Geometry of Gaussoids

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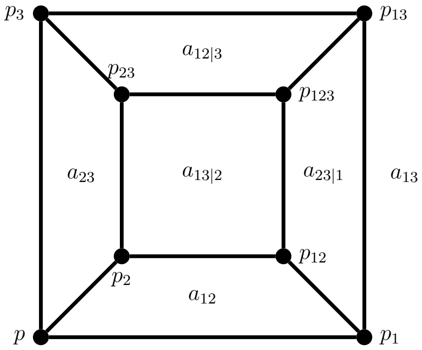
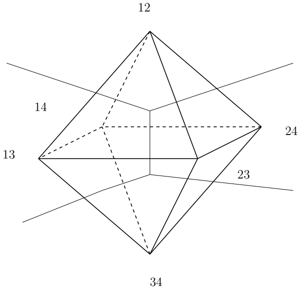


With Tobias Boege, Alessio D'Ali, and Thomas Kahle

Matroids



A matroid is a combinatorial structure that encodes independence in linear algebra and geometry. The basis axioms reflect the ideal of homogeneous relations among all minors of a rectangular matrix

$$\begin{pmatrix} 1 & 0 & \square & \square \\ 0 & 1 & \square & \square \end{pmatrix} \quad = \quad \begin{pmatrix} 1 & 0 & -p_{23} & -p_{24} \\ 0 & 1 & p_{13} & p_{14} \end{pmatrix}$$

A matroid is an assignment of 0 or $\star$ to these minors so that the quadratic Plücker relations have a chance of vanishing:

$$p_{12}p_{34} - p_{13}p_{24} + p_{14}p_{23} \;=\; 0.$$

We also like *oriented matroids*, *positroids* and *valuated matroids*.

Gaussoids

A gaussoid is a combinatorial structure that encodes independence in probability and statistics. The gaussoid axioms reflect the ideal of homogeneous relations among the *principal and almost-principal minors* of a symmetric matrix

$$\begin{pmatrix} 1 & 0 & \square & \square \\ 0 & 1 & \square & \square \end{pmatrix} \quad = \quad \begin{pmatrix} 1 & 0 & p_1 & a_{12} \\ 0 & 1 & a_{12} & p_2 \end{pmatrix}$$

A gaussoid is an assignment of 0 or $\star$ to these minors so that the quadratic Plücker relations have a chance of vanishing:

$$p \cdot p_{12} \; - \; p_1 \cdot p_2 \; + \; a_{12}^2 \; = \; 0.$$

Ditto: *oriented gaussoids*, *positive gaussoids*, *valuated gaussoids*.

The gaussoid axioms were introduced in [R. Lněnička and F. Matúš: On Gaussian conditional independence structures, *Kybernetika* (2007)]

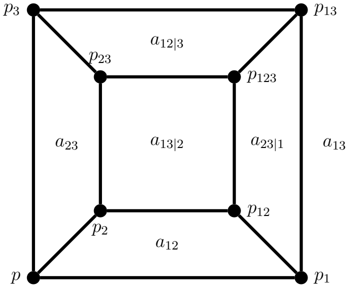
Principal and almost-principal minors

A symmetric $n \times n$-matrix Σ has 2^n principal minors p_I
one for each subset I of $[n] = \{1, 2, \ldots, n\}$.

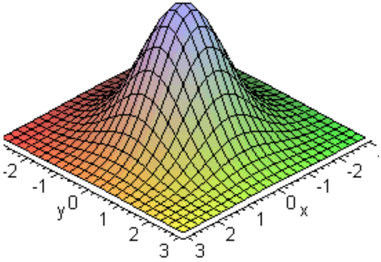
The matrix Σ has $2^{n-2}\binom{n}{2}$ almost-principal minors $a_{ij|K}$.
This is the subdeterminant of Σ with row indices $\{i\} \cup K$ and column indices $\{j\} \cup K$, where $i, j \in [n]$ and $K \subseteq [n] \backslash \{i, j\}$.

Principal minors are in bijection with the vertices of the n-cube.
Almost-principal minors are in bijection with the 2-faces of the n-cube.

$$\Sigma = \begin{pmatrix} p_1 & a_{12} & a_{13} \\ a_{12} & p_2 & a_{23} \\ a_{13} & a_{23} & p_3 \end{pmatrix}$$



Why Gauss?



If Σ is positive definite then it is the covariance matrix of a Gaussian distribution on $\mathbb{R}^n$. In statistics: $p_I > 0$ for all $I \subseteq [n]$.

Study n random variables $X_1, X_2, \ldots, X_n$,
with the aim of learning how they are related. (Yes, data science)

Almost-principal minors $a_{ij|K}$ measure partial correlations.

We have $a_{ij|K} = 0$ if and only if X_i and X_j are conditionally independent given X_K. The inequalities $a_{ij|K} > 0$ and $a_{ij|K} < 0$ indicate whether conditional correlation is positive or negative.

Ideals, Varieties, ...

Write J_n for the homogeneous prime ideal of relations among the principal and almost-principal minors of a symmetric $n \times n$-matrix.

It lives in a polynomial ring $\mathbb{R}[p, a]$ with $N = 2^n + 2^{n-2}\binom{n}{2}$ unknowns, and defines an irreducible subvariety of $\mathbb{P}^{N-1}$.

Proposition

The projective variety $V(J_n)$ is a coordinate projection of the Lagrangian Grassmannian. They share dimension and degree:

$$\dim(V(J_n)) \;=\; \binom{n+1}{2}$$

$$\mathrm{degree}(V(J_n)) \;=\; \frac{\binom{n+1}{2}!}{1^n \cdot 3^{n-1} \cdot 5^{n-2} \cdots (2n-1)^1}.$$

The elimination ideal $J_n \cap \mathbb{R}[p]$ was studied by Holtz-St and Oeding. They found hyperdeterminantal relations of degree 4.

3-cube

The ideal J_3 is generated by 21 quadrics.

There are 9 quadrics associated with the facets of the 3-cube:

$$S_{200} \quad \begin{bmatrix} (2,0,0) & a_{23}^2 + pp_{23} - p_2p_3 \\ (0,0,0) & 2a_{23}a_{23|1} + pp_{123} + p_1p_{23} - p_2p_{13} - p_{12}p_3 \\ (-2,0,0) & a_{23|1}^2 + p_1p_{123} - p_{12}p_{13} \end{bmatrix}$$

.... and two other such weight components

There are 12 trinomials associated with the edge of the 3-cube:

$$S_{110} \quad \begin{bmatrix} (1,1,0) & a_{13}a_{23} + a_{12|3}p - a_{12}p_3 \\ (1,-1,0) & a_{13|2}a_{23} + a_{12|3}p_2 - a_{12}p_{23} \\ (-1,1,0) & a_{13}a_{23|1} + a_{12|3}p_1 - a_{12}p_{13} \\ (-1,-1,0) & a_{13|2}a_{23|1} + a_{12|3}p_{12} - a_{12}p_{123} \end{bmatrix}$$

.... and two other such weight components

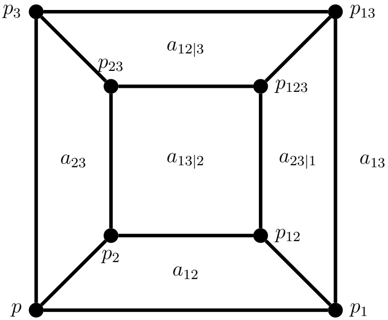
The variety $V(J_3)$ is the Lagrangian Grassmannian in $\mathbb{P}^{13}$, which has dimension 6 and degree 16. It is arithmetically Gorenstein.

Intersections with subspaces $\mathbb{P}^8$ are canonical curves of genus 9.

3-cube

Of most interest are the **12** edge trinomials:

$$p_1 a_{23} - p a_{23|1} - a_{12} a_{13} \qquad p_2 a_{13} - p a_{13|2} - a_{12} a_{23}$$
$$p_3 a_{12} - p a_{12|3} - a_{23} a_{13} \qquad p_{12} a_{13} - p_1 a_{13|2} - a_{12} a_{23|1}$$
$$p_{12} a_{23} - p_2 a_{23|1} - a_{12} a_{13|2} \qquad p_{13} a_{12} - p_1 a_{12|3} - a_{13} a_{23|1}$$
$$p_{13} a_{23} - p_3 a_{23|1} - a_{13} a_{12|3} \qquad p_{23} a_{12} - p_2 a_{12|3} - a_{23} a_{13|2}$$
$$p_{23} a_{13} - p_3 a_{13|2} - a_{23} a_{12|3} \qquad p_{123} a_{12} - p_{12} a_{12|3} - a_{23|1} a_{13|2}$$
$$p_{123} a_{13} - p_{13} a_{13|2} - a_{23|1} a_{12|3} \qquad p_{123} a_{23} - p_{23} a_{23|1} - a_{12|3} a_{13|2}$$



Gaussoid Axioms

Let $\mathcal{A}$ be the set of $\binom{n}{2}2^{n-2}$ symbols $a_{ij|K}$. Following Lněnička and Matúš, a subset $\mathcal{G}$ of $\mathcal{A}$ is a *gaussoid* on $[n]$ if it satisfies:

1. $\{a_{ij|L}, a_{ik|jL}\} \subset \mathcal{G}$ implies $\{a_{ik|L}, a_{ij|kL}\} \subset \mathcal{G}$,
2. $\{a_{ij|kL}, a_{ik|jL}\} \subset \mathcal{G}$ implies $\{a_{ij|L}, a_{ik|L}\} \subset \mathcal{G}$,
3. $\{a_{ij|L}, a_{ik|L}\} \subset \mathcal{G}$ implies $\{a_{ij|kL}, a_{ik|jL}\} \subset \mathcal{G}$,
4. $\{a_{ij|L}, a_{ij|kL}\} \subset \mathcal{G}$ implies $\left(a_{ik|L} \in \mathcal{G} \text{ or } a_{jk|L} \in \mathcal{G} \right)$.

These axioms are known as 1. *semigraphoid*, 2. *intersection*, 3. *converse to intersection*, 4. *weak transitivity*.

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These axioms are known as 1. *semigraphoid*, 2. *intersection*, 3. *converse to intersection*, 4. *weak transitivity*.

Theorem

The following are equivalent for a set $\mathcal{G}$ of 2-faces of the n-cube:

(a) *$\mathcal{G}$ is a gaussoid, i.e. the four axioms above are satisfied for $\mathcal{G}$.*

(b) *$\mathcal{G}$ is compatible with the quadratic edge trinomials in J_n.*

Duality and Minors

Let $\mathcal{G}$ be any gaussoid on $[n]$. The *dual* of $\mathcal{G}$ is

$$\mathcal{G}^* \;=\; \{\, a_{ij|L} \;:\; a_{ij|K} \in \mathcal{G} \;\text{ and }\; L = [n] \backslash (\{i,j\} \cup K) \,\}.$$

Fix an element $u \in [n]$. The *marginalization* equals

$$\mathcal{G} \backslash u \;=\; \{\, a_{ij|K} \in \mathcal{G} \;:\; u \notin \{i,j\} \cup K \,\}.$$

The *conditioning* equals

$$\mathcal{G}/u \;=\; \{\, a_{ij|K \backslash \{u\}} \;:\; a_{ij|K} \in \mathcal{G} \text{ and } u \in K \,\}.$$

Think of operations on sets of 2-faces of the n-cube.

Proposition

If $\mathcal{G}$ is a gaussoid on $[n]$, and $u \in [n]$, then $\mathcal{G}^*$, $\mathcal{G}\backslash u$ and $\mathcal{G}/u$ are gaussoids on $[n]\backslash\{u\}$. The following duality relation holds:

$$(\mathcal{G}\backslash u)^* \;=\; \mathcal{G}^*/u \quad \text{and} \quad (\mathcal{G}/u)^* \;=\; \mathcal{G}^* \backslash u.$$

If $\mathcal{G}$ is realizable (with Σ positive definite) then so are $\mathcal{G}^*$, $\mathcal{G}\backslash u, \mathcal{G}/u$.

A Pinch of Representation Theory

Fix the Lie group $G = (\mathrm{SL}_2(\mathbb{C}))^n$. Write $V_i \simeq \mathbb{C}^2$ for the defining representation of the i-th factor. The irreducible G-modules are

$$S_{d_1 d_2 \cdots d_n} \;=\; \bigotimes_{i=1}^{n} \mathrm{Sym}_{d_i}(V_i),$$

Proposition

G acts on the space W_{pr} spanned by the principal minors and the spaces W_{ap}^{ij} spanned by almost-principal minors. As G-modules,

$$W_{\mathrm{pr}} \simeq \otimes_{i=1}^{n} V_i \quad \textit{and} \quad W_{\mathrm{ap}}^{ij} \simeq \otimes_{k\in[n]\setminus\{i,j\}} V_k \quad \textit{for}\ \ 1 \le i < j \le n.$$

This defines the G-action and $\mathbb{Z}^n$-grading on our polynomial ring $\mathbb{C}[p,a]$.

The formal character of $\mathbb{C}[p,a]_1 = W_{\mathrm{pr}} \oplus \bigoplus_{i,j} W_{\mathrm{ap}}^{ij}$ is the sum of weights:

$$\prod_{i=1}^{n}(x_i + x_i^{-1}) \;+\; \sum_{1\le i<j\le n} \prod_{k\in[n]\setminus\{i,j\}}(x_k + x_k^{-1})$$

Commutative Algebra

The number of linearly independent quadrics in the ideal J_n equals

$$3^{n-2}\binom{n}{2} + 2\sum_{k=0}^{n-3} 3^k (n-k)(n-k-1)\binom{n}{k} + 2\sum_{k=2}^{\lfloor \frac{n}{2} \rfloor} k 3^{n-2k}\binom{n}{2k}$$

Derived via the lowering and raising operators in the Lie algebra $\mathfrak{g}$.

Conjecture

These quadrics generate J_n.

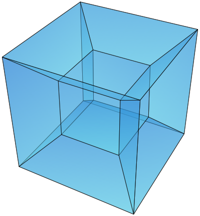
Proposition

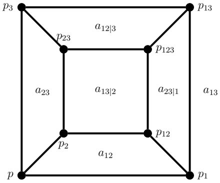
The number of face trinomials and edge trinomials equals

$$2^{n-2}\binom{n}{2} + 12 \cdot 2^{n-3}\binom{n}{3} = 2^{n-3} n(n-1)(2n-3).$$

These trinomials generate the image of J_n in $\mathbb{C}[p, a^{\pm}]$.

4-cube





There are 16 principal and 24 almost principal minors. They span

$$\mathbb{C}[p,a]_1 \;=\; S_{1111} \;\oplus\; S_{1100} \oplus S_{1010} \oplus S_{1001} \oplus S_{0110} \oplus S_{0101} \oplus S_{0011}.$$

The space of quadrics has dimension 820. As G-module, $\mathbb{C}[a,p]_2 \simeq$

$$\begin{aligned} & S_{2222} \oplus S_{2211} \oplus S_{2121} \oplus S_{2112} \oplus S_{1221} \oplus S_{1212} \oplus S_{1122} \oplus 2S_{2200} \oplus 2S_{2020} \\ & \oplus 2S_{2002} \oplus 2S_{0220} \oplus 2S_{0202} \oplus 2S_{0022} \oplus 2S_{2110} \oplus 2S_{2101} \oplus 2S_{2011} \oplus 2S_{1210} \\ & \oplus 2S_{1201} \oplus 2S_{0211} \oplus 2S_{1120} \oplus 2S_{1021} \oplus 2S_{0121} \oplus 2S_{1102} \oplus 2S_{1012} \oplus 2S_{0112} \\ & \oplus 3S_{1111} \oplus 3S_{1100} \oplus 3S_{1010} \oplus 3S_{1001} \oplus 3S_{0110} \oplus 3S_{0101} \oplus 3S_{0011} \oplus 7S_{0000}. \end{aligned}$$

The 226-dimensional submodule $(J_4)_2$ of quadrics in our ideal equals

$$\begin{aligned} & S_{2200} \oplus S_{2020} \oplus S_{2002} \oplus S_{0220} \oplus S_{0202} \oplus S_{0022} \oplus S_{2110} \oplus S_{2101} \oplus S_{2011} \\ & \oplus S_{1210} \oplus S_{1201} \oplus S_{0211} \oplus S_{1120} \oplus S_{1021} \oplus S_{0121} \oplus S_{1102} \oplus S_{1012} \\ & \oplus S_{0112} \oplus S_{1100} \oplus S_{1010} \oplus S_{1001} \oplus S_{0110} \oplus S_{0101} \oplus S_{0011} \oplus 4S_{0000}. \end{aligned}$$

Of these, 120 are trinomials: 96 edge trinomials and 24 face trinomials.

Enumeration of Gaussoids

Theorem

The number of gaussoids for $n = 3, 4, 5$ equals:

n	*all gaussoids*	*orbits for* S_n	$\mathbb{Z}/2\mathbb{Z} \rtimes S_n$	$(\mathbb{Z}/2\mathbb{Z})^n \rtimes S_n$
3	**11**	5	4	4
4	679	58	42	19
5	60,212,776	508,817	254,826	16,981

For $n = 3$, all **11** gaussoids are realizable:

$$\{\}, \{a_{12}\}, \{a_{13}\}, \{a_{23}\}, \{a_{12|3}\}, \{a_{13|2}\}, \{a_{23|1}\}, \{a_{12}, a_{12|3}, a_{13}, a_{13|2}\}, \{a_{12}, a_{12|3}, a_{23}, a_{23|1}\}, \{a_{13}, a_{13|2}, a_{23}, a_{23|1}\}, \{a_{12}, a_{12|3}, a_{13}, a_{13|2}, a_{23}, a_{23|1}\}.$$

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For $n = 4$, five of the 42 gaussoid classes are non-realizable. For instance, $\mathcal{G} = \{a_{12|3}, a_{13|4}, a_{14|2}\}$ is not realizable. *Real Nullstellensatz certificate*:

$$a_{14}\left(a_{34}^2 p_2 p_4 p_{23} + a_{23}^2 a_{34}^2 p_{24} + p_2^2 p_3 p_4 p_{34}\right)$$
$$-\left(a_{23} a_{24} a_{34} + p_2 p_3 p_4\right)\left(a_{24} p_4 a_{12|3} + a_{24} a_{23} a_{13|4} + p_3 p_4 a_{14|2}\right) \in J_4.$$

SAT Solvers

Current software for the **sat**isfiability problem is very impressive, and useful for enumerating combinatorial structures like gaussoids.

The input is a Boolean formula in conjunctive normal form (CNF).

One can specify one of the following three output options:

- **SAT**: Is the formula satisfiable?
- **#SAT**: How many satisfying assignments are there?
- **AllSAT**: Enumerate all satisfying assignments.

We found the $60,212,776$ gaussoids for $n = 5$ in about one hour using Thurley's software `bdd_minisat_all`. The input was a SAT formulation of the gaussoid axioms using 1680 clauses in the CNF.

We then analyzed the output with respect to the symmetry groups.

Oriented gaussoids

An *oriented gaussoid* is a map $\mathcal{A} \to \{0, \pm 1\}$ such that, for each edge trinomial, after setting each p_I to $+1$ and each $a_{ij|K}$ to its image, the set of signs of terms is $\{0\}$ or $\{-1, +1\}$ or $\{-1, 0, +1\}$.

Analogous to oriented matroids.

A *positive gaussoid* is an assignment $\mathcal{A} \to \{0, +1\}$ with the same compatibility requirement.

Analogous to positroids.

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Analogous to positroids.

Example Let $n = 3$. Each singleton gaussoid, like $\mathcal{G} = \{a_{12}\}$ or $\{a_{12|3}\}$ supports four oriented gaussoids, related by reorientation. We display these $24 = 6 \times 4$ oriented gaussoids by listing the six signs for $\mathcal{A}$ in the order $a_{12}, a_{13}, a_{23}, \; a_{12|3}, a_{13|2}, a_{23|1}$:

$0 - - - - -$	$0 - + + - +$	$0 + - + + -$	$0 + + - + +$
$+ 0 + + - +$	$- 0 - - - -$	$- 0 + - + +$	$+ 0 - + + -$
$+ - 0 + - +$	$- - 0 - - -$	$- + 0 - + +$	$+ + 0 + + -$
$+ - - 0 - -$	$- - + 0 - +$	$- + - 0 + -$	$+ + + 0 + +$
$- - + - 0 +$	$+ - - + 0 -$	$+ + + + 0 +$	$- + - - 0 -$
$- + - - + 0$	$+ + + + + 0$	$+ - - + - 0$	$- - + - - 0$

3-Cube and Beyond

Proposition

For $n{=}3$ *there are* 51 *oriented gaussoids in seven symmetry classes. All are realizable. This includes* 20 *uniform gaussoids* $\mathcal{A} \to \{\pm 1\}$.

The following table exhibits the seven classes. The first column gives a covariance matrix Σ that realizes the first oriented gaussoid in the class:

$(p_1,p_2,p_3, a_{12},a_{13},a_{23})$	Symmetry class of oriented gaussoids	
$(2,2,2,1,1,1)$	++++++, +−−+−−, −−+−−+, −+−−+−	
$(3,5,1,1,1,2)$	+++−++, +−−−−−, −−++−+, …, −−+−−−	
$(6,9,6,-1,-1,-7)$	−−−−−−, ++−++−, −++−++, +−++−+	
$(4,3,3,2,2,1)$	+++++0, ++++0+, …	previous page
$(2,2,2,0,-1,-1)$	0−−−−−, 0−++−+, …	previous page
$(3,2,2,0,0,1)$	00+00+, 00−00−, −00−00, … , 0+00+0	
$(1,1,1,0,0,0)$	000000	

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$(p_1, p_2, p_3, a_{12}, a_{13}, a_{23})$	Symmetry class of oriented gaussoids	
$(2, 2, 2, 1, 1, 1)$	$++++++$, $+--+--$, $--+--+$, $-+--+-$	
$(3, 5, 1, 1, 1, 2)$	$+++-++$, $+-----$, $--++-+$, $\ldots$, $--+---$	
$(6, 9, 6, -1, -1, -7)$	$------$, $++-++-$, $-++-++$, $+-++-+$	
$(4, 3, 3, 2, 2, 1)$	$+++++0$, $++++0+$, $\ldots$	previous page
$(2, 2, 2, 0, -1, -1)$	$0-----$, $0-++-+$, $\ldots$	previous page
$(3, 2, 2, 0, 0, 1)$	$00+00+$, $00-00-$, $-00-00$, $\ldots$, $0+00+0$	
$(1, 1, 1, 0, 0, 0)$	000000	

Theorem

The number of oriented gaussoids is 34,873 for $n = 4$, and it is 54936241913 for $n = 5$. Among these, 878349984 are uniform.

From Positroids to Statistics

Positroids are oriented matroids whose bases are positive. These are important in representation theory and algebraic combinatorics, and they have desirable topological properties. Positive gaussoids correspond to distributions that are of current interest in statistics:

S.Fallat, S.Lauritzen, K.Sadeghi, C.Uhler, N.Wermuth and P.Zwiernik: *Total positivity in Markov structures*, Annals of Statistics **45** (2017)

F. Mohammadi, C. Uhler, C. Wang and J. Yu: *Generalized permutohedra from probabilistic graphical models*, `arXiv:1606.01814`.

S. Lauritzen, C. Uhler and P. Zwiernik: *Maximum likelihood estimation in Gaussian models under total positivity*, `arXiv:1702.04031`.

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Ardila, Rincón and Williams (2017) proved a 1987 conjecture of Da Silva by showing that all positroids are realizable.

We derive the analogue for gaussoids: *all positive gaussoids are realizable and their realization spaces are very nice*.

Positive Gaussoids are Graphical

Every graph $\Gamma = ([n], E)$ defines a gaussoid $\mathcal{G}_\Gamma$ via CI statements that hold for the graphical model Γ. Here, $a_{ij|K}$ lies in $\mathcal{G}_\Gamma$ iff every path from i to j in Γ passes through K. Thus $a_{ij} \in \mathcal{G}_\Gamma$ when i and j are disconnected in Γ, and $a_{ij \big| [n]\setminus\{i,j\}} \in \mathcal{G}_\Gamma$ when $\{i, j\} \notin E$.

Theorem

For $n \geq 2$, there are precisely $2^{\binom{n}{2}}$ positive gaussoids. All are realizable from graphs as above. The space of covariance matrices Σ that realize $\mathcal{G}_\Gamma$ is homeomorphic to a ball of dimension $|E| + n$.

- The concentration matrices Σ^{-1} are M-matrices with support Γ. [S. Karlin and Y. Rinott: *M-matrices as covariance matrices of multinormal distributions*, Linear Algebra Appl. (1983)]
- Positive gaussoids satisfy the axiomatic requirements in [K. Sadeghi: *Faithfulness of probability distributions and graphs*, `arXiv:1701..`]

Conclusion

Matroids are cool. And so are gaussoids.

Positivity is crucial in algebraic combinatorics. And in statistics.

On this journey, let the quadratic equations be your guide.
Hitch a fast ride using SAT solvers and representation theory.

$p_1 a_{23} - p a_{23|1} - a_{12} a_{13}, \; p_2 a_{13} - p a_{13|2} - a_{12} a_{23}, \; p_3 a_{12} - p a_{12|3} - a_{23} a_{13}, \; p_{12} a_{13} - p_1 a_{13|2} - a_{12} a_{23|1}, \; p_{12} a_{23} - p_2 a_{23|1} - a_{12} a_{13|2}, \ldots$

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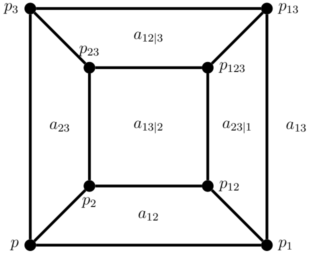
$p_1 a_{23} - p a_{23|1} - a_{12} a_{13},\ p_2 a_{13} - p a_{13|2} - a_{12} a_{23},\ p_3 a_{12} - p a_{12|3} - a_{23} a_{13},\ p_{12} a_{13} - p_1 a_{13|2} - a_{12} a_{23|1},\ p_{12} a_{23} - p_2 a_{23|1} - a_{12} a_{13|2}, \ldots$



Thank You

Stay tuned for valuated gaussoids via tropical Lagrangian Grassmannian.