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The Gaussian CI inference problem

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MATHEMATISCHE
KOMPLEXITÄTSREDUKTION

Gaussian conditional independence

Consider random variables $(\xi_i)_{i \in N} \sim \mathcal{N}(\mu, \Sigma)$. The *conditional independence (CI) statement* $\xi_i \perp\!\!\!\perp \xi_j \mid \xi_K$ conveys, informally, that if ξ_K is known, then learning the value of ξ_i does not give any information about ξ_j.

Definition

The polynomial $\Sigma[K] \coloneqq \det \Sigma_{K,K}$ is a *principal minor* of Σ and $\Sigma[ij|K] \coloneqq \det \Sigma_{iK,jK}$ is an *almost-principal minor*.

If Σ is positive-definite, then $\Sigma[K] > 0$, and $\xi_i \perp\!\!\!\perp \xi_j \mid \xi_K$ holds if and only if $\Sigma[ij|K] = 0$.

Almost-principal minors

$$
\begin{aligned}
\Sigma[ij|] &= x_{ij} \\
\Sigma[ij|k] &= x_{ij}x_{kk} - x_{ik}x_{jk} \\
\Sigma[ij|kl] &= x_{ij}x_{kk}x_{ll} - x_{il}x_{jl}x_{kk} + x_{il}x_{jk}x_{kl} + x_{ik}x_{jl}x_{kl} - x_{ij}x_{kl}^2 - x_{ik}x_{jk}x_{ll} \\
\Sigma[ij|klm] &= x_{ij}x_{kk}x_{ll}x_{mm} + x_{im}x_{jm}x_{kl}^2 - x_{im}x_{jl}x_{kl}x_{km} - x_{il}x_{jm}x_{kl}x_{km} + x_{il}x_{jl}x_{km}^2 \\
&\quad - x_{im}x_{jm}x_{kk}x_{ll} + x_{im}x_{jk}x_{km}x_{ll} + x_{ik}x_{jm}x_{km}x_{ll} - x_{ij}x_{km}^2x_{ll} \\
&\quad + x_{im}x_{jl}x_{kk}x_{lm} + x_{il}x_{jm}x_{kk}x_{lm} - x_{im}x_{jk}x_{kl}x_{lm} - x_{ik}x_{jm}x_{kl}x_{lm} \\
&\quad - x_{il}x_{jk}x_{km}x_{lm} - x_{ik}x_{jl}x_{km}x_{lm} + 2x_{ij}x_{kl}x_{km}x_{lm} + x_{ik}x_{jk}x_{lm}^2 \\
&\quad - x_{ij}x_{kk}x_{lm}^2 - x_{il}x_{jl}x_{kk}x_{mm} + x_{il}x_{jk}x_{kl}x_{mm} + x_{ik}x_{jl}x_{kl}x_{mm} \\
&\quad - x_{ij}x_{kl}^2x_{mm} - x_{ik}x_{jk}x_{ll}x_{mm} \\
&\;\;\vdots
\end{aligned}
$$

Gaussian CI models

Definition

A *CI constraint* is a CI statement $\xi_i \perp\!\!\!\perp \xi_j \mid \xi_K$ or its negation $\neg(\xi_i \perp\!\!\!\perp \xi_j \mid \xi_K)$. They are *algebraic conditions* on the entries of Σ, equivalent to vanishing or non-vanishing of the almost-principal minors $\Sigma[ij|K]$.

Definition

The *model* of a set of CI constraints is the set of all positive-definite matrices which satisfy the constraints.

Gaussian CI models

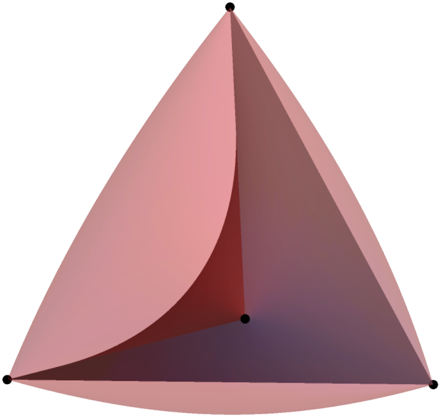

Figure: Gaussian model $\Sigma[12|3] = 0$ inside the elliptope.

Models and inference

Consider two sets of CI statements $\mathcal{P}$ and $\mathcal{Q}$:

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Reasoning about relevance statements in normally distributed random variables is the same as reasoning about the vanishing of very special kinds of determinants on very special kinds of varieties inside the positive-definite matrices.

Examples of CI inference

Consider a general positive-definite 3×3 correlation matrix

$$\Sigma = \begin{pmatrix} 1 & a & b \\ a & 1 & c \\ b & c & 1 \end{pmatrix}.$$

- If $\Sigma[12|3] = a - bc$ and $\Sigma[13|] = b$ vanish, then $\Sigma[12|] = a$ and $\Sigma[13|2] = b - ac$ must vanish as well:

$$(12|3) \wedge (13|) \Rightarrow (12|) \wedge (13|2).$$

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- If $\Sigma[12|] = a$ and $\Sigma[12|3] = a - bc$ vanish, then $bc = \Sigma[13|] \cdot \Sigma[23|]$ must vanish:

$$(12|) \wedge (12|3) \;\Rightarrow\; (13|) \vee (23|).$$

No finite set of axioms

"There is no finite complete axiomatization of Gaussian CI":

Theorem (Sullivant 2009)

As the matrix size n grows, there exist valid inference rules for Gaussians which need arbitrarily many antecedents.

$$(12|3) \wedge (23|4) \wedge (34|1) \wedge (14|2) \;\Rightarrow\; (12|) \qquad (n = 4)$$

$$(12|3) \wedge (23|4) \wedge (34|5) \wedge (45|1) \wedge (15|2) \;\Rightarrow\; (12|) \qquad (n = 5)$$

$$(12|3) \wedge (23|4) \wedge (34|5) \wedge (45|6) \wedge (56|1) \wedge (16|2) \;\Rightarrow\; (12|) \qquad (n = 6)$$

$$\vdots$$

Complexity bounds (upper)

Let $f_1, \dots, f_r \in \mathbb{Z}[t_1, \dots, t_k]$ be integer polynomials in finitely many variables. We consider a system of polynomial constraints "$f_i \bowtie_i 0$" where $\bowtie_i \in \{=, \neq, <, \leq, \geq, >\}$.

Theorem (Tarski's transfer principle)

If a polynomial system $\{f_i \bowtie_i 0\}$ has a solution over $\mathbb{R}$, then it has a solution in a finite real extension of $\mathbb{Q}$.

Theorem (Real Nullstellensatz)

A polynomial F vanishes on the semialgebraic set $\mathcal{K} = \{f_i \bowtie_i 0\}$ if and only if $F \in \sqrt[\mathbb{R}]{\mathcal{J}(f_i \bowtie_i 0)}$.

Keyword for this decision problem: *existential theory of the reals*.

Complexity bounds (lower)

Theorem (B. 2021)

For every finite real extension $\mathbb{K}/\mathbb{Q}$ there exists a Gaussian CI model $\mathcal{M}_{\mathbb{K}}$ such that: for every $\mathbb{L}/\mathbb{Q}$, $\mathcal{M}_{\mathbb{K}}$ has an $\mathbb{L}$-rational point if and only if $\mathbb{K} \subseteq \mathbb{L}$.

Theorem (B. 2021)

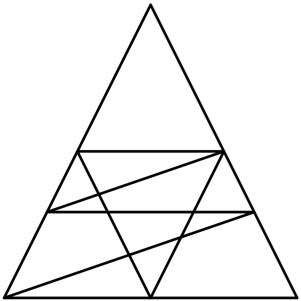
For every system of polynomials F defining a semialgebraic set $\mathcal{K} = \{f_i \bowtie_i 0\}$ one can compute a set of CI constraints $\mathcal{I}_F$ such that $\mathcal{I}_F$ has a model if and only if $\mathcal{K}$ contains a real point.

Proof idea (1): Algebra ⊆ Synthetic geometry

Point and line configuration for the equation $x^2 - 2 = 0$.

The configuration is specified by incidences between points and lines and also the parallelities of lines.

It is realizable over $\mathbb{Q}(\sqrt{2})$ but not over $\mathbb{Q}$.



Keyword for the general technique: *von Staudt constructions*.

Proof idea (2): Synthetic geometry ⊆ Gaussian CI

$$\Sigma[ij|] = x_{ij} \quad \to \text{impose } x_{kl} = x_{km} = x_{lm} = 0, \text{ then:}$$

$$\begin{aligned}
\Sigma[ij|klm] = {} & x_{ij} x_{kk} x_{ll} x_{mm} + x_{im} x_{jm} \underline{x_{kl}^2} - x_{im} x_{jl} \underline{x_{kl} x_{km}} - x_{il} x_{jm} \underline{x_{kl} x_{km}} + x_{il} x_{jl} \underline{x_{km}^2} \\
& - x_{im} x_{jm} x_{kk} x_{ll} + x_{im} x_{jk} \underline{x_{km}} x_{ll} + x_{ik} x_{jm} \underline{x_{km}} x_{ll} - x_{ij} \underline{x_{km}^2} x_{ll} \\
& + x_{im} x_{jl} x_{kk} \underline{x_{lm}} + x_{il} x_{jm} x_{kk} \underline{x_{lm}} - x_{im} x_{jk} \underline{x_{kl} x_{lm}} - x_{ik} x_{jm} \underline{x_{kl} x_{lm}} \\
& - x_{il} x_{jk} \underline{x_{km} x_{lm}} - x_{ik} x_{jl} \underline{x_{km} x_{lm}} + 2 x_{ij} \underline{x_{kl} x_{km} x_{lm}} + x_{ik} x_{jk} \underline{x_{lm}^2} \\
& - x_{ij} x_{kk} \underline{x_{lm}^2} - x_{il} x_{jl} x_{kk} x_{mm} + x_{il} x_{jk} \underline{x_{kl}} x_{mm} + x_{ik} x_{jl} \underline{x_{kl}} x_{mm} \\
& - x_{ij} \underline{x_{kl}^2} x_{mm} - x_{ik} x_{jk} x_{ll} x_{mm} \\
= {} & x_{ij} - \sum_{k=k,l,m} x_{ik} x_{jk} \quad = \quad x_{ij} - \left\langle \begin{pmatrix} x_{ik} \\ x_{il} \\ x_{im} \end{pmatrix}, \begin{pmatrix} x_{jk} \\ x_{jl} \\ x_{jm} \end{pmatrix} \right\rangle .
\end{aligned}$$

Approximations to the inference problem

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Theorem (Matúš 2005)

The following relations hold for every symmetric matrix Σ:

$$\Sigma[ij|L]^2 = \Sigma[iL] \cdot \Sigma[jL] - \Sigma[L] \cdot \Sigma[ijL]$$
$$\Sigma[kL] \cdot \Sigma[ij|L] = \Sigma[L] \cdot \Sigma[ij|kL] + \Sigma[ik|L] \cdot \Sigma[jk|L]$$

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$$\Sigma[ij|L]^2 = \Sigma[iL] \cdot \Sigma[jL] - \Sigma[L] \cdot \Sigma[ijL] \quad \to \textit{semimatroids}$$
$$\Sigma[kL] \cdot \Sigma[ij|L] = \Sigma[L] \cdot \Sigma[ij|kL] + \Sigma[ik|L] \cdot \Sigma[jk|L] \quad \to \textit{gaussoids}$$

These relations define essential geometric properties of symmetric matrices in principal and almost-principal minor coordinates. Study their combinatorics!

The multiinformation region

$$\Sigma[ij|L]^2 = \Sigma[iL] \cdot \Sigma[jL] - \Sigma[L] \cdot \Sigma[ijL]$$

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Multiinformation vectors $m = m(\Sigma) \in \mathscr{M}$ satisfy the following *linear information inequalities*:

$$\triangle_{ij|K}(m) := m_{iK} + m_{jK} - m_{ijK} - m_K \ \geq \ 0. \qquad \text{(Submodularity)}$$

Moreover $\triangle_{ij|K}(m(\Sigma)) = 0$ if and only if $\Sigma[ij|K] = 0$.

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→ This is a polyhedral condition on the vector m.

Information inequalities

Idea: Take a polyhedral cone C inside of the convex cone $\mathscr{M}^\vee$ and consider $C^\vee \supseteq \mathscr{M}$ as an outer approximation and derive CI inference rules from it.

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Linear information inequalities at the region $\mathscr{M}$ of the form

$$\sum_{\beta \in \mathcal{Q}} c_\beta \triangle_\beta (m) \le \sum_{\alpha \in \mathcal{P}} c_\alpha \triangle_\alpha (m), \text{ with } c_\alpha, c_\beta > 0,$$

encode inference rules

$$\bigwedge_{\alpha \in \mathcal{P}} \alpha \Rightarrow \bigwedge_{\beta \in \mathcal{Q}} \beta.$$

Semimatroids

The cone of *tight polymatroids* in $\mathbb{R}^{2^n}$ is given by

$$m_\emptyset = 0, \quad m_N = m_{N \setminus i}, \text{ for all } i \in N,$$
$$\triangle_{ij|K}(m) \geq 0, \text{ for all } (ij|K).$$

Each $\triangle_{ij|K} \geq 0$ gives rise to a unique facet which is identified with the CI statement $(ij|K)$.

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CI inference $\bigwedge \mathcal{P} \Rightarrow \bigwedge \mathcal{Q}$ means "if it lies on every facet $\alpha \in \mathcal{P}$, then does it lie on every facet $\beta \in \mathcal{Q}$ as well?" $\to$ Study the face lattice!

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Each face corresponds to the set of $(ij|K)$ statements of the facets it lies on.
These CI structures are *semimatroids*.

CI inference via linear programming

Inspecting the face lattice of the tight polymatroid cone in $\mathbb{R}^{2^5}$ with the LP solver `SoPlex` proves, for instance,

$$(12|) \wedge (13|4) \wedge (14|5) \wedge (15|23) \wedge (23|5) \wedge (24|135) \wedge (34|12) \wedge (35|1) \wedge (45|2)$$
$$\Rightarrow (12|5) \wedge (13|5) \wedge (14|3) \wedge (15|3) \wedge (15|4) \wedge (23|) \wedge (35|12)$$

for all Gaussian distributions.

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for all Gaussian distributions.

Theorem (Matúš 1997)

Semimatroids have no finite complete axiomatization.

The Gaussian CI configuration space

$$\Sigma[kL] \cdot \Sigma[ij|L] = \Sigma[L] \cdot \Sigma[ij|kL] + \Sigma[ik|L] \cdot \Sigma[jk|L]$$

The *Gaussian CI configuration space* $\mathscr{G} \subseteq \mathbb{R}^{2^n} \times \mathbb{R}^{\binom{n}{2}2^{n-2}}$ consists of all vectors of principal and almost-principal minors of $\Sigma \in \mathrm{PD}_n$.

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Very wasteful encoding of a matrix, but this creates simple and useful relations on configuration vectors. The CI structure of Σ is encoded in the *zero pattern* of $c(\Sigma) \in \mathscr{G}$.

Combinatorial compatibility

$$\Sigma[kL] \cdot \Sigma[ij|L] = \Sigma[L] \cdot \Sigma[ij|kL] + \Sigma[ik|L] \cdot \Sigma[jk|L]$$

Combinatorial compatibility means "fulfilling of relations under incomplete information": What if we only knew that all $\Sigma[K] \neq 0$ and whether or not $\Sigma[ij|K] = 0$ for every $(ij|K)$?

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$$\begin{aligned} (ij|L) \wedge (ij|kL) &\Rightarrow (ik|L) \vee (jk|L) \\ (ik|L) \wedge (ij|kL) &\Rightarrow (ij|L) \\ &\vdots \end{aligned}$$

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(ik|L) \wedge (ij|kL) &\Rightarrow (ij|L) \wedge (ik|jL) \\
(ij|kL) \wedge (ik|jL) &\Rightarrow (ij|L) \wedge (ik|L) \\
(ij|L) \wedge (ik|L) &\Rightarrow (ij|kL) \wedge (ik|jL)
\end{aligned}$$

This yields the definition of *gaussoids*.

CI inference via SAT solvers

Since gaussoids have a finite axiomatization, a SAT solver like `CaDiCaL` can deduce implications under the gaussoid axioms:

$$(12|) \wedge (13|4) \wedge (14|5) \wedge (15|23) \wedge (23|5) \wedge (24|135) \wedge (34|12) \wedge (35|1) \wedge (45|2)$$
$$\Rightarrow \text{ nothing.}$$

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$$\Rightarrow \text{ nothing.}$$

The structure on the left is a gaussoid. In this case, the semimatroid axioms were stronger and deduced more CI statements which hold on *every* Gaussian distribution which satisfies the left-hand side statements.

Oriented gaussoids

$$\Sigma[kL] \cdot \Sigma[ij|L] = \Sigma[L] \cdot \Sigma[ij|kL] + \Sigma[ik|L] \cdot \Sigma[jk|L]$$

What if we only knew that all $\operatorname{sgn} \Sigma[K] = +1$ and the value of $\operatorname{sgn} \Sigma[ij|K]$ for every $(ij|K)$?

$$+(ij|L) \wedge -(ij|kL) \;\Rightarrow\; [+(ik|L) \wedge +(jk|L)] \vee [-(ik|L) \wedge -(jk|L)]$$

→ *Oriented* and *orientable* gaussoids.

Oriented gaussoids

$$\Sigma[kL] \cdot \Sigma[ij|L] = \Sigma[L] \cdot \Sigma[ij|kL] + \Sigma[ik|L] \cdot \Sigma[jk|L]$$

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→ *Oriented* and *orientable* gaussoids.

$$\begin{aligned}
(ij|L) \wedge (kl|L) \wedge (ik|jL) \wedge (jl|ikL) &\Rightarrow (ik|L) \\
(ij|L) \wedge (kl|iL) \wedge (kl|jL) \wedge (ij|klL) &\Rightarrow (kl|L) \\
(ij|L) \wedge (jl|kL) \wedge (kl|iL) \wedge (ik|jlL) &\Rightarrow (ik|L) \\
(ij|kL) \wedge (ik|lL) \wedge (il|jL) &\Rightarrow (ij|L) \\
(ij|kL) \wedge (ik|lL) \wedge (jl|iL) \wedge (kl|jL) &\Rightarrow (ij|L)
\end{aligned}$$

CI inference via SAT solvers II

Running the SAT solver `CaDiCaL` on the definition of oriented gaussoids confirms that on their supports

$$(12|) \wedge (13|4) \wedge (14|5) \wedge (15|23) \wedge (23|5) \wedge (24|135) \wedge (34|12) \wedge (35|1) \wedge (45|2)$$
$$\Rightarrow \text{ everything except } (25|K) \text{ for all } K.$$

This inference rule is valid for all Gaussian distributions and as strong as possible.

Theorem (B. 2021+)

Orientable gaussoids have no finite complete axiomatization.

The search for inference rules

Inference rules help characterize the *realizable* CI structures:

- 3-variate: 11 out of 64 by Matúš 2005.
- 4-variate: 629 out of 16 777 216 by Lněnička and Matúš 2007.
- 5-variate: *open!*
  - 254 826 gaussoids modulo symmetry
  - 87 792 of which are orientable semimatroids
  - 84 434 of which are *selfadhesive* orientable semimatroids.

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Help wanted:

- Use finer approximations to $\mathscr{M}^\vee$ from the literature.
- Non-linear information inequalities → Ahmadieh and Vinzant 2021.
- Tropical approximations and valuated gaussoids.
- Compute algebraic realization spaces.
- Find and certify real solutions to polynomial systems.

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