12. Variational Quantum Algorithms

Isaac H. Kim (UC Davis)

Switching Topics

So far we focused on various fault-tolerant quantum algorithms.

Pros: We know they will work for sure. We're also pretty confident that they provide speedups, asymptotically.

Cons: These are not going to be implemented anytime soon.

Recently, there has been a huge amount of activities on variational quantum algorithms.

Pros: We can implement them now.

Cons: We don't know if they will work. It's unclear if we can get a speedup.

QAOA

QAOA = Quantum Approximate Optimization Algorithm [Farhi, Goldstone, and Gutmann (2014)]

Problem: Find the minimum-energy configuration of $H = \sum_{\alpha=1}^{m} C_\alpha(z)$, where $C_\alpha(z)$ is an Ising-like (few-body) Hamiltonian depending on a bit string z.

Idea: Discrete version of quantum adiabatic algorithm.

Quantum Adiabatic Algorithm

[Farhi, Goldstone, Gutmann, Sipser (2000)]

Adiabatically evolve $H(s) = sH + (1-s)H'$ from $s = 0$ to 1, where $H' = \sum_i X_i$.

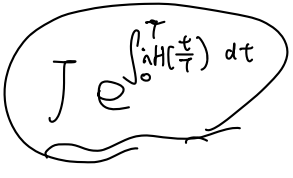
* If the evolution time is large compared to the inverse gap along the path, you will arrive at the right answer.

Trotterized Quantum Adiabatic Algorithm

[Farhi, Goldstone, Gutmann, Sipser (2000)]

Adiabatically evolve $H(s) = s\underset{\sim}{H} + (1-s)\underset{\frown}{H'}$ from $s = 0$ to 1, where $H' = \sum_i X_i$.

* Using the Trotter-Suzuki method, we can of course approximate the time evolution.



QAOA

[Farhi, Goldstone, Gutmann, Sipser (2000)]

Adiabatically evolve $H(s) = sH + (1-s)H'$ from $s = 0$ to 1, where $H' = \sum_i X_i$.

Apply $e^{i\theta_1 H} e^{i\phi_1 H'} \ldots e^{i\theta_N H} e^{i\phi_N H'}$ for finite N.

The hope is that you will get a "good enough" answer for a small N.

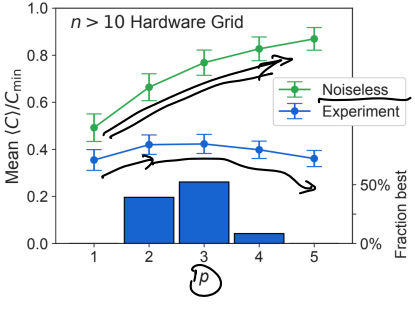
QAOA: Some history

1. 2014: QAOA proposed
2. 2014: QAOA shown to outperform the best known classical algorithm for MAX-3-LIN-2 (at the time)
3. 2015: Barak et al. comes up with a classical algorithm that beats QAOA.
4. 2019: Hastings provides evidence that finite-depth QAOA unlikely to beat “global” classical algorithms.

An interesting possibility: QAOA using logarithmic-depth.

Experiment

Since its proposal, QAOA has been implemented in a variety of setups. The largest implementation to date uses 23 qubits. [Harrigan et al. (2021)]



* From [Harrigan et al., Nature Physics **17**, 332-336 (2021)]

Challenges

1. Larger depth → more noise
2. Short depth → classically tractable
3. Unclear if a speedup is possible, even in principle
4. Finding good angles

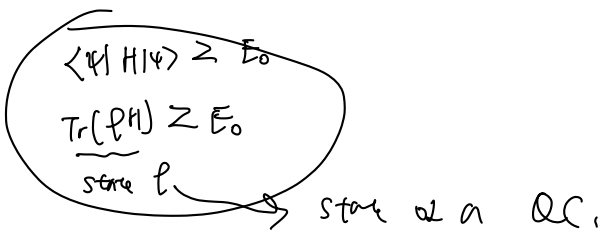
   An interesting idea: “Good angles” generalize well [Brandao et al. (2018)].

VQE

VQE = Variational Quantum Eigensolver [Peruzzo et al. (2014)]

Problem: Find the ground state energy of a Hamiltonian H.

Idea: Variational Principle



VQE vs. QPE

VQE

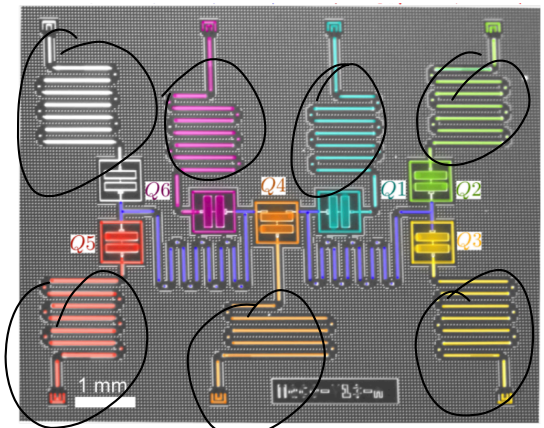
1. Easy to implement.
2. Need to begin with a state that is close to the ground state.
3. Scaling in error: $O(1/\epsilon^2)$

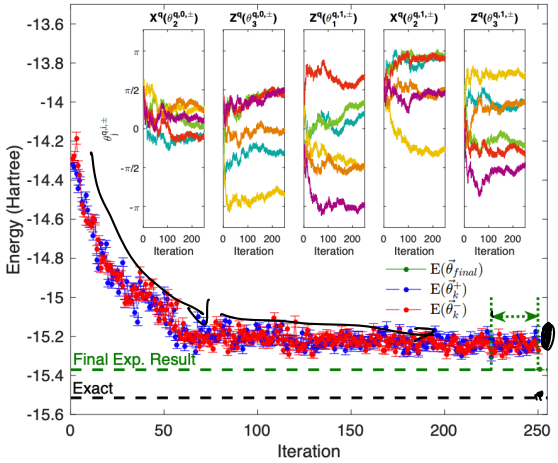
QPE

1. More complicated
2. All you need is a *constant (e.g., 0.3)* overlap with the ground state.
3. Scaling in error: $O(1/\epsilon)$

VQE: Experiment

[Kandala et al. (2017)]





$\theta_1, \cdots, \theta_N$

$E(\theta_1, \cdots, \theta_N) \rightarrow E(\theta_1 + \delta_1, \cdots, \theta_N + \delta_N) \rightarrow$ Gradient descent

$E(\theta_1 - \delta_1, \cdots, \theta_N - \delta_N)$

$H = \sum_i \alpha_i P_i \qquad \langle H \rangle = \sum_i \alpha_i \langle P_i \rangle$

$q_1\ q_2\ q_3$

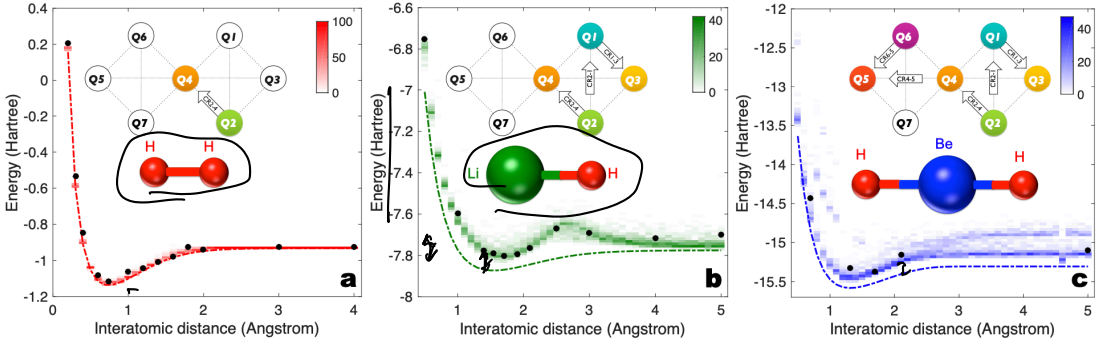
$Z \otimes Z \otimes Z$

$|0\rangle : (-1)^2$

$|1\rangle : (-1)^1$

VQE: Experiment

[Kandala et al. (2017)]



Chemists: "Chemical Accuracy": 1.6 mHa

Key Ingredients

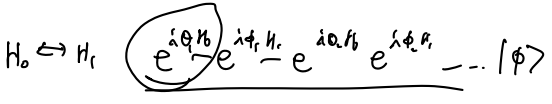
- Ansatz
- (Classical) Optimization Algorithm

Ansatz

- General unitary
- UCC
- Hamiltonian Variational Method
- Tensor Network

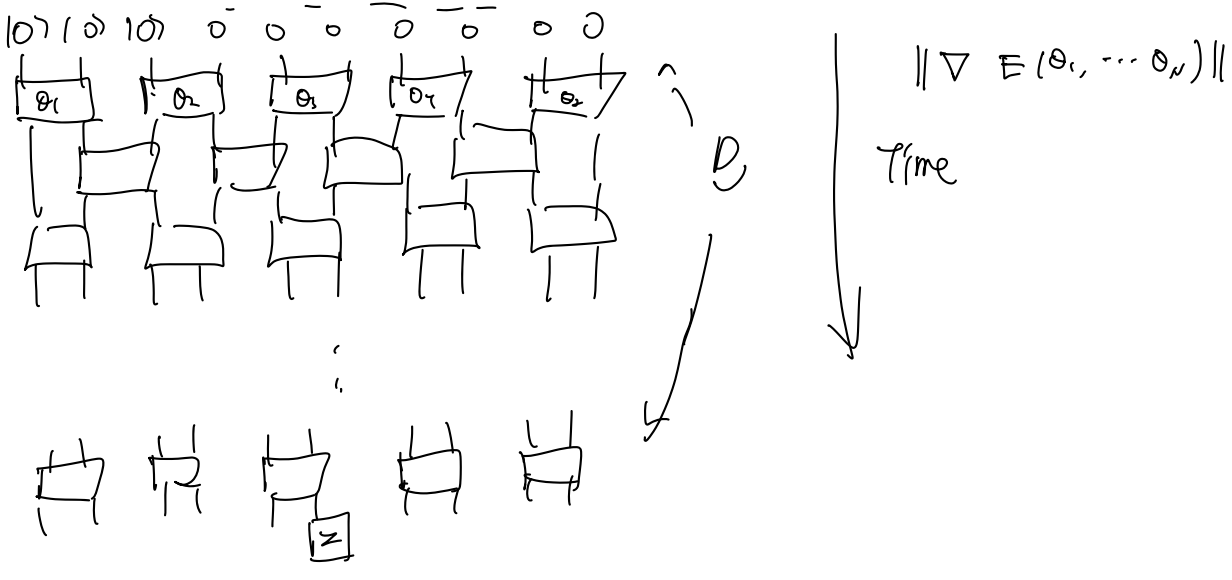
Ansatz: Approximation

- General unitary: Good for anything
- UCC: Quantum Chemistry Hamiltonians
- Hamiltonian Variational Method: States adiabatically connected to another state.
- Tensor Network: Locally interacting many-body systems



Barren Plateau

Warning: If the circuit depth becomes too large, the gradient vanishes exponentially!
[McClean et al. (2018)]

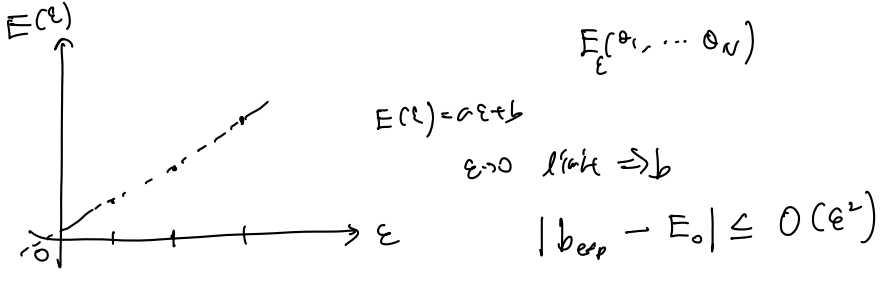


Optimization Algorithms

- A wide variety of methods have been worked out: SPSA, Gradient descent, Adam, …
- Spurious local minima may occur, and we need to understand how to avoid them!

Error mitigation

- [Temme et al. (2016), Li and Benjamin (2016)].
- Idea: *Increase* error and extrapolate.



VQE: Wishlists

- More error mitigation techniques
- Rigorous analysis on the approximation error
- Error scaling, in terms of the circuit geometry and gates
- Energy landscape

Summary

With the recent experimental progress, a great attention is given to algorithms that can be implemented in the near term. We currently do not know if these algorithms will end up being useful, because we can say very little about them rigorously.

But this could mean that there is an opportunity. With experiments, we will be able to get data which are theoretically too difficult to predict. Perhaps a new theory can be developed from these data.

A rigorous theoretical understanding of issues like approximation error, noise, and optimization, will be important.