Quantum Marginal Problems

David Gross (Colgone)

Joint with: Christandl, Doran, Lopes, Schilling, Walter
Outline

- Overview: Marginal problems
- Overview: Entanglement
- Main Theme: Entanglement Polytopes
- Shortly: Beyond the Pauli principle.
Overview: Marginal Problems
A marginal is obtained by integrating out parts of high-dim object.
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Not every set of marginals is compatible
Marginals

- A marginal is obtained by integrating out parts of high-dim object

- Not every set of marginals is compatible
- Deciding compatibility is the marginal problem
Marginals in classical probability

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One classical marginal prob well-known in quantum:
Marginals in classical probability

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One classical marginal prob well-known in quantum: Bell tests.
Bell tests as marginal problems

There are four random variables:
polarization along two axes, as seen by Alice/Bob

- Only certain pairs accessible
- Q: Are these marginals compatible with classical distribution?
- Compatible marginals form convex polytope
- Facets are Bell inequalities

Testing locality NP-hard $\Rightarrow$ so is classical marginal problem
Bell tests as marginal problems

- There are four random variables: polarization along two axes, as seen by Alice/Bob.
- Only certain pairs accessible.
- Q: Are these marginals compatible with classical distribution?

Compatible marginals form a convex polytope, with facets being Bell inequalities. Testing locality is NP-hard, so is the classical marginal problem.
Bell tests as marginal problems

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Marginals in quantum theory

- For subset $S_i$ specify state $\rho_i$.
- Q: Are these compatible:

$$\rho_i = \text{tr}_{S_i} \rho$$

for some global $\rho$?
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Would solve all finite-dim. few-body ground-state probs!
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Would solve all finite-dim. few-body ground-state probs!

E.g.: For two-body Hamiltonian

$$H = \sum_{i,j=1}^{n} h_{i,j},$$

compute

$$\min_{\rho} \text{tr} H \rho = \min_{\rho} \sum_{i,j} \text{tr} h_{i,j} \rho = \min_{\{\rho_{i,j}\} \text{ comp.}} \sum_{i,j} \text{tr} h_{i,j} \rho_{i,j}.$$
Marginals in quantum theory: Ground States

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Remarks:

- Left-hand side optimizes over \(O(d^n)\) variables.
- R.h.s. over \(O(n^2 d^4)\). Exponential improvement!
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General theory of convex optimization \( \Rightarrow \) Computational complexity of 2-RDM method dominated by deciding compatibility of \( \rho_{i,j} \)’s.

Two directions:
- Progress on q. marginal prob. \( \Rightarrow \) info about ground states
- Hardness of ground-states \( \Rightarrow \) hardness of q. marginals.
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Natural Question:
Is there subproblem with enough structure to be tractable?
1-RDM marginal problem

1-RDM subproblem: marginals do not overlap, global state pure

\[ \begin{array}{cccc}
\circ & \circ & \circ & \circ \\
S_1 & S_2 & S_3 & S_4
\end{array} \]

Classical version:

\[ \text{Globally pure} \iff \text{no global randomness} \implies \text{no local randomness}. \]

Quantum version:

\[ \text{Globally pure} \not\implies \text{no local randomness} \text{ (in presence of entanglement)}. \]

\[ \text{. . . seems non-trivial, but tractable!} \]
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- ⇒ no local randomness.
- ... trivial.

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- Globally pure
  - \(\nRightarrow\) no local randomness (in presence of entanglement).
- ... seems non-trivial, but tractable!
1-RDM marginal problem

Questions to be asked:

- Structure of set of 1-RDMs?
- What info about global $\psi$ accessible from 1-RDM?
- Computational complexity of 1-RDM marginal prob.?
- Practical uses?
Structure of 1-RDMs.
Reduction to eigenvalues

- Local basis change does not affect compatibility
- ⇒ can assume $\rho_i$ are diagonal ⇒ described by eigenvalues

$$\langle \vec{\lambda}^{(1)}, \ldots, \vec{\lambda}^{(n)} \rangle \in \mathbb{R}^{dn}.$$
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- Compatible spectra form *convex polytope*
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\[ \text{[Klyachko, Kirwan, Christandl, Mitchison, Harrow, Daftuar, Hayden, \ldots]} \]
Reduction to eigenvalues

- Local basis change does not affect compatibility
- $\Rightarrow$ can assume $\rho_i$ are diagonal $\Rightarrow$ described by *eigenvalues*

$$\langle \tilde{\lambda}^{(1)}, \ldots, \tilde{\lambda}^{(n)} \rangle \in \mathbb{R}^{dn}.$$ 

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  [Klyachko, Kirwan, Christandl, Mitchison, Harrow, Daftuar, Hayden, ...]

- No *conceptually simple* proof known to me!
Example: $d = n = 2$

Warm up: work out solution for two qubits.
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- Schmidt-decomposition:

\[ |\psi\rangle = \sqrt{\lambda^{(1)}} |e_1\rangle \otimes |f_1\rangle + \sqrt{\lambda^{(2)}} |e_2\rangle \otimes |f_2\rangle \]

- With

\[ \rho_1 = \lambda^{(1)} |e_1\rangle \langle e_1| + \lambda^{(2)} |e_2\rangle \langle e_2|, \quad \rho_2 = \lambda^{(1)} |f_1\rangle \langle f_1| + \lambda^{(2)} |f_2\rangle \langle f_2|. \]
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▸ So eigenvalues must be equal: $\vec{\lambda}_1 = \vec{\lambda}_2$.

In terms of largest eigenvalue, get simple polytope:
Further examples

Three qubits:

Three fermions on 6 modes ("Dennis-Borland"): (c.f. M. Christandl’s talk)
Summary: Structure of 1-RDM’s

- Compatible 1-RDMs described by convex polytopes of spectra.
Summary: Structure of 1-RDM's

- Compatible 1-RDMs described by convex polytopes of spectra.
- If this doesn’t surprise you, I’m terribly sad.
Computational aspects.
List inequalities?

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$\langle \vec{D}, x \rangle \leq c.$

- Polytopes characterized by finitely many linear ineqs

[Klyachko, Altunbulak]
List inequalities?

Polytopes characterized by finitely many linear ineqs

\[ \langle \vec{D}, x \rangle \leq c. \]

Ansatz so far: Compute all ineqs

→ Altunbulak’s talk

Doesn’t seem to scale: too many ineqs as \( n, d \) go up.

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[Klyachko, Altunbulak]
List inequalities?

There might be better algorithm than “checking all ineqs”.

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</tr>
<tr>
<td>$\lambda_1 + \lambda_2 - 2\lambda_3 - \lambda_4 - \lambda_5 \leq 0$</td>
</tr>
<tr>
<td>$\lambda_1 - \lambda_2 - \lambda_3 + \lambda_6 - 2\lambda_7 \leq 0$</td>
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<td>$2\lambda_1 - \lambda_2 + \lambda_3 - 2\lambda_4 - 2\lambda_5 - \lambda_6 + \lambda_8 \leq 1$</td>
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</tbody>
</table>

[Klyachko, Altunbulak]

- There might be better algorithm than “checking all ineqs”.  
- Ex.: $\ell_1$-unit ball in $\mathbb{R}^n$ has $2^n$ linear ineqs, but membership equivalent to $\|x\|_{\ell_1} = \sum_{i=1}^{n} |x_i| \leq 1$. 

\[ \|x\|_{\ell_1} = \sum_{i=1}^{n} |x_i| \leq 1. \]
Thus, central open question:

Q.: Is there a poly-time algorithm that decides the 1-RDM quantum marginal problem?
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Progress Nov. 2015 [Burgisser, Christandl, Mulmuley, Walter]:

- Problem in $\text{NP} \cap \text{coNP}$
  - Virtually guarantees that it can’t be proven hard
  - Suggests it might be in $\text{P}$. 

Info about global state from 1-RDMs.

Selection rules

Selection rule, “Generalized Hartree-Fock”:

If a state $\psi$ maps to the boundary of the polytope, only few, special Slater determinants can appear in an expansion of $\psi$. 

Stated by Klyachko (2009). He didn’t feel proof was necessary.
True for general scenarios – stated here for Fermions.

[Schilling, DG, Christandl, PRL ’13]
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If the eigenvalues of $\psi$ saturate the ineq. $\langle D, \lambda \rangle = c$, then (1) only contains Slater dets whose eigenvalues do so as well.
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Trick:

- Introduce operator $\hat{D} = \sum_i D_i a_i^{\dagger} a_i$.

- Then

  $$\langle D, \lambda \rangle = \text{tr} \hat{D} \rho^{(1)} = \text{tr} \hat{D} \psi \langle \psi |.$$
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Proof: Blackboard.
Info about global state from 1-RDMs.

Part 2: Entanglement.
Entanglement

- Two pure states $\psi, \phi$ are in same *entanglement class* if they can be converted into each other with finite probability of success using local operations and classical communication.
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Entanglement

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▶ Often referred to as SLOCC classes. But that sounds too unpleasant.

▶ Formally:

$$\psi \sim \phi \iff \psi = (g_1 \otimes \cdots \otimes g_n)\phi$$

with $g_i$ local invertible matrices (filtering operations).

▶ Mathematically: We’re looking at $SL(\mathbb{C}^d)^\times \times^n$-orbits in $(\mathbb{C}^d)^n$. 
SLOCC, SLOCC! – Who’s There?

- For three qubits \((d = 2, n = 3)\), equivalence classes known since mid-1800s. Re-discovered in 2000 to great effect:

> **Three qubits can be entangled in two inequivalent ways**
> Abstract: Invertible local transformations of a multipartite system are used to define equivalence classes in the set of entangled states. This classification concerns the entanglement properties of a single copy of the state. Accordingly, we say that two states ...
> Cited by 1683 - Related articles - BL Direct - All 22 versions - Import into BibTeX

> **Four qubits can be entangled in nine different ways**
> F Verstraete, J Dehaene, B De Moor... - Physical Review A, 2002 - APS
> ... to the singlet state by SLOCC operations 3. In the case of three entangled qubits, it was shown 2,4,5 that each state can be converted by SLOCC operations either to the GHZ-state \((000 111)\)/& or to the W-state \((001 010 100 \rangle\), leading to two inequivalent ways of entangling ...
> Cited by 350 - Related articles - BL Direct - All 12 versions - Import into BibTeX

> **Control and measurement of three-qubit entangled states**
> CF Roos, M Riebe, H Häffner, W Hänsel... - Science, 2004 - sciencemag.org
> ... The ions’ electronic qubit states are initialized in the S state by optical pumping. Three qubits can be entangled in only two inequivalent ways, represented by the Greenberger-Horne-Zeilinger (GHZ) state, and the W state, (17). ...
> Cited by 273 - Related articles - All 13 versions - Import into BibTeX
Examples

Classes:

- Products $\psi = \phi_1 \otimes \phi_2 \otimes \phi_3$.
- Three classes of *bi-separable* states: $\psi = \phi_1 \otimes \phi_{2,3}$.
- The W-class:

  $$|W\rangle = |001\rangle + |010\rangle + |100\rangle.$$ 

- The GHZ-class:

  $$|GHZ\rangle = |000\rangle + |111\rangle.$$
Further examples

4 qubits:

- Classification apparently first obtained in QI community [Verstraete et al. (2002)].
- Nine families of four complex parameters each.
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Beyond:

- Number of parameters required to label orbits increases exponentially.
- Only sporadic facts known.
Desiderata

Can we come up with theory that

- is systematic
  (any number of particles, local dimensions, symmetry constraints),

- is efficient
  (only polynomial number of parameters have to be learned),

- experimentally feasible
  (parameters easily accessible, robust to noise)?
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Claim:
The single-site quantum marginal problem lives up to these standards.
Entanglement Polytopes
Central observation, entanglement polytopes

Set of allowed eigenvalues may depend on entanglement class of global state.

[Walter, Doran, Gross, Christandl, Science 2013]
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Thus:

- To every class $C$, associated set $\Delta_C$ of local eigenvalues of states in (closure of) $C$. 

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[Walter, Doran, Gross, Christandl, Science 2013]

- Clearly: the position of $\vec{\lambda}(\psi)$ w.r.t. the entanglement polytopes contains all local information about global entanglement class.
Examples re-visited: 3 qubit entanglement polytopes

For three qubits, polytopes resolve all 6 entanglement classes:

\[ \lambda^{(1)}_{\text{max}} + \lambda^{(2)}_{\text{max}} + \lambda^{(3)}_{\text{max}} \geq 2 \]

Any violation of that witnesses GHZ-type entanglement.

[Hang et al. (2004), Sawicki et al. (2012), our paper]
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4 qubits:

- **Entanglement classes:**
  9 families with up to four complex parameters each [Verstraete et al. (2002)].

- **Entanglement Polytopes:**
  13 polytopes, 7 of which are genuinely 4-party entangled.

- **We feel:** attractive balance between coarse-graining and preserving structure.

Example: 4-qubit W-class

\[ \mathcal{C}_W \ni |0001\rangle + |0010\rangle + |0100\rangle + |1000\rangle \]

again an “upper pyramid”:

\[ \lambda^{(1)}_{\max} + \lambda^{(2)}_{\max} + \lambda^{(3)}_{\max} + \lambda^{(4)}_{\max} \geq 3. \]
Example: 4 qubit entanglement polytopes
Example: Bosonic qubits

Consider $n$ bosonic qubits:

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- $\Rightarrow$ single number captures all: $\lambda_{\text{max}} \in [0.5, 1]$. 
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Analyze polytopes:

- $|0, \ldots, 0\rangle$ in all $\mathcal{C}$’s $\Rightarrow$ $\Delta \mathcal{C} = [\gamma \mathcal{C}, 1]$.

- Turns out: Possible choices are

$$
\gamma \mathcal{C} \in \left\{ \frac{1}{2} \right\} \cup \left\{ \frac{N - k}{N} : k = 0, 1, \ldots, \lfloor N/2 \rfloor \right\} \ldots
$$

- ... with innermost point $\gamma$ the image of $W$-type states.
A vector is \textit{genuinely }\(n\)-\textit{partite entangled} if it does not factorize \textit{w.r.t.} any bi-partition:

\[ \psi \neq \psi_1 \otimes \psi_2. \]
Example: No Solipsism

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Example:

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Interpretation:

- *no solipsism*: love needs a partner! (And entangled qubits need their counter-parts).
Example: Distillation

Entanglement measures from local information:

- (Linear) entropy of entanglement

\[ E(\psi) = 1 - \frac{1}{N} \sum_i \text{tr} \rho_i^2 \]

simple function of Euclidean distance of eigenvalue point to origin.

- “Closer to origin ⇒ more entanglement”.
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- “Closer to origin ⇒ more entanglement”.

- ⇒ can bound \textit{distillable} entanglement from local information!

- Can even give \textit{distillation procedure} without need to know state beyond local densities (generalizing [Verstraete \textit{et al.} 2002]).
Yeah, but no pure state exists in Nature.
Pure???

- Yeah, but no pure state exists in Nature.
- Results are epsilonifiable: if distance $d$ of spectrum to a polytope $\Delta$ exceeds
  \[ 4N\sqrt{1 - p}, \]
  then $\rho \not\in \text{conv}(\Delta)$.
- $p = \text{tr} \rho^2$ is purity, which an be lower-bounded from local information alone.
Summary of Entanglement Polytopes

- Locally accessible info about global entanglement encoded in *entanglement polytopes* – subpolytopes of the set of admissible local spectra.
- Provides a systematic and efficient way of obtaining information about entanglement classes.
Thank you for your attention!

David Gross (Uni Cologne)

Oxford, April 2016