Variational Quantum Algorithms

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구성

CONTENTS

Motivation

- **Why quantum algorithms?**
- Why VQAs? - NISQ Era

Motivation

Quantum Algorithms

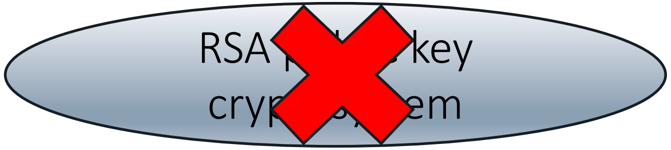
Why quantum algorithms?

- Quantum computer can theoretically solve some problems much faster than classical computers.

✓ Shor's factoring algorithm

✓ Grover's search algorithm

✓ Physics and chemistry simulations



[P. Shor, Polynomial-Time Algorithms for Prime Factorization and Discrete Logarithms on a Quantum Computer, SIAM J.Sci.Statist.Comput. 26 (1997)

Motivation

Quantum Algorithms

Resources for Shor's factoring algorithm

✓ ≈ 5,000 qubits to factor cryptographically significant numbers (without error correction)

✓ ≈ 1,000,000 qubits with error correction

✓ ≈ 100,000,000 quantum gates

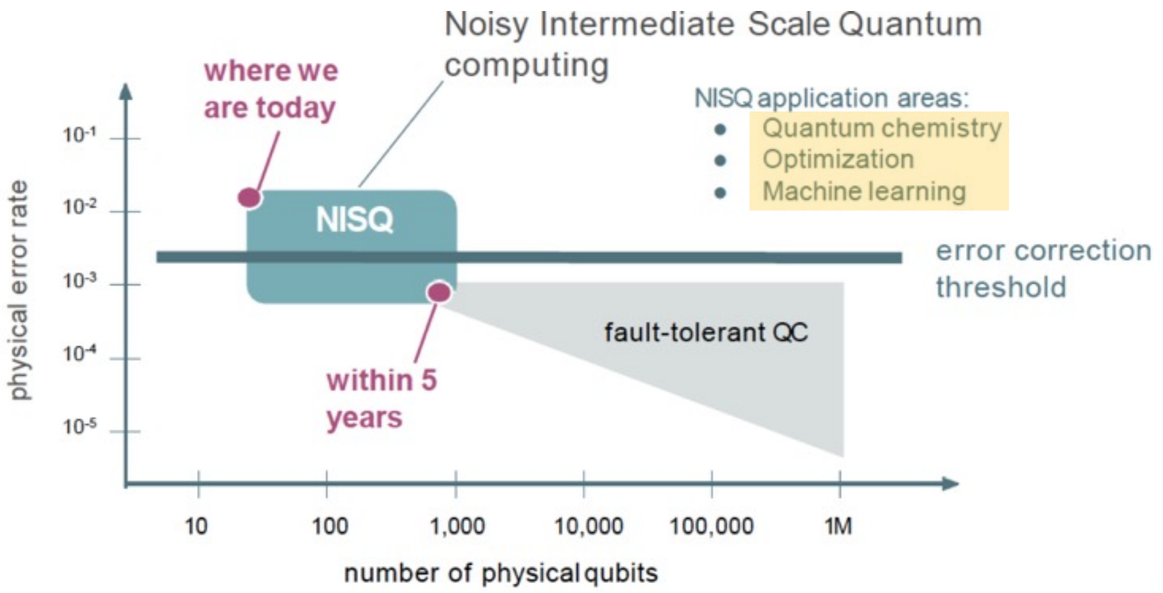
Motivation

- Why quantum algorithms?
- **Why VQAs? - NISQ Era**

Motivation

NISQ Era

NISQ (Noisy Intermediate-Scale Quantum) Era



[J. Preskill, Quantum Computing in the NISQ era and beyond, Quantum 2, 79 (2018)]

Motivation

Near-Term Quantum Algorithms

Near-Term Quantum Algorithms

✓ Algorithms run on small quantum computers

✓ Algorithms solve useful problems

✓ Low-depth, Robust to errors

✓ Efficient use of qubits

- It needs enough qubits to store the problem

For example, VQE (Variational Quantum Eigensolver) or

QAOA (Quantum Approximate Optimization Algorithm)

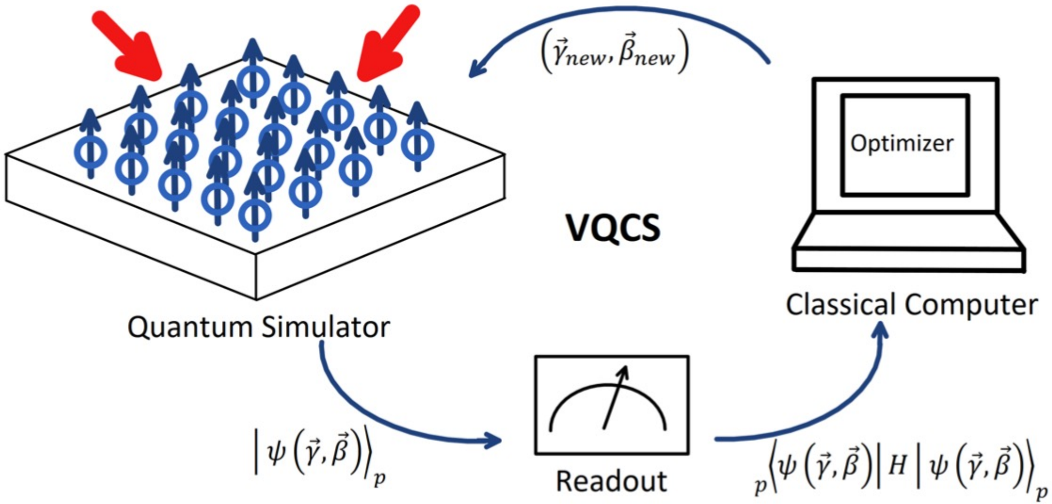
Variational Quantum Algorithms

- **What is VQAs?**
- VQE and QAOA

Variational Quantum Algorithms

What is VQAs?

Variational Quantum-Classical Simulations

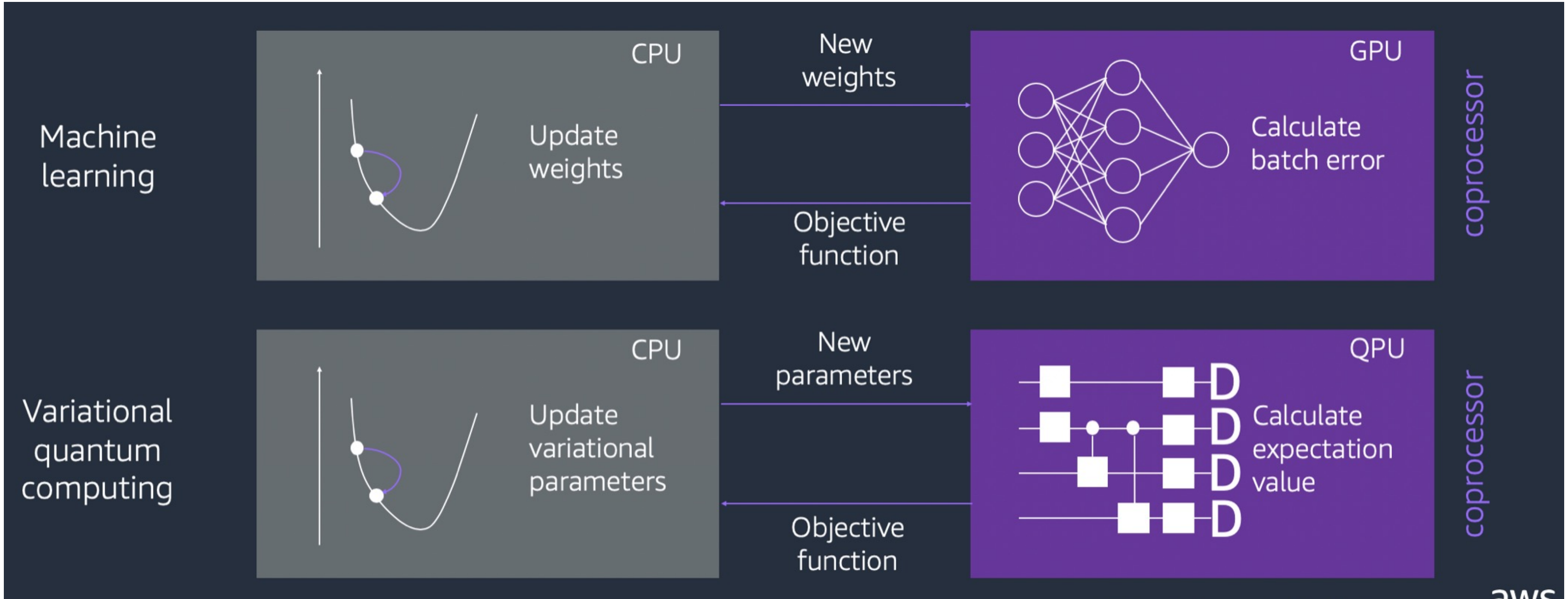


[W.W. Ho and T.H. Hsieh, Efficient variational simulation of non-trivial quantum states, SciPost Phys. 6, 029 (2019)]

Variational Quantum Algorithms

What is VQAs?

Variational Quantum-Classical Simulations



Variational Quantum Algorithms

- What is VQAs?
- **VQE** and QAOA

Variational Quantum Eigensolver (VQE)

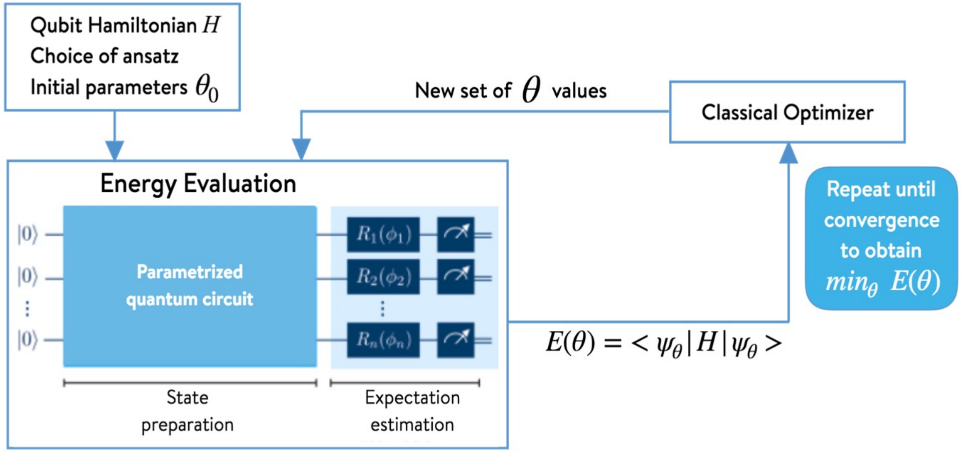
What is VQE?

- ✓ VQE is an approach to find the ground state of a quantum Hamiltonian H
- ✓ Based on the variational principle of quantum mechanics:

For all state $|\psi\rangle$,

$$\langle\psi|H|\psi\rangle \geq E_0$$

where E_0 is the ground energy of H



http://openqemist.1qbit.com/docs/_images/VQE_overview.png

[A. Peruzzo et al., A variational eigenvalue solver on a photonic quantum processor, Nature. Communications 5, (2014)]

Variational Quantum Eigensolver (VQE)

What is a good family of circuits to optimize over?

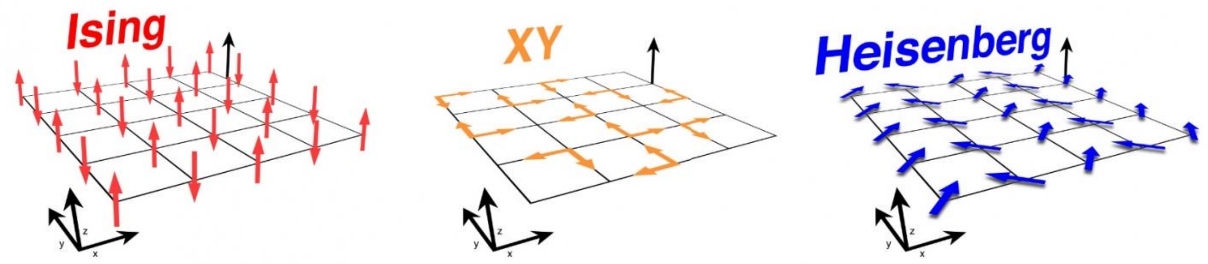
✓ k-local Hamiltonians: $H = \sum_i H_i$, and each H_i acts nontrivially on $\leq k$ qubits

Eg) Ising model : $H = \sum_{\langle i,j \rangle} Z_i Z_j$,

where $Z_i \equiv I \otimes \cdots \otimes Z \otimes \cdots \otimes I$ and $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

↑ i-th

Heisenberg model : $H = \sum_{\langle i,j \rangle} X_i X_j + Y_i Y_j + Z_i Z_j$



Variational Quantum Eigensolver (VQE)

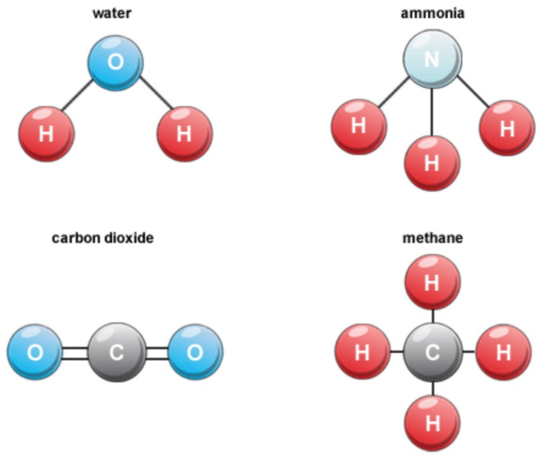
What is a good family of circuits to optimize over?

✓ Fermionic Hamiltonians (e.g. molecules):

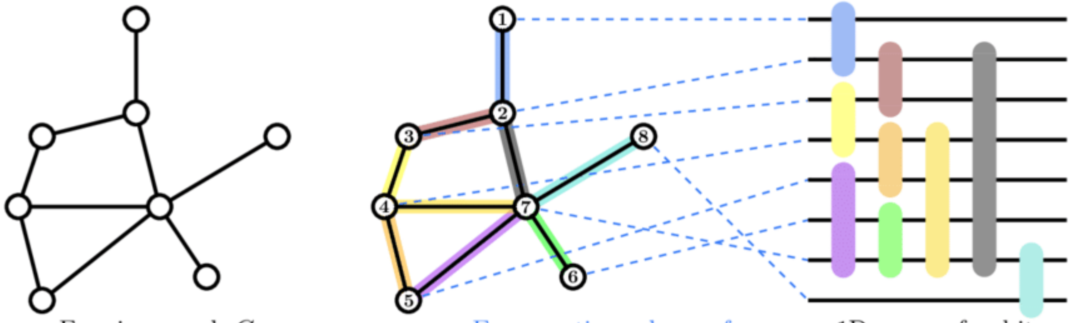
$$H = \sum_{i,j} h_{ij} a_i{}^\dagger a_j + \sum_{i,j,k,l} h_{ijkl} a_i{}^\dagger a_j a_k{}^\dagger a_l$$

Here, $a_i{}^\dagger$ and a_i are fermionic creation and annihilation operators.

$$a_i{}^\dagger \mapsto Z_1 \otimes \cdots \otimes Z_{i-1} \otimes |1\rangle\langle 0| \quad a_i \mapsto Z_1 \otimes \cdots \otimes Z_{i-1} \otimes |0\rangle\langle 1|$$



Jordan–Wigner transformation



Fermion graph G_F Enumeration scheme f 1D array of qubits

Variational Quantum Eigensolver (VQE)

Some variational ansatze – targeted at quantum simulation

✓ Hamiltonian Variational ansatz:

- Assume that: we want to find the ground state of $H = \sum_i H_i$

  we can write $H = H_A + H_B$

  ↑ easy to prepare the ground state of H_A

- Then: prepare the ground state of H_A

  For each of L layers l, implement $\prod_k e^{it_{lk}H_k}$ for some times $t_{lk} \in \mathbb{R}$

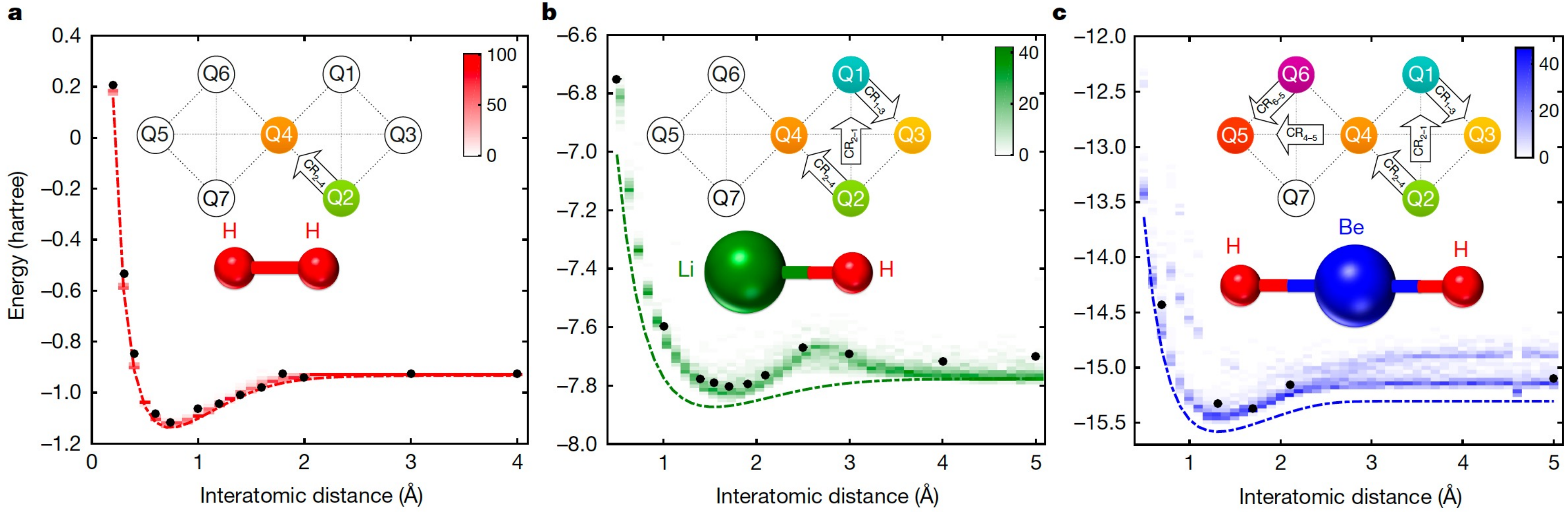
- Intuition comes from the **quantum adiabatic theorem**:

  As $L \to \infty$, this ansatz provably can represent the ground state of H.

Variational Quantum Eigensolver (VQE)

Applications of VQE

✓ Application to Quantum Chemistry

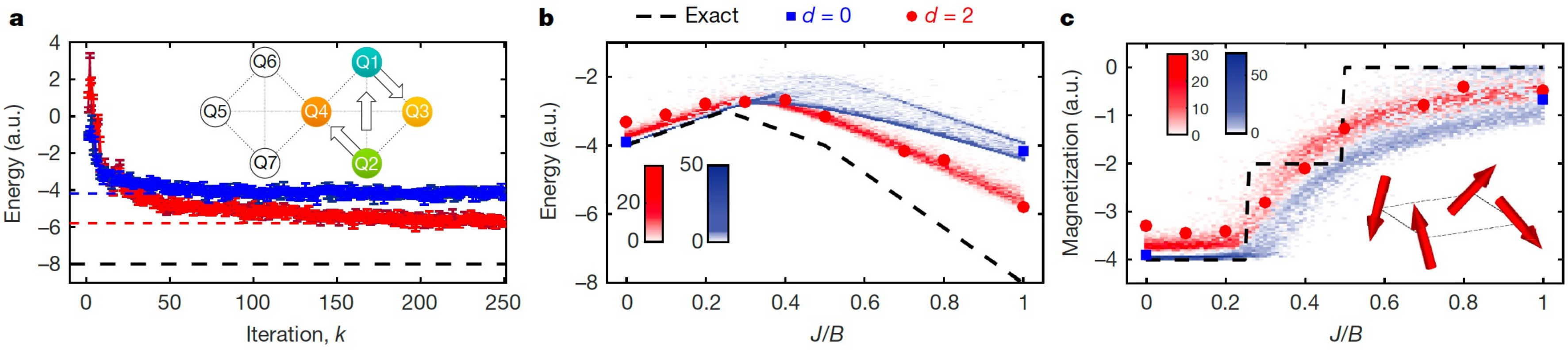


[A. Kandala et al., Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets, Nature 549, pp 242–246 (2017))]

Variational Quantum Eigensolver (VQE)

Applications of VQE

✓ Application to Quantum Magnetism



[A. Kandala et al., Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets, Nature 549, pp 242–246 (2017))]

Variational Quantum Algorithms

- What is VQAs?
- VQE and **QAOA**

Quantum Approximate Optimization Algorithm

What is QAOA?

QAOA

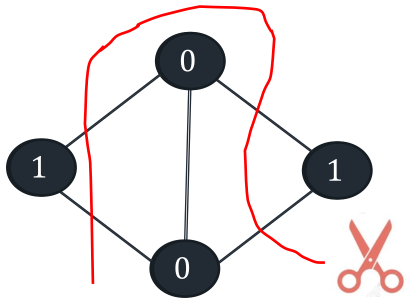
MAX-CUT Problem

- ✓ QAOA was introduced by Farhi *et al.* (2014)
- ✓ Apply VQE framework to solve classical optimization problem by setting

$$H = \sum_{x \in \{0,1\}^n} C(x) |x\rangle\langle x|$$

where $C(x)$ is a cost function.

- ✓ The ground state of H = the lowest-cost x



Cut = 4

[E. Farhi et al., A Quantum Approximate Optimization Algorithm, arXiv:1411.4028 (2014)]

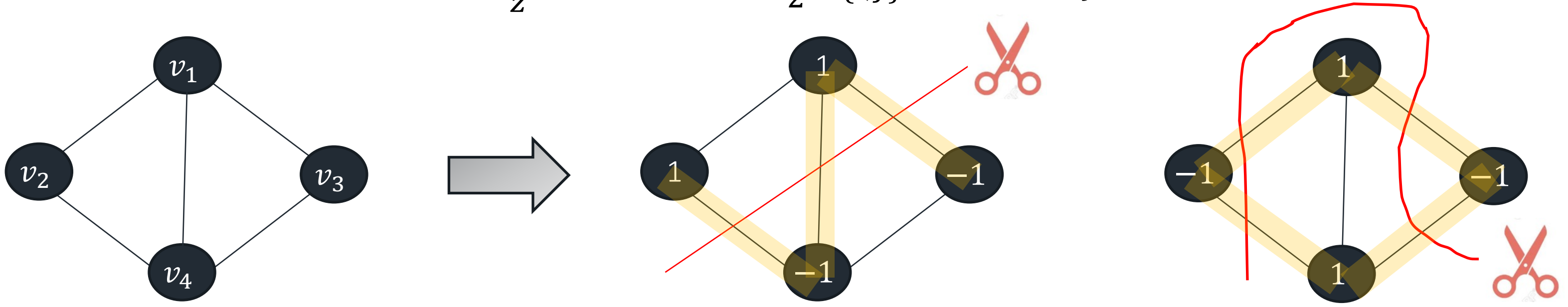
Quantum Approximate Optimization Algorithm

What is MAX-CUT problem?

MAX-CUT Problem

✓ Formulated as an optimization problem : for $z = (z_1, \cdots, z_N)$, $z_i \in \{-1,1\}\ \forall i$

$$\max_z C(z) = \max \frac{1}{2} \sum_{\{i,j\} \in E} (1 - z_i z_j)$$



$C(s) = \frac{1}{2}(2+2+2) = 3$

$C(s) = \frac{1}{2}(2+2+2+2) = 4$

Quantum Approximate Optimization Algorithm

QAOA for MAX-CUT Problem

QAOA for MAX-CUT Problem

- ✓ MAX-CUT Hamiltonian:

$$H_C = \frac{1}{2}\sum_{\{i,j\}\in E}(1 - Z_i Z_j)$$

- ✓ Note that $Z_i \equiv I\otimes\cdots\otimes Z\otimes\cdots\otimes I$ and $Z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$

  ↑ i-th

- ✓ $H_C|x\rangle = C(x)|x\rangle \quad \forall\, x \in \{0,1\}^N$

- ✓ $\max\limits_x C(x) = \max_x \frac{1}{2}\sum_{\{i,j\}\in E}(1-(-1)^{x_i}(-1)^{x_j}) = \max\limits_z C(z)$

Quantum Approximate Optimization Algorithm

What is QAOA?

Level p-QAOA

1. Initialize the quantum processor in $|+\rangle^{\otimes N}$
2. Generate a variational wavefunction

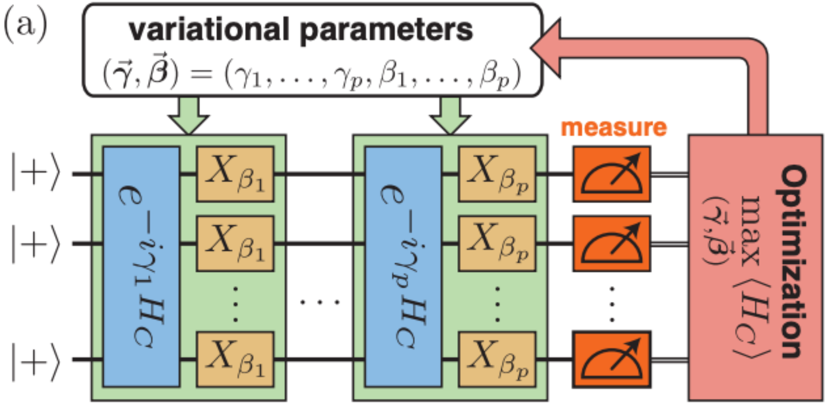
   $$|\psi_p(\vec{\gamma},\vec{\beta})\rangle = e^{-i\beta_p H_B} e^{-i\gamma_p H_C} \cdots e^{-i\beta_1 H_B} e^{-i\gamma_1 H_C} |+\rangle^{\otimes N}$$

   by applying the problem Hamiltonian H_C and a mixing Hamiltonian $H_B = \sum_{j=1}^{N} X_j$
3. Determine the expectation value

   $$F_p(\vec{\gamma},\vec{\beta}) = \langle \psi_p(\vec{\gamma},\vec{\beta}) | H_C | \psi_p(\vec{\gamma},\vec{\beta}) \rangle$$
4. Search for the optimal parameters

   $$(\vec{\gamma}^*,\vec{\beta}^*) = \arg\max_{\vec{\gamma},\vec{\beta}} F_p(\vec{\gamma},\vec{\beta})$$

   by a classical computer



[L. Zhou et al., Quantum Approximate Optimization Algorithm: Performance, Mechanism, and Implementation on Near-Term Devices, Phys. Rev. X 10, 021067, 2020]

Approximation ratio $r = \dfrac{F_p(\vec{\gamma}^*,\vec{\beta}^*)}{C_{\max}}$

Quantum Approximate Optimization Algorithm

Why should we imagine that QAOA works ?

- Intuition comes from the **quantum adiabatic theorem**:

  We start in the ground state of $H_A = \sum_j X_j$ and want to find the ground state of

$$H_B = H_C = \frac{1}{2} \sum_{\{i,j\} \in E} (1 - Z_i Z_j)$$

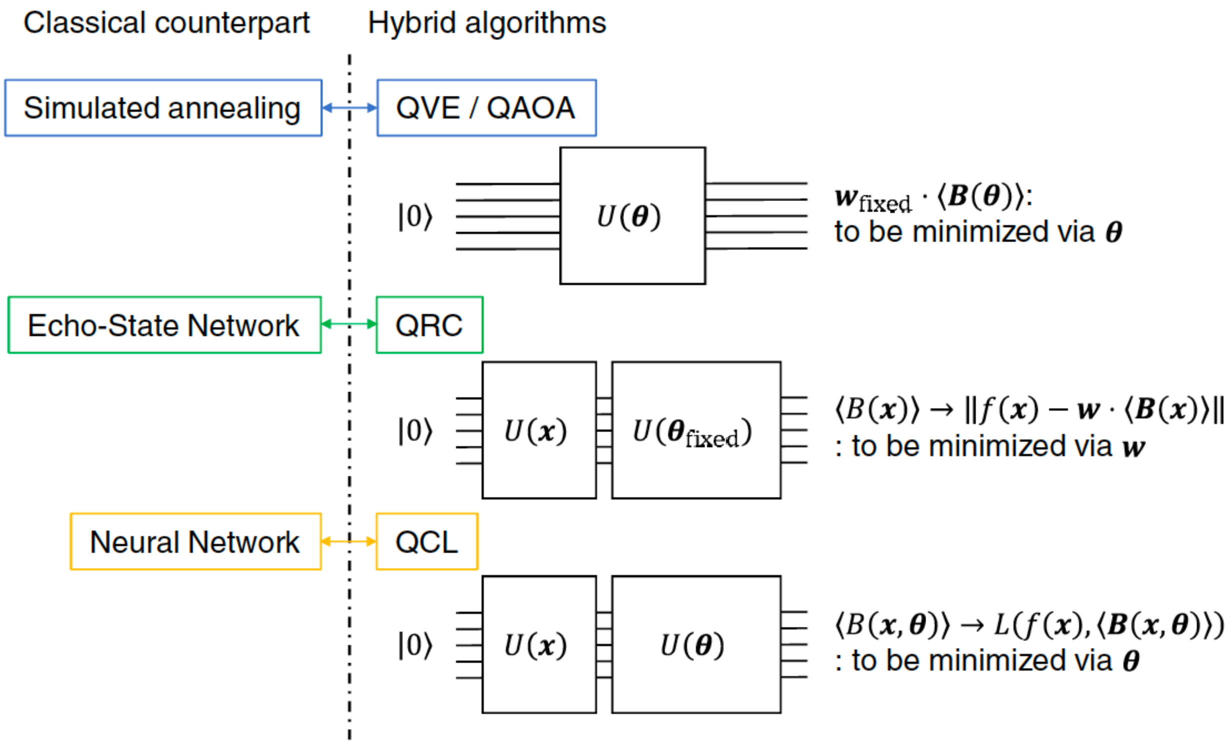
- If we smoothly change $H_A \rightarrow H_B$ slowly enough, we remain in the ground state.
- If we take **large enough p**, QAOA can find the ground state of H_C.

- QAOA essentially encompasses Grover's search algorithm.

VQAs and QML

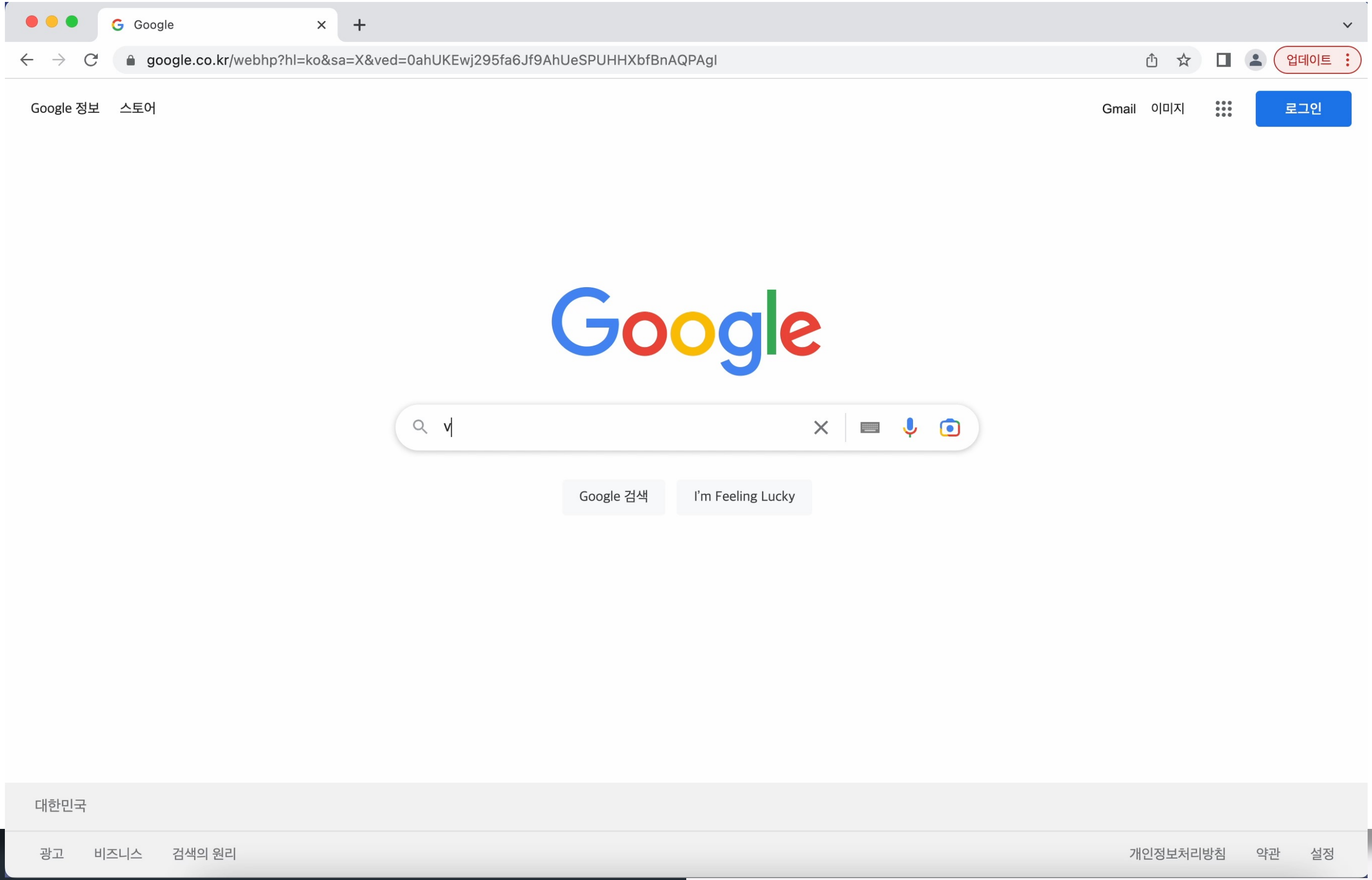
VQAs and QML

Quantum Circuit Learning



[K. Mitarai et al., Quantum circuit learning, PHYSICAL REVIEW A 98, 032309 (2018)

VQAs and QML


Google
google.co.kr/webhp?hl=ko&sa=X&ved=0ahUKEwj295fa6Jf9AhUeSPUHHXbfBnAQPAgI
업데이트
Google 정보
스토어
Gmail
이미지
로그인
Google
v
Google 검색
I'm Feeling Lucky
대한민국
광고
비즈니스
검색의 원리
개인정보처리방침
약관
설정

Thank you!