Quantum Approximate Optimization Algorithm
Part 1

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구성

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- VQE and QAOA

Variational Quantum Algorithms

What is VQAs?

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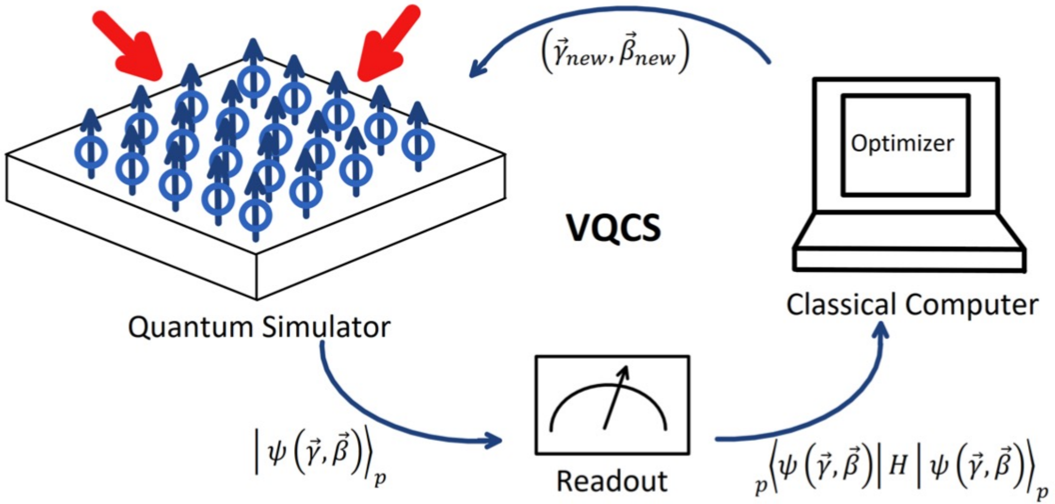
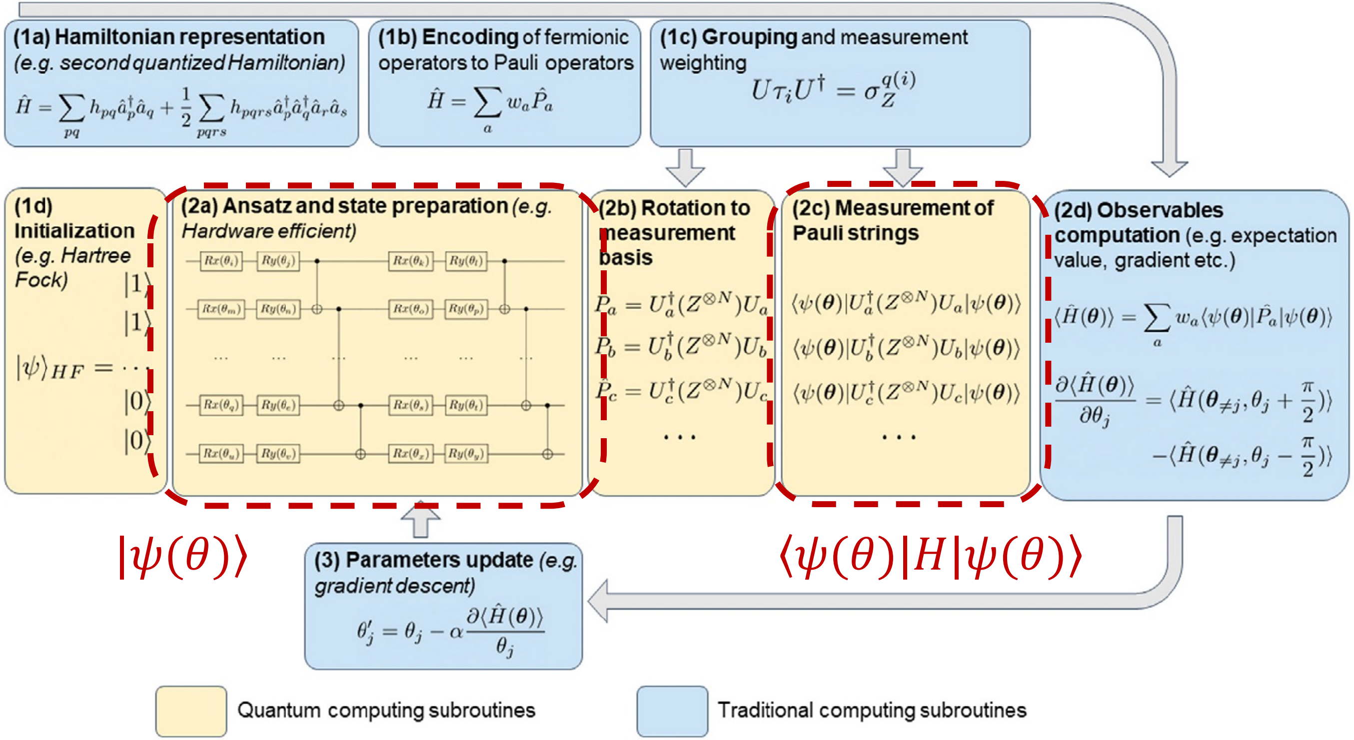


[W.W. Ho and T.H. Hsieh, Efficient variational simulation of non-trivial quantum states, SciPost Phys. 6, 029 (2019)]

Variational Quantum Eigensolver (VQE)

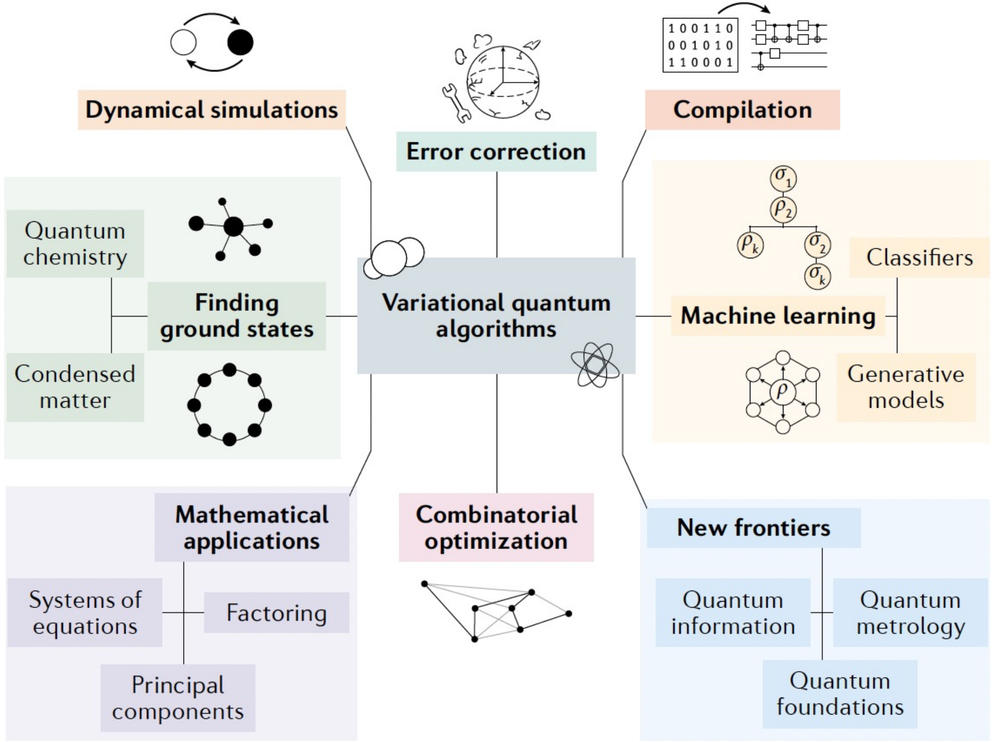
What is VQE?



[J. Tilly et al., The Variational Quantum Eigensolver: A review of methods and best practices, Physics Reports **986** 1–128 (2022)]

Variational Quantum Algorithms

What is VQAs?



[M. Cerezo et al., Variational quantum algorithms,, Nature Reviews Physics **3**, pages 625–644 (2021)]

Variational Quantum Algorithms

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

Quantum Approximate Optimization Algorithm

What is QAOA?

QAOA

- ✓ 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.

$$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}, |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

$$|0\rangle\langle 0| = \begin{pmatrix}1\\0\end{pmatrix}(1\ \ 0) = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}$$

$$|1\rangle\langle 1| = \begin{pmatrix}0\\1\end{pmatrix}(0\ \ 1) = \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix}$$

$$C(0)|0\rangle\langle 0| + C(1)|1\rangle\langle 1| = \begin{pmatrix}C(0) & 0\\0 & C(1)\end{pmatrix}$$

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

Quantum Approximate Optimization Algorithm

What is QAOA?

QAOA

- ✓ 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

$$H = C(0)|0\rangle\langle 0| + C(1)|1\rangle\langle 1| = \begin{pmatrix} C(0) & 0 \\ 0 & C(1) \end{pmatrix}$$

$$\langle 0|H|0\rangle = (1\ \ 0)\begin{pmatrix} C(0) & 0 \\ 0 & C(1) \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = C(0)$$

$$\langle 1|H|1\rangle = (0\ \ 1)\begin{pmatrix} C(0) & 0 \\ 0 & C(1) \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = C(1)$$

Generally,

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

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

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

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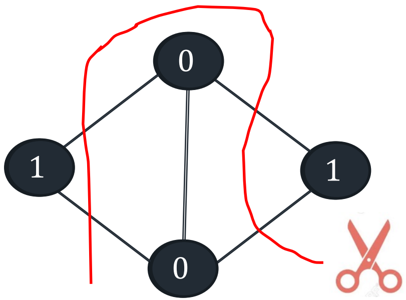


Cut = 4

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

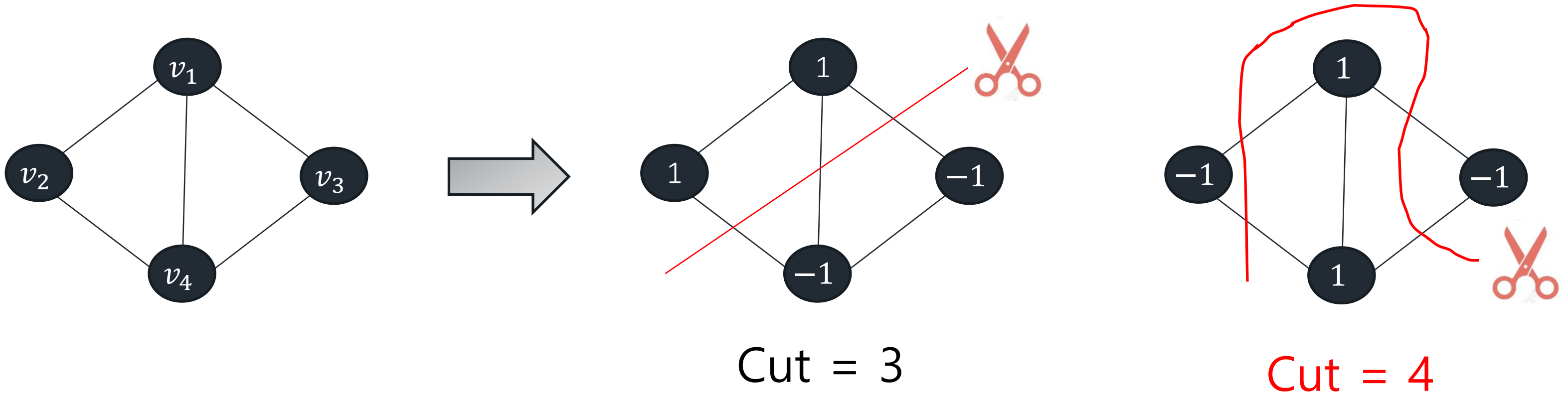
MAX-CUT problem

MAX-CUT problem

What is MAX-CUT problem?

MAX-CUT Problem

✓ **Goal**: Split the set of vertices V of a graph G into two disjoint parts such that the number of edges spanning two parts is maximized



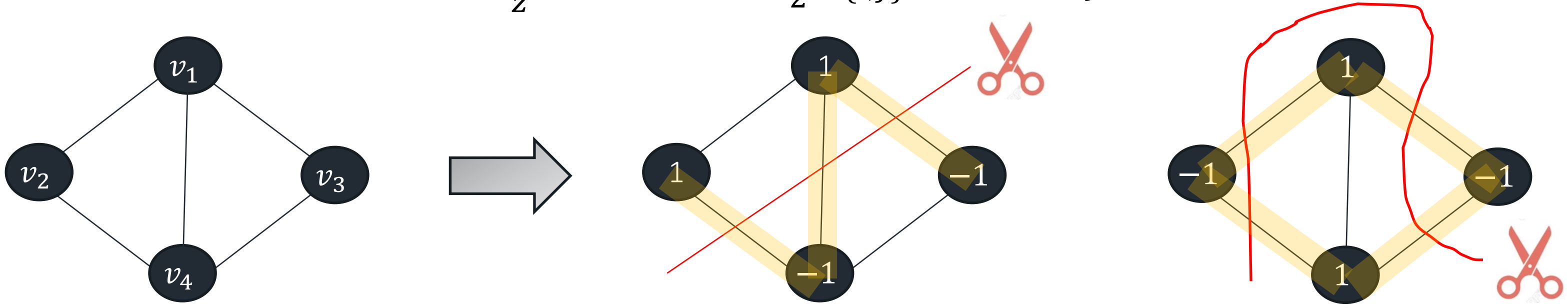
MAX-CUT problem

What is MAX-CUT problem?

MAX-CUT Problem

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

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



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

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

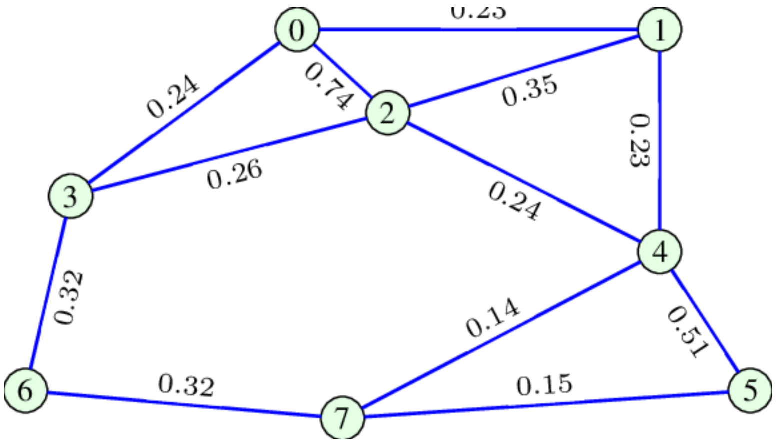
Weighted MAX-CUT problem

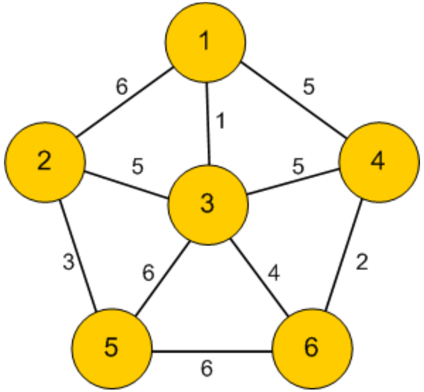
Weighted MAX-CUT problem

What is the weighted MAX-CUT problem?

Weighted MAX-CUT Problem

✓ Weighted undirected graph: $G = (V, E)$ with **edge weight $w_{ij} > 0$**, $w_{ij} = w_{ji}$ for $(i, j) \in E$





Weighted MAX-CUT problem

What is the weighted MAX-CUT problem?

Weighted MAX-CUT Problem

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

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

or, equivalently, for $\boldsymbol{x} = (x_1, \cdots, x_N)$, $x_i \in \{0,1\}\ \forall i$

$$\max_{\boldsymbol{x}} C(\boldsymbol{x}) = \max \frac{1}{2} \sum_{\{i,j\} \in E} \boldsymbol{w_{ij}} (1 - (-1)^{x_i} (-1)^{x_j})$$

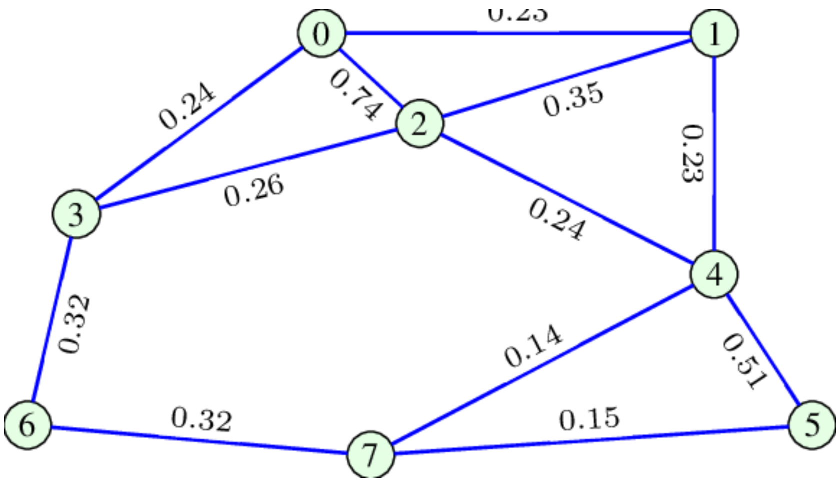
$$= \max \sum_{\{i,j\} \in E} \boldsymbol{w_{ij}} (1 - x_i) x_j$$

Weighted MAX-CUT problem

Applications of the weighted MAX-CUT problem

✓ Marketing model :

w_{ij} = probability that the person j will buy a product after i gets a free one



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
- ✓ $H_C|x\rangle = C(x)|x\rangle \quad \forall\, x \in \{0,1\}^N$
- ✓ $\max_x C(x) = \max_x \frac{1}{2}\sum_{\{i,j\}\in E}(1 - (-1)^{x_i}(-1)^{x_j}) = \max_z C(z)$

Pauli matrices

$$X = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, Y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, Z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

$$Z|0\rangle = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix} = |0\rangle, \qquad Z|1\rangle = -|1\rangle$$

$$Z_i Z_j = I\otimes\cdots\otimes Z\otimes\cdots\otimes Z\otimes\cdots\otimes I$$

↑ i-th ↑ j-th

$$Z_0 Z_2|1000\rangle = Z|1\rangle\otimes|0\rangle\otimes Z|0\rangle\otimes|0\rangle$$
$$= -|1000\rangle$$
$$= (-1)^{x_0}(-1)^{x_2}|1000\rangle$$

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 $H = H_B + H_C$

  ↑ easy to prepare the ground state of H_B

- 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**:

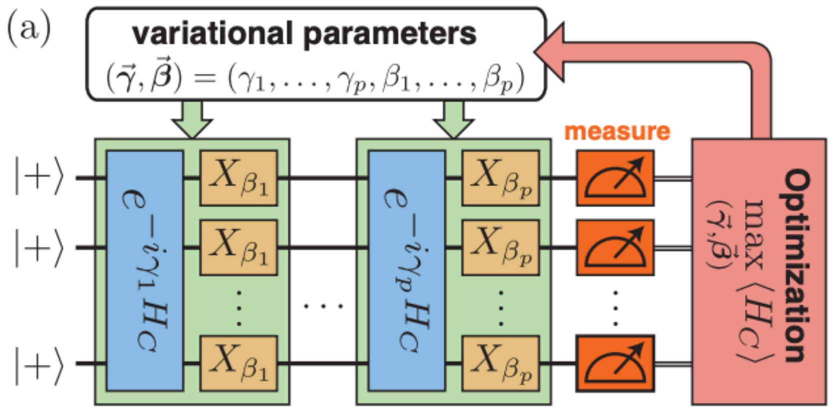
  As $L \to \infty$, this ansatz provably can represent the ground state of H.

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

Limitations of QAOA

Quantum Approximate Optimization Algorithm

What is QAOA?

Level p-QAOA

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

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

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$$F_p(\vec{\gamma},\vec{\beta}) = \langle\psi_p(\vec{\gamma},\vec{\beta})|H_C|\psi_p(\vec{\gamma},\vec{\beta})\rangle$$

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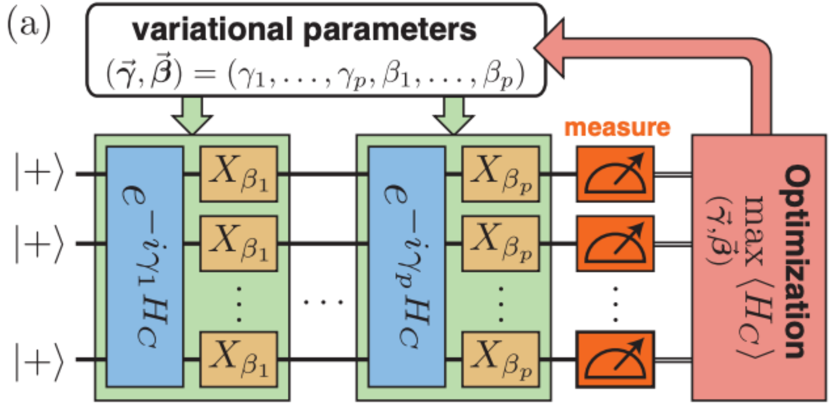

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Approximation ratio $r = \frac{F_p(\vec{\gamma}^*,\vec{\beta}^*)}{C_{max}}$

Quantum Approximate Optimization Algorithm

Limitations of QAOA

Bipartite D-regular graph (2019)

For every integer $D \geq 3, \exists$ an infinite family of bipartite D-regular graphs $\{G_n\}$ such that

$$\frac{1}{|E|}\langle +^n | U^{-1} H_n U | +^n \rangle \leq \frac{5}{6} + \frac{\sqrt{D-1}}{3D}$$

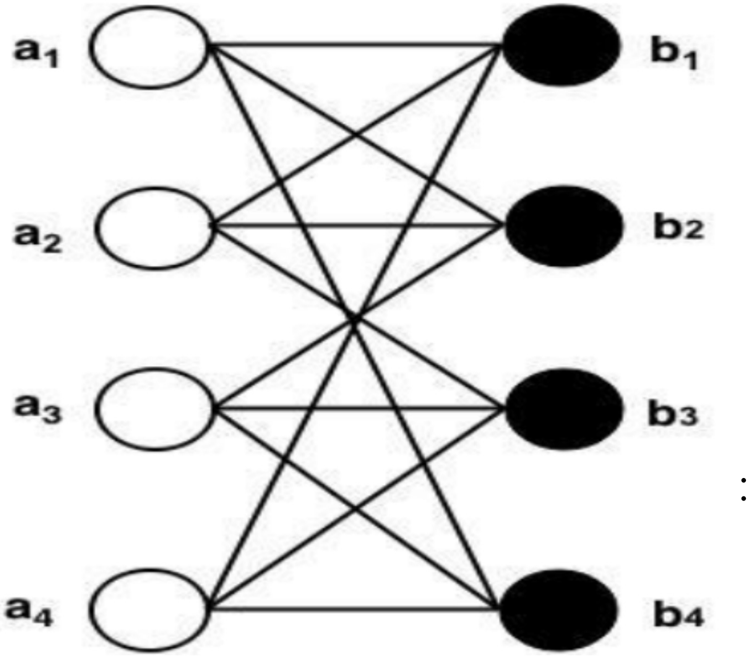
for any level-p QAOA circuit $U \equiv U(\beta, \gamma)$

as long as

$$p < (1/3 \log_2 n - 4) D^{-1},$$

where

$$H_n = \frac{1}{2} \sum_{(u,v)\in E} (I - Z_u Z_v).$$



[S. Bravyi *et al.*, Obstacles to State Preparation and Variational Optimization from Symmetry Protection, Phys. Rev. Lett. 125, 260505 (2019)]

Quantum Approximate Optimization Algorithm

Limitations of QAOA

Ring of disagrees (2019)

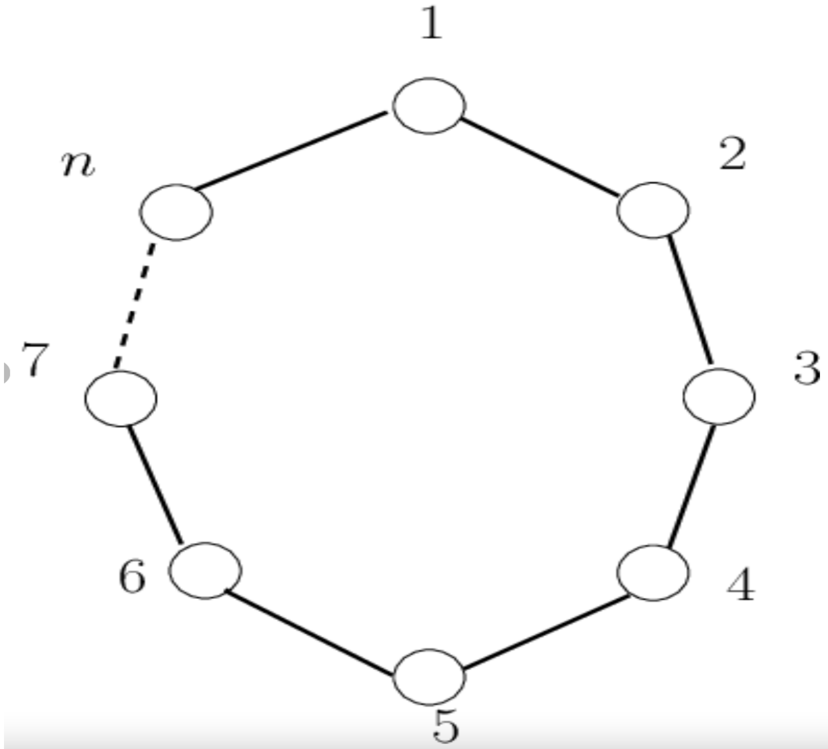
Let H_n be the ring of disagrees Hamiltonian

$$H_n = \frac{1}{2} \sum_{p \in \mathbb{Z}_n} (I - Z_p Z_{p+1}),$$

when n is even.

Let U be a Z_2-symmetric unitary with range $R < n/4$. Then

$$\frac{1}{n} \langle +^n | U^\dagger H_n U | +^n \rangle \leq \frac{2R + 1/2}{2R + 1}.$$



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Thank you!

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