Ideals of Gaussian Graphical Models

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October 25, 2019

Gaussian Graphical Models

- Let $G = ([m], E)$ be an undirected graph.
- Consider the set

$$PD(G) = \{K \in PD_m : K_{ij} = 0 \text{ if } i \neq j \text{ and } i - j \notin E\}.$$

- Let

$$\mathcal{M}_G = \{\Sigma = K^{-1} : K \in PD(G)\}.$$

- The set of covariance matrices $\mathcal{M}_G$ are from the centered Gaussian graphical model associated to G: those distributions with density function

$$f(x|\Sigma) = \frac{1}{|\Sigma|^{1/2}(2\pi)^{m/2}} \exp(-\tfrac{1}{2}x^T\Sigma^{-1}x)$$

Uses of Graphical Models

- Unifying framework for many classes of multivariate statistical models
  - Markov models/Hidden Markov models
  - Ising model/Spatial Models
- Useful for discussion of conditional independence structures
- Uses:
  - Artificial Intelligence/Machine Learning
  - Causal Inference
  - Computational Biology

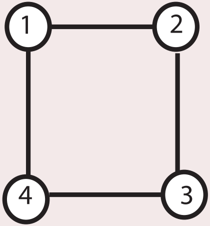
Ideals of Gaussian Graphical Models

$$I_G = \mathcal{I}(\mathcal{M}_G) \subseteq \mathbb{R}[\sigma_{ij} : 1 \leq i \leq j \leq m] = \mathbb{R}[\sigma]$$
$$= \langle f \in \mathbb{R}[\sigma] : f(\Sigma) = 0 \text{ for all } \Sigma \in \mathcal{M}_G \rangle$$

Problem

Determine I_G for all graphs G. What are the generating sets and/or Gröbner bases of these ideals?

Example



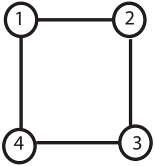
$$\Sigma^{-1} = K = \begin{pmatrix} k_{11} & k_{12} & 0 & k_{14} \\ k_{12} & k_{22} & k_{23} & 0 \\ 0 & k_{23} & k_{33} & k_{34} \\ k_{14} & 0 & k_{34} & k_{44} \end{pmatrix}$$

$$I_{C_4} = \langle |\Sigma_{124,234}|, |\Sigma_{123,134}| \rangle$$

Conditional Independence Constraints

Definition

Let $G = ([n], E)$ a graph and A, B, C be disjoint subsets of $[n]$. C separates A and B if every path from some $a \in A$ to some $b \in B$ passes through a $c \in C$.



$\{2, 4\}$ separates $\{1\}$ from $\{3\}$.

Proposition

Let G be a graph and suppose that C separates A and B in G. Then for all $\Sigma \in \mathcal{M}_G$

$$\operatorname{rank} \Sigma_{A \cup C, B \cup C} = \#C.$$

In particular all $\#C + 1$ subdeterminants of $\Sigma_{A \cup C, B \cup C}$ belong to I_G.

Conditional Independence Ideal

Definition

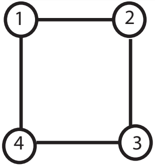
Let $G = ([n], E)$ be a graph. Let $CI_G \subseteq \mathbb{R}[\sigma]$ be the ideal generated by all $\#C + 1$ subdeterminants of $\Sigma_{A\cup C, B\cup C}$ where A, B, C range over all sets such that C separates A and B in G.

CI_G is the conditional independence ideal of G.

- Always have $CI_G \subseteq I_G$.
- In fact, $V(CI_G) \cap PD_m = V(I_G) \cap PD_m$.

Question

Is it always true that $CI_G = I_G$?



$$CI_{C_4} = I_{C_4} = \langle |\Sigma_{124,234}|, |\Sigma_{123,134}| \rangle$$

Why is I_G interesting?

- The variety $V(CI_G) \cap PSD_n$ has extraneous solutions that correspond to SINGULAR multivariate Gaussians that satisfy the conditional independence constraints of G but are not limits of distributions that factor.
  - Using I_G removes these extraneous solutions.
- If we care about hidden variable models, the elimination $CI_G \cap \mathbb{R}[\Sigma_A]$ potentially has higher dimensional solutions that are not in the model (projections of distributions outside of $V(I_G) \cap PD_n$.
  - Using I_G removes these bad higher dimensional components.
- Interesting connections to problems in classical algebraic geometry.

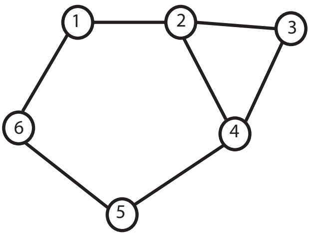
For Discrete Random Variables

Theorem (Geiger-Meek-Sturmfels(2006))

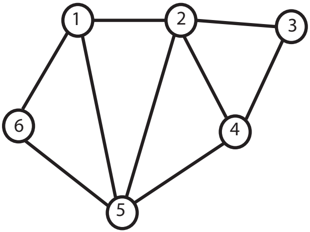
Let G be a graph and let I_G the vanishing ideal of the discrete graphical model and CI_G the conditional independence ideal. Then $I_G = CI_G$ if and only if G is a chordal graph.

- A graph G is chordal if every cycle in G of length ≥ 4 has a chord.

Not Chordal Graph



Chordal Graph



The question

Question

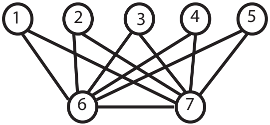
For which graphs G is $CI_G = I_G$ for Gaussian graphical models?

Conjecture

If C_n is an n cycle graph then $CI_{C_n} = I_{C_n}$ is generated by degree 3 determinants.

Proposition

The chordal graph $G = \hat{K}_{2,5}$ has $CI_G \neq I_G$.



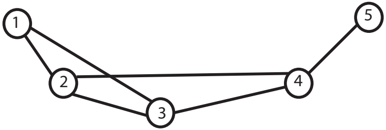
$$\sigma_{12}\sigma_{13}\sigma_{24}\sigma_{35}\sigma_{45} - \sigma_{12}\sigma_{13}\sigma_{25}\sigma_{34}\sigma_{45} - \sigma_{12}\sigma_{14}\sigma_{23}\sigma_{35}\sigma_{45}$$
$$+\sigma_{12}\sigma_{14}\sigma_{25}\sigma_{34}\sigma_{35} + \sigma_{12}\sigma_{15}\sigma_{23}\sigma_{34}\sigma_{45} - \sigma_{12}\sigma_{15}\sigma_{24}\sigma_{34}\sigma_{35}$$
$$+\sigma_{13}\sigma_{14}\sigma_{23}\sigma_{25}\sigma_{45} - \sigma_{13}\sigma_{14}\sigma_{24}\sigma_{25}\sigma_{35} - \sigma_{13}\sigma_{15}\sigma_{23}\sigma_{24}\sigma_{45}$$
$$+\sigma_{13}\sigma_{15}\sigma_{24}\sigma_{25}\sigma_{34} - \sigma_{14}\sigma_{15}\sigma_{23}\sigma_{25}\sigma_{34} + \sigma_{14}\sigma_{15}\sigma_{23}\sigma_{24}\sigma_{35}$$

$$\in I_G \setminus CI_G$$

Fat Path Graphs

Definition

A graph G is a fat path graph if, for every $i < j$ with $i - j \in E$, and for all k, l such that $i \leq k < l \leq j$ then $k - l \in E$.



Theorem (Fink-Rajchgot-S 2016)

If G is a fat path graph then $I_G = CI_G$.

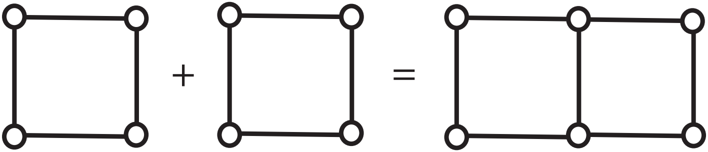
- Fat path graphs are chordal graphs.
- Uses connection between (some instances of) gaussian graphical models and matrix Schubert varieties.

Gluing Graphs: Discrete Graphical Models

Theorem (Geiger-Meek-Sturmfels(2006))

Let G be a graph and let I_G the vanishing ideal of the discrete graphical model and CI_G the conditional independence ideal. Then $I_G = CI_G$ if and only if G is a chordal graph.

- Proof idea: Show that $I_G = CI_G$ is preserved when doing decompositions of graphs.



- More generally, for reducible graphs generators of I_G can be obtained from I_{G_1} and I_{G_2} plus conditional independence conditions from the overlap.
- Can anything like this be true for Gaussian graphical models?

Gluing Graphs: Gaussians Graphical Models??

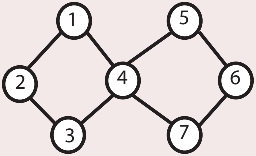
- If G is the k-clique sum of G_1 and G_2 is

$$I_G = \mathrm{Lift}(I_{G_1}) + \mathrm{Lift}(I_{G_2}) + k + 1 \text{ minors from overlap?}$$

- "Obvious" if $k = 0$.
- $G = \hat{K}_{2,5}$ shows that can't be true for $k \geq 2$.
- Sturmfels and Uhler (2009) asked if true of $k = 1$.

Example (Misra-Sullivant(2019))

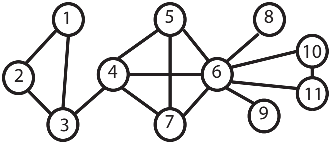
For the graph $G = C_4 \# C_4$, I_G has a minimal generator of degree 4 that is not in CI_G.



Does anything work out nicely for ideals of GGMs?!?

Conjecture (Sturmfels-Uhler(2010))

I_G is generated in degree 2 if and only G is a chordal graph that can be built by 1-clique sums of complete graphs. In this case $I_G = CI_G$.



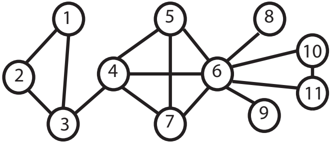
Theorem (Misra-Sullivant (2019))

The Sturmfels-Uhler conjecture is true.

Chordal Graphs that are 1-clique Sums

Theorem (Misra-Sullivant (2019))

I_G is generated in degree 2 if and only G is a chordal graph that can be built by 1-clique sums of complete graphs. In this case $I_G = CI_G$.



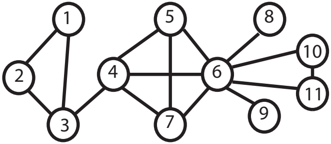
Proof idea:

- All these 2×2 minors means I_G must be toric in this case.
- These chordal 1-sum graphs are precisely the geodesic graphs.
- Use the combinatorics of the toric structure to analyze ideal.

The Shortest Path Map

Proposition

A graph G is a 1 clique sum of complete graphs if and only if for every connected induced subgraph H of G and every pair of vertices i j in H, there is a unique locally shortest path between i and j in H.



- For this reason we call 1 clique sum of complete graphs geodesic graphs.

Shortest Path Map

Let $G = ([n], E)$ be a geodesic graph.

- Let $i \leftrightarrow j$ denote the unique shortest path between i and j in G.
- For each $i \in [n]$ introduce a parameter a_i.
- For each $i \to j \in E$ introduce a parameter λ_{ij}.
- Consider the shortest path parametrization

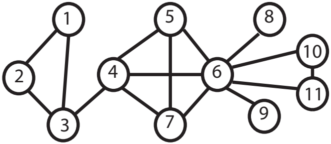
$$\phi(a, \lambda) = (\sigma_{ij})_{1 \leq i \leq j \leq n}$$

  where

$$\sigma_{ij} = a_i a_j \prod_{i' - j' \in i \leftrightarrow j} \lambda_{i'j'}$$

- Let $SP_G = \mathcal{I}(\mathrm{im}(\phi)) \subseteq \mathbb{R}[\sigma]$.

Example



$$\sigma_{17} = a_1 a_7 \lambda_{13} \lambda_{34} \lambda_{47} \qquad \sigma_{26} = a_2 a_6 \lambda_{23} \lambda_{34} \lambda_{46}$$

$$\sigma_{16} = a_1 a_6 \lambda_{13} \lambda_{34} \lambda_{46} \qquad \sigma_{27} = a_2 a_7 \lambda_{23} \lambda_{34} \lambda_{47}$$

$$\sigma_{17}\sigma_{26} - \sigma_{16}\sigma_{27} \in SP_G$$

Proof Sketch

Theorem (Misra-Sullivant (2019))

I_G is generated in degree 2 if and only G is a chordal graph that can be built by 1-clique sums of complete graphs. In this case $I_G = CI_G$.

- Find a quadratic Gröbner basis of SP_G.
  - Depends on combinatorics of path systems in geodesic graphs.
- Show that $SP_G = CI_G$, all the quadratic generators of come from conditional independence statement.
- Since SP_G is prime, has the same dimension as I_G, and $SP_G = CI_G \subseteq I_G$, these ideals must be equal.

Summary

- The vanishing ideals of undirected Gaussian graphical models seem difficult to describe.
- When are these ideals generated by the conditional independence constraints?
- True in the case of 1-clique sums of complete graphs.
- Other cases: Fat Path Graphs (Fink-Rajchgot-Sullivant (2016))
- What about non-determinantal constraints?

$$\begin{aligned}
&\sigma_{12}\sigma_{13}\sigma_{24}\sigma_{35}\sigma_{45} - \sigma_{12}\sigma_{13}\sigma_{25}\sigma_{34}\sigma_{45} - \sigma_{12}\sigma_{14}\sigma_{23}\sigma_{35}\sigma_{45} \\
&+\sigma_{12}\sigma_{14}\sigma_{25}\sigma_{34}\sigma_{35} + \sigma_{12}\sigma_{15}\sigma_{23}\sigma_{34}\sigma_{45} - \sigma_{12}\sigma_{15}\sigma_{24}\sigma_{34}\sigma_{35} \\
&+\sigma_{13}\sigma_{14}\sigma_{23}\sigma_{25}\sigma_{45} - \sigma_{13}\sigma_{14}\sigma_{24}\sigma_{25}\sigma_{35} - \sigma_{13}\sigma_{15}\sigma_{23}\sigma_{24}\sigma_{45} \\
&+\sigma_{13}\sigma_{15}\sigma_{24}\sigma_{25}\sigma_{34} - \sigma_{14}\sigma_{15}\sigma_{23}\sigma_{25}\sigma_{34} + \sigma_{14}\sigma_{15}\sigma_{23}\sigma_{24}\sigma_{35}
\end{aligned}$$

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