Maximum likelihood thresholds of linear covariance models

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j.w.w. Shlomo Gortler and Louis Theran: https://arxiv.org/abs/2305.06280

j.w.w. Sean Dewar, Shlomo Gortler, Tony Nixon, Meera Sitharam, and Louis Theran: https://arxiv.org/abs/2210.11081 https://arxiv.org/abs/2108.02185

> j.w.w. Hayden Outlaw https://arxiv.org/pdf/2312.03145

- Definitions
- Reformulation of the MLT of a graphical model as a rigidity-theoretic property of the graph and implications
- What is the "expected" MLT of a Gaussian graphical model?
- Generalize the rigidity-theoretic picture, determine MLTs of "generic" linear concentration models

tl;dr:

Linear concentration model = linear space of symmetric matrices that contains a positive definite matrix

- A statistical model is a family of joint probability distributions
- The *n*-**variate normal distribution** with mean $\mu \in \mathbb{R}^n$ and covariance $\Sigma \succ 0$ is the normal distribution with density function

$$f_{\mu,\Sigma}(x) := \frac{\exp(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu))}{\sqrt{(2\pi)^{\nu} \det(\Sigma)}}$$

- An *n*-variate *linear concentration model* is the family of multivariate normal distributions whose inverse covariance matrix lies in a particular linear subspace of *n* × *n* symmetric matrices
- Covariance matrices are positive definite, so if $L \subseteq S^n$ does not have a positive definite matrix, the statistical model is empty

Definition

Let G be a graph on vertex set $\{1, ..., n\}$. Consider the following subspace $L_G \subseteq S^n$ of $n \times n$ symmetric matrices

 $L_G := \{M \in S^n : M_{ij} = 0 \text{ whenever } ij \text{ is not an edge of } G\}.$



Definition

The **Gaussian graphical model** \mathcal{M}_G associated to a graph G is the linear concentration model associated to L_G .

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Suppose we are given:

- A linear subspace $L \subseteq S^n$ of $n \times n$ symmetric matrices, and
- a matrix $X \in \mathbb{R}^{n \times d}$, columns supposedly iid from a distribution in \mathcal{M}_L

The *maximum likelihood estimate (MLE)* is the solution to the following optimization problem, if it exists:

$$\begin{array}{ll} \max & \operatorname{Tr}(XX^{T}K) + \log \det K \\ \text{s.t.} & K \succ 0 \quad \text{and} \quad K \in L. \end{array}$$

The *maximum likelihood threshold of L* is the minimum *n* such that the above optimization problem has a solution for any generic $X \in \mathbb{R}^{n \times d}$.

Rigidity theory basics

Definition

A **bar and joint framework in** *d* **dimensions** consists of a graph *G*, and a map $p: V(G) \to \mathbb{R}^d$. Such a framework is **independent** if the edge-lengths can be independently perturbed.



Theorem (Asimov and Roth 1978)

Given a graph G, if $p: V(G) \to \mathbb{R}^d$ is "generic," then whether the framework (G, p) is independent in \mathbb{R}^d does not depend on p.

One says that G is (generically) independent in \mathbb{R}^d if (G, p) is independent for all generic $p : V(G) \to \mathbb{R}^d$.

Definition (Generic completion rank)

The **generic completion rank of** G, denoted GCR(G), is the minimum d such that G is generically independent in \mathbb{R}^{d-1} .

Theorem (Uhler 2012, Gross and Sullivant 2018)

 $MLT(G) \leq GCR(G).$

GCR(G) can be computed in RP time, so it would be great if the above inequality were sharp. However...

Theorem (Blekherman and Sinn 2019)

 $MLT(K_{5,5}) = 4 \text{ but } GCR(K_{5,5}) = 5.$ MLT(K_{n,n}) = $O(\sqrt{n})$ whereas $GCR(K_{n,n}) = O(n).$

Definition

Two frameworks (G, p) and (G, q) on the same graph G are **equivalent** if the following holds for every edge uv of G

$$\|p(u) - p(v)\| = \|q(u) - q(v)\|.$$

(G, p) in \mathbb{R}^k has *full affine span* if $\{p(v) : v \in V(G)\}$ affinely spans \mathbb{R}^k .

Theorem (BDGNST)

Let G be a graph with n vertices. MLT(G) is the smallest d such that every generic framework in \mathbb{R}^{d-1} is equivalent to a framework in \mathbb{R}^{n-1} with full affine span.



Definition

Two frameworks (G, p) and (G, q) on the same graph G are **equivalent** if the following holds for every edge uv of G

$$||p(u) - p(v)|| = ||q(u) - q(v)||.$$

They are moreover *congruent* if the above holds for all pairs uv of vertices of G.

Definition

A framework (G, p) in \mathbb{R}^d is **globally rigid** if all equivalent frameworks in \mathbb{R}^d are congruent.



Theorem (Connelly 2005; Gortler, Healy, and Thurston 2010)

Given a graph G, if $p: V(G) \to \mathbb{R}^d$ is "generic," then whether the framework (G, p) is globally rigid in \mathbb{R}^d does not depend on p.

One says that G is (generically) globally rigid in \mathbb{R}^d if (G, p) is globally rigid for all generic $p: V(G) \to \mathbb{R}^d$.

Theorem (BDGNST)

If a subgraph of G on at least d + 1 vertices is generically globally rigid in \mathbb{R}^{d-1} , then MLT(G) > d.

Theorem (BDGNST)

MLT(G) = GCR(G) in all of the following cases:

- GCR(G) ≤ 4
- MLT(G) ≤ 3
- G has 9 or fewer vertices.

The MLT of an Erdös-Renyi random graph

Let c > 0 be fixed and let G(n, n/c) denote the Erdös-Renyi random graph model with expected edge density c.

Conjecture (BDGNST)

Let c > 0 be fixed. If $G \sim G(n, n/c)$ then MLT(G) = GCR(G) with high probability. In this case, $MLT(G) \approx \lfloor c/2 \rfloor + 2$ with high probability.



$$\max_{K} \quad \operatorname{Tr}(XX^{T}K) + \log \det K + \alpha \|K\|_{1}$$

s.t. $K \succ 0$.

Given *n* datapoints, i.i.d. from a "reasonable" distribution, with what probability does GraphLasso pick a graphical model with MLT $\leq n$?



More rigidity: stress matrices

Given a graph G = (V, E) and $p \in (\mathbb{R}^d)^n$, a *stress* of the framework (G, p) is a vector $\omega \in \mathbb{R}^E$ such that

$$\sum_{:ij\in E} \omega_{ij}(p(j) - p(i)) = 0 \quad \text{for all } i \in V.$$

The associated **stress matrix** Ω is defined by

$$\Omega_{ij} = \begin{cases} \omega_{ij} & \text{if } ij \in E \\ 0 & \text{if } i \neq j \text{ and } ij \notin E \\ -\sum_{k: ik \in E} \omega_{ik} & \text{if } i = j. \end{cases}$$

By construction, if ω is a stress of (G, p) with stress matrix Ω , then

$$\Omega \begin{pmatrix} 1 & -p(1) - \\ 1 & -p(2) - \\ \vdots & \vdots \\ 1 & -p(n) - \end{pmatrix} = 0$$

So rank $(\Omega) \leq n - d - 1$ if p is generic. This inequality can be strict.

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Stress matrix example



$$\begin{pmatrix} 0 & 1 & 0 & 1 & -2 \\ 1 & 0 & 1 & 0 & -2 \\ 0 & 1 & 0 & 1 & -2 \\ 1 & 0 & 1 & 0 & -2 \\ -2 & -2 & -2 & -2 & 8 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ 1 & 2 & 2 \\ 1 & 0 & 2 \\ 1 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Theorem (Connelly 2005; Gortlear-Healy-Thurston 2010)

A graph G on n vertices is generically globally rigid in \mathbb{R}^d iff there exists $p \in (\mathbb{R}^d)^n$ such that (G, p) has a stress matrix of rank n - d - 1.

Theorem (Alfakih 2011)

If G is a graph on n vertices and $p \in (\mathbb{R}^d)^n$, and (G, p) has a PSD stress matrix of rank n - (d + k) - 1, then any framework equivalent to (G, p) in \mathbb{R}^{n-1} has an affine span of dimension at most d + k.

Theorem (BDGNST)

Let G be a graph with n vertices. MLT(G) is the smallest d such that every generic framework in \mathbb{R}^{d-1} is equivalent to a framework in \mathbb{R}^{n-1} with full affine span.

The upshot: the MLT of G is the minimum d such that no generic d-dimensional framework (G, p) has a nonzero PSD stress.

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Maximum likelihood thresholds

Generalizing to linear concentration models

Let $L \subseteq S^n$ be a linear subspace of symmetric matrices and let $d \le n$. Does there exist an open neighborhood $U \subseteq \mathbb{R}^{n \times d}$ such that for each $X \in U$, there exists a **nonzero PSD** $\Omega \in L$ such that $\Omega X = 0$?

Theorem (BGT)

The minimum d for which the above answer is "no" is the MLT of L.

Rigidity-theoretic interpretation:

- L is like a graph, X is a point configuration
- projecting XX^T onto L is recording edge-lengths of a framework
- each $\Omega \in L$ satisfying $\Omega X = 0$ is a stress of X

When $L = L_G$, we are literally asking if there exists an open neighborhood of (d-1)-dimensional frameworks on G that all have a PSD stress.

Does there exist an open neighborhood $U \subseteq \mathbb{R}^{n \times d}$ such that for each $X \in U$, there exists a **nonzero PSD** $\Omega \in L$ such that $\Omega X = 0$?

Let $S^n(d)$ denote the variety of $n \times n$ symmetric matrices of rank d.

Proposition (BGT)

If the projection of $S^n(d)$ onto L is dim(L)-dimensional, the answer is "no."

- dim(L) ≤ dn (^d₂) = dim(Sⁿ(d)) is neccessary for this projection to be full-dimensional.
- When $L = L_G$, this projection is full-dimensional iff G is independent in the (d 1)-rigidity matroid.
- Answer for $L = L_G$ can still be "no" even when G is **not** independent (Blekherman and Sinn).

Generic linear spaces

Theorem (BGT)

Let $L \subseteq S^n$ be a **generic** linear subspace. The following are equivalent:

$$1 \quad \text{dim}(L) \leq nd - \binom{d}{2}.$$

- Interprojection of Sⁿ(d) onto L is dim(L)-dimensional,
- There does **not** exist an open neighborhood U ⊆ ℝ^{n×d}, and such that for every X ∈ U, there exists a nonzero PSD Ω ∈ L such that ΩX = 0.

Corollary

Let $L \subseteq S^n$ be a **generic** linear subspace. The MLT of L is the minimum d such that dim $(L) \leq dn - {d \choose 2}$.

- This is the behavior one would expect from a dimension count. Not obvious since we're working over the reals!
- Proof uses tools from convexity theory and differential topology.

Lemma

Let $L \subseteq S^n$ be a generic linear subspace. Assume dim $(L) > nd - {d \choose 2}$. Then there exists an open neighborhood $U \subseteq \mathbb{R}^{n \times d}$ such that for every $X \in U$, there exists a nonzero PSD $\Omega \in L$ such that $\Omega X = 0$.

 ${\it L}$ being "generic" excludes the following two possibilities, neither of which is robust to perturbation

• L does not contain a PSD matrix of rank n - d, where d satisfies

$$m \ge dn - \binom{d}{2} - n + d + 1$$

L contains a PSD matrix of the above rank, but for every such matrix Ω, L non-transversely intersects the space of matrices sharing a kernel with Ω.

Lemma

Let $L \subseteq S^n$ be a generic linear subspace. Assume dim $(L) \leq nd - {d \choose 2}$. Then the projection of $S^n(d)$ onto L is full-dimensional in L.

This also holds when $L = L_G$ for a graph G that is independent in the (d-1)-dimensional rigidity matroid.

Proof idea:

- generic normal spaces of $S^n(d)$ have dimension $\binom{n-d+1}{2}$
- dimension count says intersection with L expected to be trivial
- if *L* and normal space have larger than expected dimension, a perturbation of *L* does not.

Definition

The **weak** maximum likelihood threshold of a linear concentration model $L \subseteq S^n$ is the minimum d such that **some** open set $U \subseteq \mathbb{R}^{n \times d}$ satisfies the property that for every $X \in U$, the following has a solution

$$\begin{array}{ll} \max & \operatorname{Tr}(XX^{T}K) + \log \det K \\ \mathrm{s.t.} & K \succ 0 \quad \mathrm{and} \quad K \in L. \end{array}$$

Conjecture

The weak maximum likelihood threshold of a graph G is 2 if and only if it has at least one edge, and an acyclic orientation with no "stretched cycles"



Thank you for your attention!

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