Mixtures of Discrete Decomposable Graphical Models

Yulia Alexandr (UCLA)

joint work with Jane Ivy Coons and Nils Sturma

AMS Sectional Meeting
California Polytechnic, San Luis Obispo, CA
May 3, 2025

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)
⋆ $\boxed{\textit{computational biology}}$ (protein interaction networks)
⋆ $\boxed{\textit{phylogenetics}}$ (gene trees)
⋆ economics (dependencies between financial entities)
⋆ computer vision (image structures and relationships within scenes)

Undirected Graphical Models

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

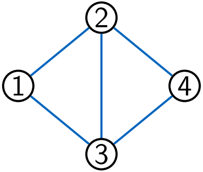
The graph G specifies dependencies between random variables.

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:



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

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 $d_A := \#\mathcal{R}_A = \prod_{v \in A} d_v$.

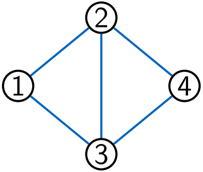
Definition

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

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

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

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.

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

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

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

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

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

$I^{(r)}_{j_C; A \perp\!\!\!\perp B}$ = 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?

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:

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

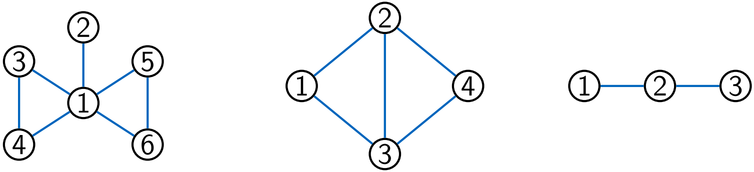
Shout-out: `MultigradedImplicitization.m2` by Joe Cummings and Ben Hollering

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 $C_i = \widetilde{C}_i \setminus S$.

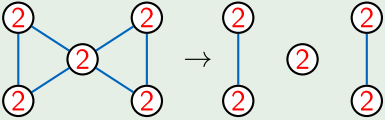
Examples:



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



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

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

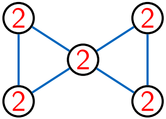
Theorem (A.-Coons-Sturma, 2024)

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.

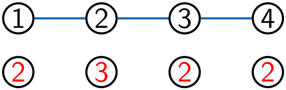
Question: Are the secants of $\mathcal{M}_{P_n}$ defective for $n > 3$?

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 $n > 3$? **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

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?