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Second order cone relaxations for quantum Max Cut

arXiv:2411.04120

joint work with:

Ojas Parekh & Kevin Thompson, Sandia National Laboratory

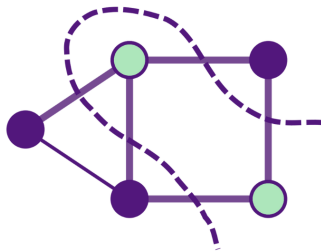
Sevag Gharibian, Paderborn University

Max Cut

Let $G = (V, E)$ be a graph. A *cut* is a subset $K \subseteq V$.
Denote by $E(K)$ the edges crossing from K to $\bar{K} = V \setminus K$.

Task: Find a *maximum cut*, so that the the number of edges between the subsets is maximal.

$$\text{MaxCut}(G) = \max_{K \subseteq V} |E(K)|$$



Max Cut II

Some Facts:

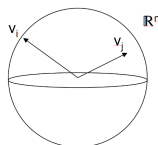
- ▶ MaxCut is NP-hard.
- ▶ Polynomial time approximation algorithm by Goemans and Williamson. Finds cut with approximation ratio

$$\frac{\text{MaxCut}(G)^{\text{approx}}}{\text{MaxCut}(G)^{\text{true}}} \geq 0.878$$

through randomized rounding of a semidefinite program.

J. ACM, 42 (6), 1115–1145 (1995)

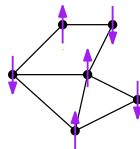
- ▶ GW is the optimal polynomial-time algorithm if the Unique Games Conjecture holds.



Physics of Max Cut

Max Cut is also a physics problem: find ground state energy of system with anti-ferromagnetic interactions (Ising model).

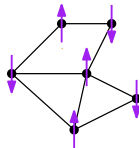
$$\text{MaxCut}(G) = \max \frac{1}{2} \sum_{(ij) \in E} (1 - z_i z_j)$$



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“Quantum Ising model” = quantum Heisenberg model

$$H = -\frac{1}{2} \sum_{(i,j) \in E} (\mathbb{1} - X_i X_j - Y_i Y_j - Z_i Z_j)$$

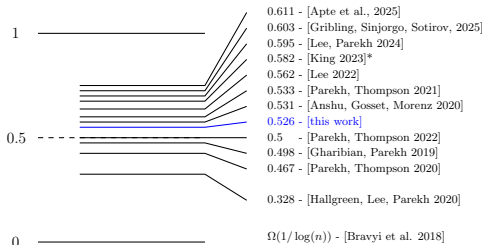
$$\text{QMaxCut}(G) = -\min_{\varrho} \text{tr}(H\varrho)$$

Quantum Max Cut

Quantum Max Cut: find ground state on graph

$$H = -\frac{1}{2} \sum_{(i,j) \in E} (\mathbb{1} - X_i X_j - Y_i Y_j - Z_i Z_j)$$

- ▶ QMA-complete.
- ▶ Practically challenging: diagonalize matrices of size $2^n \times 2^n$.
- ▶ Variational upper bounds / SDP lower bounds.
- ▶ Approximation algorithms (NPA + randomized rounding):
provides lower bound and upper bound with guarantee.



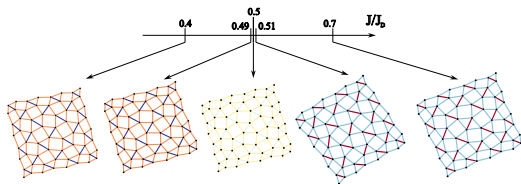
Main result

Previous* approximation algorithms require a semidefinite program of size $n^2 \times n^2$.

SDP of $n \times n$ matrix with second order cone constraints.
Approximation ratio of 0.526.

FH, Kevin Thompson, Ojas Parekh, Sevag Gharibian, arXiv:2411.04120

- ▶ Factor $\times 10$ in size to previous methods.
- ▶ Recovers phases of Shastry-Sutherland model.
- ▶ Good scaling (256-qubit systems).



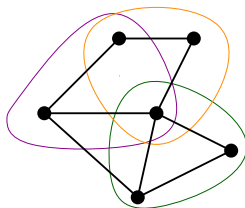
* all entangled approximations.

Key idea

How to obtain a practically useful relaxation + approximation algorithm?

Combine

- ▶ Optimization over moment matrix (SDP): Pauli-NPA.
- ▶ Optimization over three-qubit marginals (SOCP).



3-qubit marginals

Some facts:

- ▶ QMC is real: $H = -\frac{1}{2} \sum_{(i,j) \in E} (1 - X_i X_j - Y_i Y_j - Z_i Z_j) = H^T$
- ▶ QMC is $SU(2)$ invariant:

$$U^{\otimes n} H (U^{\otimes n})^\dagger = H \quad \text{for all } U \in SU(2)$$

How to use this?

- ▶ Use the representation theory of the symmetric group / $SU(2)$.
- ▶ Define permutation operators $\pi \in S_n$ acting on $(\mathbb{C}^d)^{\otimes n}$:

$$\pi |v_1\rangle \otimes \dots \otimes |v_n\rangle = |v_{\pi^{-1}(1)}\rangle \otimes \dots \otimes |v_{\pi^{-1}(n)}\rangle$$

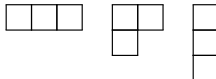
Some Representation theory

- ▶ A $U^{\otimes n}$ -invariant operator A can be expanded as

$$A = \sum_{\pi \in S_n} a_{\pi} \pi$$

- ▶ The subspaces that are invariant under $SU(2)$ are labeled by *partitions* $\lambda \vdash n$.
- ▶ For $n = 3$, there are the partitions (3) , $(2, 1)$, and $(1, 1, 1)$.

Visually,



- ▶ That is, one can block-diagonalize an invariant A .

Three-qubit marginals

Consider a three-qubit marginal of the ground state of H .

$$\varrho_{123} = \sum_{\pi \in S_3} r_{\pi} \pi \quad \longleftarrow \quad \text{six parameters}$$

Further simplifications:

- ▶ On $(\mathbb{C}^2)^{\otimes 3}$, the partition $(1, 1, 1)$ vanishes, i.e.

$$\mathbb{1} - (12) - (13) - (23) + (123) + (132) = 0$$

- ▶ If $H = H^T$, then also $\varrho_{ijk}^T = \varrho_{ijk}$.
- ▶ Write $\langle \pi \rangle = \text{tr}(\pi \varrho)$.
Because $(123)^T = (123)^{-1} = (132)$, we have

$$\langle (123) \rangle = \langle (132) \rangle$$

Let's count: We are left with $6 - 1 - 1 - 1 = 3$ parameters.

Three-qubit marginals

⇒ Describe real $U^{\otimes n}$ -invariant three-qubit state by:

$$x = \langle \text{SWAP}_{12} \rangle, \quad y = \langle \text{SWAP}_{23} \rangle, \quad z = \langle \text{SWAP}_{13} \rangle,$$

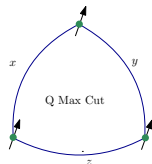
Lieb-Mattis (1962) and Parekh-Thompson (2022) conditions:

$$0 \leq x + y + z \leq 3, \quad (\text{LM})$$

$$(x^2 + y^2 + z^2) - 2(xy + xz + yz) + 2(x + y + z) \leq 3. \quad (\text{PT})$$

A real $U^{\otimes 3}$ -invariant operator on $(\mathbb{C}^2)^{\otimes 3}$ is a state, if and only if LM and PT hold.

FH, Kevin Thompson, Ojas Parekh, Sevag Gharibian, arXiv:2411.04120



Deriving Lieb-Mattis and Parekh-Thompson

A basis for the invariant subspace:

$$R_+ = \frac{1}{6} (\text{id} + (12) + (23) + (13) + (123) + (132)) ,$$

$$R_- = \frac{1}{6} (\text{id} - (12) - (23) - (13) + (123) + (132)) ,$$

$$R_0 = \frac{1}{3} (2 \text{id} - (123) - (132)) ,$$

$$R_1 = \frac{1}{3} (2(23) - (13) - (12)) ,$$

$$R_2 = \frac{1}{\sqrt{3}} ((12) - (13)) ,$$

$$R_3 = \frac{i}{\sqrt{3}} ((123) - (132)) .$$

Eggeling-Werner, PRA 63, 042111 (2001)

Note:

- ▶ R_+ is (up to multiplicities) one-dimensional.
- ▶ R_0, R_1, R_2, R_3 behave like Pauli I, X, Y, Z . $\implies$ Bloch ball!
- ▶ R_- is the anti-symmetric subspace, vanishes on qubits.

Second order cone programming

Second-order cone programs (SOCP) have the form

$$\begin{aligned} \min_x \quad & f^T x \\ \text{subject to} \quad & \|A_i x + b_i\| \leq c_i^T x + d_i, \quad i = 1, \dots, N, \end{aligned}$$

Here:

- ▶ $\|\cdot\|$ the Euclidean norm.
- ▶ variable: $x \in \mathbb{R}^n$
- ▶ problem parameters:
 $f \in \mathbb{R}^n$, $A_i \in \mathbb{R}^{n_i-1 \times n}$, $b_i \in \mathbb{R}^{n_i-1}$, $c_i \in \mathbb{R}^n$, and $d_i \in \mathbb{R}$.

... In practise, SOCP's are much more efficient to solve than SDP's.

Second order cone relaxation for Quantum Max Cut

Our real invariant three-qubit state constraint is a second order cone constraint!

Combining level-1 from Pauli-NPA and second order constraints together:

$$\max_{x_{ij}} \quad \frac{1}{2} \sum_{(i,j) \in E} (1 - x_{ij})$$

$$\begin{aligned} \text{subject to} \quad & 0 \leq x_{ij} + x_{jk} + x_{ik} \leq 3, \\ & (x_{ij}^2 + x_{ik}^2 + x_{jk}^2) - 2(x_{ij}x_{ik} + x_{ij}x_{jk} + x_{ik}x_{jk}) + 2(x_{ij} + x_{ik} + x_{jk}) \leq 3 \\ & M \succeq 0, \quad M_{ii} = 3, \quad M_{ij} = 2x_{ij} - 1. \end{aligned}$$

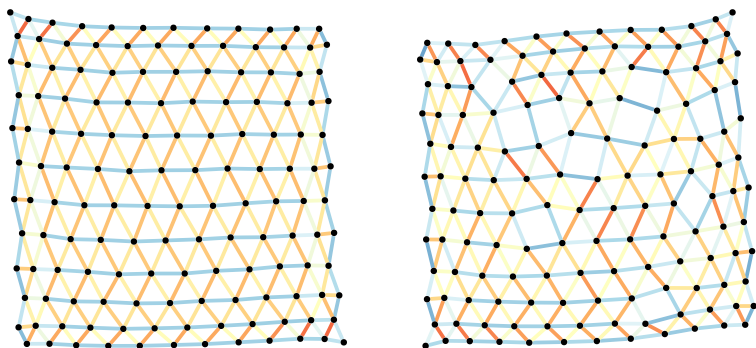
- ▶ Upper *and* lower bounds. Efficient in practise.
- ▶ Flexible: gives bounds where other methods fail (random graphs, deformed lattices, spin glass).
- ▶ However: weak on sparse graphs and highly structured lattices.

Approximation ratio

- ▶ Key idea: Take x_{ij} values from level 1 of the Pauli-hierarchy, and compute a maximal matching of G^* .
- ▶ Set of non-overlapping edges on graph that maximizes the sum of $\sum_{(ij) \in E} x_{ij}$.
- ▶ Place singlet for every edge in matching, place product state for unmatched vertices.
- ▶ Reasoning with the constraints from LM and PT yields an approximation ratio of 0.526 to the true ground state energy.

*A matching of G is a subset of edges such that no two edges in the subset share a common vertex.

Lower bounds for lattice with defects



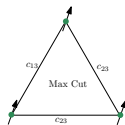
- ▶ Lower bounds on GS energy.
- ▶ cold blue = singlet, red hot = orthogonal to singlet.
- ▶ Lattice defects break boundary effects.

Summary

- ▶ New approach for lower bounds: combination of moment matrices and marginal approximations.
- ▶ Symmetry reduction is powerful. SOCP are efficient.

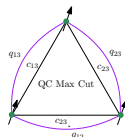
Outlook

- ▶ Similar analysis for classical-quantum Max Cut
 $H = \sum_{(ij) \in E} J(XX + YY)_{ij} + ZZ_{ij}, J \in \mathbb{R}$
- ▶ SOCP for arbitrary Hamiltonians with Lovasz bounds.
- ▶ Entanglement characterization of classical-quantum 3-RDM



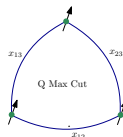
$J = 0$

Z_2



$J > 0$

$U(1) \times Z_2$



$J = 1$

$SU(2)$