Algebraic Geometry of Quantum Graphical Models

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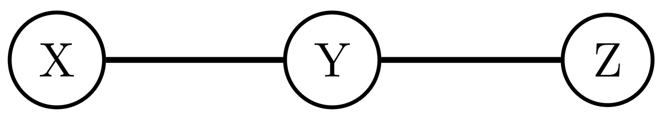
(Classical) Graphical Models

In a (classical) graphical model, a graph encodes conditional independence statements between random variables represented by the nodes. Example: the 3-chain graph



encodes the statement $X \perp\!\!\!\perp Z \mid Y$. For binary random variables X, Y and Z, this defines a statistical model described by the algebraic variety

$$\mathcal{M}_G = \mathcal{V}(p_{001}p_{100} - p_{000}p_{101}, p_{011}p_{110} - p_{010}p_{111}) \subseteq \mathbb{P}^7_{p_{ijk}}.$$

Goal

Our goal is to associate algebraic varieties to quantum graphical models. We propose three such varieties:

- Quantum conditional mutual information (QCMI) varieties
- Petz varieties
- Gibbs varieties from families of Hamiltonians

In each of these cases, one recovers the classical graphical model when restricting to diagonal quantum states.

Hammersley–Clifford Theorem

- **Classical [3]:** A probability distribution $p > 0$ satisfies the pairwise Markov property on a graph G if and only if it factors as a product of potential functions, each depending only on a clique of G:

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

- **Quantum [4]:** Let $G = (V, E)$ be a tree and let $\rho > 0$ be a quantum state satisfying $I(v_i : v_k \mid v_j) = 0$ for all $(v_i, v_j, v_k) \in V^3$ such that v_j separates v_i from v_k in G. Then ρ is the exponential of a sum of local commuting Hamiltonians:

$$\rho = \exp(H) \quad \text{with} \quad H = \sum_{C \in \mathcal{C}(G)} h_C, \quad [h_C, h_{C'}] = 0 \ \forall C, C' \in \mathcal{C}(G).$$

Gibbs Varieties from Hamiltonians

- **Definition.** Let $X \subseteq \mathbb{S}^n$ be a unirational variety of $n \times n$ symmetric matrices. Its Gibbs manifold is $\mathrm{GM}(X) := \exp(X)$, the Gibbs variety $\mathrm{GV}(X)$ is the Zariski closure $\mathrm{GV}(X) := \overline{\mathrm{GM}(X)} \subseteq \mathbb{S}^n$.
- In general, sums of local commuting Hamiltonians do not form a unirational variety. However, one can consider suitable subsets, e.g. sums of local decomposable tensors $X_G := \sum_{C \in \mathcal{C}(G)} X_C$.

Quantum Information Projection

- Let $\mathcal{Q}$ be a family of quantum states. Given an arbitrary state ρ, what is the state $\tilde{\rho} \in \mathcal{Q}$ "closest" to ρ? (Analogue of MLE)

Definition. The quantum relative entropy is

$$D(\rho \| \sigma) := \begin{cases} \mathrm{tr}(\rho(\log(\rho) - \log(\sigma))) & \text{if } \mathrm{supp}(\rho) \subseteq \mathrm{supp}(\sigma) \\ +\infty & \text{otherwise.} \end{cases}$$

Definition. The quantum information projection of ρ to $\mathcal{Q}$ is

$$\tilde{\rho} := \underset{\rho' \in \mathcal{Q}}{\operatorname{argmin}} \ D(\rho \| \rho').$$

Theorem. Let $\mathfrak{H} = \langle H_1, \dots, H_k \rangle \subseteq \mathbb{S}^d_{\mathbb{R}}$ be a span of commuting Hamiltonians, fix $\rho \in \mathbb{S}^d_{\mathbb{R}}$, $\rho > 0$, and let $b_i := \mathrm{tr}(H_i \rho)$ for $i = 1, \dots, k$. Let $M_\rho := \{A \in \mathbb{S}^d_{\mathbb{R}} \mid \langle H_i, A \rangle = b_i \text{ for } i = 1, \dots, k\}$. Then $M_\rho \cap \mathrm{GM}(\mathfrak{H})$ consists of a unique point ρ^*. It is the maximiser of the von Neumann entropy inside M_ρ and the quantum information projection of ρ to $\mathrm{GM}(\mathfrak{H})$. (Analogue of Birch's Theorem)

Quantum Information Theory Basics

- A quantum state on N qudits is represented by a unit length vector $|\psi\rangle \in \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N$, $\quad \mathcal{H}_i \cong \mathbb{C}^d$.
- An ensemble of quantum states is a collection $\{p_i, |\psi_i\rangle\}_i$, where $\{p_i\}_i$ is a discrete probability distribution. It is described by its density matrix

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \in \mathrm{End}(\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N).$$

We think of quantum states as real positive-semidefinite matrices with trace one.

- The partial trace is an operation to obtain the state of a subsystem from the state of a multipartite system, analogous to marginalisation in statistics. For a bipartite state ρ_{AB} on $\mathcal{H}_A \otimes \mathcal{H}_B$, it is defined on elementary tensors via

$$\mathrm{tr}_B(|a_i\rangle\langle a_j| \otimes |b_k\rangle\langle b_l|) := |a_i\rangle\langle a_j| \cdot \mathrm{tr}(|b_k\rangle\langle b_l|) = |a_i\rangle\langle a_j| \cdot \langle b_l \mid b_k\rangle$$

and is extended linearly. We write $\rho_A := \mathrm{tr}_B \, \rho_{AB}$; this is a quantum state on $\mathcal{H}_A$.

Quantum Conditional Mutual Information Variety

- **Definition.** The von Neumann entropy $S(\rho)$ of a quantum state ρ is $S(\rho) := -\mathrm{tr}(\rho \log \rho)$.
- **Definition.** For a tripartite state ρ_{ABC}, the quantum conditional mutual information (QCMI) between A and C given B is

$$I(A{:}C \mid B) := S(\rho_{AB}) + S(\rho_{BC}) - S(\rho_{ABC}) - S(\rho_B).$$

The vanishing $I(A{:}C \mid B) = 0$ is analogous to classical conditional independence $A \perp\!\!\!\perp C \mid B$.

- **Theorem [2].** A state ρ_{ABC} satisfies $I(A{:}C \mid B) = 0$ if and only if it admits a factorisation

$$\rho_{ABC} = \Lambda_{AB}\Lambda_{BC} \quad \text{with} \quad [\Lambda_{AB}, \Lambda_{BC}] = 0,$$

where $\Lambda_{AB}, \Lambda_{BC}$ are symmetric matrices acting nontrivially only on $\mathcal{H}_A \otimes \mathcal{H}_B$ resp. $\mathcal{H}_B \otimes \mathcal{H}_C$.

Construction. Let $G = (V = \{S_1, \dots, S_N\}, E)$ be a tree.

- For each triple of vertices (S_i, S_j, S_k) such that S_j separates S_i and S_k in G, impose the QCMI statement

$$\mathrm{tr}_{V \setminus \{S_i, S_j, S_k\}} \rho_V = \Lambda_{S_i S_j} \Lambda_{S_j S_k} \text{ with } \left[\Lambda_{S_i S_j}, \Lambda_{S_j S_k}\right] = 0.$$

- For any two QCMI statements $I(S_i : S_k \mid S_j) = I(S_{i'} : S_{k'} \mid S_{j'}) = 0$, impose compatibility constraints

$$\mathrm{tr}_{\mathcal{T} \setminus (\mathcal{T} \cap \mathcal{T}')} \rho_{\mathcal{T}} = \mathrm{tr}_{\mathcal{T}' \setminus (\mathcal{T} \cap \mathcal{T}')} \rho_{\mathcal{T}'} \quad \text{where} \quad \mathcal{T} = (S_i, S_j, S_k), \ \mathcal{T}' = (S_{i'}, S_{j'}, S_{k'}).$$

- Via elimination of the Λ parameters, this gives rise to a variety, the QCMI variety.

Petz Variety

- The Petz recovery map for the 3-chain graph is

$$\mathcal{R}(\rho_{AB}, \rho_{BC}) = (\rho_{AB}^{1/2} \otimes \mathrm{Id}_C)(\mathrm{Id}_A \otimes \rho_B^{-1/2} \otimes \mathrm{Id}_C)(\mathrm{Id}_A \otimes \rho_{BC})(\mathrm{Id}_A \otimes \rho_B^{-1/2} \otimes \mathrm{Id}_C)(\rho_{AB}^{1/2} \otimes \mathrm{Id}_C);$$

it recovers a state ρ_{ABC} satisfying $I(A : C \mid B) = 0$ from two compatible two-body marginals.

- Let $V = \{(X, Y, Z) \in \mathbb{S}^4_{\mathbb{R}} \times \mathbb{S}^4_{\mathbb{R}} \times \mathbb{S}^2_{\mathbb{R}} \mid \mathrm{tr}_A(X^2) = \mathrm{tr}_C(Y^2) = Z^2\}$; then define the rational Petz map

$$R : V \dashrightarrow \mathbb{S}^8_{\mathbb{R}}, \quad (x, y, z) \mapsto (x \otimes \mathrm{Id}_C)(\mathrm{Id}_A \otimes z^{-1} \otimes \mathrm{Id}_C)(\mathrm{Id}_A \otimes y)(\mathrm{Id}_A \otimes z^{-1} \otimes \mathrm{Id}_C)(x \otimes \mathrm{Id}_C).$$

- This map can be generalised to arbitrary trees G by iteratively applying the procedure for 3-chains of G.
- **Definition.** The Petz variety is the Zariski closure of R. It is an irreducible variety.

Example: 3-chain Graph

Let G be the 3-chain graph and consider the qubit case, i.e. $\mathcal{H}_i \cong \mathbb{C}^2$ for $i = 1, 2, 3$.

- The QCMI variety of G is an irreducible, 12-dimensional variety inside $\mathbb{S}^8$ of degree 110, cut out by 735 equations in degrees one to five.
- For $X_G = \{K \otimes L \otimes \mathrm{Id}_2 + \mathrm{Id}_2 \otimes M \otimes N \mid K, L, M, N \in \mathbb{S}^2\}$, the Gibbs variety $\mathrm{GV}(X_G) \subseteq \mathbb{S}^8$ is an irreducible, 14-dimensional variety cut out by nine linear forms and 66 quadratic equations with coefficients ± 1.

References

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