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Quantum Approximate Optimization Algorithm (QAOA) on Constrained Optimization Problems

Jaimie Stephens, Ciaran Ryan-Anderson, and Ojas Parekh

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Optimization Problems

Types of Binary Optimization Problems

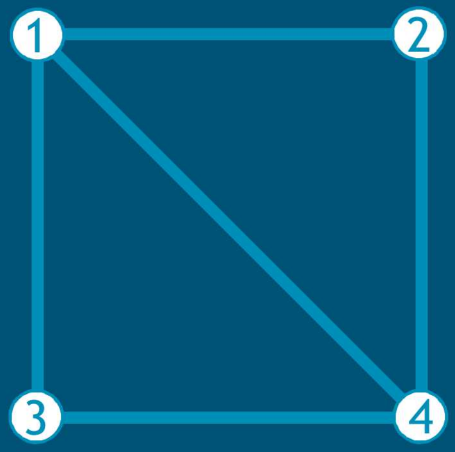
- Unconstrained Optimization
  - MaxCut
  - MaxE3Lin2

- Constrained Optimization
  - MinVertexCover

MaxCut

- Given a graph $G = (V, E)$, we want to partition the vertices into two sets $V' \subseteq V$ and V/V', s.t. the number of edges, $\{u, v\} \in E$, that have $u \in V'$ and $v \in V/V'$ is maximized.

- Example: MAXCUT = ?



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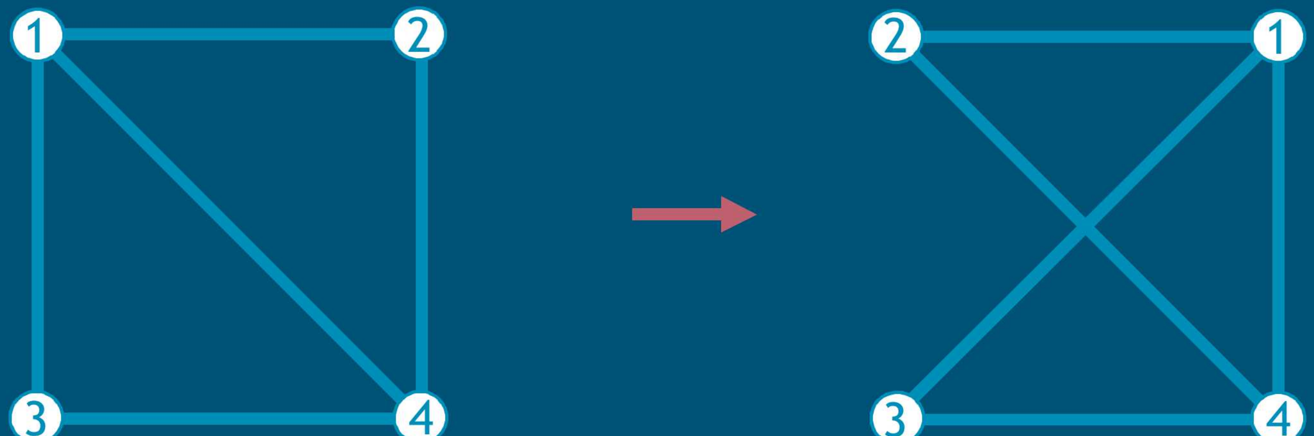
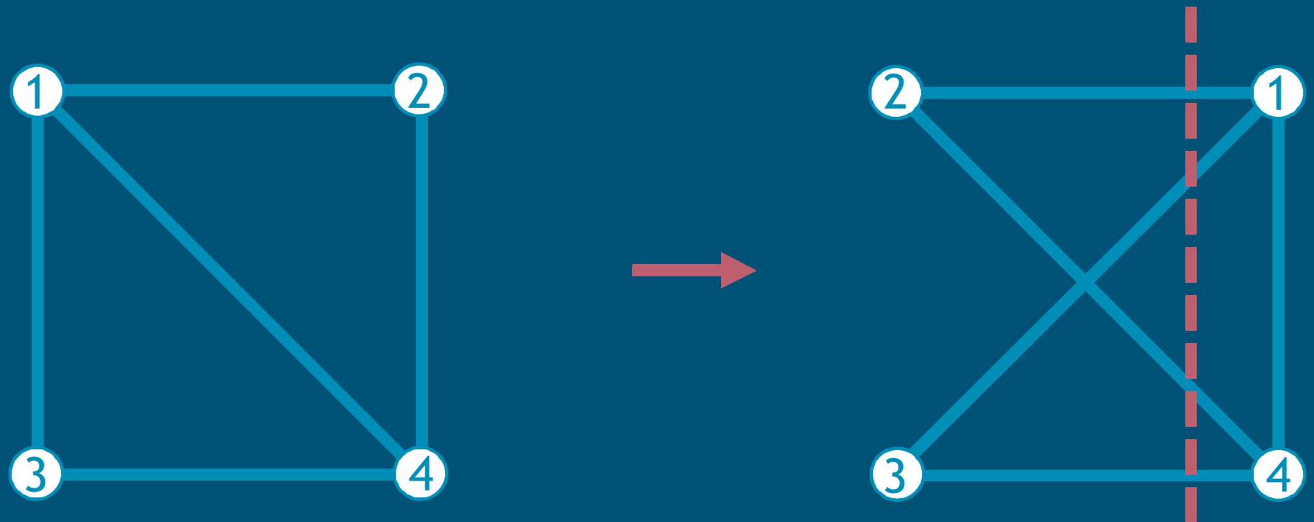


MAXCUT

- Given a graph $G = (V, E)$, we want to partition the vertices into two sets $V' \subseteq V$ and V/V', s.t. the number of edges, $\{u, v\} \in E$, that have $u \in V'$ and $v \in V/V'$ is maximized.

- Example: MAXCUT = 4



MaxE3Lin2

Given a system of linear equations $E_1, E_2, \ldots, E_n$, over $\mathbb{Z}_2$ where each linear equation, E_j, has exactly three variables, $(x_j, x_k, x_l) \in \{0,1\}$. We want to find variables, $x_1, \ldots, x_m$, s.t. the maximum number of equations are satisfied.

MaxE3Lin2

Example: MAXE3LIN2 = ?

$$E_1:\ x_1 + x_2 + x_3 = 1$$
$$E_2:\ x_1 + x_3 + x_5 = 0$$
$$E_3:\ x_2 + x_4 + x_6 = 1$$
$$E_4:\ x_4 + x_5 + x_6 = 1$$

MaxE3Lin2

Example: MAXE3LIN2 = ?

$$E_1\colon\ x_1 + x_2 + x_3 = 1$$
$$E_2\colon\ x_1 + x_3 + x_5 = 0$$
$$E_3\colon\ x_2 + x_4 + x_6 = 1$$
$$E_4\colon\ x_4 + x_5 + x_6 = 1$$

If we let $x_1 = x_2 = x_3 = x_5 = 1$ and $x_4 = x_6 = 0$ then E_1, E_3, and E_4 are satisfied, but not E_2.

MAXE3LIN2

Example: MAXE3LIN2 = ?

$$E_1 \colon x_1 + x_2 + x_3 = 1$$
$$E_2 \colon x_1 + x_3 + x_5 = 0$$
$$E_3 \colon x_2 + x_4 + x_6 = 1$$
$$E_4 \colon x_4 + x_5 + x_6 = 1$$

Note that the LHS adds up to 0 while the RHS adds up to 1. Thus we cannot satisfy all four clauses simultaneously.

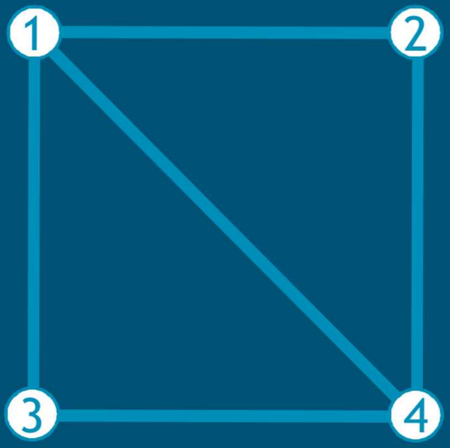
MaxE3Lin2

Example: MAXE3LIN2 = 3

$$E_1:\ x_1 + x_2 + x_3 = 1$$
$$E_2:\ x_1 + x_3 + x_5 = 0$$
$$E_3:\ x_2 + x_4 + x_6 = 1$$
$$E_4:\ x_4 + x_5 + x_6 = 1$$

VertexCover

Given a graph $G = (V, E)$, we want to find a subset of vertices $V' \subseteq V$, s.t. $\forall$ edges $\{u, v\} \in E$, $u \in V'$ or $v \in V'$.



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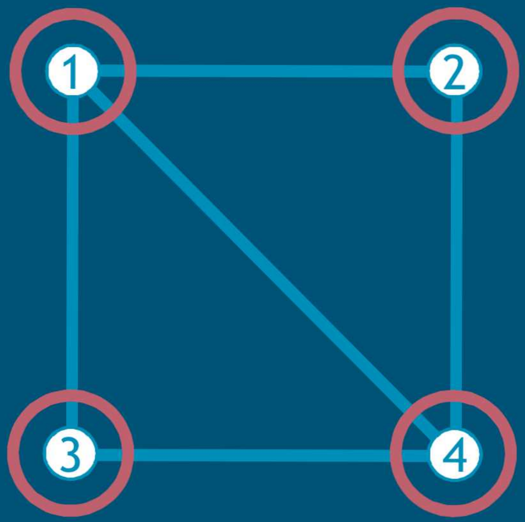

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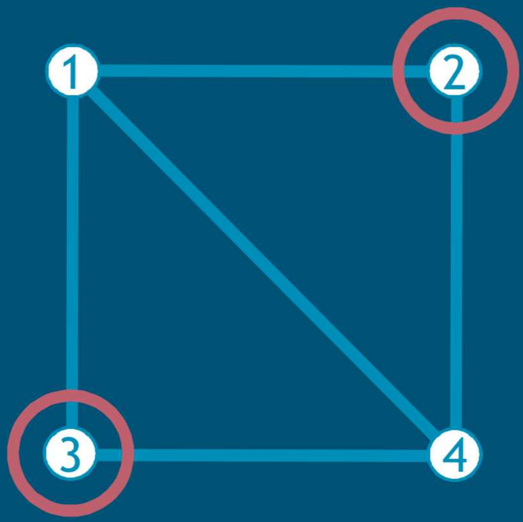

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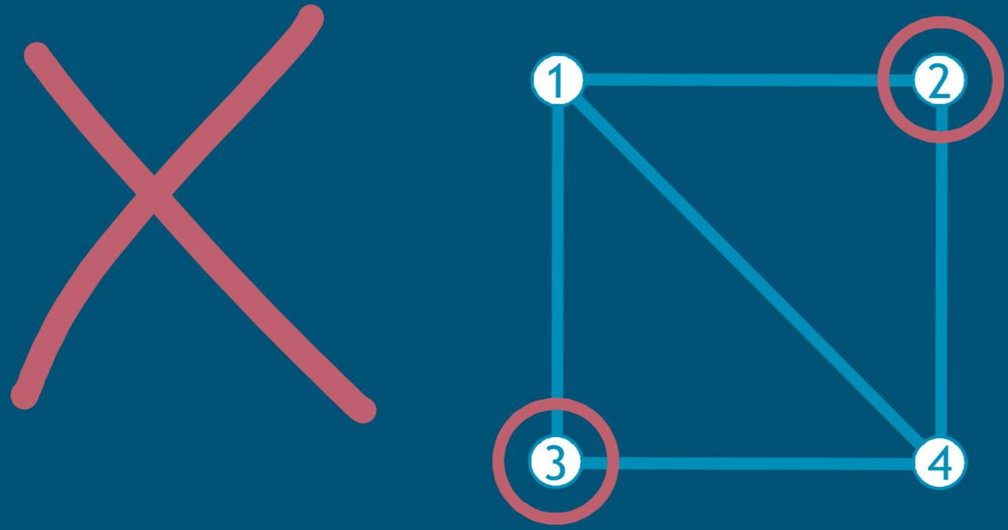

VertexCover

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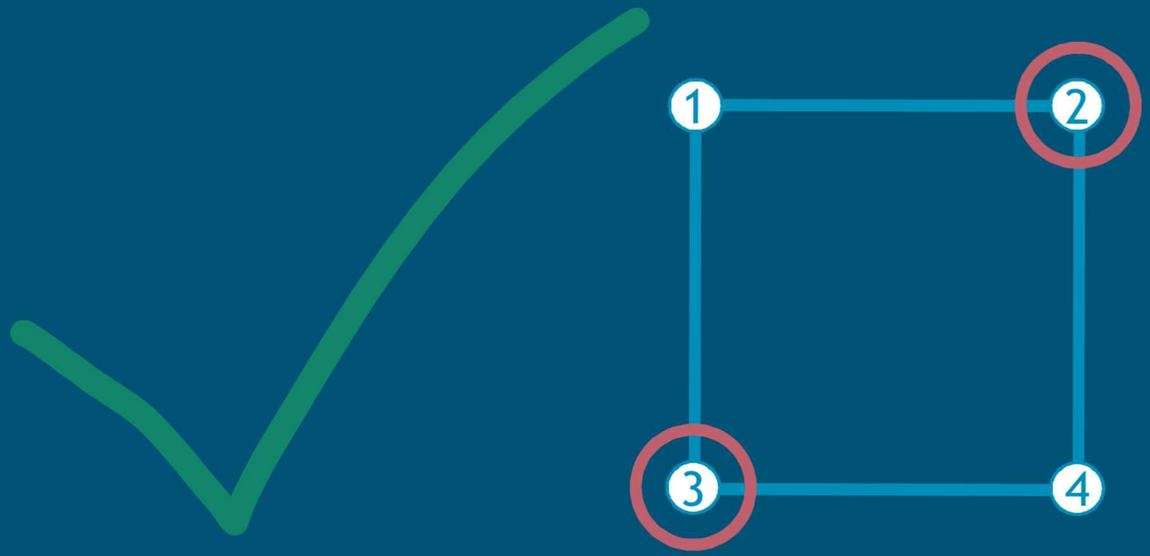
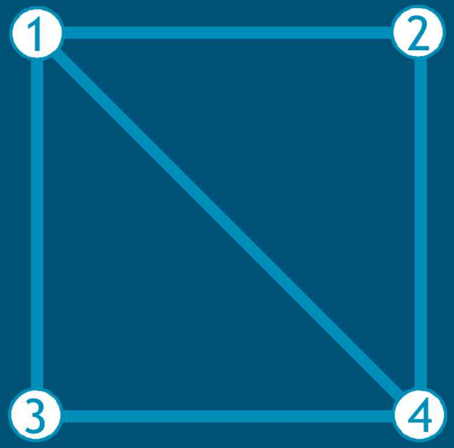


MINVERTEXCOVER

- Given a graph $G = (V, E)$, we want to find the minimum subset of vertices $V' \subseteq V$, s.t. for all edges $\{u, v\} \in E$, $u \in V'$ or $v \in V'$.

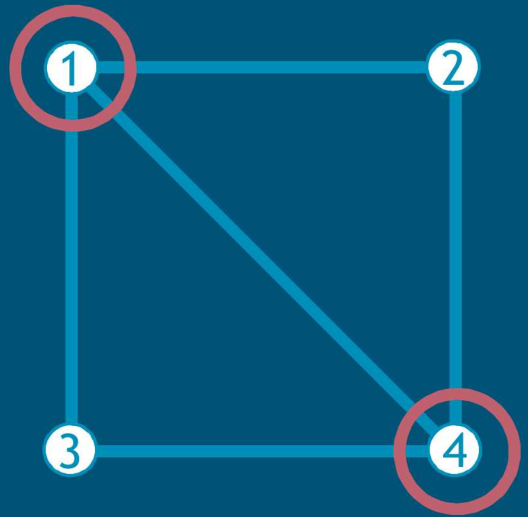
- Example: MINVERTEXCOVER = ?



MinVertexCover

- Given a graph $G = (V, E)$, we want to find the minimum subset of vertices $V' \subseteq V$, s.t. for all edges $\{u, v\} \in E$, $u \in V'$ or $v \in V'$.

- Example: MinVertexCover $= 2$



Quantum Approximate Optimization Algorithm (QAOA)[1]

[1] Farhi and Goldstone (2014)

What is QAOA?

- The goal of QAOA is to approximate hard optimization problems on a quantum computer.

- Given $f: \{0,1\}^n \rightarrow \mathbb{R}$, find $x \in \{0,1\}^n$ s.t. $f(x)$ is a minimum (maximum).

- We can represent $f(x)$ as a problem Hamiltonian,

$$H_P|x\rangle = f(x)|x\rangle.$$

Inspiration

QAOA was inspired by Trotterization of Adiabatic Quantum Computing (AQC)

AQC

- In AQC we start in a ground state of a driver Hamiltonian that is easy to prepare i.e.

$|s\rangle = |+\rangle^{\otimes n}$, the ground state of $H_D = -\sum_{j=1}^{n} X_j$

- We then evolve under the Hamiltonian,

$$H(t) = s(t)H_P + \big(1 - s(t)\big)H_D$$

where $s = s(t)$ is a smooth function of t, $s(t = 0) = 0$, and $s(t = \mathrm{T}) = 1$.

Trotterization

$$U(T,0) = U(T,T-\Delta t)U(T-\Delta t, T-2\Delta T)\ldots U(\Delta t, 0) = \prod_{k=1}^{N} U(k\Delta t, (k-1)\Delta t)$$

where $\Delta t = {}^{T}/_{N}$ and,

$$U(t_2, t_1) = \mathcal{T}\exp\left[-i\int_{t_1}^{t_2} H(t)dt\right].$$

Trotterization

For $\Delta t \ll T$, $H(t)$ is approximately constant over the time interval Δt.

$$U(T,0) \approx \prod_{k=1}^{N} e^{-i\Delta t H(k\Delta t)}$$

Lie-Trotter-Suzuki

We now use the Lie-Trotter-Suzuki decomposition,

$$e^{\delta(A+B)} \approx e^{\delta A} e^{\delta B} + O(\delta^2\ )$$

with the assumption that $\Delta t \ll T$ to make the approximation

$$U(T,0) \approx \prod_{k=0}^{N} e^{-i\Delta t\left[s(k\Delta t)H_P + \left(1-s(k\Delta t)\right)H_D\right]}$$

$$\approx \prod_{k=0}^{N} e^{-i\Delta t\left(1-s(k\Delta t)\right)H_D} e^{-i\Delta t s(k\Delta t)H_P} .$$

QAOA

- Now for QAOA we let N become p where $p \ll N$.
- We then define $\boldsymbol{\beta} = \beta_1\beta_2 \dots \beta_p$ and $\boldsymbol{\gamma} = \gamma_1\gamma_2 \dots \gamma_p$ as free parameters.
- We let $\Delta t\big(1 - s(k\Delta t)\big)$ go to β_k and $\Delta t s(k\Delta t)$ go to γ_k.
- Now we define the $QAOA_p$ operator

$$Q_p(\boldsymbol{\beta}, \boldsymbol{\gamma}) = \prod_{k=0}^{p} e^{-i\beta_k H_D} e^{-i\gamma_k H_P} .$$

Goal

We want to find optimal times $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ for some number of iterations $p \ll \infty$ such that the expectation value of the problem Hamiltonian is minimized.

$$\min_{\boldsymbol{\beta},\boldsymbol{\gamma}} \langle \boldsymbol{\beta}, \boldsymbol{\gamma} | H_P | \boldsymbol{\beta}, \boldsymbol{\gamma} \rangle$$

Does it work?

- From Trotterization, it follows that we obtain the optimal solution when $p \to \infty$. Due to the curse of dimensionality, it is difficult to analyze $p > 1$.

- For MaxE3Lin2, Farhi and Goldstone showed $QAOA_1$ made a better approximation than the best known classical algorithm only to inspire a better classical algorithm. [1]

[1] Farhi and Goldstone (2014)

Approximating Constrained Optimization Problems

QAOA++[1][2]

- Problem Hamiltonian:

$$H_P = \sum_{x=0}^{2^n-1} f(x)|x\rangle\langle x|$$

- Driving Hamiltonian:

$$H_D|x\rangle = \sum_j c_j|x_j\rangle \;\forall\; |x\rangle \in \mathcal{F}$$

where $\{|x_j\rangle\}$ is the basis for $\mathcal{F}$, and $\mathcal{F}$ is the space of feasible solutions.

- Initial state: $|s\rangle \in \mathcal{F}$

[1] Hadfield et. al. (2017) [2] Marsh and Wang (2018)

Constrained Quantum Annealing[1] (CQA)

- Problem Hamiltonian:

$$H_P = \sum_{x=0}^{2^n-1} f(x)|x\rangle\langle x|$$

- Driving Hamiltonian: Choose H_D s.t. $[H_D, H_F] = 0$ where for the computational basis $\{|x_j\rangle\}$,

$$H_F|x_j\rangle = \begin{cases} 0 & \text{if } |x_j\rangle \in \mathcal{F} \\ \lambda_j|x_j\rangle \text{ s.t. } \lambda_j \gg 0 & \text{if } |x_j\rangle \notin \mathcal{F} \end{cases}.$$

- Initial state: $|s\rangle \in \mathcal{F}$

[1] Hen and Spedalieri (2016)

QAOA with Penalties

- Problem Hamiltonian:

$$H_P = \sum_{x=0}^{2^n-1} f(x)|x\rangle\langle x| + \alpha H_F$$

- Driving Hamiltonian:

$$H_D = \sum_{j=0}^{2^n} X_j$$

- Initial state: $|s\rangle = |+\rangle^{\otimes n}$

QAOA++ $\Leftrightarrow$ CQA

$(\Longrightarrow)$

- Suppose $\forall\ |f\rangle \in \mathcal{F}$,

$$H_D\Big|f\rangle = \sum_j c_j\Big|f_j\rangle.$$

- Define

$$H_F = \sum_{x=0}^{2^n-1} c_x|x\rangle\langle x| \text{ where } c_x = \begin{cases} 0\ if\ |x\rangle \in \mathcal{F} \\ 1 \qquad\qquad o.w. \end{cases}.$$

QAOA++ $\Leftrightarrow$ CQA

$(\Longrightarrow)$

If $\langle x|H_D H_F|y\rangle = \langle x|H_F H_D|y\rangle$ $\forall$ basis vectors $|x\rangle$ and $|y\rangle$ of the full space then $[H_D, H_F] = 0$.
There are three cases:

- $|x\rangle \in \mathcal{F}$ and $|y\rangle \in \mathcal{F}$
- Either $|x\rangle$ or $|y\rangle \in \mathcal{F}$, but not both.
- $|x\rangle \notin \mathcal{F}$ and $|y\rangle \notin \mathcal{F}$.

QAOA++ $\Leftrightarrow$ CQA

$(\Longrightarrow)$

- Case 1: $|x\rangle \in \mathcal{F}$ and $|y\rangle \in \mathcal{F}$.

$$H_F|x\rangle = H_F|y\rangle = 0$$

$$\Rightarrow \langle x|H_D H_F|y\rangle = \langle x|H_F H_D|y\rangle = 0.$$

QAOA++ $\Leftrightarrow$ CQA

$(\Longrightarrow)$

- Case 2: Either $|x\rangle$ or $|y\rangle \in \mathcal{F}$, but not both.

  WLOG let $|x\rangle \in \mathcal{F}$.

  Then $H_D|x\rangle \in \mathcal{F}$.

  $\Longrightarrow H_F|x\rangle = H_F(H_D|x\rangle) = 0.$

  Thus $\langle x|H_D H_F|y\rangle = \langle x|H_F H_D|y\rangle = 0.$

QAOA++ $\Leftrightarrow$ CQA

$(\Longrightarrow)$

- Case 3: $|x\rangle \notin \mathcal{F}$ and $|y\rangle \notin \mathcal{F}$.

  $H_F|x\rangle = |x\rangle$ and $H_F|y\rangle = |y\rangle$.

  $\Longrightarrow \langle x|H_D H_F|y\rangle = \langle x|H_D|y\rangle = \langle x|H_F H_D|y\rangle$.

QAOA++ $\Leftrightarrow$ CQA

$(\Leftarrow)$

- Suppose $[H_D, H_F] = 0$, and let the feasible subspace be the ground state of the feasible Hamiltonian

$$H_F|x\rangle = 0 \text{ iff } |x\rangle \in \mathcal{F}.$$

- Let $|x\rangle \in \mathcal{F}$. Then

$$H_F(H_D|x\rangle) = H_D H_F|x\rangle = 0.$$

- Thus $H_D|x\rangle \in \mathcal{F} \;\; \forall \, |x\rangle \in \mathcal{F}$.

QAOA++ ⇔CQA

Therefore if you have a driving Hamiltonian for QAOA++ you can use it for CQA and if you have a driving Hamiltonian for CQA you can use it for QAOA++. ■

Future Work

How does QAOA with penalties compare?

- Look at MinVertexCover.
- Then look at the general case.

MinVertexCover Mapping[1]

- Given a graph, $G = (V, E)$, assign each qubit to a vertex $v \in V$.

- If a qubit is in the -1 eigenstate of Z, $|1\rangle$, the vertex represented by that qubit is in the vertex cover. If a qubit is in the $+1$ eigenstate of Z, $|0\rangle$, the vertex represented by that qubit is not in the vertex cover.

[1] Hadfield et. al. (2017)

QAOA++ [1]

- Problem Hamiltonian:

$$H_P = \sum_{u \in V} W_u$$

where $W_u = |1\rangle\langle 1|_u$

- Driving Hamiltonian:

$$H_D = \sum_{u \in V} \left(X_u \sum_{\substack{v \in V \\ s.t.\{u,v\} \in E}} W_v \right)$$

- Initial state:

$$|s\rangle = |1\rangle^{\otimes |V|}$$

[1] Hadfield et. al. (2017)

QAOA with penalties

- Problem Hamiltonian:

$$H_P = \sum_{u \in V} W_v + \sum_{\{u,v\} \in E} (I - W_u - W_v + W_u W_v)$$

- Driving Hamiltonian:

$$H_D = -\sum_{u \in V} X_u$$

- Initial state:

$$|s\rangle = |+\rangle^{\otimes |V|}$$

Goal

- Compare how these two techniques perform on MinVertexCover using numerical approaches.

- Try to gain intuition to show connection analytically for MinVertexCover, and in general.

- Finding a connection between QAOA++ and QAOA with penalties could allow us to show that if good values of $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ can be found for one of these techniques, they can also be found for the other one.

Thanks!