Treks, tetrads & third-order tensors of moments

Polynomial relations for linear graphical models beyond covariance matrices

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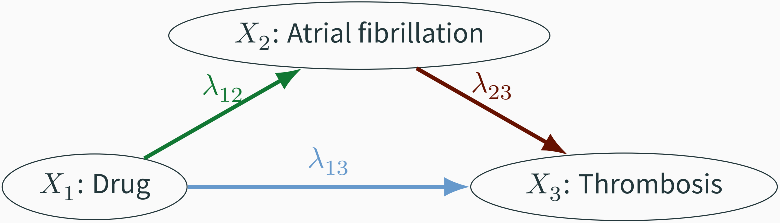
Directed arrows capture causal relations between random variables



translating to equations

$$
\begin{aligned}
X_1 &= && && \varepsilon_1 \\
X_2 &= \lambda_{12} X_1 && && + \varepsilon_2 \\
X_3 &= \lambda_{13} X_1 && + \lambda_{23} X_2 && + \varepsilon_3
\end{aligned}
$$

Structural equation models

A graph $G = (V, E)$ gives rise to structural equations

$$X_i = \sum_{j \in \text{pa}(i)} \lambda_{ji} X_j + \varepsilon_i, \quad i \in V,$$

- ε_i represent stochastic errors with $\mathbb{E}[\varepsilon_i] = 0$,
- λ_{ji} are unknown parameters forming a matrix $\Lambda = (\lambda_{ij})$.

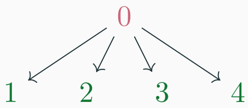
The corresponding moment tensor model is

$$\begin{aligned}\mathcal{M}^{(2,3)}(G) = \{(S = (I-\Lambda)^{-T}\Omega^{(2)}(I-\Lambda)^{-1},\\ T = \Omega^{(3)} \bullet (I-\Lambda)^{-1} \bullet (I-\Lambda)^{-1} \bullet (I-\Lambda)^{-1}) :\\ \Omega^{(2)} \text{ is } n \times n \text{ positive definite diagonal matrix},\\ \Omega^{(3)} \text{ is } n \times n \times n \text{ diagonal 3-way tensor, and } \Lambda \in \mathbb{R}^E\}.\end{aligned}$$

This makes (statistical) sense for non-Gaussian random variables.

Goal: characterize polynomial relations among elements in the model.

Let 0 be a hidden variable and $1, 2, 3, 4$ be observed ones.



Then the following tetrad relations [Drton, Sturmfels, Sullivant 05; Peters, Janzing, Schölkopf 17] hold among the elements of the covariance matrix

$$s_{12}s_{34} - s_{13}s_{24} \quad s_{12}s_{34} - s_{14}s_{23} \quad s_{13}s_{24} - s_{14}s_{23}.$$

Proof Evaluate the expressions via

$$s_{ij} \mapsto \omega_0 \lambda_{0i} \lambda_{0j}.$$

They all evaluate to zero.

Why higher moments?

The covariance matrix structure reveals statistical information, e.g.

has covariance ideal $I = \langle s_{13}s_{22} - s_{12}s_{23} \rangle$ corresponding to the statement $X_1 \perp\!\!\!\perp X_3 | X_2$...

Proposition One can deduce the skeleton and the colliders of the graph from the covariance matrix.

...but so do the graphs

Proposition [Wang, Drton 18] The whole graph can be reconstructed from covariance matrices and 3^{rd}-order tensors.

A *trek* with top v between i and j is formed by joining two paths sharing a source v

$$i = i_l \leftarrow \cdots \leftarrow i_1 \leftarrow v \rightarrow j_1 \rightarrow \ldots \rightarrow j_r = j$$

and gives rise to a monomial

$$a_v(\lambda_{vi_1}\lambda_{i_1i_2}\ldots\lambda_{i_{l-1}i_l})(\lambda_{vj_1}\lambda_{j_1j_2}\ldots\lambda_{j_{r-1}j_r}).$$

An n-*trek* between vertices $k_1, \ldots, k_n$ is a collection of directed paths $T = (P_1, \ldots, P_n)$, where P_r has sink k_r and they all share the same top vertex as source $v = \mathrm{top}(T)$.

$$\begin{array}{lllllll} & \nearrow & k_{11} \longrightarrow k_{12} \longrightarrow \cdots \rightarrow k_{1l_1} = k_1 \\ v & \longrightarrow & k_{21} \longrightarrow k_{22} \longrightarrow \cdots \rightarrow k_{2l_2} = k_2 \\ & \searrow & k_{31} \longrightarrow k_{32} \longrightarrow \cdots \rightarrow k_{3l_2} = k_3 \end{array}$$

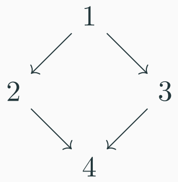
A trek is minimal if the top node is the only one that appears in all paths of the trek. For a graph G, let $T(i_1, \ldots, i_n)$ be the set of minimal n-treks between $i_1, \ldots, i_n$.

Consider the polynomial map ϕ_G:

$$\begin{aligned}
\mathbb{C}[s_{ij}, t_{ijk} \mid 1 \le i \le j \le k \le n] &\to \mathbb{C}[a_i, b_i, \lambda_{ij} \mid i \to j \in E] \\
s_{ij} &\mapsto \sum_{\tau \in T(i,j)} a_{\mathrm{top}(\tau)} \prod_{k \to l \in \tau} \lambda_{kl}, \\
t_{ijk} &\mapsto \sum_{\tau \in T(i,j,k)} b_{\mathrm{top}(\tau)} \prod_{m \to l \in \tau} \lambda_{ml}.
\end{aligned}$$

Example

$$\begin{aligned}
s_{ii} &\mapsto a_i \quad t_{iii} \mapsto b_i \\
s_{13} &\mapsto a_1 \lambda_{13} \\
s_{14} &\mapsto a_1 \lambda_{12} \lambda_{24} + a_1 \lambda_{13} \lambda_{34} \\
t_{123} &\mapsto b_1 \lambda_{12} \lambda_{13}
\end{aligned}$$



$$\begin{aligned} s_{ij} &\mapsto \sum_{\tau \in T(i,j)} a_{\mathrm{top}(\tau)} \prod_{k \to l \in \tau} \lambda_{kl} \\ t_{ijk} &\mapsto \sum_{\tau \in T(i,j,k)} b_{\mathrm{top}(\tau)} \prod_{m \to l \in \tau} \lambda_{ml} \end{aligned}$$

Proposition [Sullivant 08; Améndola, Drton, G, Homs & Robeva 22] For a directed graph G, let ϕ_G be the map given by the simple trek rule. Then the vanishing ideal $I^{(2,3)}(G) := \mathcal{J}(\mathcal{M}^{(2,3)}(G))$ of the model is

$$I^{(2,3)}(G) = \ker \phi_G.$$

Corollary [Améndola, Drton, G, Homs & Robeva 22] If G is a tree, $I^{(2,3)}(G)$ is a toric ideal, i.e. it is generated by binomials.

Vanishing minors

Let $i, j \in V$ be two vertices such that a 2-trek between i and j exists. Define

$$A_{ij} := \begin{bmatrix} s_{ik_1} & \cdots & s_{ik_r} & t_{i\ell_1 m_1} & \cdots & t_{i\ell_q m_q} \\ s_{jk_1} & \cdots & s_{jk_r} & t_{j\ell_1 m_1} & \cdots & t_{j\ell_q m_q} \end{bmatrix},$$

where

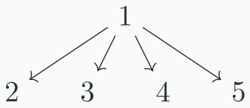
- $k_1, \dots, k_r$ are all vertices such that $\text{top}(i, k_a) = \text{top}(j, k_a)$ and
- (l_1, m_1),... ,(l_q, m_q) are all pairs of vertices such that $\text{top}(i, l_b, m_b) = \text{top}(j, l_b, m_b)$.

Proposition [Améndola, Drton, G, Homs & Robeva 22] For a tree G, the following polynomials are in $I^{(2,3)}(G)$:

- s_{ij} such that there is no 2-trek between i and j,
- t_{ijk} such that there is no 3-trek between i, j and k,
- the 2-minors of A_{ij}, for all (i, j) with a 2-trek between them.

Proposition [Améndola, Drton, G, Homs & Robeva 22] All quadratic binomials in $I^{(2,3)}(G)$ are linear combinations of 2-minors of matrices A_{ij}.

Example The binomial $f = s_{23}t_{145} - s_{45}t_{123}$ lies in $I^{(2,3)}(G)$. It is a sum of minors from A_{13}, A_{14} and A_{15}.

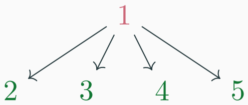


Theorem [Améndola, Drton, G, Homs & Robeva 22] All binomials in $I^{(2,3)}(G)$ are generated by quadratic binomials, i.e. $I^{(2,3)}(G)$ is generated by the matrices A_{ij} (plus vanishing indeterminates).

Proof A distance reduction argument for binomials in the ideal, showing that matrix minors are a Markov basis.

Application: trees with hidden variables

Let $H \cup O$ be a partition of the nodes of the DAG G. The hidden nodes H are said to be *upstream* from the observed nodes O in G if there are no edges $o \to h$ in G with $o \in O$ and $h \in H$.



Lemma The ideal $I^{(2,3)}(G)$ is homogeneous w.r.t. the grading:

$$\begin{aligned} \deg s_{ij} &= (1, 1 + \text{number of elements in the multiset } \{i, j\} \text{ in } O) \\ \deg t_{ijk} &= (1, \text{number of elements in the multiset } \{i, j, k\} \text{ in } O). \end{aligned}$$

Proposition For a tree G, the observed variable ideal $I_O^{(2,3)}(G)$ is generated by the minors of the submatrices of A_{ij} with i, j both in O, with columns indexed by k and (l, m) where k, l, m are all in O.

Theorem [Améndola, Drton, G, Homs & Robeva 22] Let J be the ideal generated by the linear generators of $I^{(2,3)}(G)$ and matrices A_{ij} such that there is a directed path between i and j. Then

$$\mathcal{M}^{(2,3)}(G) = V(J) \cap PD(n).$$

In particular, pick $(S,T) \in \mathcal{M}^{(2,3)}(G)$. For $i \to j \in E$, let $\lambda_{ij} = \frac{s_{ij}}{s_{ii}}$, coming from A_{ij}. Then one can show

$$S' = (I-\Lambda)^T S (I-\Lambda) \quad \text{and} \quad T' = T \bullet (I-\Lambda) \bullet (I-\Lambda) \bullet (I-\Lambda)$$

are diagonal.

Example Let G be $1 \to 2$, $1 \to 3$, $1 \to 4$, $1 \to 5$. Computations show

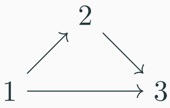
$$I^{(2,3)}(G) = (J : s_{11}^{\infty})$$

and

$$\mathcal{M}^{(2,3)}(G) = V(I^{(2,3)}(G)) \cap PD(5) = V(J) \cap PD(5).$$

A forest of non-trees

The ideal of the 3×3 minors of



$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \end{array} \begin{array}{c} \begin{array}{ccccccc} 1 & 2 & 11 & 12 & 13 & 22 & 23 \end{array} \\ \begin{pmatrix} s_{11} & s_{12} & t_{111} & t_{112} & t_{113} & t_{122} & t_{123} \\ s_{12} & s_{22} & t_{112} & t_{122} & t_{123} & t_{222} & t_{223} \\ s_{13} & s_{23} & t_{113} & t_{123} & t_{133} & t_{223} & t_{223} \end{pmatrix} \end{array}$$

is given by

the 2×2 minors of

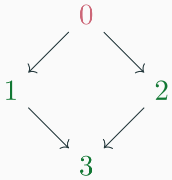
$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 11 & 12 & 13 \end{array} \\ \begin{pmatrix} s_{11} & t_{111} & t_{112} & t_{113} \\ s_{12} & t_{112} & t_{122} & t_{123} \\ s_{13} & t_{113} & t_{123} & t_{133} \end{pmatrix} \end{array}$$

and the determinant of

$$\begin{array}{c} \\ \emptyset \\ 2 \\ 3 \end{array} \begin{array}{c} \begin{array}{ccc} 13 & 22 & 23 \end{array} \\ \begin{pmatrix} s_{13} & s_{22} & s_{23} \\ t_{123} & t_{222} & t_{223} \\ t_{133} & t_{223} & t_{223} \end{pmatrix} \end{array}$$

A forest on non-trees

The ideal of the graph



is given by the maximal minors of

$$
\begin{array}{c} \\ 1 \\ 2 \\ 3 \end{array}
\begin{array}{c}
\begin{array}{ccccccc} 1 & 2 & 11 & 12 & 13 & 22 & 23 \end{array} \\
\begin{pmatrix}
s_{11} & s_{12} & t_{111} & t_{112} & t_{113} & t_{122} & t_{123} \\
s_{12} & s_{22} & t_{112} & t_{122} & t_{123} & t_{222} & t_{223} \\
s_{13} & s_{23} & t_{113} & t_{123} & t_{133} & t_{223} & t_{233}
\end{pmatrix}
\end{array}.
$$

Given a polytree G, the third-order moment polytope is

$P_G^{(3)} = \mathrm{conv}\left(e_{ijk} : i, j, k \text{ such that a 3-trek between } i, j \text{ and } k \text{ exists}\right)$

where $e_{ijk} \in \mathbb{R}^{|V|+|E|}$ is the vector of exponents of the monomial $\phi_G(t_{ijk}) = b_{\mathrm{top}(i,j,k)} \prod_{l \to m \in \mathcal{T}(i,j,k)} \lambda_{lm} \in \mathbb{R}[b_l, \lambda_{lm}]$.

Theorem The third-order moment polytope $P_G^{(3)}$ is the solution to

$$z_l \geq 0 \text{ for all } l \in V,$$

$$y_{lm} \geq 0 \text{ for all } l \to m \in E,$$

$$\sum_{l \in V} z_l = 1,$$

$$2z_l + \sum_{h \in pa(l)} y_{hl} - y_{lm} \geq 0 \text{ for all m such that } l \to m \in E,$$

$$3z_l + \sum_{h \in pa(l)} y_{hl} - \sum_{m \in ch(l)} y_{lm} \geq 0 \text{ for all } l \in V.$$

Open problems

- What about non-trees?
- Sparse latent factor analysis (current project with Drton, Portakal, Sturma)
- Latent factor analysis in higher dimensions (see also Ardiyansyah, Sodomaco 22)
- Euclidean distance degrees to the varieties
- **[Your favorite graphical model here]**

Summary

- Graphical models are richer in the non-Gaussian setting, it is meaningful to study higher-order moment tensors
- The trek rules can be extended for h.o.m. and one can obtain binomial (matrix minors) descriptions of the ideals
- The hidden variable ideals are given by some of the binomials
- Lots of open questions …

Reference:
Améndola, Drton, G, Homs & Robeva
Third-Order Moment Varieties of Linear Non-Gaussian Graphical Models

Thank you!