Mixtures of Discrete Decomposable Graphical Models

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joint work with Jane Ivy Coons and Nils Sturma

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Graphical models

Graphical models encode relationships between random variables using a graph structure:

- Vertices $\rightarrow$ random variables
- Edges $\rightarrow$ conditional dependence relations

Any graphical model adopts a natural parametrization which can be read from the structure of the underlying graph.

Widely used in:

⋆ statistics (causal inference)
⋆ machine learning (Bayesian networks, generative models)
⋆ computational biology (protein interaction networks)
⋆ phylogenetics (gene trees)
⋆ economics (dependencies between financial entities)
⋆ computer vision (image structures and relationships within scenes)

Example

Three random variables:

X_1 : length of a person's hair (bald, short, medium, and long).
X_2 : how often a person watches soccer (never, sometimes, and often).

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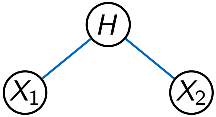
H : a person's gender!



The random variable G could be hidden or observed.

We write $X_1 \perp\!\!\!\perp X_2 | H$.

Parametric vs. implicit description

Given a model, parametrized by

$$\varphi : \theta = (\theta_1, \ldots, \theta_n) \mapsto \big(f_1(\theta), f_2(\theta), \ldots f_m(\theta)\big),$$

we are interested in describing the polynomials defining $\overline{\text{image}}(\varphi)$. This process is called *implicitization*.

Parametric vs. implicit description

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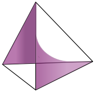
Example: the independence model.

Parametrization:

$$(\theta_1, \theta_2) \;\mapsto\; \big(\underbrace{\theta_1\theta_2}_{p_1},\; \underbrace{\theta_1(1-\theta_2)}_{p_2},\; \underbrace{(1-\theta_1)\theta_2}_{p_3},\; \underbrace{(1-\theta_1)(1-\theta_2)}_{p_4}\big).$$



Implicit ideal: $I = \langle p_1 p_4 - p_2 p_3, \;\; p_1 + p_2 + p_3 + p_4 - 1\rangle$.

The generators of the ideal I are called *model invariants*.

Undirected Graphical Models

Setup: Random variables $(X_v)_{v \in V}$ and undirected graph $G = (V, E)$.

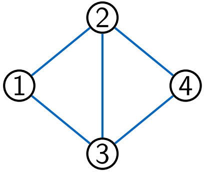
The graph G specifies dependencies between random variables.

Global Markov Property of G: all conditional independence statements

$$X_A \perp\!\!\!\perp X_B | X_C$$

for all disjoint sets A, B, and C such that C separates A and B in G.

Example:



$$X_1 \perp\!\!\!\perp X_4 | (X_2, X_3)$$

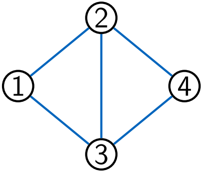
Parametrized Graphical Models

Factorization:

$$p(x) = \frac{1}{Z} \prod_{C \in \mathcal{C}(G)} \psi_C(x_C),$$

where $\mathcal{C}(G)$ is the collection of maximal cliques of G.

Example:



$$p(x_1, x_2, x_3, x_4) \propto \psi_{123}(x_1, x_2, x_3) \cdot \psi_{234}(x_2, x_3, x_4)$$

Theorem (Hammersley-Clifford)

A positive probability density satisfies the global Markov property on the graph G if and only if it factorizes according to G.

Discrete Undirected Graphical Models

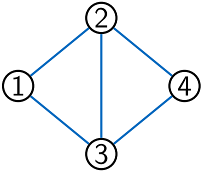
Finite state space $\mathcal{R} = \prod_{v \in V}[d_v]$. For $A \subset V$, let $\mathcal{R}_A = \prod_{v \in A}[d_v]$ and $d_A := \#\mathcal{R}_A = \prod_{v \in A} d_v$.

Definition

The discrete log-linear graphical model $\mathcal{M}_G$ consists of all probability distributions $p \in \Delta_{|\mathcal{R}|}$ such that

$$p_i = \frac{1}{Z(\theta)} \prod_{C \in \mathcal{C}(G)} \theta_{i_C}^{(C)}.$$

Example



$$p_{i_1 i_2 i_3 i_4} \propto \theta_{i_1 i_2 i_3}^{(C_1)} \cdot \theta_{i_2 i_3 i_4}^{(C_2)}$$

This is a log-linear model! It is parametrized by monomials and its Zariski closure is a toric variety.

Log-linear (toric) models

Every *log-linear model* is specified by an integer matrix $A \in \mathbb{Z}^{d \times n}$ with the vector of all ones in its rowspan.

Let $A = [A_1 \; A_2 \; \ldots \; A_n]$ and $\theta^{A_j} := \theta_1^{a_{1j}} \ldots \theta_d^{a_{dj}}$.

The log-linear model $\mathcal{M}_A$ is parametrized as

$$\theta \mapsto (\theta^{A_1}, \theta^{A_2}, \ldots, \theta^{A_n}).$$

The implicit description of this model is given as

$$I_A = \langle p^u - p^v : u - v \in \ker_{\mathbb{Z}}(A) \rangle.$$

Example:

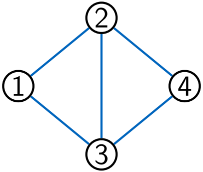
$$A = \begin{bmatrix} 2 & 1 & 0 \\ 0 & 1 & 2 \end{bmatrix}$$

Parametrization: $(\theta_1, \theta_2) \mapsto (\theta_1^2, \quad \theta_1\theta_2, \quad \theta_2^2).$

Ideal: $I_A = \langle p_1 p_3 - p_2^2 \rangle.$

Diamond graph, binary variables.

	0000	0001	0010	0011	0100	0101	0110	0111	1000	1001	1010	1011	1100	1101	1110	1111
000•	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
001•	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0
010•	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0
011•	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0
100•	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0
101•	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0
110•	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0
111•	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1
•000	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
•001	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0
•010	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0
•011	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0
•100	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0
•101	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0
•110	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0
•111	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1



Mixture Models

We use the rth **mixture** to model a situation where the population is split into r subpopulations.

$$\mathrm{Mixt}^r(\mathcal{M}) = \{\pi_1 \boldsymbol{p}^1 + \ldots + \pi_r \boldsymbol{p}^r : \pi \in \Delta_r, \boldsymbol{p}^i \in \mathcal{M} \text{ for all } i \in [r]\}$$

Secant varieties: Given a variety W

$$\mathrm{Sec}^r(W) := \overline{\{\alpha_1 w^1 + \ldots + \alpha_r w^r : \sum \alpha_i = 1 \text{ and } w^i \in W \text{ for all } i \in [r]\}}$$

Parameterization of $\mathrm{Mixt}^r(\mathcal{M}_G)$:

$$p_i = \frac{1}{Z(\theta)} \sum_{j=1}^{r} \prod_{C \in \mathcal{C}} \theta_{i_C}^{(j,C)}$$

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Questions: Dimension? Ideal $I_G^{(r)}$?

Expected dimension: $\min\{r \dim(\mathcal{M}_G) + (r-1), \quad \prod_{i \in V(G)} d_i - 1\}$.

Mixtures of the independence model

Independence model

= graphical model with empty graph,

= intersection of the probability simplex with the set of tensors of nonnegative rank at most 1.

Ideal of mixtures:

$r = 2$: Generated by all 3×3 minors of all flattenings. [Allman et al., 2015].

$r \geq 3$: Minors are not enough ("Salmon conjecture").

Dimension of mixtures:

- When the tensors are matrices, these are always defective.
- The dimension of the set of all rank r $m \times n$ matrices is $r(m + n - r) < r(m + n - 1) + (r - 1)$ when $r > 1$.
- Otherwise, "usually" of expected dimension, for details see [Landsberg, 2015, Section 5.5].

Sub-Ideals via Conditional Independence

Notation:

- For $S \subset V$, let $\mathcal{R}_S := \prod_{v \in S} [d_v]$ be the state space restricted to S
- For $i_S \in \mathcal{R}_S$, define the marginal

$$p_{i_S +} := \sum_{j \in \mathcal{R}_{V-S}} p_{i_S j}$$

- $I^{(r)}_{j_C; A \perp\!\!\!\perp B}$ = ideal of $(r+1) \times (r+1)$ minors of the matrix whose rows/columns are indexed by i_A / i_B and whose (i_A, i_B) entry is $p_{i_A i_B j_C +}$

Proposition (A.-Coons-Sturma, 2024)

Let $A, B, C \subset V$ be disjoint sets such that C separates A and B in G. Then for each $j_C \in \mathcal{R}_C$, $I^{(r)}_G$ contains $I^{(r)}_{j_C; A \perp\!\!\!\perp B}$.

$$\rightarrow \begin{bmatrix} p_{111} & p_{112} \\ p_{211} & p_{212} \end{bmatrix} \text{ and } \begin{bmatrix} p_{121} & p_{122} \\ p_{221} & p_{222} \end{bmatrix} \rightarrow \begin{matrix} p_{111}p_{212} - p_{112}p_{211} \\ p_{121}p_{222} - p_{122}p_{221} \end{matrix}.$$

Ideals

Question: Is $I_G^{(r)}$ the sum of these sub-ideals?

Ideals

Question: Is $I_G^{(r)}$ the sum of these sub-ideals? No!

Example (Second Mixture of the Binary 5-path)

By the proposition, the ideal $I_G^{(2)}$ contains 32 minimal cubic generators. However it also has 57 minimal quartic generators of the form:

$$p_{11222}p_{21112}p_{22121}p_{22211} - p_{11112}p_{21222}p_{22121}p_{22211} - p_{11221}p_{21112}p_{22122}p_{22211} + p_{11112}p_{21221}p_{22122}p_{22211} -$$
$$p_{11222}p_{21111}p_{22121}p_{22212} + p_{11111}p_{21222}p_{22121}p_{22212} + p_{11221}p_{21111}p_{22122}p_{22212} - p_{11111}p_{21221}p_{22122}p_{22212} -$$
$$p_{11212}p_{21122}p_{22111}p_{22221} + p_{11122}p_{21212}p_{22111}p_{22221} + p_{11211}p_{21122}p_{22112}p_{22221} - p_{11122}p_{21211}p_{22112}p_{22221} +$$
$$p_{11212}p_{21121}p_{22111}p_{22222} - p_{11121}p_{21212}p_{22111}p_{22222} - p_{11211}p_{21121}p_{22112}p_{22222} + p_{11121}p_{21211}p_{22112}p_{22222}.$$

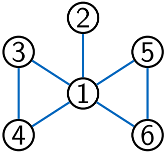
Shout-out: `MultigradedImplicitization.m2` by Joe Cummings and Ben Hollering

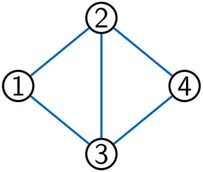
Clique-Stars

Definition

A graph G is a *clique star* if it is a union of cliques, $G = \cup_{i=1}^{k} \widetilde{C}_i$, and there is another clique S such that $\widetilde{C}_i \cap \widetilde{C}_j = S$ for all $i \neq j$.
Moreover, we write $C_i = \widetilde{C}_i \setminus S$.

Examples:

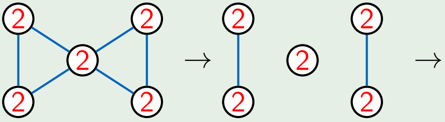




Clique-Stars: Ideal

Notation: $I^{(r)}_{j_S, d_{C_1} \times \cdots \times d_{C_k}}$ denotes the vanishing ideal of the rth mixture of the k-way independence model with the states $\prod_{i \in C} d_i$ for each clique C, with the fixed value $X_S = j_S \in \mathcal{R}_S$.

Example



$$\begin{bmatrix} p_{11111} & p_{12111} & p_{21111} & p_{22111} \\ p_{11112} & p_{12112} & p_{21112} & p_{22112} \\ p_{11121} & p_{12121} & p_{21121} & p_{22121} \\ p_{11122} & p_{12122} & p_{21122} & p_{22122} \end{bmatrix}$$

Theorem (A.-Coons-Sturma, 2024)

Let $G = (C_1 \cup \cdots \cup C_k \cup S, E)$ be a clique-star. Then

$$I^{(r)}_G = \sum_{j_S \in \mathcal{R}_S} I^{(r)}_{j_S, d_{C_1} \times \cdots \times d_{C_k}}.$$

Clique-Stars: Dimension

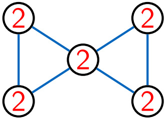
Theorem (A.-Coons-Sturma, 2024)

Let $G = (C_1 \cup \cdots \cup C_k \cup S, E)$ be a clique-star. Then

$$\dim(Sec^r(\overline{\mathcal{M}_G})) = \min\left\{ d_S \cdot \dim(\overline{\mathcal{T}^r_{d_{C_1}\times\cdots\times d_{C_k}}}) - 1, \prod_{v\in V} d_v - 1 \right\},$$

where $\mathcal{T}^r_{d_{C_1}\times\cdots\times d_{C_k}}$ is the set of $d_{C_1}\times\cdots\times d_{C_k}$ tensors of nonnegative rank at most r.

Example:



If $r = 2$ and all variables are binary, then

$$\dim(\mathrm{Sec}^2(\overline{\mathcal{M}_G})) = \min\{2\cdot 2\cdot(4+4-2)-1, 31\} = 23.$$

Expected dimension is 27 (similar for 3-path).

Proof: Restructure Jacobian of parametrization s.t. it is block-diagonal.

Dimensions

Let P_n denote the path with n vertices. We have seen that the secants of $\mathcal{M}_{P_3}$ are defective.

Question: Are the secants of $\mathcal{M}_{P_n}$ defective for $n > 3$?

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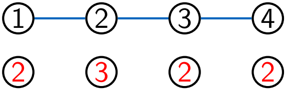
Question: Are the secants of $\mathcal{M}_{P_n}$ defective for $n > 3$? **No!**

Surprising Example



The dimension of the toric model $\mathcal{M}_{P_4}$ with $d_1 = d_3 = d_4 = 2$ and $d_2 = 3$ is 10. Its second secant has dimension

$$21 = 2 \times 10 + (2 - 1),$$

which is the expected dimension.

Dimensions of Second Secants for Decomposable Graphs

Theorem (A.-Coons-Sturma 2024)

Let G be a decomposable graph that is not a clique star with $d_v \geq 2$ for all $v \in V$. Then

$$\dim(\mathrm{Mixt}^2 \mathcal{M}_G) = 2\dim(\mathcal{M}_G) + 1.$$

In particular, the secant variety has the expected dimension.

Why do we care?

- This means the parameters are "as identifiable as possible"
- In other words, they can be identified to the same extent as they can be for the log-linear model

Proof Strategy: Slicing Point Configurations

Theorem (Theorem 2.3, Draisma 2008)

- *Let* V_A *be the toric variety specified by integer matrix* $A \in \mathbb{Z}^{d \times n}$.
- *Let* $\mathbf{v} \in (\mathbb{R}^d)^*$.
- *Let* A_+ *denote the columns of* A *such that* $\mathbf{v} \cdot \mathbf{a} > 0$.
- *Similarly,* A_- *consists of the columns of* A *such that* $\mathbf{v} \cdot \mathbf{a} < 0$.

Then

$$\dim\big(\mathrm{Sec}^2(V_A)\big) \geq \mathrm{rank}(A_+) + \mathrm{rank}(A_-) - 1.$$

In particular, if we can separate the vertices of conv(A) with a hyperplane so that the columns on either side have full rank, then the secant has the expected dimension.

Proof Strategy

Graphs with three maximal cliques:

- we show that we can extend a hyperplane normal $\mathbf{v}$ for G to $\mathbf{v}'$ for G' when G' is obtained by:
  - adding a vertex without changing the clique structure, or
  - increasing d_v by 1 for some vertex v.
- Any such graph can be obtained from P_4 or $P_3 \sqcup P_1$ by a sequence of these operations, so we find hyperplanes for these two graphs.

Graphs with more than three maximal cliques:

- Find a separating hyperplane for a subgraph with three cliques
- Show that extending by zeros on the rest of the graph gives a separating hyperplane for all of G

Future Work

Conjecture (A.-Coons-Sturma, 2024)

If G is **any** *graph that is not a clique star with $d_v \geq 2$ for all $v \in V$, then its second mixture has the expected dimension.*

Question

Draisma's theorem can also be applied when

- we take r-mixtures for arbitrary r and/or
- we take mixtures of several different graphs (join varieties).

What happens then?

Question

Dimensions of mixtures of your favorite log-linear model?

Acknowledgements

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- Applied Algebra Seminar organizers,
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