Geometry of Marginals of Small Quantum Systems

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Abstract

We discuss two basic problems of marginals of small quantum systems. We then present new methods for the analysis of quantum marginals and indicate how the methods could be extended to Boson or Fermion density matrices.

While quantum marginals are in the focus of computationally hard problems of quantum chemistry, basic questions about small systems are already hard to understand. For example, Werner [1] used Bell's inequalities to show that two two-qubit states coinciding in one of their one-qubit marginals may not be the marginals of a three-qubit state. Another example is the discovery of a six-qubit pure state uniquely determined by its two-body marginals which is not the unique ground state of a two-local Hamiltonian [2]. Towards a systematic analysis of marginals, we show how to analyze the lattice of exposed faces (intersections with supporting hyperplanes) employing an algebraic characterization [3], and we explain some recent results obtained for three qubits. Finally, we indicate how the methods could be extended to Boson or Fermion density matrices using the projection onto the symmetric or anti-symmetric subspace.

[1] Reinhard F. Werner, *An application of Bell's inequalities to a quantum state extension problem*, Letters in Mathematical Physics **17** (1989), 359-363.

[2] Salini Karuvade et al., *Uniquely determined pure quantum states need not be unique ground states of quasi-local Hamiltonians*, Physical Review A **99** (2019), 062104.

[3] S. W., *A variational principle for ground spaces*, Reports on Mathematical Physics **82** (2018), 317-336.

PART I. Introduction to Marginal Problems

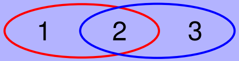
Subsystems of a Many-Body System

Definition

We consider a many-body system of N units. A family of subsets $\mathfrak{g}$ of $\{1, \ldots, N\}$ denotes a family of subsystems. If we compare different subsystems we choose an ordering on the subsets.

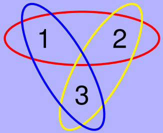
Examples *(Families of Subsystems)*

1) Path graph on three nodes $\mathfrak{g} = \{\{1, 2\}, \{2, 3\}\}$



The ordering $\mathfrak{g} = \{(2, 1), (2, 3)\}$ will be convenient.

2) Complete graph on three nodes $\mathfrak{g} = \{\{1, 2\}, \{2, 3\}, \{3, 1\}\}$



Algebra of a Quantum System

Definition

- Let M_d denote the set of complex $d \times d$ matrices. Let $\mathcal{A} \subset M_d$ be a *-subalgebra with the inner product $\langle A, B \rangle = \mathrm{tr}(A^* B)$, $A, B \in \mathcal{A}$.
- The state space of $\mathcal{A}$ comprises the positive semi-definite matrices of trace one, called states or density matrices,

$$\mathcal{D}(\mathcal{A}) = \{\rho \in \mathcal{A} : \rho \succeq 0, \mathrm{tr}(\rho) = 1\}.$$

- A state $\rho \in \mathcal{D}(\mathcal{A})$ is a pure state if and only if ρ is an extreme point of $\mathcal{D}(\mathcal{A})$ if and only if ρ lies on no open segment in $\mathcal{D}(\mathcal{A})$.

Examples

- Given a projection $P = P^2 = P^*$ in $\mathcal{A}$, we shall consider the *-algebra $P\mathcal{A}P = \{PAP : A \in \mathcal{A}\}$ with multiplicative identity P.
- The pure states of $\mathcal{D}(M_d)$ are the projections of rank one.
- We identify $\mathbb{C}^d \subset M_d$ with the diagonal matrices. The state space $\mathcal{D}(\mathbb{C}^d)$ is the simplex of probability distributions on $\{1, \ldots, d\}$.

Marginals of a Quantum Many-Body System

Definition

- Let $\mathfrak{a} = (\mathcal{A}_1, \ldots, \mathcal{A}_N)$ be a sequence of *-algebras $\mathcal{A}_i \subset M_{d_i}$, $i = 1, \ldots, N$. Let $\nu \subset \{1, \ldots, N\}$. The *-algebra of the subsystem with units in ν is the tensor product $\mathcal{A}_\nu := \bigotimes_{i \in \nu} \mathcal{A}_i$. We denote the multiplicative identity of $\mathcal{A}_\nu$ by $\mathbb{1}_\nu$ and write $\mathcal{A} = \mathcal{A}_{\{1,\ldots,N\}}$.
- Let $\mu \subset \nu$. The partial trace $\mathrm{tr}_{\nu\setminus\mu} : \mathcal{A}_\nu \to \mathcal{A}_\mu$ over the subsystem $\nu \setminus \mu$ is the hermitian adjoint to $\mathcal{A}_\mu \to \mathcal{A}_\nu$, $A \mapsto A \otimes \mathbb{1}_{\nu\setminus\mu}$. The state $\rho_\mu = \mathrm{tr}_{\nu\setminus\mu}(\rho) \in \mathcal{D}(\mathcal{A}_\mu)$ is called the μ-marginal ρ_μ of $\rho \in \mathcal{D}(\mathcal{A}_\nu)$.
- Let $\bar{\nu} = \{1, \ldots, N\} \setminus \nu$. The marginal map with respect to the algebras $\mathfrak{a}$ and the subsystems $\mathfrak{g}$ is

$$\mathrm{mar}_{(\mathfrak{a},\mathfrak{g})} : \quad \mathcal{A} \to \bigtimes_{\nu \in \mathfrak{g}} \mathcal{A}_\nu, \qquad A \mapsto (\mathrm{tr}_{\bar{\nu}}(A))_{\nu \in \mathfrak{g}}.$$

  The marginal set $\mathrm{mar}_{(\mathfrak{a},\mathfrak{g})}(\mathcal{D}(\mathcal{A}))$ is also known as the set of reduced density matrices (Erdahl 1972, Zeng et al. 2019).

- Robert M. Erdahl, JMP **13** (1972), 1608–1621.
- Bei Zeng et al., Quantum Information Meets Quantum Matter, New York: Springer, 2019.

Marginal Problems

Definition

Let $\mathcal{D}(\mathfrak{a},\mathfrak{g}) = \bigtimes_{\nu\in\mathfrak{g}} \mathcal{D}(\mathcal{A}_\nu)$ denote the set of families of states on the subsystems specified by $\mathfrak{g}$. The marginal problem is the task to decide whether a family $\rho(\nu)_{\nu\in\mathfrak{g}} \in \mathcal{D}(\mathfrak{a},\mathfrak{g})$ lies in the marginal set, that is to say, whether there is $\sigma \in \mathcal{D}(\mathcal{A})$ such that $\rho(\nu)_{\nu\in\mathfrak{g}} = \mathrm{mar}_{(\mathfrak{a},\mathfrak{g})}(\sigma)$, or equivalently, such that $\rho(\nu) = \sigma_\nu$ for all $\nu \in \mathfrak{g}$.

Physicists have studied various restrictions of the marginal problem.

Definition

Let $P \in \mathcal{A}$ be a projection. We call P-restricted marginal problem the task to decide whether a family $\rho(\nu)_{\nu\in\mathfrak{g}} \in \mathcal{D}(\mathfrak{a},\mathfrak{g})$ is the family of marginals of a state in $\mathcal{D}(P\mathcal{A}P)$, that is to say, whether there is $\sigma \in \mathcal{D}(P\mathcal{A}P)$ such that $\rho(\nu)_{\nu\in\mathfrak{g}} = \mathrm{mar}_{(\mathfrak{a},\mathfrak{g})}(\sigma)$.

Examples: Symmetrization $P_S : (\mathbb{C}^d)^{\otimes r} \to (\mathbb{C}^d)^{\otimes r}$, $v \mapsto \frac{1}{N!}\sum_{\pi\in S_N} \pi(v)$

Antisymmetrization $P_A : (\mathbb{C}^d)^{\otimes r} \to (\mathbb{C}^d)^{\otimes r}$, $v \mapsto \frac{1}{N!}\sum_{\pi\in S_N} \mathrm{sgn}(\pi)\pi(v)$

Examples of Marginal Problems

Theorem *(1-Body N-Representability Problem)*

This is the P_A-restricted marginal problem for $\mathcal{A}_i = M_d$, $i = 1, \dots, N$, and for $\mathfrak{g} = \{\{1\}\}$. The states in $\mathcal{D}(P_A \mathcal{A} P_A)$ are called Fermion states. It has been shown in Quantum Chemistry in the 1960's that a one-body state $\rho \in \mathcal{D}(M_d)$ lies in the marginal set $\operatorname{mar}_{(\mathfrak{a},\mathfrak{g})}(\mathcal{D}(P_A \mathcal{A} P_A))$, if and only if all eigenvalues of ρ are less than or equal to $1/N$. (Schur-Horn orbitope)

Most marginal problems are difficult to solve (for exceptions see, e.g., Klyachko 2006). A necessary condition for $\rho(\nu)_{\nu \in \mathfrak{g}} \in \mathcal{D}(\mathfrak{a}, \mathfrak{g})$ to lie in the marginal set is that $\rho(\nu)_{\nu \in \mathfrak{g}}$ is compatible in the sense that for all $\mu, \nu \in \mathfrak{g}$ we have $\rho(\mu)_{\mu \cap \nu} = \rho(\nu)_{\mu \cap \nu}$.

Theorem

Let $\mathfrak{a} = (\mathbb{C}^{d_1}, \dots, \mathbb{C}^{d_N})$ and let $\mathfrak{g}$ be the set of edges of a graph without cycles on the nodes $\{1, \dots, N\}$. Then $\rho(\nu)_{\nu \in \mathfrak{g}} \in \mathcal{D}(\mathfrak{a}, \mathfrak{g})$ lies in the marginal polytope $\operatorname{mar}_{(\mathfrak{a},\mathfrak{g})}(\mathcal{D}(\mathcal{A}))$ if and only if $\rho(\nu)_{\nu \in \mathfrak{g}}$ is compatible.

A Pair of Overlapping Two-Qubit States

Note *(Zeng et al. 2019)*

Marginal problem of $\mathfrak{a} = (M_2, M_2, M_2)$, $\mathfrak{g} = \{(2,1),(2,3)\}$ is still open.

Partial results:

Theorem *(Bell-Inequalities, Werner 1989)*

If $\rho \in \mathcal{D}(M_2 \otimes M_2)$ and $(\rho, \rho) \in \mathrm{mar}_{(\mathfrak{a},\mathfrak{g})}(\mathcal{D}(\mathcal{A}))$, then for all $A_i, B_i \in \mathcal{H}(M_2)$, $i \in \{0,1\}$, of operator norm at most one we have

$$\mathrm{tr}\left(\rho(A_0 \otimes B_0 + A_0 \otimes B_1 + A_1 \otimes B_0 - A_1 \otimes B_1)\right) \leq \sqrt{6}.$$

The maximum of the LHS is $\sqrt{8}$ without the condition $(\rho, \rho) \in \mathrm{mar}_{(\mathfrak{a},\mathfrak{g})}(\mathcal{D}(\mathcal{A}))$.

Theorem *(Symmetric Extension Problem, Chen et. al 2014)*

If $\rho \in \mathcal{D}(\mathcal{A}_{\{2,1\}})$ then $(\rho, \rho) \in \mathrm{mar}_{(\mathfrak{a},\mathfrak{g})}(\mathcal{D}(\mathcal{A}))$ if and only if

$$\mathrm{tr}(\rho_{\{1\}}^2) \geq \mathrm{tr}(\rho^2) - 4\sqrt{\det \rho}.$$

Jianxin Chen, et al., *Symmetric extension of two-qubit states*, PRA **90** (2014), 032318.

PART II. Lattices of Ground Projections

Local Hamiltonians

Definition

- The space of local Hamiltonians with respect to the algebras $\mathfrak{a}$ and with interactions specified by a family $\mathfrak{g}$ of subsets of $\{1, \ldots, N\}$ is

$$U_{(\mathfrak{a},\mathfrak{g})} = \left\{ \sum_{\nu \in \mathfrak{g}} A(\nu) \otimes \mathbb{1}_{\bar{\nu}} : A(\nu) \in \mathcal{H}(\mathcal{A}_\nu), \nu \in \mathfrak{g} \right\}.$$

- We endow the (real) vector space $\mathcal{H}(\mathcal{A})$ of the hermitian matrices in $\mathcal{A}$ with the scalar product $\langle A, B \rangle = \mathrm{tr}(AB)$, $A, B \in \mathcal{H}(\mathcal{A})$.
- Let $\pi_U : \mathcal{H}(\mathcal{A}) \to \mathcal{H}(\mathcal{A})$ be the orthogonal projection to a subspace $U \subset \mathcal{H}(\mathcal{A})$. We call $W(U) = \pi_U(\mathcal{D}(\mathcal{A}))$ the numerical range of U.

Lemma

The marginal map factors through $\mathbb{C}U_{(\mathfrak{a},\mathfrak{g})}$ and restricts to the linear isomorphism $W(U_{(\mathfrak{a},\mathfrak{g})}) \xrightarrow{\mathrm{mar}_{(\mathfrak{a},\mathfrak{g})}} \mathrm{mar}_{(\mathfrak{a},\mathfrak{g})}(\mathcal{D}(\mathcal{A}))$ onto the marginal set.

Idea: Study the geometry of numerical ranges of subspaces $U \subset \mathcal{H}(\mathcal{A})$.

Pure State Quantum Tomography

Definition

- A state $\rho \in \mathcal{D}(\mathcal{A})$ is uniquely determined among all states (UDA) with respect to U if for all $\sigma \in \mathcal{D}(\mathcal{A})$ the equality $\pi_U(\sigma) = \pi_U(\rho)$ implies $\sigma = \rho$.
- The ground projection of $A \in \mathcal{H}(\mathcal{A})$ is the spectral projection of A corresponding to the smallest eigenvalue.
- A state $\rho \in \mathcal{D}(\mathcal{A})$ is the unique ground state (UGS) of $A \in \mathcal{H}(\mathcal{A})$ if ρ is the ground projection of A. A state $\rho \in \mathcal{D}(\mathcal{A})$ is a UGS of U if ρ is the UGS of a matrix in U.

Lemma

- If $\rho \in \mathcal{D}(\mathcal{A})$ is a UGS of U, then ρ is *UDA* with respect to U.
- If a pure state $\rho \in \mathcal{D}(\mathcal{A})$ is UDA with respect to U then $\pi_U(\rho)$ is an extreme point of the numerical range $W(U)$.
- If $\rho \in \mathcal{D}(\mathcal{A})$ is the UGS of $A \in U$ then $B = \pi_U(\rho)$ is an exposed point of $W(U)$. In fact, $\pi_U(\rho) = \operatorname{argmin}_{B \in W(U)} \langle A, B \rangle$.

Tomography From Quantum Marginals

Question *(Chen et al. 2012)*

Is there a pure state that is UDA with respect to $U_{(\mathfrak{a},\mathfrak{g})}$ and that is not a UGS of $U_{(\mathfrak{a},\mathfrak{g})}$? Does the numerical range $W(U_{(\mathfrak{a},\mathfrak{g})})$ have a non-exposed point?

Jianxin Chen, et al., *Comment on some results of Erdahl and the convex structure of reduced density matrices*, Journal of Mathematical Physics **53** (2012), 072203.

Theorem *(Karuvade et al. 2019)*

Consider a six-qubit system with two-local interactions, that is to say, $\mathfrak{a} = (M_2, M_2, M_2, M_2, M_2, M_2)$ and $\mathfrak{g}$ consists of the two-element subsets of $\{1, \ldots, 6\}$. Then there exists a pure state that is UDA with respect to $U_{(\mathfrak{a},\mathfrak{g})}$ and that is not a UGS of $U_{(\mathfrak{a},\mathfrak{g})}$.

Idea: a) Study the exposed faces of the numerical range $W(U_{(\mathfrak{a},\mathfrak{g})})$.
b) Find non-exposed points of $W(U_{(\mathfrak{a},\mathfrak{g})})$ for systems with less than six qubits.

Lattices of Exposed Faces

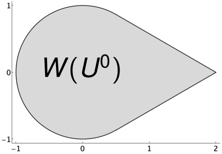
Definition

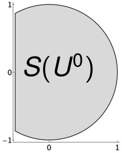
- Let $\mathbb{1} \in U$ and put $U^0 = U \cap \mathbb{1}^\perp = \{A \in U : \mathrm{tr}(A) = 0\}$.
- Spectrahedron $S(U^0) = \{A \in U^0 : \mathbb{1} + A \succeq 0\}$.
- An exposed face of a convex set $C \subset U^0$ has the form $\mathrm{argmin}_{B \in C} \langle A, B \rangle$ for some $A \in U^0$. Let $\mathcal{F}(C)$ denote the set of exposed faces.
- Let $\mathcal{P}(U)$ denote the set of ground projections of matrices in U.

Theorem

- $S(U^0)$ is the polar convex set to the numerical range $W(U^0)$.
- There are lattice isomorphisms $\mathcal{P}(U) \to \mathcal{F}(W(U^0)) \to \mathcal{F}(S(U^0))$, $P \mapsto \pi_{U^0}(\mathcal{D}(P\mathcal{A}p))$, $F \mapsto$ (inner normal cone of F) $\cap\, \partial S(U^0)$.

Example:





Lattice of Ground Projections

Definition

A coatom of a lattice $\mathcal{L}$ with greatest element 1 is a maximal element of $\mathcal{L}\setminus\{1\}$. $\mathcal{L}$ is coatomistic if any element is the infimum of a set of coatoms.

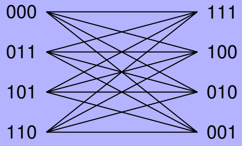
Theorem *(W. 2018)*

- The lattices $\mathcal{P}(U) = \mathcal{F}(W(U^0))$ are coatomistic.
- A projection $P \in \mathcal{P}(U)$ is a coatom if and only if $P'\mathcal{A}^+P' \cap U$ is a ray. Thereby, $\mathcal{A}^+$ is the cone of positive semi-definite matrices in $\mathcal{A}$.

Commutative Example

2-local 3-bit Hamiltonians: $\mathfrak{a} = (\mathbb{C}^2, \mathbb{C}^2, \mathbb{C}^2)$, $\mathfrak{g} = \{\{1,2\},\{2,3\},\{3,1\}\}$.

The coatoms of $\mathcal{P}(U_{(\mathfrak{a},\mathfrak{g})})$ all have rank six. They are the complements of the edges in the complete bipartite graph with vertices $\{0,1\}^{\times 3}$, the bipartition being defined by the even resp. odd number of 1's.



Three Qubits

Let $\mathfrak{a} = (M_2, M_2, M_2)$ and $\mathfrak{g} = \big\{\{1,2\},\{2,3\},\{3,1\}\big\}$.

Lemma

The lattice $\mathcal{P}(U_{(\mathfrak{a},\mathfrak{g})})$ has no coatom of rank seven.

The lattice isomorphism $\mathcal{F}(W(U^0)) \cong \mathcal{F}(S(U^0))$ is antitone. The coatoms of $\mathcal{P}(U)$ are in one-to-one correspondence with the exposed points of $S(U^0)$.

Experimental Maths

The exposed points of the spectrahedron $S(U^0)$ can be explored numerically using semi-definite programming. Candidates can be verified using the preceding theorem.

Example *(Coatom of Rank Five)*

Kernel projection of $6III + 3IIZ + IZI + 2ZII + 4IZX - 4ZIX + 3ZIZ - 3ZZI$

Indistinguishable Particles

In principle, the algebraic approach works also for quantum marginals of bosonic and fermionic states.

Lemma

Let $P \in \mathcal{A}$ be a projection and $U \subset \mathcal{H}(\mathcal{A})$ a vector space of hermitian matrices. Then $\pi_U|_{\mathcal{H}(P\mathcal{A}P)}$ factors through PUP and restricts to the linear isomorphism $W(PUP) = \pi_{PUP}(\mathcal{D}(P\mathcal{A}P)) \xrightarrow{\pi_U} \pi_U(\mathcal{D}(P\mathcal{A}P))$.

S. W., *Quantum convex support*, Linear Algebra and its Applications **435** (2011), 3168–3188.

Observation: The P-restricted marginal problem is equivalent to the membership problem of the numerical range $W(PUP)$.

Study the membership problem of the numerical range $W(PUP)$ where $P = P_S$ is the symmetrization (resp. $P = P_A$ is the antisymmetrization) and $U = U_{(\mathfrak{a},\mathfrak{g})}$ is a space of local Hamiltonians.

Gracias por su atención!

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