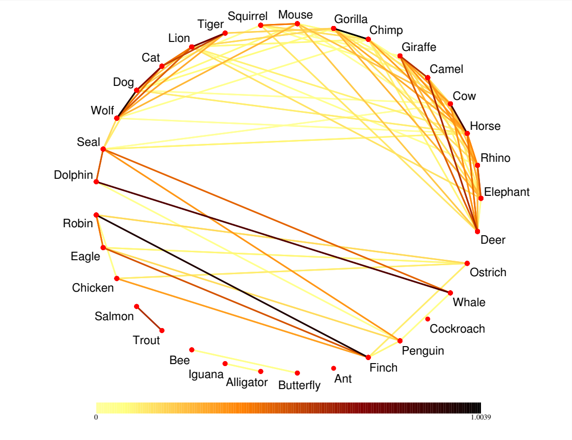
Applications

Animals data [2]

- $p = 33$ animals
- $n = 102$ questions: "has lungs?", "is warm-blooded?" ...
- Each entry is a true-false answer to the question
- Analyze the relation among animals

	Bee	Cat	Lion	... $p = 33$
has lungs?	0	1		
is warm-blooded?	0	1		
live in groups?	1	0		
.				
.				
.				
$n = 102$				

Animals similarity



Dolphin -- Whale

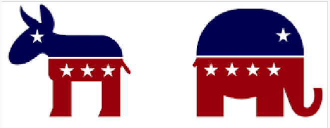
Robin -- Finch

Similar animals are connected with edges of large weights

Politician network [3]

- $p = 50$ politicians (Democratic / Republican senators)

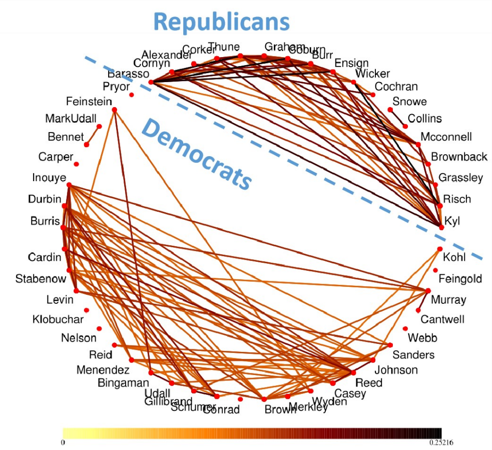
Democrats vs Republicans



- $n = 293$ voting records for the 111th United States Congress (2009-2011)
- Each entry is a yes-no vote
- Analyze the networks from politician's behaviors

$$
\begin{array}{cc}
 & \text{Alexander} \quad \text{Bennet} \ \ldots \ p = 50 \\
n = 293 & \begin{array}{|cc|} 0 & 1 \\ 0 & 1 \\ 1 & 0 \\ & \\ & \end{array}
\end{array}
$$

Politician network



A clear divide between Democrats (bottom left nodes) and Republicans (top right nodes)

The senators are clustered into two parties

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