Algebraic Approaches to Colored Gaussian Graphical Models

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Symmetry, Stability, and Computations

Storyline

1. Colored Gaussian Graphical (CGG) models

2. CGG models with toric vanishing ideals

based on the paper *Symmetrically colored Gaussian graphical models with toric vanishing ideals*, SIAM Journal on Applied Algebra and Geometry 7.1 (2023): 133-158. with

Jane Ivy Coons (University of Oxford)

Pratik Misra (TU Munich)

Miruna Stefana Sorea (SISSA)

3. CGG models toric after a linear change of variables

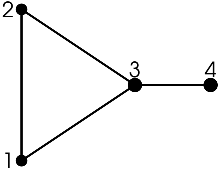
based on *Symmetry Lie algebras of varieties with applications to algebraic statistics*, arXiv:2309.10741, with

Arpan Pal (University of Idaho)

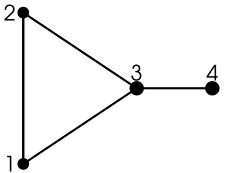
4. Ongoing and future work

An ideal $I \subseteq \mathbb{R}[x_1, \ldots, x_n]$ is **toric** if one of the equivalent properties holds:

I is a prime binomial ideal $\iff$ I is the kernel of a monomial map $\mathbb{R}[x_1, \ldots, x_n] \to \mathbb{R}[y_1^{\pm 1}, \ldots, y_m^{\pm 1}]$



$$\mathcal{L}_G = \left\{ K = \begin{bmatrix} k_{11} & k_{12} & k_{13} & 0 \\ k_{12} & k_{22} & k_{23} & 0 \\ k_{13} & k_{23} & k_{33} & k_{34} \\ 0 & 0 & k_{34} & k_{44} \end{bmatrix} \mid k_{11}, k_{12}, \ldots, k_{44} \in \mathbb{R} \right\}$$



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A random vector X is distributed according to a **multivariate Gaussian distribution** $\mathcal{N}_n(\mathbf{0}, \Sigma)$ with mean $\mathbf{0}$ if it has probability density function

$$\varphi_\Sigma(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^n \det(\Sigma)}} \exp(-\frac{1}{2}\mathbf{x}^T\Sigma^{-1}\mathbf{x}),$$

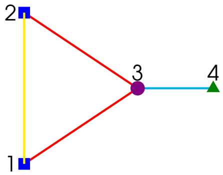
where Σ is a symmetric positive definite matrix.

- $\Sigma =$ **covariance matrix**
- $K := \Sigma^{-1} =$ **concentration matrix**

The **Gaussian graphical model** for G is the set of $\mathcal{N}_n(\mathbf{0}, \Sigma)$ with $\Sigma \in \mathcal{L}_G^{-1} \cap PD_4$

Here,

$$\mathcal{L}_G^{-1} = \overline{\{\Sigma \in \mathrm{Sym}_n(\mathbb{R}) \mid \Sigma^{-1} \in \mathcal{L}_G\}}.$$



$$\mathcal{L}_{\mathcal{G}} = \left\{ K = \begin{bmatrix} k_b & k_y & k_r & 0 \\ k_y & k_b & k_r & 0 \\ k_r & k_r & k_v & k_c \\ 0 & 0 & k_c & k_g \end{bmatrix} \mid k_b, k_y, \ldots, k_g \in \mathbb{R} \right\}$$

colors: b, v, g, y, r, c.

The **colored Gaussian graphical model** for $\mathcal{G}$ is the set of Gaussian distribution $\mathcal{N}_n(\mathbf{0}, \Sigma)$ such that $\Sigma \in \mathcal{L}_{\mathcal{G}}^{-1} \cap PD_4$.

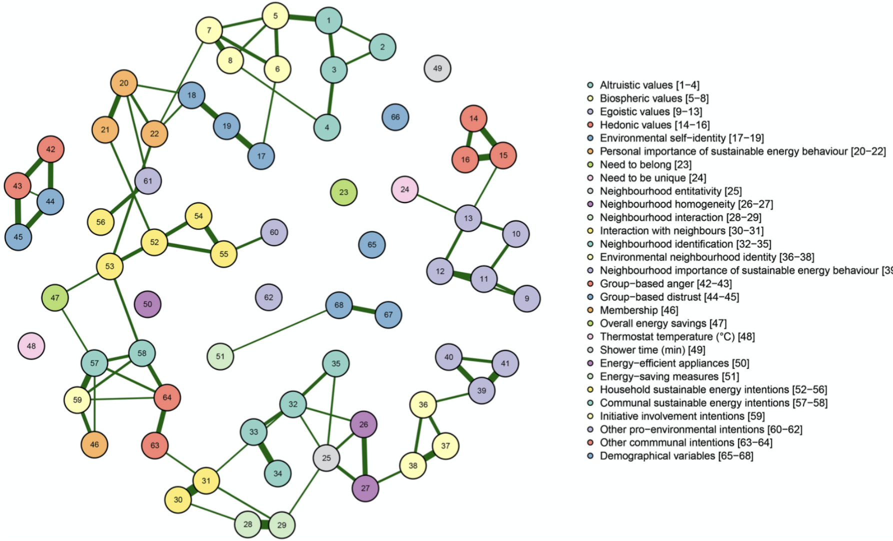
Høsgaard and Lauritzen. "Graphical Gaussian models with edge and vertex symmetries." *Journal of the Royal Statistical Society, Series B. Statistical Methodology* **70** (2008), no.5, 1005-1027.

Objective: $\mathcal{L}_{\mathcal{G}}^{-1}$ gives the set of covariance matrices. Understand its algebraic structure and contributions to applications.

$$\mathcal{L}_{\mathcal{G}}^{-1} = \{\Sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} & \sigma_{14} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} & \sigma_{24} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} & \sigma_{34} \\ \sigma_{14} & \sigma_{24} & \sigma_{34} & \sigma_{44} \end{bmatrix} \mid \sigma_{11} = \sigma_{22}, \sigma_{13} = \sigma_{23}, \sigma_{14} = \sigma_{24}, \sigma_{24}\sigma_{33} = \sigma_{23}\sigma_{34}\}$$

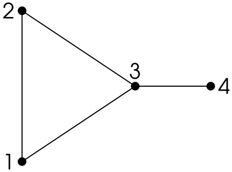
$$= V(\underbrace{\langle \sigma_{11} - \sigma_{22}, \sigma_{13} - \sigma_{23}, \sigma_{14} - \sigma_{24}, \sigma_{24}\sigma_{33} - \sigma_{23}\sigma_{34} \rangle}_{I_{\mathcal{G}}})$$

not linear, but toric

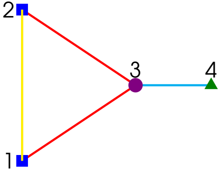


[1] Hiroyuki Toh and Katsuhisa Horimoto. "Inference of a genetic network by a combined approach of cluster analysis and graphical Gaussian modeling." Bioinformatics 18.2 (2002): 287-297.
[2] Ernst Wit and Antonino Abbruzzo. "Factorial graphical models for dynamic networks." Network Science 3.1 (2015): 37-57.
[3] Bhushan, Nitin, Florian Mohnert, Daniel Sloot, Lise Jans, Casper Albers, and Linda Steg. "Using a Gaussian graphical model to explore relationships between items and variables in environmental psychology research." Frontiers in psychology 10 (2019)

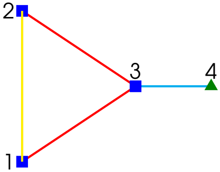
Objective: When is $\mathcal{L}^{-1}$ toric? Can we compute its defining binomials?



$$I_G = \langle \sigma_{24}\sigma_{33} - \sigma_{23}\sigma_{34}, \sigma_{14}\sigma_{33} - \sigma_{13}\sigma_{34} \rangle$$



$$I_{\mathcal{G}} = \langle \sigma_{11} - \sigma_{22}, \sigma_{13} - \sigma_{23}, \sigma_{14} - \sigma_{24}, \sigma_{24}\sigma_{33} - \sigma_{23}\sigma_{34} \rangle$$



$$\begin{aligned} I_{\mathcal{G}'} = \langle &\sigma_{11} - \sigma_{22}, \sigma_{13} - \sigma_{23}, \sigma_{14} - \sigma_{24}, \sigma_{24}\sigma_{33} - \sigma_{23}\sigma_{34}, \\ &2\sigma_{12}\sigma_{24}^2 - 2\sigma_{22}\sigma_{24}^2 - \sigma_{23}\sigma_{24}\sigma_{34} + \sigma_{22}\sigma_{34}^2 + \\ &\sigma_{12}^2\sigma_{44} + \sigma_{22}^2\sigma_{44} - \sigma_{23}^2\sigma_{44} - \sigma_{22}\sigma_{33}\sigma_{44} \rangle \end{aligned}$$

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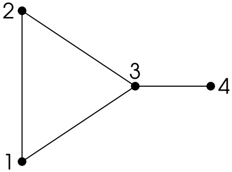

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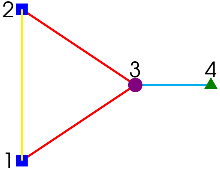

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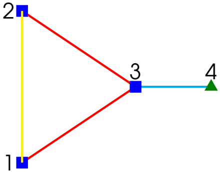

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The answer is in **symmetrically colored graphs**.

Equations vanishing in $\mathcal{L}_{\mathcal{G}}^{-1}$: a first recipe

The space $\mathcal{L}_{\mathcal{G}}^{-1}$ is the variety of the kernel $I_{\mathcal{G}}$ of the rational map

$$\rho_{\mathcal{G}} : \mathbb{R}[\Sigma] \to \mathbb{R}(K),\ \rho_{\mathcal{G}}(\sigma_{ij}) = \frac{(-1)^{i+j} K_{ij}}{\det(K)},$$ NOT a monomial map!!!

where K_{ij} is the ij-th minor of the symmetric matrix K.

$I_{\mathcal{G}}$ is the **vanishing ideal of the colored Gaussian graphical model for** $\mathcal{G}$.

Theorem [Misra & Sullivant, 2021][a]: Let G be a block graph. Then I_G is a toric ideal generated by quadratics.

[a] Misra and Sullivant. "Gaussian graphical models with toric vanishing ideals." *Annals of the Institute of Statistical Mathematics* **73** (2021), no. 4, 757-785.

Theorem Coons, M, Misra & Sorea, 2023: Let $\mathcal{G}$ be a block graph with RCOP coloring. Then $I_{\mathcal{G}}$ is a toric ideal. Moreover,

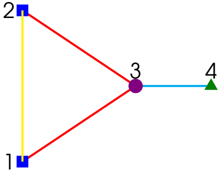
$$I_{\mathcal{G}} = I_G + I_{\overline{\mathcal{G}}},$$

where

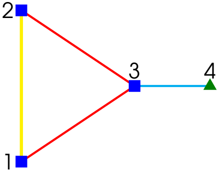
- I_G is the ideal of the uncolored Gaussian graphical model, and
- $I_{\overline{\mathcal{G}}} = \langle \sigma_{ij} - \sigma_{uv},\ \text{for Colors}(i \leftrightarrow j) = \text{Colors}(u \leftrightarrow v) \rangle$.

Let $\mathrm{Aut}(\mathcal{G})$ be the group of graph automorphisms of $\mathcal{G}$ that preserve its vertex and edge colors.

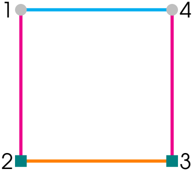
The colored graph $\mathcal{G}$ is an **RCOP graph*** if there exists a subgroup $\Gamma \subset \mathrm{Aut}(\mathcal{G})$ whose vertex and edge orbits are exactly the vertex and edge color classes of $\mathcal{G}$, respectively.



$\Gamma = \mathrm{Aut}(\mathcal{G}) = \{(), (12)\}$



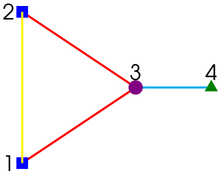
$\mathrm{Aut}(\mathcal{G}') = \{(), (12)\}$

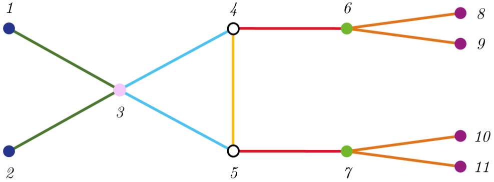


$\Gamma = \mathrm{Aut}(\mathcal{G}') = \{(), (14)(23)\}$

***** Høsgaard and Lauritzen. "Graphical Gaussian models with edge and vertex symmetries." *Journal of the Royal Statistical Society, Series B. Statistical Methodology* **70** (2008), no.5,

Intuitive idea: **Block graphs** are formed by inductively gluing complete graphs at a single vertex.



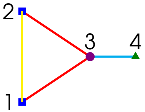


Key Property: Any two vertices in a block graph have a unique shortest path connecting them.

A key idea

The **shortest path map** $\varphi_{\mathcal{G}}$ for colored block graph $\mathcal{G}$ is

$$\begin{aligned}\varphi_{\mathcal{G}} : \mathbb{C}[\sigma_{ij} \mid 1 \le i \le j \le n] &\to \mathbb{C}[t_\lambda \mid \lambda \in \mathrm{Colors}(\mathcal{G})], \\ \sigma_{ij} &\mapsto t_{\lambda(i)} t_{\lambda(j)} \prod_{e \in E(i \leftrightarrow j)} t_{\lambda(e)}.\end{aligned}$$



$$\begin{aligned}\varphi_{\mathcal{G}}(\sigma_{11}) &= t_b{}^2 \\ \varphi_{\mathcal{G}}(\sigma_{12}) &= t_b{}^2 t_y \\ \varphi_{\mathcal{G}}(\sigma_{22}) &= t_b{}^2 \\ \varphi_{\mathcal{G}}(\sigma_{13}) &= t_b t_v t_r \\ \varphi_{\mathcal{G}}(\sigma_{23}) &= t_b t_v t_r\end{aligned}$$

$$\begin{aligned}\varphi_{\mathcal{G}}(\sigma_{33}) &= t_v{}^2 \\ \varphi_{\mathcal{G}}(\sigma_{14}) &= t_b t_g t_r t_c \\ \varphi_{\mathcal{G}}(\sigma_{24}) &= t_b t_g t_r t_c \\ \varphi_{\mathcal{G}}(\sigma_{34}) &= t_v t_g t_c \\ \varphi_{\mathcal{G}}(\sigma_{44}) &= t_g{}^2\end{aligned}$$

$\ker \varphi_{\mathcal{G}} = \langle \sigma_{11} - \sigma_{22}, \sigma_{13} - \sigma_{23}, \sigma_{14} - \sigma_{24}, \sigma_{24}\sigma_{33} - \sigma_{23}\sigma_{34} \rangle$

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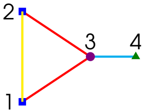


$$\varphi_{\mathcal{G}}(\sigma_{11}) = t_b{}^2$$
$$\varphi_{\mathcal{G}}(\sigma_{12}) = t_b{}^2 t_y$$
$$\varphi_{\mathcal{G}}(\sigma_{22}) = t_b{}^2$$
$$\varphi_{\mathcal{G}}(\sigma_{13}) = t_b t_v t_r$$
$$\varphi_{\mathcal{G}}(\sigma_{23}) = t_b t_v t_r$$

$$\varphi_{\mathcal{G}}(\sigma_{33}) = t_v{}^2$$
$$\varphi_{\mathcal{G}}(\sigma_{14}) = t_b t_g t_r t_c$$
$$\varphi_{\mathcal{G}}(\sigma_{24}) = t_b t_g t_r t_c$$
$$\varphi_{\mathcal{G}}(\sigma_{34}) = t_v t_g t_c$$
$$\varphi_{\mathcal{G}}(\sigma_{44}) = t_g{}^2$$

$$\ker \varphi_{\mathcal{G}} = \langle \sigma_{11} - \sigma_{22}, \sigma_{13} - \sigma_{23}, \sigma_{14} - \sigma_{24}, \sigma_{24}\sigma_{33} - \sigma_{23}\sigma_{34} \rangle = I_{\mathcal{G}}$$

Note: linear forms: $I_{\overline{\mathcal{G}}} = \langle \sigma_{ij} - \sigma_{k\ell}$, for $\mathrm{Colors}(i \leftrightarrow j) = \mathrm{Colors}(k \leftrightarrow \ell)\rangle$.
quadratic forms:
$I_G = \langle \sigma_{ij}\sigma_{k\ell} - \sigma_{i\ell}\sigma_{kj}$, for $\mathrm{Colors}(i \leftrightarrow j, k \leftrightarrow \ell) = \mathrm{Colors}(i \leftrightarrow \ell, k \leftrightarrow j)\rangle$.

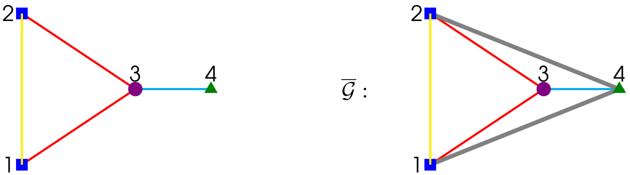
Theorem Coons, M, Misra & Sorea, 2023: Let $\mathcal{G}$ be a block graph with RCOP coloring. Then $I_{\mathcal{G}} = \ker \varphi_{\mathcal{G}} = I_G + I_{\overline{\mathcal{G}}}$.

Proof Idea:

1. $I_{\overline{\mathcal{G}}}$ is the vanishing of a complete colored graph $\overline{\mathcal{G}}$. It forms a Jordan algebra; that is, $\mathcal{L}_{\overline{\mathcal{G}}} = \mathcal{L}_{\overline{\mathcal{G}}}^{-1}$

$\mathcal{G}$:

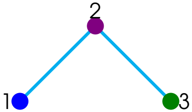
$\overline{\mathcal{G}}$:



$$\boldsymbol{I_{\overline{\mathcal{G}}}} = \langle \sigma_{11} - \sigma_{22}, \sigma_{13} - \sigma_{23}, \sigma_{14} - \sigma_{24} \rangle \subseteq \boldsymbol{I_{\mathcal{G}}}$$

2. $\ker \varphi_{\mathcal{G}} = I_G + I_{\overline{\mathcal{G}}}$ (*the hard work is here*)
3. $\ker \varphi_{\mathcal{G}} \subseteq I_{\mathcal{G}}$ and $\dim(\ker \varphi_{\mathcal{G}}) = \dim(I_{\mathcal{G}})$
4. Since $\ker \varphi_{\mathcal{G}}, I_{\mathcal{G}}$ are both prime ideals, (2)+(3) implies $\ker \varphi_{\mathcal{G}} = I_{\mathcal{G}}$

Some colored GGM are toric after a linear change of variables



$$I_{\mathcal{G}} = \langle \sigma_{23}\sigma_{11} - \sigma_{12}\sigma_{13},\ \sigma_{12}(\sigma_{23} + \sigma_{33}) - \sigma_{13}(\sigma_{22} + \sigma_{23}) \rangle.$$

The change of variables

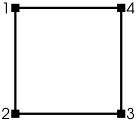
$$p_{22} = \sigma_{22} + \sigma_{23}$$
$$p_{33} = \sigma_{33} + \sigma_{23}$$
$$p_{ij} = \sigma_{ij} \text{ for all other } i, j$$

yields

$$I_{\mathcal{G}} = \langle p_{23}p_{11} - p_{12}p_{13},\ p_{22}p_{13} - p_{12}p_{23} \rangle.$$

Question: to what extend this happens?

... and some not under any linear change of variables



$$I_G = \langle$$

$$\sigma_{23}\sigma_{14}\sigma_{24} - \sigma_{13}\sigma_{24}^2 - \sigma_{22}\sigma_{14}\sigma_{34} + \sigma_{12}\sigma_{24}\sigma_{34} + \sigma_{22}\sigma_{13}\sigma_{44} - \sigma_{12}\sigma_{23}\sigma_{44},$$

$$\sigma_{13}\sigma_{23}\sigma_{14} - \sigma_{24}\sigma_{13}^2 - \sigma_{12}\sigma_{33}\sigma_{14} + \sigma_{11}\sigma_{33}\sigma_{24} + \sigma_{12}\sigma_{13}\sigma_{34} - \sigma_{11}\sigma_{23}\sigma_{34}\rangle$$

Sketch of the proof [M, Pal 2023]:

1. Determine a group action of $\mathrm{GL}_n(\mathbb{C})$ on $\mathbb{C}[x] = \mathbb{C}[x_1, \ldots, x_n]$ by

$$\text{for } g = \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix} \in \mathrm{GL}_n(\mathbb{C}), p \in \mathbb{C}[x], \quad g \cdot p(x_1, \ldots, x_n) = p(g_1 \cdot x, \ldots, g_n \cdot x).$$

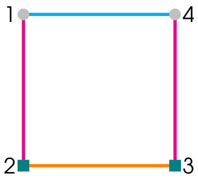
2. The stabilizer $G_I = \{g \in \mathrm{GL}_n(\mathbb{C}) \mid g \cdot p \in I, \forall p \in I\}$ of a prime homogeneous ideal in $I \subseteq R$ is a Lie group.
3. If I is toric, then the torus acting on $V(I)$ is embedded in G_I. So, $\dim(G_I) \geq \dim(I)$.

3′ If $\dim(G_I) < \dim(I)$, then I cannot be turned toric under any linear change of variables.

In our case $\dim(G_I) = 4 < 8 = \dim(I)$.

Project initiated in conversations with JM Landsberg at 2022 Texas Algebraic Geometry Symposium at Texas A&M

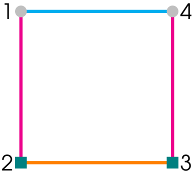
Good news



Its vanishing ideal is

$$
\begin{aligned}
I_{\mathcal{G}} = \langle & \sigma_{13} - \sigma_{24}, \sigma_{22} - \sigma_{33}, \sigma_{12} - \sigma_{34}, \sigma_{11} - \sigma_{44}, \\
& \sigma_{23}\sigma_{14}\sigma_{24} - \sigma_{24}^3 - \sigma_{33}\sigma_{14}\sigma_{34} + \sigma_{24}\sigma_{34}^2 + \sigma_{33}\sigma_{24}\sigma_{44} - \sigma_{23}\sigma_{34}\sigma_{44}\rangle \\
& = I_{\overline{\mathcal{G}}} + I_G
\end{aligned}
$$

Good news



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&= I_{\overline{\mathcal{G}}} + I_G
\end{aligned}
$$

Theorem [Coons, M 2023+]: Let $\mathcal{G}$ be an RCOP graph. Then $I_{\mathcal{G}}$ is a minimal prime for $I_{\overline{\mathcal{G}}} + I_G$.

The algebra, especially its toric structure, of CGG models, contributes to:

the Maximum Likelihood (ML) estimates and ML degrees

ongoing work with Jane Ivy Coons

Høsgaard and Lauritzen. "Graphical Gaussian models with edge and vertex symmetries." *Journal of the Royal Statistical Society, Series B. Statistical Methodology* **70** (2008), no.5, 1005-1027.

the ML threeshold

leading a working group at IMSI with Roser Homs Poons

model selection and identifiability

unexplored

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Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the NSF.

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–long program "Algebraic Statistics and Our Changing World

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Thank you!

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