On the Existence of the Maximum Likelihood Estimator for Undirected Gaussian Models

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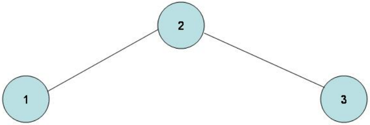
1. vertices are represented by random variables,
2. edges correspond to the conditional independence constraints.

Example

For three random variables x_1, x_2, x_3 the conditional independence relation $x_1 \perp\!\!\!\perp x_3 | x_2$ can be represented by the following graph.



Gaussian Graphical Models

Let $\mathbf{x} = (x_1, \ldots, x_n)^T$ be a random vector in $\mathbb{R}^n$ with

- $\mathbf{x} \sim \mathcal{N}_n(\mu, \Sigma)$
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Then

$$x_i \perp\!\!\!\perp x_j | \text{rest} \quad \Leftrightarrow k_{ij} = 0.$$

[Lauritzen, S. Graphical Models]

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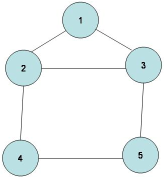

can equivalently be expressed by the concentration matrix

$$K = \begin{pmatrix} k_{11} & k_{12} & k_{13} & 0 & 0 \\ k_{21} & k_{22} & k_{23} & k_{24} & 0 \\ k_{31} & k_{32} & k_{33} & 0 & k_{35} \\ 0 & k_{42} & 0 & k44 & k_{45} \\ 0 & 0 & k_{53} & k_{54} & k_{55} \end{pmatrix}$$

The Maximum Likelihood Estimation

Saturated Gaussian model

$$\mathcal{M} : (\mathcal{N}_n(\mathbf{0}, \Sigma) \in \mathcal{P}(\mathbb{R}^n) : \Sigma \in \mathbf{PD}_n(\mathbb{R}))\,.$$

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- $\mathbf{x}_\nu = (x_{\nu 1}, \ldots, \mathbf{x}_{\nu n})^T \in \mathbb{R}^n \quad \nu \in [N]$
- Sample data as an N by n matrix

$$X := \begin{pmatrix} x_{11} & \ldots & x_{1n} \\ & \ddots & \\ x_{N1} & \ldots & x_{Nn} \end{pmatrix}$$

- The MLE exists $\Leftrightarrow \quad S := X^T X \in \mathbf{PD}_n(\mathbb{R})$
- $\widehat{\Sigma} = \dfrac{S}{N}$
- In general, $\mathrm{rank}(X^T X) = N$ with probability 1.

Likelihood Inference For Gaussian Graphical Models

Observations $\mathbf{x}_1, \ldots, \mathbf{x}_N$ are taken from the Gaussian graphical model

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The MLE is determined by

$$\widehat{\Sigma}_{ij} = \frac{1}{N}(X^T X)_{ij} \quad \text{if } i \backsim j, \text{or } i = j,$$

and restriction $\widehat{\Sigma}^{-1} \in \mathbf{S}^+(\mathcal{G})$.

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   Iterative proportional scaling [Speed & Kiivery, 1986].
2. Under what conditions the existence of the MLE is guaranteed?
   - Necessary condition: The size of the sample data, $N \geq$ the size of the largest complete subgraph.
   - Sufficient condition: $N \geq$ the tree-width of the Graph.

Undirected graphs

Let $\mathcal{G} = (V, E)$ be a loopless undirected graph, were

- V the set of vertices,
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- $\mathcal{G}_1$ is an induced subgraph of $\mathcal{G}$ if $E_1 = E \cap V_1 \times V_1$.

- A path $P = (I, F)$ is

$$I = \{v_0, v_1 \ldots, v_k\} \quad F = \{(v_0, v_1), (v_1, v_2, \ldots (v_{k-1}, v_k)\},$$

  where all the v_i's are distinct. P is called a path between v_0 and v_k.
- Two paths between u, v are called independent if the intersection of their vertex sets is only u, v.

- A cycle is defined similar to a path, however v_k is v_0 and $k > 2$.

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- For an edge e, $\mathcal{G} - e$ is the subgraph of G obtained by removing this edge from E.

Contacting an edge

let $e = \{u, v\}$ be an edge of $\mathcal{G}$. By $\mathcal{G}/e$ we denote the graph obtained from $\mathcal{G}$ by contracting the edge e, where

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1. two vertices u, v are replaced by a new vertex v_e,
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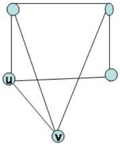
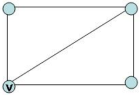
3. the new v_e becomes adjacent to all former neighbors of u, v.





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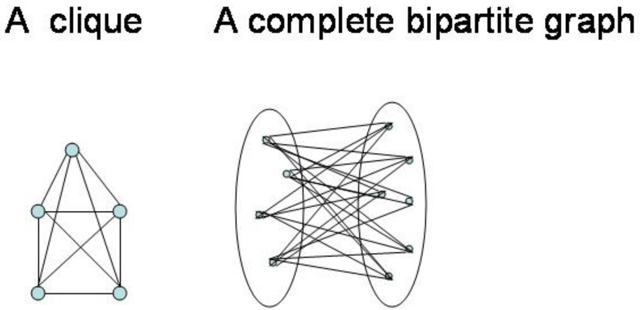
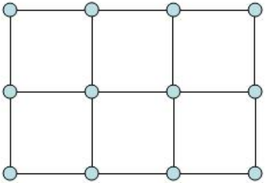
- A graph $\mathcal{G}_1$ is a topological minor of $\mathcal{G}$, $\mathcal{G}_1 \preccurlyeq_T \mathcal{G}$, if $\mathcal{G}$ is obtained from $\mathcal{G}_1$ by replacing edges with independent paths. In such case we also say that $\mathcal{G}$ is a subdivision of $\mathcal{G}_1$.

Some graphs



A grid graph



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  We write

  $$\mathcal{G} = \mathcal{G}_1 \oplus_k \mathcal{G}_2,$$

  where k is the size of the common clique.

Decomposable graphs

A graph is decomposable if it can be written as clique sums of complete graphs.
A graph is decomposable $\Leftrightarrow$ it is triangulated.

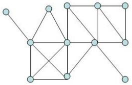

Figure: A triangulated graph

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- $tw(\mathcal{G}_1 \oplus_k \mathcal{G}_2) = max\{tw(\mathcal{G}_1), tw(\mathcal{G}_2)\}$.

Some examples

1. $tw(K_n) = n - 1$
2. $tw(K_{n,m}) = min(n, m)$
3. $tw(T) = 1$, for any tree T
4. $tw(Gr_{n,m}) = min(n, m)$
5. $tw(C_n) = 2$

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- We write $A \overset{\mathcal{G}}{=} B$ for two matrices $A = (a_{ij}), B = (b_{ij})$ if

$$a_{ij} = b_{ij} \text{ whenever } (i, j) \in E, \text{or } i = j.$$

Gaussian rank

Definition

The Gaussian rank of $\mathcal{G}$, denoted by $r(\mathcal{G})$, is the smallest integer r with this property:
If A is a positive definite matrix in $\mathbf{PSD}_n(\mathbb{R})$ with $rank(A) = \overline{\overline{r}}(A) = r$ (i.e $A \in H(n, r)$), then there exists a positive definite matrix $M \in \mathbf{PD}_n(\mathbb{R})$ such that $A \stackrel{\mathcal{G}}{=} M$.

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Example

1. $r(K_n) = \omega(K_n) = n$
2. For any tree T $r(T) = 2$
3. $r(C_n) = 3$ [Buhl, 1993] . More generally, if $tw(G) = 2$, then $r(\mathcal{G}) = 3$

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- $\omega(\mathcal{G}) \leq r(\mathcal{G}) \leq tw(\mathcal{G}) + 1$
- $r(\mathcal{S}(K_n)) \leq n$

- If v is a vertex of $\mathcal{G}$, then we have

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- Similarly, if e is and edge of $\mathcal{G}$, then

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Proof.

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- $r(K_{n,m}) \leq \min(n, m) + 1$.

Proof.

Let $X, Y \subset V$ with $|X| = m, |Y| = n$ and $E = \{(u, v) : u \in X, v \in Y)\}$. Suppose $m \leq n$. Let $\tilde{\mathcal{G}}$ be the graph with the same vertex set as $\mathcal{G}$ and the set of edges $\tilde{E} = E \cup \{(u, w) : u, w \in X\}$. Then $\tilde{\mathcal{G}}$ is triangulated and $\omega(\tilde{\mathcal{G}}) = m + 1$. Therefore $r(\mathcal{G}) \leq r(\tilde{\mathcal{G}}) = m + 1$. □

Harder problems

Definition

The clique contraction number of a graph $\mathcal{G}$, denoted by $\eta(\mathcal{G})$, is the size of largest clique that one can get from contacting some of the edges of $\mathcal{G}$.

It is known that $\eta(\mathcal{G}) \leq tw(\mathcal{G}) + 1$.

Conjecture

For any graph $\mathcal{G}$ we have

1. $r(\mathcal{G}) \leq \eta(\mathcal{G})$,
2. $r(\mathcal{G}) \geq \delta(\mathcal{G}) := \min\{d_{\mathcal{G}}(v) : v \in V\}$.