The Quantum Marginal Problem

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This paper aims to give a brief introduction to the quantum marginal problem. It provides an overview of several important results and a bibliography for more in-depth reading.

INTRODUCTION: A CLASSICAL ANALOGY

Given a multivariate probability distribution, we can easily compute marginal distributions in one or more of its variables. The reverse process - given a set of (putative) marginal distributions, to find a joint distribution having such margins - is known as the classical marginal problem. In general it is not easy. For marginals involving two or more variables such a distribution does not necessarily exist; thus one part of the problem is determining compatibility conditions that will guarantee the existence of a solution. When such conditions are met we may ask the nontrivial question, "is the solution unique?" - and, if the answer is "no" we can try to describe all possible joint distributions having the given marginals, and to determine whether there exists a solution having specific properties (e.g.: in the discrete case, a joint distribution whose entries are multiples of a given fraction).

THE QUANTUM MARGINAL PROBLEM

This problem has a close quantum mechanical analog. Given a multi-component system in a pure state we can take partial traces to find density matrices for the states of subsystems of one or more components. The pure quantum marginal problem consists of "reverse engineering" this: i.e., determining whether a given set of density matrices is the set of "marginals" (partial traces) of some larger, global pure state density matrix. A variant of this problem asks the question for a global matrix with a given spectrum (i.e., not necessarily pure - which would have the spectrum (1,0,...,0) - but having some prescribed mixed state). Yet another variant is the question of whether a system with a given number of components has an absolutely maximally entangled (AME) state (pure global state such that any bipartition is maximally entangled - i.e., having maximally mixed marginals). Naturally, when a solution exists there are the questions about how to construct it and whether or not it is unique.[1]

These questions have practical applications in quantum chemistry, condensed matter physics, and quantum error-correcting codes.[2,3,4]

In the broadest sense, both the classical and quantum marginal problems are concerned with using information about parts of a system to deduce some of its global properties .

As with the classical case, the quantum marginal problem is more difficult than the reverse process of computing marginals. A natural first question is whether the problem lends itself to a brute force computational approach. For small systems (say, two or three qubits) or special cases this might work; however,in general the problem is known to be computationally hard, making this approach not feasible. (In fact, it has been shown that the problem remains computationally hard even for a quantum computer.)[5] Thus we have to resort to cleverness.

SOME KNOWN RESULTS

Compatibility conditions (i.e., necessary conditions for a set of putative marginals to correspond to a global state matrix with given properties) typically take the form of inequalities involving eigenvalues or functions thereof. This is intuitive: given a set of marginals compatible with a particular global state, one would expect that slightly perturbing the eigenvalues of the marginal and global matrices would preserve compatibility(at least in some directions of perturbation), and so the problem boils down to determining boundaries beyond which the compatibility no longer holds.

For bivariate marginals, strong subadditivity of the von Neumann entropy [6] gives a compatibility constraint:

$$S(\rho_{ABC}) \leq S(\rho_{AB}) + S(\rho_{BC}) - S(\rho_B).$$

(Note that although this is a necessary condition, it is by no means necessarily sufficient!)

A few basic results can be deduced from facts about tensor products:

1) For a pure state $\psi \in \mathcal{H}_A \otimes \mathcal{H}_B$ the marginals ρ_A and ρ_B have the same spectra (up to having more or fewer zero eigenvalues when $\mathcal{H}_A$ and $\mathcal{H}_B$ have different dimensions). Conversely, if ρ_A and ρ_B have the same spectra (again, up to more/fewer zeros), then a pure state with marginals ρ_A and ρ_B exists and is given by $\psi = \sum_i \lambda_i \alpha_i \otimes \beta_i$, where α_i and β_i are the respective eigenbasis vectors of ρ_A and ρ_B with eigenvalue λ_i (this is the Schmidt decomposition).

2) In the univariate marginal case (i.e., when the given local density matrices describe non-overlapping components) the existence of a global state with a given spectrum depends only on the spectra of the local density matrices, since these can be diagonalized by local unitaries. In particular, to answer the question whether an n-qubit system with given density matrices for each qubit could have a (global) density matrix with a given spectrum, we need only concern ourselves with the compatibility of the global spectrum with the local (individual qubit) spectra.

In 2004 Klyachko solved the compatibility problem for a multi-component system with given global state spectrum and univariate marginals. Prior to this there were several partial results, e.g.:

Theorem (Higuchi et al. [7] Bravyi [8])
A pure n-qubit state with univariate margins ρ_i exists iff their minimal eigenvalues λ_i satisfy the inequalities

$$\lambda_i \leq \sum_{j \neq i} \lambda_j.$$

Theorem (Bravyi [8])
A mixed two-qubit state ρ_{AB} with spectrum $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ and marginals ρ_A, ρ_B exists iff the minimal eigenvalues λ_A, λ_B of these marginals satisfy the inequalities

$$\lambda_A \geq \lambda_3 + \lambda_4, \quad \lambda_B \geq \lambda_3 + \lambda_4$$

$$\lambda_A + \lambda_B \geq \lambda_2 + \lambda_3 + 2\lambda_4$$

$$|\lambda_A - \lambda_B| \leq min\{\lambda_1 - \lambda_3, \lambda_2 - \lambda_4\}.$$

Higuchi [9] established conditions for compatibility of a pure state $\psi \in \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ with marginals ρ_A, ρ_B, and ρ_C. These conditions take the form of 7 inequalities (up to permutation of A, B, and C).

The significance of Klyachko's 2004 paper is that it established a "general recipe for producing marginal inequalities" for these kinds of systems. As an appendix, it includes 19 pages (!) of inequalities giving compatibility requirements for some of the smaller systems (3 qubits, 4 qubits, 2 qutrits, etc).

The paper presents two methods of approach, one involving algebraic geometry and the other representation theory of symmetric groups. The gist of the first approach is, for a 2-component system, to consider the set of possible spectra a and b of Hermitian matrices on the two components $\mathcal{H}_A$ and $\mathcal{H}_B$, taken modulo an equivalence relation (preserving ordering of sums of their eigenvalues); partition the resulting space into "cubicles" and "edges", and establish that a mixed state ρ_{AB} with margins ρ_A and ρ_B exists if and only if the spectra of ρ_{AB}, ρ_A, and ρ_B satisfy inequalities involving (representatives of equivalence classes of) eigenvalues of spectra a and b in certain cubicles. (See Theorem 4.1.3 in [10].) It is a rather involved argument, but the examples on p. 11 of the paper demonstrate the idea nicely. This approach generalizes to systems with more than two components.

The gist of the second approach is to associate Young diagrams to spectra of ρ_{AB}, ρ_A, and ρ_B. Since each Young diagram with n cells corresponds to a particular conjugacy class - and hence a particular irreducibe representation - of S_n, this associates an irreducible representation of S_n (for some $n \in N$) to each spectrum. Theorem 5.3.1 then establishes that the following are equivalent:

1) For some $m > 0$ the Kronecker coefficient $g(m\lambda, m\nu, m\mu)$ is nonzero,

2) There exists a mixed state ρ_{AB} with spectrum ν and marginals ρ_A, ρ_B with spectra λ, μ,

3) There exists a pure state ρ_{ABC} with marginals ρ_A, ρ_B, and ρ_C having spectra λ, μ, ν.

The Kronecker coefficient $g(\lambda, \mu, \nu)$ gives the number of times an irreducible representation S_λ of S_n appears in the direct sum decomposition of $S_\mu \otimes S_\nu$ for irreducible representations S_μ and S_ν of S_n. This is a very interesting result; however, at present Kronecker coefficients are not well understood (i.e., there is no known algorithm for computing them). Thus the value of the theorem lies in establishing the theoretical connection between representation theory and the marginal problem rather than in practical application. This connection has subsequently been elaborated upon and used to prove facts about symmetric groups in connection with the quantum marginal problem.[10,11]

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