Maximum likelihood threshold of a graph

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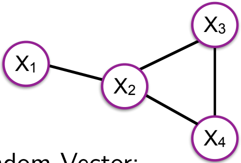
Gaussian graphical models



Random Vector:

$$X = (X_1, X_2, X_3, X_4)$$

Let $X \sim \mathcal{N}(0, \Sigma)$.

The non-edges of G record the conditional independence structure of X:

$$X_1 \perp\!\!\!\perp X_4 \mid (X_2, X_3)$$

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$$\Rightarrow (\Sigma^{-1})_{14} = 0,\ (\Sigma^{-1})_{13} = 0.$$

$\mathbb{S}^m$ = $m \times m$ symmetric real matrices

$\mathbb{S}^m_{>0}$ = pos. def. matrices in $\mathbb{S}^m$.

$\mathbb{S}^m_{\geq 0}$ = psd matrices in $\mathbb{S}^m$

Let $G = (V, E)$ with $|V| = m$.

$$\mathcal{M}_G = \{\Sigma \in \mathbb{S}^m_{>0} : (\Sigma^{-1})_{ij} = 0 \text{ for all } i, j \text{ s.t. } i \neq j, ij \notin E\}$$

Definition

The centered **Gaussian graphical model** associated to the graph G is the set of all multivariate normal distributions $\mathcal{N}(0, \Sigma)$ such that $\Sigma \in \mathcal{M}_G$.

Maximum likelihood estimation

Goal: Find Σ that best explains data

Observations: $Y_1, \ldots, Y_n$
Sample covariance matrix: $S = \frac{1}{n}\Sigma_{i=1}^{n} Y_i Y_i^T$

If the MLE exists, it is the unique positive definite matrix Σ that satisfies:

$$\Sigma_{ij} = S_{ij} \text{ for } ij \in E \text{ and } i = j$$

$$(\Sigma)_{ij}^{-1} = 0 \text{ for } ij \notin E \text{ and } i \neq j$$

When $n \geq m$, the MLE exists with probability one. What about the case when $m >> n$?

Question (Lauritzen)

For a given graph G what is the smallest n such that the MLE exists with probability one?

Maximum likelihood threshold

Definition

We call the smallest n such that the MLE exists with probably one (i.e. for generic data) the **maximum likelihood threshold**, or, **mlt**.

- **Clique number:** $\omega(G) =$ size of a largest clique of G
- **Chordal graph:** A graph with no induced cycle of length ≥ 4.
- **Chordal cover of $G = (V, E)$:** A graph $H = (V, E')$ such that H is chordal and $E \subseteq E'$.
- **Tree width:** $\tau(G) = \min\{\omega(H) - 1 \ : \ H \text{ is a chordal cover of } G\}$.

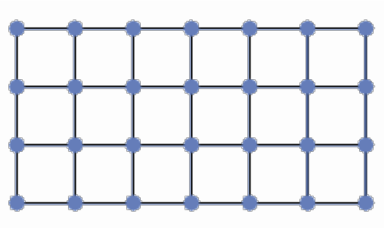
Proposition (Buhl 1993)

$$\omega(G) \leq mlt(G) \leq \tau(G) + 1$$

Bounds

Notice that these bounds can be far away from each other.

Consider for example, $G = Gr_{k_1,k_2}$, the $k_1 \times k_2$ grid graph:



$\omega(G)$ = size of largest clique = 2
$\tau(G)$ = tree width = $\min(k_1, k_2)$

Proposition (Uhler 2012)

The maximum likelihood threshold of the 3×3 grid graph is 3.

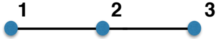
Rank of a graph

Let

$$\phi_G : \mathbb{S}^m \to \mathbb{R}^{V+E}$$

$$\phi_G(\Sigma) = (\sigma_{ii})_{i \in V} \oplus (\sigma_{ij})_{ij \in E}$$

G:



$$\phi_G\left(\begin{bmatrix} 1 & 2 & 3 \\ 2 & 1 & 2 \\ 3 & 2 & 1 \end{bmatrix}\right)$$

$$= (1, 1, 1, 2, 2)^T$$

Cone of sufficient statistics:
$\mathcal{C}_G := \phi_G(\mathbb{S}^m_{\succ 0})$.

Remark: For a given $S \in \mathbb{S}^m_{\succeq 0}$, the MLE exists if and only if $\phi_G(S) \in \operatorname{int}(\mathcal{C}_G)$.

Let $S(m, n) = \{\Sigma \in \mathbb{R}^{m \times m} \ : \ \Sigma = \Sigma^T, \operatorname{rank}(\Sigma) \leq n\}$.

Definition

The **rank of a graph** G is the minimal n such that $\dim \phi_G(S(m, n)) = \dim \mathcal{C}_G = |V| + |E|$

Proposition (Uhler 2012) $\operatorname{mlt}(G) \leq \operatorname{rank}(G)$

Algebraic Matroids

Definition

Let $I \subset \mathbb{K}[x_1, \ldots, x_n]$ be a prime ideal. This defines an **algebraic matroid** with ground set $\{x_1, \ldots, x_n\}$, and $K \subseteq \{x_1, \ldots, x_n\}$ an independent set if and only if $I \cap \mathbb{K}[K] = \langle 0 \rangle$.

$I_n \subseteq \mathbb{K}[\sigma_{ik} \;\; 1 \leq i \leq j \leq m]$: ideal defining $S(m, n)$.

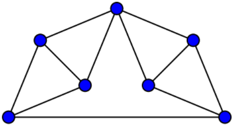
If $\phi_G(S(m,n)) = \dim \mathcal{C}_G$, then $\mathrm{mlt}(G) \leq n$

$\Rightarrow$

Elimination criterion *(Uhler 2012): If*
$I_n \cap \mathbb{K}[\sigma_{ij} \; : \; ij \in E, i = j]$, *then*
$mlt(G) \leq n$

Corollary (Matroidal interpretation of elimination criterion)

If $\{\sigma_{ij} \; : \; ij \in E, i = j\}$ is an independent set in the algebraic matroid associated to I_{n+1} then $mlt(G) \leq n$.



G is called **rigid** if, for generic points $\mathbf{p}_1, \ldots, \mathbf{p}_m \in \mathbb{R}^n$, the set of distances $||\mathbf{p}_i - \mathbf{p}_j||_2$ for $ij \in E$, determine all the other distances $||\mathbf{p}_i - \mathbf{p}_j||_2$ with $ij \in \binom{[m]}{2}$

Consider the map $\psi_n \; : \mathbb{R}^{n\times m} \to \mathbb{R}^{m(m-1)/2}$

$$(\mathbf{p}_1, \ldots, \mathbf{p}_m) \mapsto (||\mathbf{p}_i - \mathbf{p}_j||_2^2 \; : \; 1 \leq i < j \leq m).$$

Let $J_n = I(\mathrm{im}(\psi_n)) \subseteq \mathbb{K}[x_{ij} \;\; 1 \leq i < j \leq m]$.

n - dimensional generic rigidity matroid: the algebraic matroid associated to the ideal J_n, is called the denoted $\mathcal{A}(n)$.

Rigidity Matroid $\cong$ Symmetric Minor Matroid

Theorem (Gross-Sullvant 2014)

- *A graph $G = (V, E)$ has rank$(G) = n$ if and only if E is an independent set in $\mathcal{A}(n-1)$ and not an independent set in $\mathcal{A}(n-2)$.*
- *The matroid $\mathcal{A}(n-1)$ is isomorphic to the contraction of the rank n symmetric minor matroid via the diagonal elements.*

Proof.

Compare the Jacobian of the map

$$(\mathbf{p}_1, \ldots, \mathbf{p}_m) \mapsto (||\mathbf{p}_i - \mathbf{p}_j||_2^2 \; : \; 1 \leq i < j \leq m)$$

to the Jacobian of the map

$$(\mathbf{p}_1, \ldots, \mathbf{p}_m) \mapsto (\mathbf{p}_i \cdot \mathbf{p}_j \; : \; 1 \leq i < j \leq m)$$

□

Laman's Theorem

Theorem (Laman's condition)

Let $G = (V, E)$ be a graph, and suppose that $\mathrm{rank}(G) \leq n$. Then, for all subgraphs $G' = (V', E')$ of G such that $\#V' \geq n - 1$ we must have

$$\#E' \leq \#V'(n-1) - \binom{n}{2}. \tag{1}$$

Laman's Theorem states that the condition above is both necessary and sufficient for a set to be independent in $\mathcal{A}(2)$.

Corollary

Let $G = (V, E)$ be a graph, if for all subgraphs $G' = (V', E')$ of G

$$\#E' \leq 2(\#V') - 3,$$

then $mlt(G) \leq 3$.

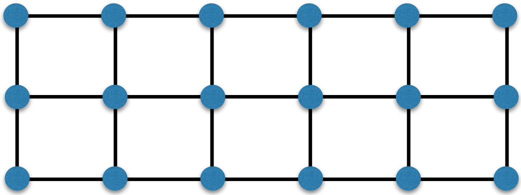
Definition

Let G be a graph and $r \in \mathbb{N}$. The r-**core** of G is the graph obtained by successively removing vertices of G of degree$< r$.

Theorem (Gross-Sullivant 2014, Ben-David 2014)

Let G have an empty n-core, then $rank(G) \leq n$.

$\Rightarrow$ **mlt**$(Gr_{k_1,k_2}) = 3$



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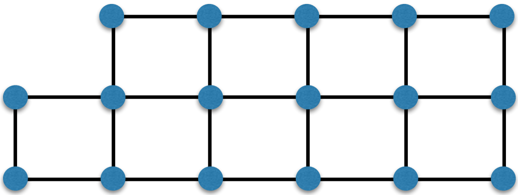

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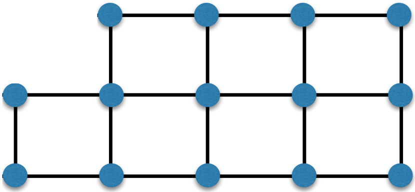

r-cores

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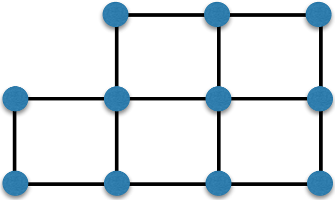

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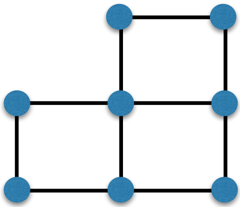

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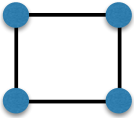

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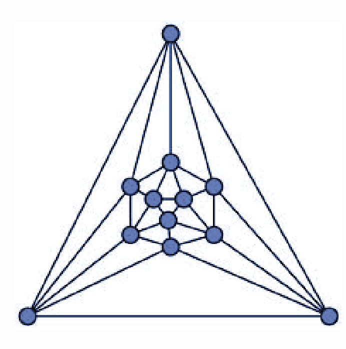
Planar graphs



Theorem (Gross-Sullivant 2014)

If G is a planar graph then $mlt(G) \leq 4$.

Some questions

- Find an example of a graph where $\text{mlt}(G) < \text{rank}(G)$.
  - A graph where $\dim \phi_G(S(m,n)) \neq |V| + |E|$ but $\phi_(S(m,n) \cap \mathbb{S}_{\geq 0})$ is not in the algebraic boundary of $\mathcal{C}_G$.
- How are the boundary components of $\mathcal{C}_G$ related to the circuits in the rigidity matroid?
- Maximum likelihood threshold has a natural rigidity theory analogue: are they equivalent?

Thank you

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