No voodoo here! Learning discrete graphical models via inverse covariance estimation

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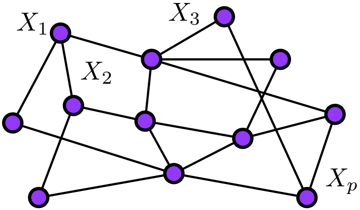
Joint work with Martin Wainwright

Introduction: Graphical models

- Graph $G = (V, E)$
- Represents joint distribution of $(X_1, \ldots, X_p)$, where $|V| = p$



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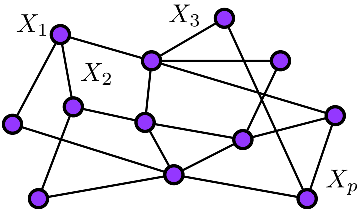

- Absent edges indicate conditional independence:

$$(s, t) \notin E \implies X_s \perp\!\!\!\perp X_t \mid X_{\setminus\{s,t\}}$$

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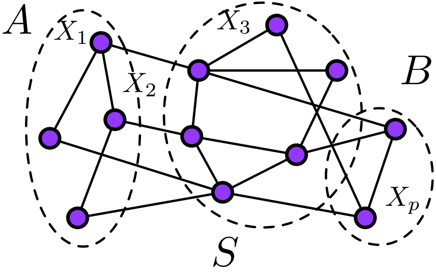

- More generally, $X_A \perp\!\!\!\perp X_B \mid X_S$ whenever $S \subseteq V$ separates A from B

Introduction: Graphical models

- Wide applications in computer vision, civil engineering, political science, epidemiology ...
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- Wide applications in computer vision, civil engineering, political science, epidemiology ...
- **Goal:** Edge recovery from n samples: $\left\{(X_1^{(i)}, X_2^{(i)}, \dots, X_p^{(i)})\right\}_{i=1}^n$
- High-dimensional setting: $p \gg n$
- Samples may be non-i.i.d. or corrupted by noise/missing data

Structure learning for Gaussians

- When $(X_1, \dots, X_p) \sim N(0, \Sigma)$, Hammersley-Clifford implies

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- Numerous methods for edge recovery by estimating $\Theta = \Sigma^{-1}$:
  - Nodewise regression with Lasso (Meinshausen & Bühlmann '06)
  - Global estimation of Θ with penalized MLE (Yuan & Lin '07)
  - Nonparanormal (Liu et al. '09, '12)

Non-Gaussian distributions

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Main contributions:

- Establish relationship between **augmented** inverse covariance matrices and edge structure in discrete graphical models
- Propose two new algorithms for structure learning in discrete graphs

A curious example

- Binary Ising model:

$$\mathbb{P}_\theta(x_1, \ldots, x_p) \;\propto\; \exp\left(\sum_{s \in V} \theta_s x_s + \sum_{(s,t) \in E} \theta_{st} x_s x_t\right),$$

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$$\theta \in \mathbb{R}^{p + \binom{p}{2}}, \qquad (x_1, \ldots, x_p) \in \{0, 1\}^p$$

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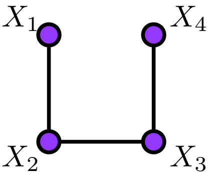

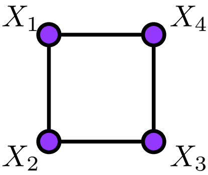

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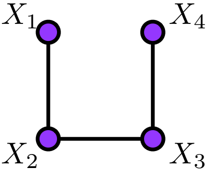
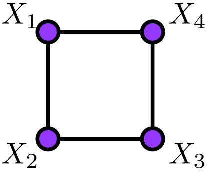


$$\Theta_{\text{chain}} = \begin{bmatrix} 9.80 & -3.59 & 0 & 0 \\ -3.59 & 34.30 & -4.77 & 0 \\ 0 & -4.77 & 34.30 & -3.59 \\ 0 & 0 & -3.59 & 9.80 \end{bmatrix}$$



$$\Theta_{\text{loop}} = \begin{bmatrix} 51.37 & -5.37 & -0.17 & -5.37 \\ -5.37 & 51.37 & -5.37 & -0.17 \\ -0.17 & -5.37 & 51.37 & -5.37 \\ -5.37 & -0.17 & -5.37 & 51.37 \end{bmatrix}$$

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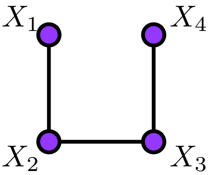

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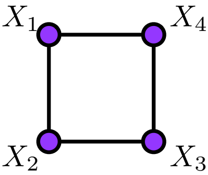

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- Θ is graph-structured for chain, but not loop

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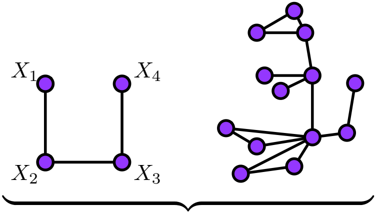
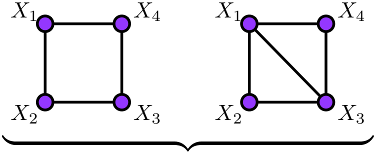


Θ graph-structured



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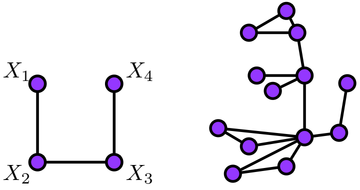

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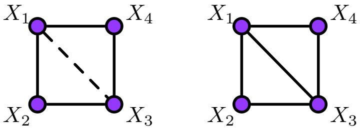

Θ **not** graph-structured

- However, letting $\Gamma_{\text{aug}} = \text{Cov}(X_1, X_2, X_3, X_4, X_1X_3)^{-1}$ for loop:

$$\Gamma_{\text{aug}} \propto \begin{bmatrix} 115 & -2 & 109 & -2 & -114 \\ -2 & 5 & -2 & 0 & 1 \\ 109 & -2 & 114 & -2 & -114 \\ -2 & 0 & -2 & 5 & 1 \\ -114 & 1 & -114 & 1 & 119 \end{bmatrix}$$

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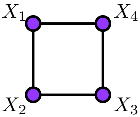
- **Ex:** When $U = \{1\}$, $\phi_U = (\mathbb{I}\{x_1 = 1\}, \ldots, \mathbb{I}\{x_1 = m-1\})$

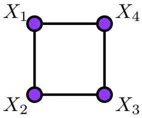
Augmenting covariance matrix



G

Augmenting covariance matrix

- Triangulate G



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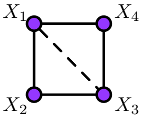
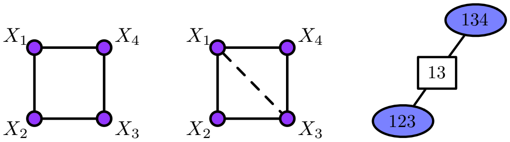


triangulated

Augmenting covariance matrix

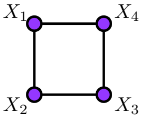
- Triangulate G
- Form junction tree with separator sets



G triangulated junction tree

Augmenting covariance matrix

- Triangulate G
- Form junction tree with separator sets
- Let $\mathcal{S}^+$ = nodes + separator sets



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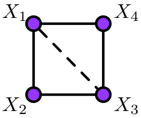

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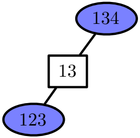

junction tree

$$
\begin{array}{c c}
 & \begin{array}{ccccc} X_1 & X_2 & X_3 & X_4 & X_1X_3 \end{array} \\
\begin{array}{c} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_1X_3 \end{array} & \left[\begin{array}{c} \\ \\ \mathrm{Cov}(\phi_{\mathcal{S}^+}) \\ \\ \\ \end{array} \right]
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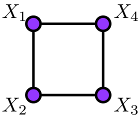

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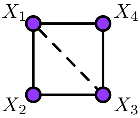

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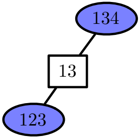

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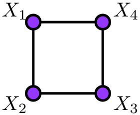
augmented matrix

Theorem

The inverse covariance matrix of $\{\phi_U : U \in \mathcal{S}^+\}$ from any junction tree is graph-structured



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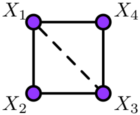

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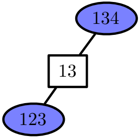

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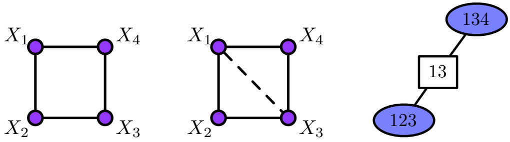
Example: Binary Ising model



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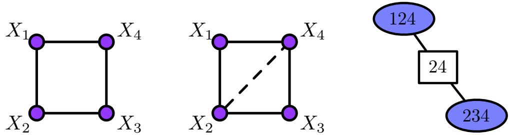
G triangulated junction tree augmented matrix

- Statistics included in $\phi_{\mathcal{S}^+}$ depend on triangulation



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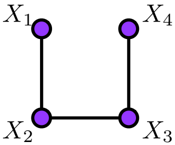

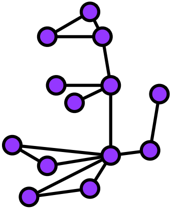

$$(\mathrm{Cov}(X_1, \ldots, X_p))^{-1}$$

Structure learning

Structure learning

- Graphical Lasso for Gaussian graphical models:

$$\widehat{\Theta} \in \arg\min_{\Theta \succeq 0} \left\{ \operatorname{trace}(\widehat{\Sigma}\Theta) - \log\det(\Theta) + \lambda \sum_{s \neq t} |\Theta_{st}| \right\}$$

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- Based on penalized MLE for Gaussians

- **When does graphical Lasso succeed for non-Gaussians?**

Graphical Lasso

Corollary

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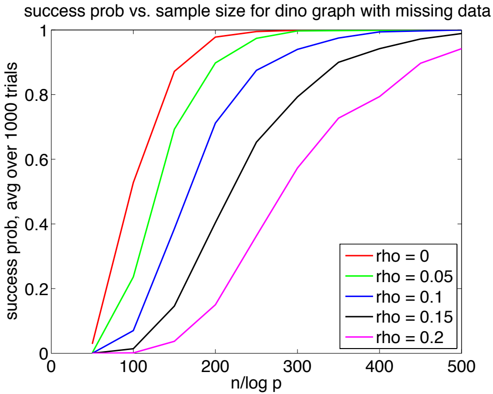
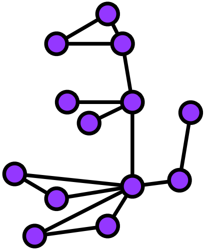
- Group graphical Lasso for $m > 2$
- Easily accommodates additive noise/missing data (modify $\widehat{\Sigma}$)

Simulation study

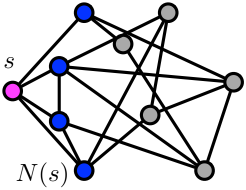
- Graphical Lasso for dinosaur graph: probability of success for recovering 15 edges vs. rescaled sample size (with missing data)





Inference methods for non-trees

- Nodewise method: recovers neighborhood $N(s)$ for any fixed $s \in V$



G

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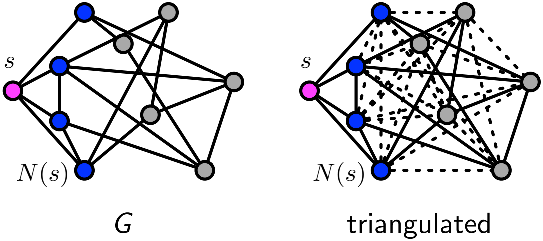

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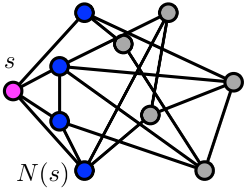

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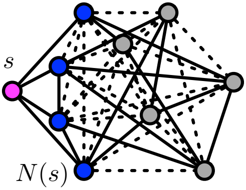
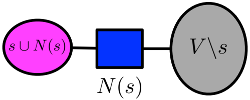


triangulated



junction tree

More details at poster!

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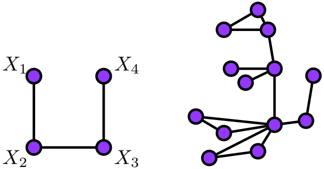

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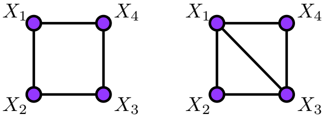

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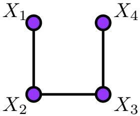
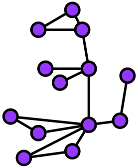
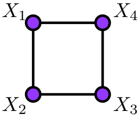
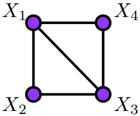




vs.

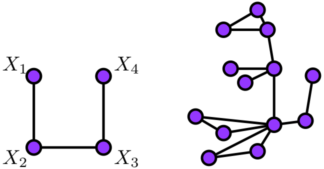




- Proposed structure learning methods for arbitrary discrete graphs

Summary

- Established relationship between augmented inverse covariance matrices and edge structure in discrete graphical models
- Demystified relationship between



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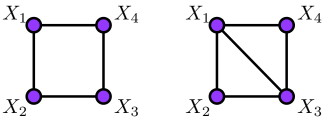

- Proposed structure learning methods for arbitrary discrete graphs
- Methods are theoretically rigorous and easily adapted to corrupted observations