(Oriented) Gaussoids

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based on joint work with T. Boege, A. D'Ali, F. Röttger and B. Sturmfels.

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Journal of Algebraic Statistics

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- development of new statistical models and methods with interesting algebraic or geometric properties;
- novel applications of algebraic and geometric methods in statistics.

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An example

Consider a vector

$$X = (X_1, X_2, X_3)$$

with multivariate normal distribution $N(0, \Sigma)$.

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Answer: For $0 < \epsilon < 1/2$

$$\Sigma = \begin{pmatrix} 1 & -\epsilon & -\epsilon \\ -\epsilon & 1 & -\epsilon \\ -\epsilon & -\epsilon & 1 \end{pmatrix} \text{ is positive definite,}$$

has negative off-diagonal entries and negative almost principal minors.

Minors and correlations

Let $\Sigma \in \mathrm{PD}_n$ be an $n \times n$ covariance matrix.
The principal minor for $L \subseteq [n]$ is $p_L = \det \Sigma_{L \times L}$.
The almost principal minor for $i \neq j \in [n]$, $K \subseteq [n] \setminus \{i, j\}$ is

$$a_{ij|K} = \det \Sigma_{iK \times jK}$$

Sign convention $iK = [i, k_1, \ldots, k_m]$ where $k_1 < \cdots < k_m$.

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Fact

- $X_i \perp\!\!\!\perp X_j \,|X_K \;\Leftrightarrow\; a_{ij|K} = 0$
- partial correlations $\rho_{ij|K} = \frac{a_{ij|K}}{\sqrt{p_{\{i\} \cup K}\, p_{\{j\} \cup K}}}$.

Example

For $0 < \epsilon < 1/2$

$$\Sigma = \begin{pmatrix} 1 & -\epsilon & -\epsilon \\ -\epsilon & 1 & -\epsilon \\ -\epsilon & -\epsilon & 1 \end{pmatrix} \in \mathrm{PD}_n$$

- correlation $\rho_{12} = a_{12} = -\epsilon$
- partial correlation $\rho_{12|3}$:

$$\rho_{12|3} = \frac{a_{12|3}}{\sqrt{p_{13}p_{23}}} = \frac{\begin{vmatrix} a_{12} & a_{13} \\ a_{23} & a_{33} \end{vmatrix}}{1-\epsilon^2} = \frac{-\epsilon-\epsilon^2}{1-\epsilon^2} < 0$$

Another question

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NO!

Let $\Sigma \in \mathrm{PD}_3$ have negative off-diagonal entries: $a_{ij} = a_{ij|\emptyset} < 0$. Then, writing out the 2×2 determinant:

$$a_{ij|k} = p_{\{k\}} a_{ij} - a_{ik} a_{jk} \quad \Rightarrow \quad a_{ij|k} < 0.$$

Oriented gaussoids capture combinatorial constraints on covariance signs.

Edge relations and (oriented) gaussoids

Relations among the p_L and $a_{ij|K}$

- For each $i, j, k \in [n]$ and $L \subseteq [n] \setminus \{i, j, k\}$ we have

$$p_{kL}a_{ij|L} - a_{ik|L}a_{jk|L} - a_{ij|kL}p_L = 0$$

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Definition

Write $\mathcal{A} = \{a_{ij|K} : i, j \in [n], K \subseteq [n] \setminus \{i, j\}\}$

- A gaussoid is a map $\mathcal{A} \to \{0, *\}$ consistent with all trinomials.

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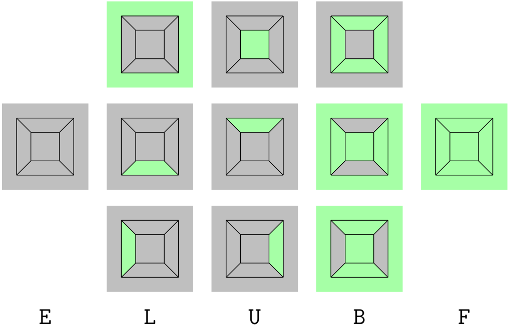
- A gaussoid is a map $\mathcal{A} \to \{0, *\}$ consistent with all trinomials.
- An oriented gaussoid is a consistent map $\mathcal{A} \to \{0, +, -\}$.
- A positive gaussoid is one with image in $\{0, +\}$.
- A uniform gaussoid is one with image in $\{+, -\}$.

An ...oid is realizable if there exists Σ whose minors realize the map.

Examples

For $n = 3$ there are six symbols $\mathcal{A}_3 = \{a_{12}, a_{13}, a_{23}, a_{12|3}, a_{13|2}, a_{23|1}\}$.

There are 11 gaussoids among the $2^6 = 64$ subsets. They are all realizable.

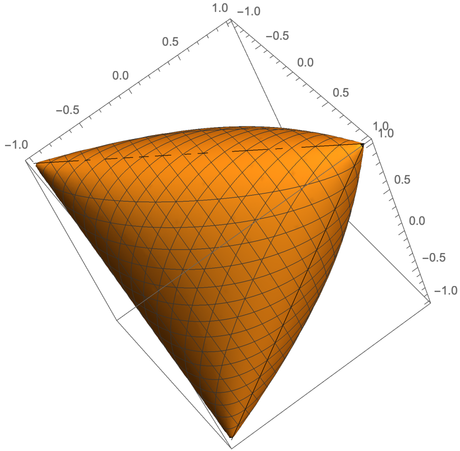


Example: oriented 3-gaussoids

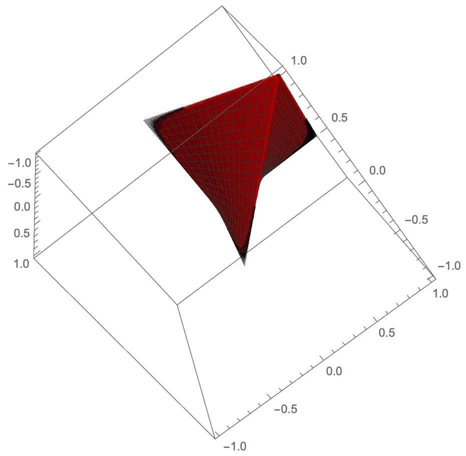
Consider the variable ordering $a_{12}, a_{13}, a_{23}, a_{12|3}, a_{13|2}, a_{23|1}$

There are 51 oriented gaussoids in 7 natural symmetry classes:

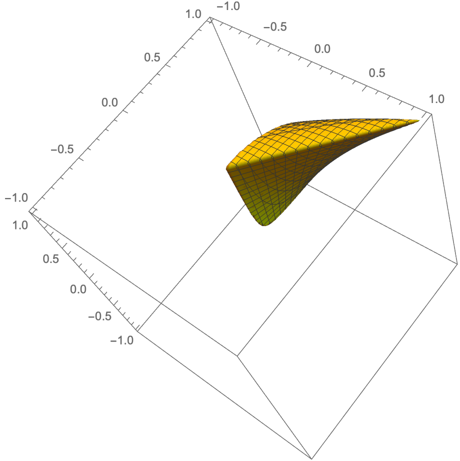
$(p_1, p_2, p_3, a_{12}, a_{13}, a_{23})$	Symmetry class
$(2, 2, 2, 1, 1, 1)$	$++++++$, $+--+--$, $--+--+$, $-+--+-$
$(3, 5, 1, 1, 1, 2)$	$+++-++$, $+-----$, $--++-+$, $\ldots$, $--+---$
$(6, 9, 6, -1, -1, -7)$	$------$, $++-++-$, $-++-++$, $+-++-+$
$(4, 3, 3, 2, 2, 1)$	$+++++0$, $++++0+$, $+++0++$,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



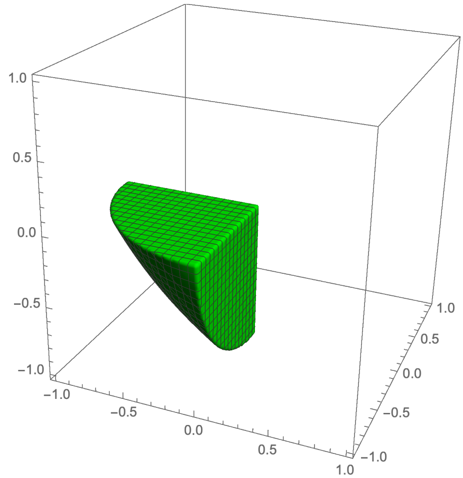
The set of of all PD 3×3-matrices with diagonal $(1, 1, 1)$ is the elliptope.



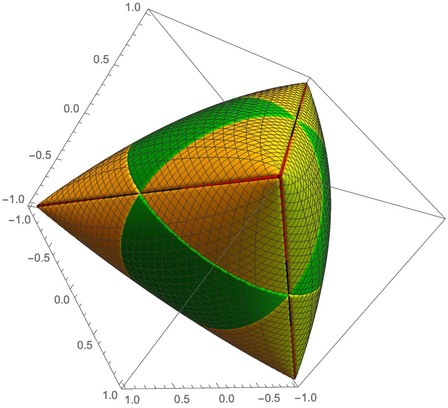
$$(a_{12}, a_{13}, a_{23}, a_{12|3}, a_{13|2}, a_{23|1}) = (+ + + + + +)$$



$$(a_{12}, a_{13}, a_{23}, a_{12|3}, a_{13|2}, a_{23|1}) = (+ + + - + +)$$



$$(a_{12}, a_{13}, a_{23}, a_{12|3}, a_{13|2}, a_{23|1}) = (- - - - - -)$$


1.0
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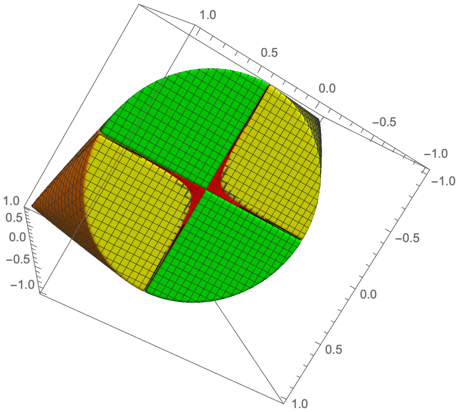
1.0
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Realizability

The signs of partial correlations of any multivariate Gaussian always form an oriented gaussoid.

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Non-realizable oriented gaussoids

For $n = 4$ there is a non-realizable uniform oriented gaussoid:

$$+ + + + + + + + + + + + + + - - + - + - + - + -$$

- The realization space of an oriented gaussoid is semi-algebraic.
- Positivstellensatz certificate for non-realizability.
- Non-realizable 4-gaussoids characterized in [LM07].
- There exists (many) 5-gaussoids not realizable over $\mathbb{C}$.

Matroid theory as a cue

...oid axioms = synthetic conditional independence

- Counting → `https://www.gaussoids.de`.
- Minors correspond to conditioning and marginalization.
- Descriptive power of gaussoid axioms
  - Sullivant, Šimeček: No finite axiomatization for Gaussian CI.
- Complexity of testing orientability: NP-complete ?

Matroid theory as a cue

Study realizations of ...oids.

- Are realization spaces universal semi-algebraic sets?
- What do graphical models realize?
  - Thm. All positive gaussoids are realized by undirected GM.
- What do structural equation models realize ?
- What happens close to the identity ?
- Positivity on the Lagrangian Grassmannian

What happens close to the identity?

In 2007 Lněnička and Matúš characterized the realizable 4-gaussoids. (50 out of 679 are not realizable)

i	$A^{(i)}$	i	$A^{(i)}$	i	$A^{(i)}$	i	$A^{(i)}$
1	$\begin{pmatrix} 1 & \varepsilon & \varepsilon & \varepsilon^2 \\ \varepsilon & 1 & 0 & \varepsilon \\ \varepsilon & 0 & 1 & 0 \\ \varepsilon^2 & \varepsilon & 0 & 1 \end{pmatrix}$	2	$\begin{pmatrix} 1 & \varepsilon & \varepsilon & \varepsilon \\ \varepsilon & 1 & 0 & \varepsilon^2 \\ \varepsilon & 0 & 1 & 0 \\ \varepsilon & \varepsilon^2 & 0 & 1 \end{pmatrix}$	3	$\begin{pmatrix} 1 & \varepsilon & \varepsilon & 1\text{-}\varepsilon^2 \\ \varepsilon & 1 & 0 & \varepsilon \\ \varepsilon & 0 & 1 & 0 \\ 1\text{-}\varepsilon^2 & \varepsilon & 0 & 1 \end{pmatrix}$	4	$\begin{pmatrix} 1 & 1\text{-}\varepsilon^2 & \varepsilon^2 & 0 \\ 1\text{-}\varepsilon^2 & 1 & 0 & \varepsilon \\ \varepsilon^2 & 0 & 1 & \text{-}\varepsilon \\ 0 & \varepsilon & \text{-}\varepsilon & 1 \end{pmatrix}$
6	$\begin{pmatrix} 1 & \varepsilon^2 & \varepsilon^2 & 0 \\ \varepsilon^2 & 1 & 0 & \varepsilon \\ \varepsilon^2 & 0 & 1 & \text{-}\varepsilon \\ 0 & \varepsilon & \text{-}\varepsilon & 1 \end{pmatrix}$	7	$\begin{pmatrix} 1 & \varepsilon & \varepsilon & 0 \\ \varepsilon & 1 & 0 & \varepsilon \\ \varepsilon & 0 & 1 & \text{-}\varepsilon \\ 0 & \varepsilon & \text{-}\varepsilon & 1 \end{pmatrix}$	8	$\begin{pmatrix} 1 & \varepsilon & \varepsilon^2 & \varepsilon \\ \varepsilon & 1 & 0 & \varepsilon \\ \varepsilon^2 & 0 & 1 & \varepsilon \\ \varepsilon & \varepsilon & \varepsilon & 1 \end{pmatrix}$	9	$\begin{pmatrix} 1 & \varepsilon & \varepsilon & \varepsilon^2 \\ \varepsilon & 1 & 0 & \varepsilon^2 \\ \varepsilon & 0 & 1 & \varepsilon \\ \varepsilon^2 & \varepsilon^2 & \varepsilon & 1 \end{pmatrix}$
10	$\begin{pmatrix} 1 & \varepsilon & \varepsilon^2 & \varepsilon \\ \varepsilon & 1 & 0 & \varepsilon^2 \\ \varepsilon^2 & 0 & 1 & \varepsilon \\ \varepsilon & \varepsilon^2 & \varepsilon & 1 \end{pmatrix}$	11	$\begin{pmatrix} 1 & \varepsilon & \varepsilon^3 & \varepsilon^2 \\ \varepsilon & 1 & 0 & \varepsilon \\ \varepsilon^3 & 0 & 1 & \varepsilon \\ \varepsilon^2 & \varepsilon & \varepsilon & 1 \end{pmatrix}$	12	$\begin{pmatrix} 1 & \varepsilon & \varepsilon & \varepsilon^2 \\ \varepsilon & 1 & 0 & \varepsilon \\ \varepsilon & 0 & 1 & \varepsilon \\ \varepsilon^2 & \varepsilon & \varepsilon & 1 \end{pmatrix}$	13	$\begin{pmatrix} 1 & \text{-}\varepsilon & \varepsilon & \varepsilon \\ \text{-}\varepsilon & 1 & 0 & \varepsilon \\ \varepsilon & 0 & 1 & \varepsilon \\ \varepsilon & \varepsilon & \varepsilon & 1 \end{pmatrix}$
14	$\begin{pmatrix} 1 & \text{-}\varepsilon & \varepsilon & \varepsilon^2 \\ \text{-}\varepsilon & 1 & 0 & \varepsilon \\ \varepsilon & 0 & 1 & \varepsilon \\ \varepsilon^2 & \varepsilon & \varepsilon & 1 \end{pmatrix}$	16	$\begin{pmatrix} 1 & \varepsilon & \varepsilon & 2\varepsilon^2 \\ \varepsilon & 1 & 0 & \varepsilon \\ \varepsilon & 0 & 1 & \varepsilon \\ 2\varepsilon^2 & \varepsilon & \varepsilon & 1 \end{pmatrix}$	17	$\begin{pmatrix} 1 & 1\text{-}\varepsilon^2 & \varepsilon^2 & \varepsilon \\ 1\text{-}\varepsilon^2 & 1 & 0 & \varepsilon \\ \varepsilon^2 & 0 & 1 & \varepsilon \\ \varepsilon & \varepsilon & \varepsilon & 1 \end{pmatrix}$	18	$\begin{pmatrix} 1 & g_\varepsilon & \varepsilon f_\varepsilon & \varepsilon \\ g_\varepsilon & 1 & 0 & \varepsilon g_\varepsilon \\ \varepsilon f_\varepsilon & 0 & 1 & f_\varepsilon \\ \varepsilon & \varepsilon g_\varepsilon & f_\varepsilon & 1 \end{pmatrix}$
19	$\begin{pmatrix} 1 & \varepsilon & \varepsilon^3 & \varepsilon^4 \\ \varepsilon & 1 & 0 & \varepsilon \\ \varepsilon^3 & 0 & 1 & \text{-}\varepsilon \\ \varepsilon^4 & \varepsilon & \text{-}\varepsilon & 1 \end{pmatrix}$	20	$\begin{pmatrix} 1 & 2\text{-}\delta^{\text{-}2} & \delta & \delta \\ 2\text{-}\delta^{\text{-}2} & 1 & 0 & \delta \\ \delta & 0 & 1 & \delta^2 \\ \delta & \delta & \delta^2 & 1 \end{pmatrix}$	21	$\begin{pmatrix} 1 & \varepsilon & \varepsilon f_\varepsilon & \varepsilon \\ \varepsilon & 1 & 0 & \varepsilon^2 \\ \varepsilon f_\varepsilon & 0 & 1 & 2\varepsilon \\ \varepsilon & \varepsilon^2 & 2\varepsilon & 1 \end{pmatrix}$	23	$\begin{pmatrix} 1 & \varepsilon^2 & \varepsilon & \varepsilon \\ \varepsilon^2 & 1 & \varepsilon & \text{-}\varepsilon \\ \varepsilon & \varepsilon & 1 & \varepsilon \\ \varepsilon & \text{-}\varepsilon & \varepsilon & 1 \end{pmatrix}$
24	$\begin{pmatrix} 1 & \varepsilon^2 & \varepsilon & \varepsilon \\ \varepsilon^2 & 1 & \varepsilon & \varepsilon \\ \varepsilon & \varepsilon & 1 & \varepsilon \\ \varepsilon & \varepsilon & \varepsilon & 1 \end{pmatrix}$	25	$\begin{pmatrix} 1 & \varepsilon^2 & \varepsilon & \varepsilon \\ \varepsilon^2 & 1 & \varepsilon & \text{-}\varepsilon \\ \varepsilon & \varepsilon & 1 & \varepsilon^2 \\ \varepsilon & \text{-}\varepsilon & \varepsilon^2 & 1 \end{pmatrix}$	26	$\begin{pmatrix} 1 & \varepsilon^3 & \varepsilon^2 & \varepsilon \\ \varepsilon^3 & 1 & \varepsilon & \varepsilon \\ \varepsilon^2 & \varepsilon & 1 & \varepsilon \\ \varepsilon & \varepsilon & \varepsilon & 1 \end{pmatrix}$	27	$\begin{pmatrix} 1 & \varepsilon^3 & \varepsilon & \varepsilon \\ \varepsilon^3 & 1 & \varepsilon^2 & \varepsilon^2 \\ \varepsilon & \varepsilon^2 & 1 & \varepsilon^2 \\ \varepsilon & \varepsilon^2 & \varepsilon^2 & 1 \end{pmatrix}$
28	$\begin{pmatrix} 1 & \varepsilon^3 & \varepsilon^2 & \varepsilon \\ \varepsilon^3 & 1 & \varepsilon & \varepsilon^4 \\ \varepsilon^2 & \varepsilon & 1 & \varepsilon \\ \varepsilon & \varepsilon^4 & \varepsilon & 1 \end{pmatrix}$	30	$\begin{pmatrix} 1 & \varepsilon^2 & \varepsilon & \varepsilon \\ \varepsilon^2 & 1 & \varepsilon & \varepsilon \\ \varepsilon & \varepsilon & 1 & \varepsilon^2 \\ \varepsilon & \varepsilon & \varepsilon^2 & 1 \end{pmatrix}$				

Table 1

Definition

A . . .oid is ϵ-realizable if there exist $a_{ij} \in \mathbb{N}, c_{ij} \in \mathbb{Q}$ such that

$$A_\epsilon = \begin{pmatrix} 1 & & & & \\ & 1 & & c_{ij}\epsilon^{a_{ij}} & \\ & & \ddots & & \\ & & & 1 & \\ & & & & 1 \end{pmatrix} \in \mathrm{PD}_n$$

realizes it for all sufficiently small ϵ.

Facts about ϵ-realizability

- ϵ-realizability is minor closed
- Šimeček: ϵ-realizability is not finitely axiomatizable

Proof. Let us consider a Gaussian distribution $\boldsymbol{\xi} = (\xi_a)_{a\in\{1,\ldots,n\}}$ with a variance matrix $\boldsymbol{\Sigma} = (\sigma_{a\cdot b})_{a,b\in\{1,\ldots,n\}}$ such that

$$\begin{aligned} \sigma_{a\cdot a} &= 1, \\ \forall a > 1: \ \sigma_{1\cdot a} &= \sigma_{a\cdot 1} = \epsilon^{n-a+1}, \\ \forall a, b > 1, a \neq b: \ \sigma_{a\cdot b} &= \sigma_{b\cdot a} = \epsilon, \end{aligned}$$

where $\epsilon > 0$ is any sufficiently small number. Apparently, $\boldsymbol{\Sigma} > 0$ because $|\boldsymbol{\Sigma}| = 1 + \epsilon(\cdots) > 0$, where "$\ldots$" stands for some polynom in ϵ.

- There exist non-ϵ-realizable gaussoids
- LM_{20} is an example that is far from the identity:

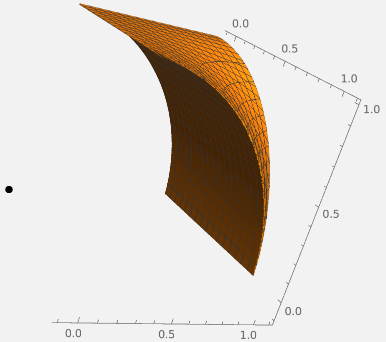
$$++--+++0++++0---+++++0++$$

Proof

Write out realization space to find

$$1 + \sigma_{12}\sigma_{14}\sigma_{24} = \sigma_{14}^2 + \sigma_{24}^2$$

This implies a Euclidean distance of 1 from the identity.



- There exist non-ϵ-realizable gaussoids close to the identity.
- LM_{21} is an example.

++++++−0++++0−−−+0++++++

Proof

LM realization is

$$\mathsf{LM}_{21} = \begin{pmatrix} 1 & \epsilon & \epsilon f_\epsilon & \epsilon \\ \epsilon & 1 & 0 & \epsilon^2 \\ \epsilon f_\epsilon & 0 & 1 & 2\epsilon \\ \epsilon & \epsilon^2 & 2\epsilon & 1 \end{pmatrix}, \text{ where } f_\epsilon = 2\epsilon/(1+\epsilon^2).$$

Assuming an ϵ-realization can be shown to lead to a contradiction.

Quo vadis?

- ϵ-realizability is practical and has been used in proofs.
- What is the (tropical) geometry of ϵ-realization spaces?
- Are uniform gaussoids ϵ-realizable?
- Does there exist a gaussoid that has no rational realization?
  - (all ϵ-realizable gaussoids do!)

Outlook

Matroid theory is connected to the geometry of the Grassmannian.

- A totally positive matrix is a matrix all of whose minors are positive.
- Positivity on the Grassmannian leads to cluster algebras, ...

Gaussoid theory is connected to the Lagrangian Grassmannian.

- A realization of a positive gaussoid is a symmetric matrix all of whose principal and almost principal minors are positive.
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- A realization of a positive gaussoid is a symmetric matrix all of whose principal and almost principal minors are positive.
- Positivity of Plücker coordinates on the Lagrangian Grassmannian leads to interesting math (e.g. Coxeter matroids)!

Thanks for your attention!