Overparameterization in the quantum approximate optimization algorithm

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Outline of Presentation

- Motivation
- QAOA Background
- ma-QAOA
  - Theoretical results
  - Determining parameters
- Symmetry and ma-QAOA

Why quantum?

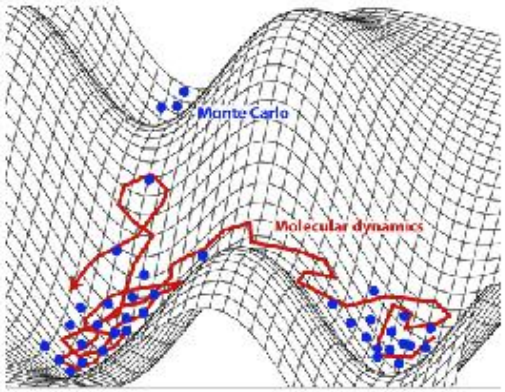

Figure: Image from Wikipedia

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QAOA Background

- Quantum approximate optimization algorithm (QAOA)
- Introduced in 2014 by Farhi, Goldstone, and Gutmann to approximately solve combinatorial optimization problems [3]
  - MaxCut, MaxIndSet are two commonly studied ones
- Algorithm has gained a lot of attention in recent years [4, 2, 7]
  - Promising experimental results
  - Lots of open problems

What is a combinatorial optimization problem?

- Specified by n bits and m clauses.
  - Clauses are constraints on a subset of bits
- Define an objective function, which is the number of clauses satisfied:

$$C(z) = \sum_{\alpha=1}^{m} C_\alpha(z)$$

  where $z = x_1 ... x_n$ is a bit string.
  - $C_\alpha(z) = 1$ if clause α is satisfied, else it is 0
- Is there a bit string that satisfies all of the clauses? How can we maximize or minimize $C(z)$?

Example: MaxCut

- Let $G = (V, E)$ be a graph. We want to divide V into two sets such that the number of edges between them is maximized.
- This problem can be formulated as

$$\min_{x \in \{0,1\}^n} \sum_{ij \in E(G)} x_j(x_i - 1) + x_i(x_j - 1) = \min_{x \in \{0,1\}^n} \sum_{ij \in E(G)} 2x_i x_j - x_i - x_j$$

Example: MaxCut

We will call the two sets red and blue.

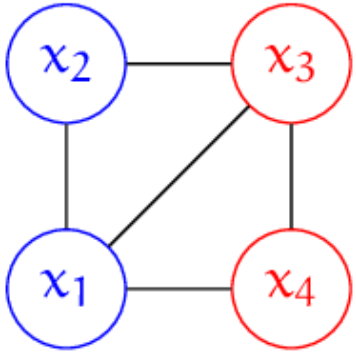


Figure: Not the best MaxCut solution. There are three edges whose endpoints are in different sets.

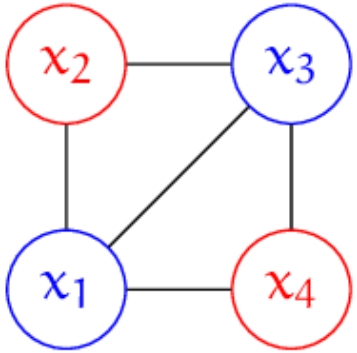


Figure: The best MaxCut solution. There are four edges whose endpoints are in different sets.

How are these problems solved with QAOA?

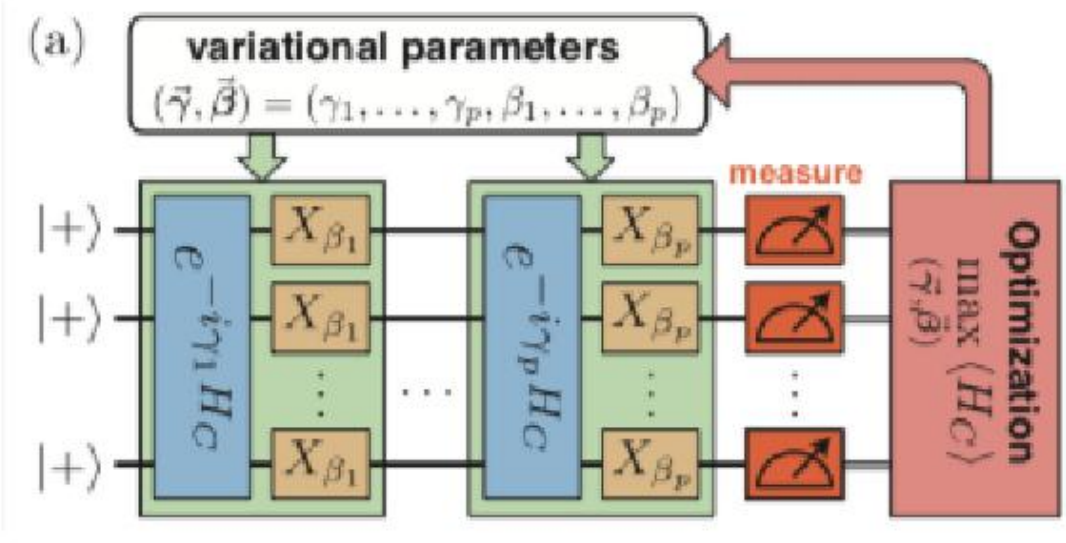


Figure: QAOA [1]

How are these problems solved with QAOA?

- We want to create a unitary operator based on C:

$$U(C,\gamma) = e^{-iC\gamma} = \prod_{\alpha} e^{-iC_\alpha \gamma}$$

- Alternate this operator with a mixing operator

$$U(B,\beta) = e^{-iB\beta}$$

  and apply to an initial state $|s\rangle$ that depends on B.
- In the end, get $|\gamma,\beta\rangle = U(B,\beta_p)U(C,\gamma_p)...U(B,\beta_1)U(C,\gamma_1)|s\rangle$ which has depth p. γ and β are angles.
- The approximation ratio is $\langle C\rangle / C_{max}$ and is primary metric for success.

Motivation

- There is a trade off between time spent using classical techniques and quantum techniques when implementing QAOA
- By shifting more burden onto classical optimization, we can design shallower quantum circuits that might be implementable in the NISQ era

Multi-angle QAOA

- How much better can we do if we allow each gate to have its own angle?
- We redefine C and B so that each summand C_a and B_v has its own angle, γ_a and β_v respectively to get

$$U(C, \vec{\gamma}) = e^{-iC\vec{\gamma}} = e^{-i\sum_a C_a \gamma_a} = \prod_a e^{-i\gamma_a C_a}$$

and

$$U(B, \vec{\beta}) = e^{-iB\vec{\beta}} = e^{-i\sum_{v \in V(G)} B_v \beta_v} = \prod_{v \in V(G)} e^{-i\beta_v B_v}$$

where $\vec{\gamma} = (\gamma_{a_1}, \gamma_{a_2}, ...)$ and $\vec{\beta} = (\beta_{v_1}, \beta_{v_2}, ...)$.

Multi-angle QAOA

Theorem

[5] The multi-angle quantum approximate optimization algorithm converges to the optimal solution as $\mathrm{p} \to \infty$.

- Prove using squeeze theorem
- The theorem ignores the difficulty of optimizing angle selection.
- We don't need exact optimal, we just need to do better than the original QAOA.

Multi-angle QAOA

Theorem

[5]
Let $\beta'_u = 2\beta_u$ *and* $\beta'_v = 2\beta_v$ *The expected value of* C *after one iteration of ma-QAOA applied to MaxCut for triangle free graphs* G *is* $\sum_{uv\in E} \langle \gamma_{uv}\beta_x | C_{uv} | \gamma_{uv}\beta_x \rangle$, *where:*

$$\langle \gamma_{uv}\beta_x | C_{uv} | \gamma_{uv}\beta_x \rangle = \frac{1}{2} + \frac{1}{2}\sin\gamma_{uv}(\cos\beta'_v \sin\beta'_u \prod_w \cos\gamma_{uw} + \cos\beta'_u \sin\beta'_v \prod_x \cos\gamma_{vx})$$

where $w \in \mathrm{Nbhd}(u) \setminus v$ *and* $x \in \mathrm{Nbhd}(v) \setminus u$.

- The proof relies on the Pauli-solver algorithm
- This looks a lot like the equations for weighted graphs.

Preliminary Data

- We compare one iteration of ma-QAOA to 1-QAOA, 2-QAOA, and 3-QAOA for solving MaxCut on all non-isomorphic, connected eight-vertex graphs.

QAOA type	Average approximation ratio for all eight-vertex graphs
ma-QAOA	.9257
p=1 QAOA	.8061
p=2 QAOA	.8767
p= 3 QAOA	.9192

Table: The average approximation ratio for eight-vertex graphs.

- Used BFGS to find optimal angles
- Over 20% of graphs have an approximation ratio of 1.0 for one iteration of ma-QAOA.

Theoretical Result

- ma-QAOA has an approximation ratio of 1 for MaxCut on all star graphs
- QAOA approximation ratio tends to 0.75 for large n

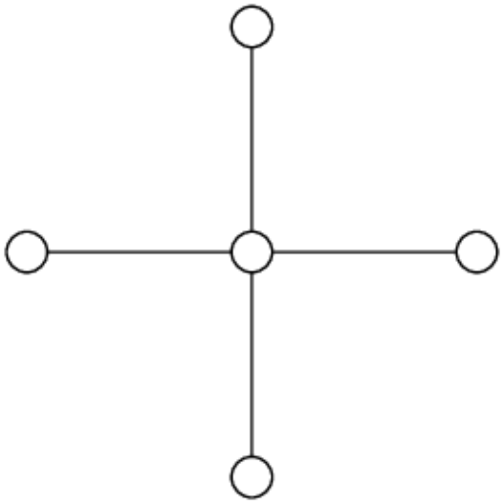


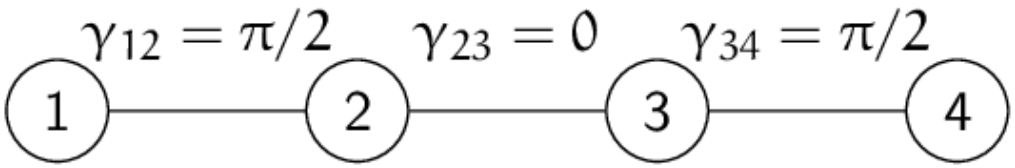
Figure: The star graph on five vertices.

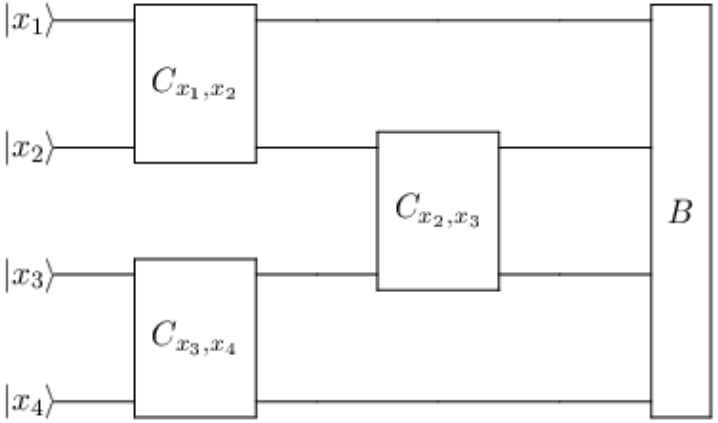
Efficient Embedding

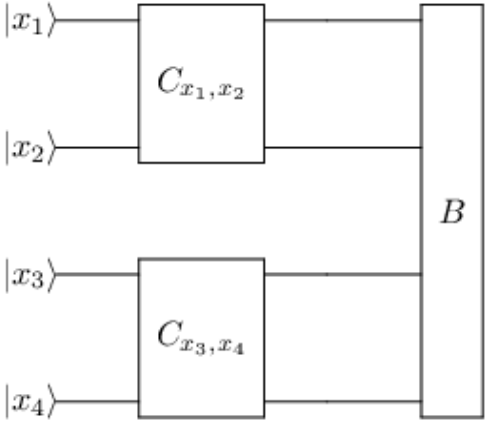
- The above results indicate that ma-QAOA may need fewer iterations than QAOA. This alone should lead to shallower circuits.
  - 15% of β angles are zero.
  - 25% of γ angles are zero.
- Zero-angle gates don't have to be implemented, leading to smaller circuits (especially on limited-connection hardware- fewer swaps).

Example: Multi-angle QAOA and circuit depth

- For example, consider P_4 .







Drawback

- Lots of angles are needed for this: n beta angles and up to $\binom{n}{2}$ gamma angles per iteration

Graph Automorphisms

- A *graph automorphism* is a permutation of the vertex set of a graph, $\sigma : V \to V$
  - Satisfies the condition that a pair of vertices, (u, v), forms an edge if and only if the pair $(\sigma(u), \sigma(v))$ also forms an edge.
- Any set of automorphisms generate a corresponding vertex and edge orbits, which are the equivalence classes of the vertices (edges) under the action of the automorphism.
- A *generator* of a group is a set of automorphisms $(\sigma_1, \ldots, \sigma_n)$ containing group elements so that application of the generators on themselves and each other can produce all elements in the group.

sym-QAOA

- **Idea:** use problem symmetry to reduce the number of parameters in ma-QAOA [6]
- sym-QAOA selects a single automorphism and assigns the same angle to all vertices in the same vertex orbit and the same angle to all edges in the same edge orbit
- best-1sym-qaoa runs sym-QAOA over all automorphisms and selects the one that gives the largest Max-Cut value
- Requires $|\mathrm{Orb}_v| + |\mathrm{Orb}_e|$ parameters
  - each element in the same vertex orbit or edge orbit receives the same parameter

max-sym-QAOA and rand-group-QAOA

- max-sym-QAOA computes the symmetry generator of G and determine the corresponding maximum vertex orbit, Orb_v, and edge orbit, Orb_e.
- Finding the generating set of the automorphism group of a graph is an extra step in max-sym-QAOA
- rand-group-qaoa groups vertices in the problem graph randomly into sets and edges randomly into sets, such that the number of parameters is the same as that of max-sym-qaoa.

best-1sym-QAOA vs. ma-QAOA

- Below figure shows the difference in approximation ratios between best-1sym-qaoa and ma-qaoa for these $5,918$ graphs.
- best-1sym-qaoa has the same approximation ratio as ma-qaoa has on $5,097$ graphs ($\sim 86.1\%$ of the studied graphs)
- On average used 28.1% fewer parameters

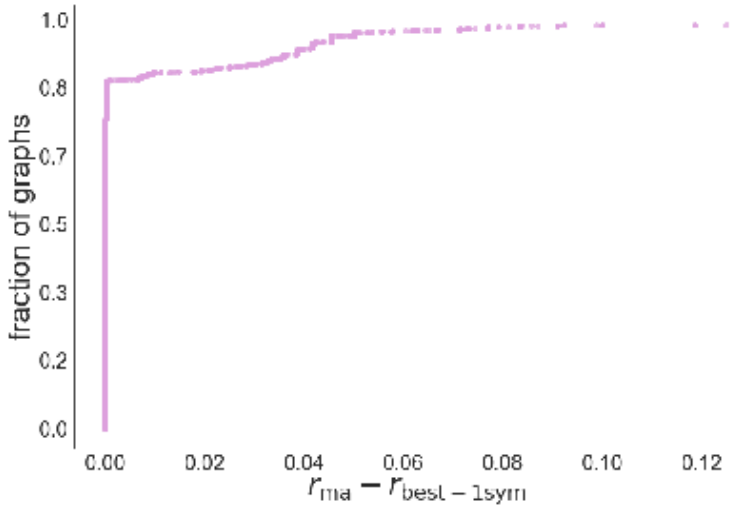


Figure: Difference in approximation ratios.

max-sym-QAOA vs. ma-QAOA

- Again, compare max-sym-QAOA to ma-QAOA on the $7,565$ graphs that contain nontrivial symmetry.
- As shown in the below figure, max-sym-QAOA performs as well as ma-QAOA on 2,713 of these graphs.

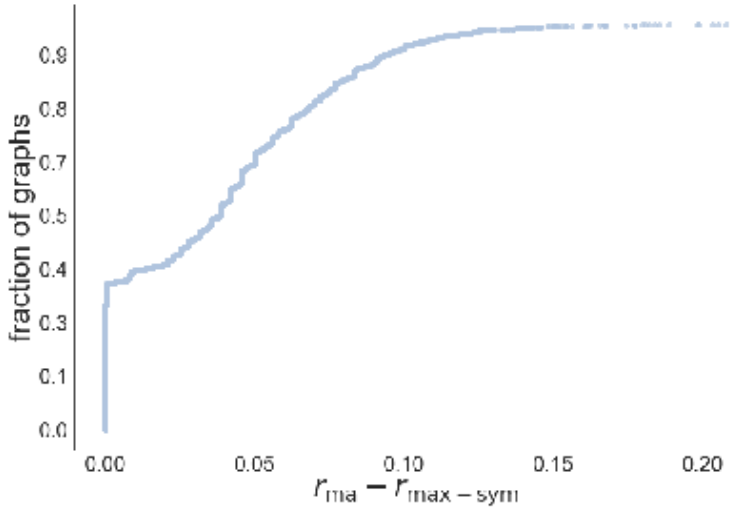


Figure: Difference in approximation ratios.

Evidence for central role of symmetries

- Compare max-sym-QAOA to rand-group-QAOA on 7,565 graphs where max-sym-QAOA does not equal ma-QAOA
- Define the ratio

$$k_{\text{var}} := \frac{f(x^*_{\text{ma}}) - f(x^*_{\text{var}})}{f(x^*_{\text{ma}}) - f(x^*)}.$$

- $k = 0$, the QAOA variant recovers ma-QAOA, and when $k = 1$, it performs the same as QAOA.

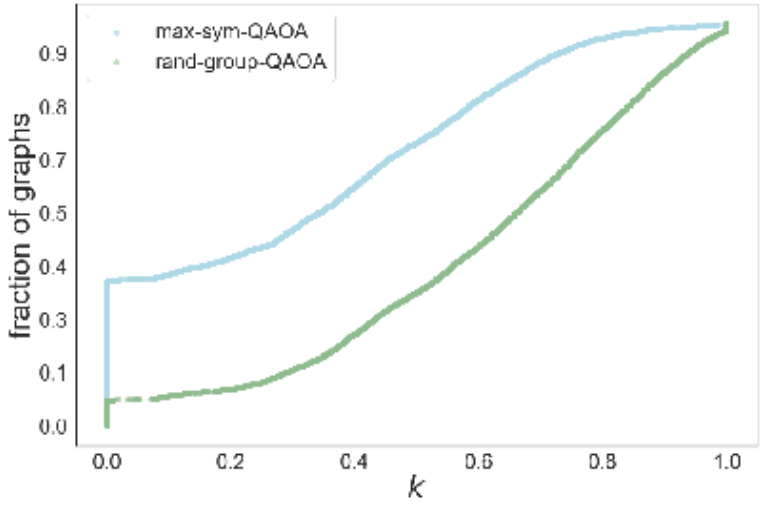


Figure: Fraction of graphs achieving ratio k.

Current work/ future directions

- Mathematically prove ma-QAOA = best-1sym-QAOA for particular kinds of graphs
- ma-QAOA performance bounds
- Are there other classes of graphs where ma-QAOA strictly outperforms QAOA?

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Thanks