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Complexity Classification of Product State Problems for Local Hamiltonians

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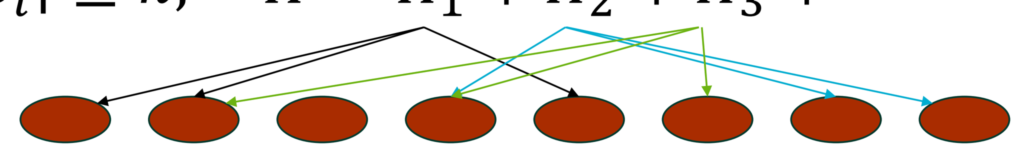
Local Hamiltonians

- An n-qubit Hamiltonian is a $2^n \times 2^n$ Hermitian matrix encoding the behavior of a physical system.
- Ground state/minimum eigenvector can encode quantum phenomena like super-fluidity, electronic structure, etc.
- Quantum constraint satisfaction problems (like Max-SAT)

$$H = \sum_i H_{S_i} \otimes \mathbb{I}_{\bar{S}_i}, \quad |S_i| \leq k, \quad H = H_1 + H_2 + H_3 + \cdots$$



Product States

Product states are unentangled tensor products of single-qubit states

$$\rho = \rho_1 \otimes \rho_2 \otimes \rho_3 \otimes \cdots \otimes \rho_n$$

- Efficiently describable classically
- Rigorously near-optimal for many natural Hamiltonians
- A popular ansatz in Hamiltonian approximation algorithms, e.g. mean-field approximations

Finding the minimum-energy product state is a typical first step when finding the ground state is difficult.

Main Question

For which Hamiltonians is estimating the minimum product state energy easy or hard?

Specifically, given a set S of allowed terms, consider the Hamiltonian family generated by S:

$$\{ H = \sum_i w_i H_i \text{ with } H_i \in S \}$$

Prior works have shown, depending on the allowed constraints,

- [Cubitt, Montanaro 2013]: estimating the ground state energy is either in P, or is NP-, StoqMA-, or QMA-complete.
- [Schaefer 1976]: families of Boolean SAT formulas are either in P or are NP-complete.

Main Result

We fully classify the complexity of estimating minimum product state energies for families of 2-local Hamiltonians.

Estimating the minimum product state energy is NP-complete iff estimating the ground state energy is NP-hard.

Equivalently: For any fixed set of 2-qubit Hamiltonian terms S,

- if every matrix in S is 1-local then the problem is in P,
- and otherwise the problem is NP-complete.

Open Problems

1. Can we use the complexity of product state problems to suggest the general ground states of a class of Hamiltonians are *not* hard?
2. Classify S-prodLH with additional restrictions, e.g. only positive weights, spatial geometry?
3. Can we classify the complexity of larger terms, e.g. 3-local?

Proof Strategy

- ✓ If every term is 1-local, then the state of each qubit can be optimized individually, so product state problems are in P.
- ✓ Product state energies can always be verified in NP.
- ❑ **To Do:** if S contains a nontrivial 2-qubit term, then can construct a Hamiltonian with an NP-hard objective embedded in its optimum product state energy.

Step 1: View product state problems as optimization over single-qubit Bloch vectors. For X, Y, Z the Pauli matrices,

$$\rho^a = \frac{1}{2}(I + a_1 X + a_2 Y + a_3 Z), \qquad \hat{a} \in \mathbb{R}^3, |\hat{a}| = 1$$

For any 2-qubit term H, $\quad \mathrm{Tr}(H\rho^u\rho^v) = \hat{u}^T \mathrm{M} \hat{v} + \hat{u}^T \hat{c} + \hat{v}^T \hat{w}$. (I)

For the particularly simple term $H = XX + YY + ZZ$, this expression is just an inner product: $\quad \mathrm{Tr}(H\rho^u\rho^v) = \hat{u} \cdot \hat{v}$. (II)

Step 2: Make the product state energy have a "nicer" form, i.e. make (I) look more like (II).

Given an arbitrary 2-qubit term, we add ancilla qubits and construct gadgets to symmetrize and delete 1-local terms:

$$H_{sym} = H^{ab} + H^{ba}$$

$$G^{uv} = H^{uv}_{sym} + H^{ab}_{sym} - H^{ua}_{sym} - H^{vb}_{sym}$$

$$\min_{\rho = \rho_1 \rho_2 \dots \rho_n} \mathrm{Tr}[\rho \sum_{uv \in E} G^{uv}] = -2 \max_{\hat{u} \in S^2} \sum_{uv \in E} \|W(\hat{u} - \hat{v})\|$$

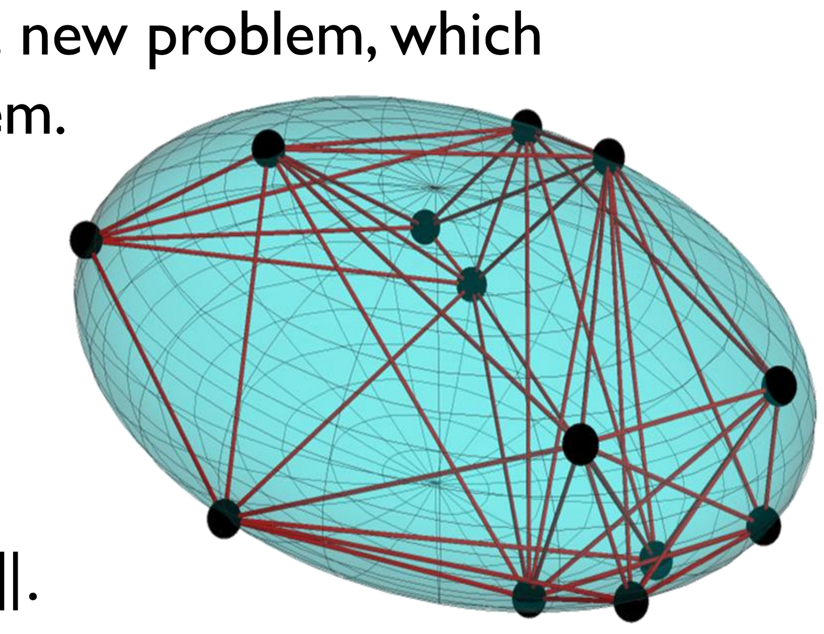
Step 3: Define this final objective as a new problem, which generalizes the famous Max-Cut problem.

Stretched linear Vector Max-Cut:

For a fixed matrix $W = \begin{bmatrix} \alpha & & \\ & \beta & \\ & & \gamma \end{bmatrix}$,

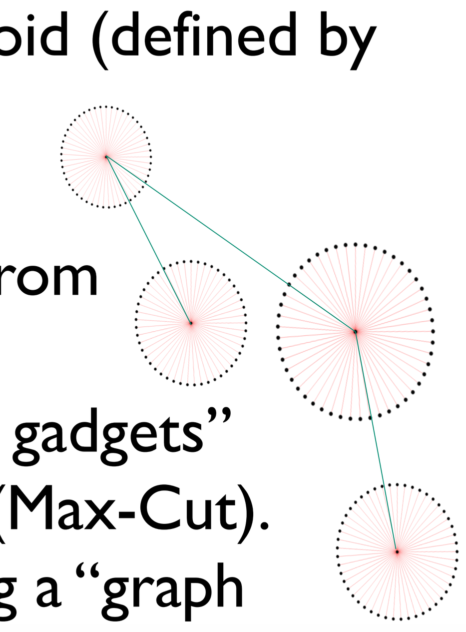
given a graph $G = (V, E)$, estimate

$$\mathrm{MC}^{\mathrm{L}}_W(G) = \frac{1}{2} \max_{\hat{u} \in S^{k-1}} \sum_{uv \in E} \|W\hat{u} - W\hat{v}\|.$$

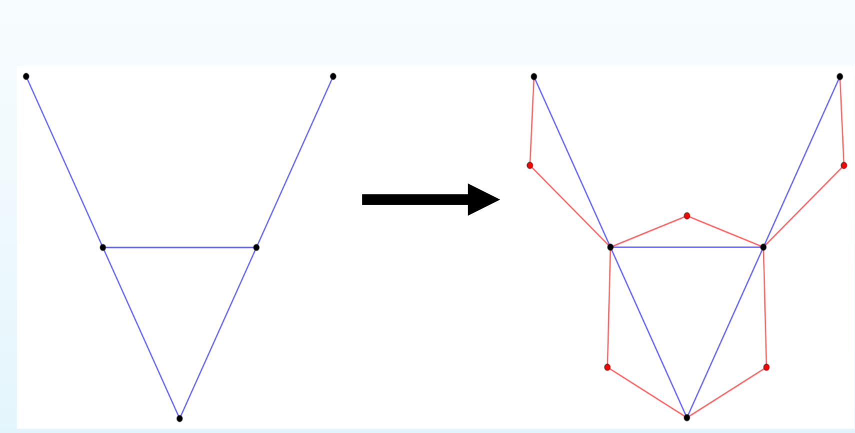


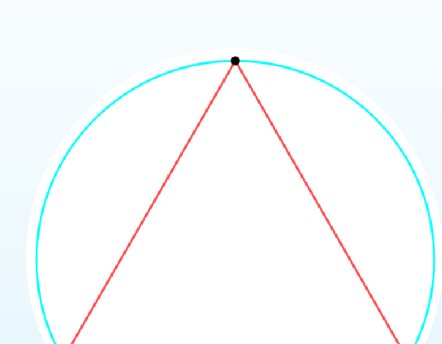
Equivalently: embed vertices of a graph onto an ellipsoid (defined by W) to maximize the sum of the edge lengths.

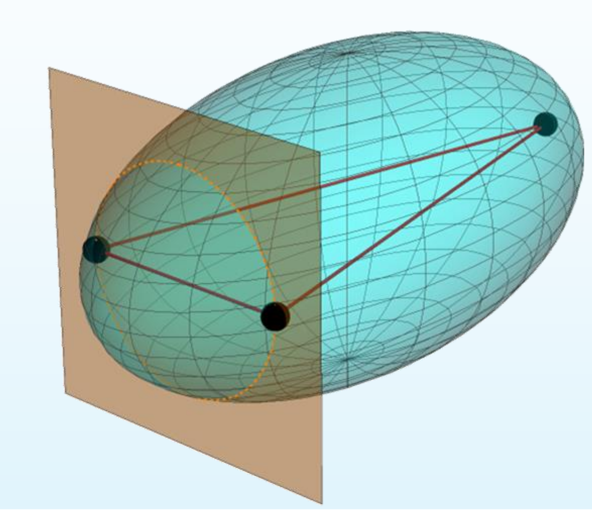
Step 4: Show $\mathrm{MC}^{\mathrm{L}}_W$ is NP-complete by reductions from 3-Coloring or Max-Cut.



- For W with unique maximum weight, we use "star gadgets" to force maximal solutions to live in 1 dimension (Max-Cut).
- For other W, we use 3-clique gadgets, constructing a "graph of triangles". A maximal vector assignment must be maximal on *every* gadget. Maximal-length triangles in ellipsoids are somewhat unique, so once a set of 3 vectors is assigned to one gadget, they must be used for *all* gadgets (3-Coloring).







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