

QAOA and its Applications

Johannes Weidenfeller

IBM Quantum Research Intern

Recap

Hermitian Matrix

A matrix H that is equal to its own conjugate transpose $H = H^\dagger$.

Eigenvalue and Eigenvector

A vector v is an eigenvector of a matrix M with eigenvalue λ , if $Mv = \lambda v$.

Quantum System

The state of a quantum system is described by a vector $|\psi\rangle$ in a complex Hilbert space \mathcal{H} .

Observables

Physical observables are described by a Hermitian operator H and the expectation value of the corresponding measurement is given by $\langle\psi|H|\psi\rangle$.

Content

- 1) Variational Quantum Eigensolvers
- 2) QUBOs and MaxCut
- 3) The QAOA Circuit
- 4) Adiabatic Quantum Computing
- 5) Recent Results and Caveats

Variational Quantum Eigensolvers

Hamiltonian

Operator corresponding to the total energy of a quantum system described by Hermitian matrix

$$H = H^\dagger$$

Energy of system in state $|\psi\rangle$ given by expectation value

$$E(|\psi\rangle) = \langle\psi|H|\psi\rangle$$

Ground State

The lowest energy state $|\psi^*\rangle$ of a quantum system

$$|\psi^*\rangle = \underset{|\psi\rangle \in \mathcal{H}}{\operatorname{argmin}} E(|\psi\rangle)$$

The variational method

- Method for approximating ground state $|\psi^*\rangle$ and lowest energy E_{min} of a quantum system
 - 1.) Choose **ansatz** or **trial state** parameterized by θ

$$|\psi(\theta)\rangle$$

- 2.) Vary parameters θ to minimize the energy value

$$E(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle$$

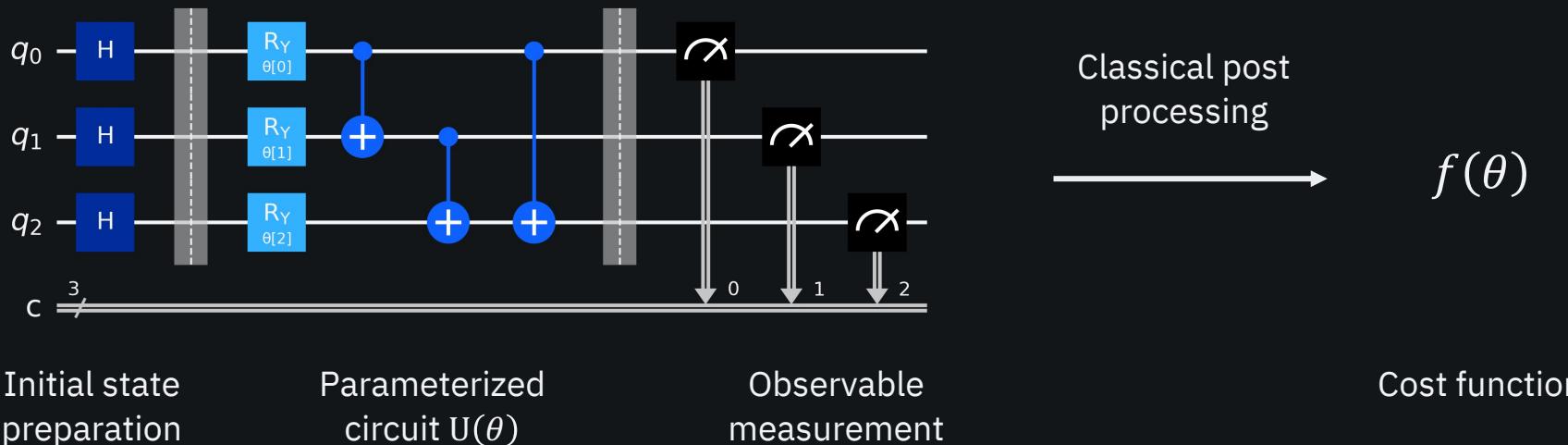
$$\theta^* = \operatorname{argmin}_{\theta} E(\theta)$$

- $E(\theta^*)$ is an upper bound for E_{min} and $|\psi(\theta^*)\rangle$ approximates $|\psi^*\rangle$

Variational Quantum Circuits

Variational Quantum Circuit

A quantum circuit that depends on parameters θ_i



Initial state preparation

Parameterized circuit $U(\theta)$

Observable measurement

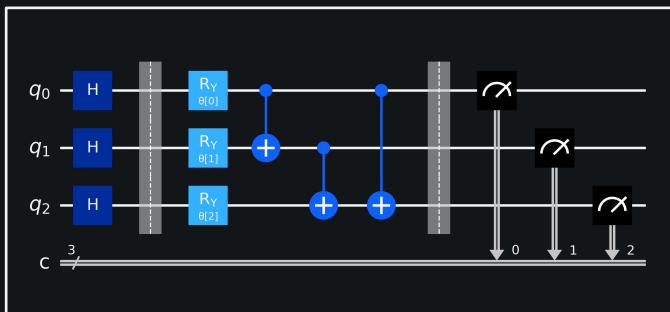
Cost function

Variational Quantum Eigensolvers

Idea: Prepare quantum state with variational quantum circuit $U(\theta)$

$$|\psi(\theta)\rangle = U(\theta)|\psi_0\rangle$$

Variational Quantum Circuit



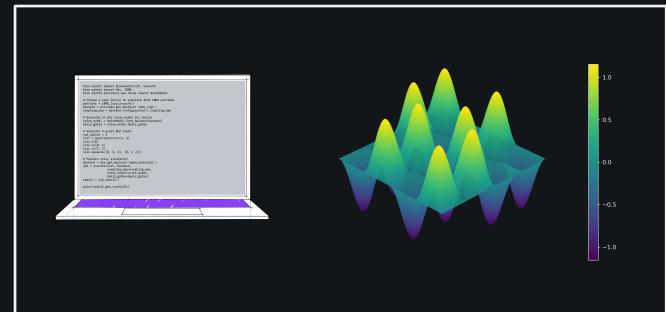
Measurement

$$E(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle$$

Parameter update

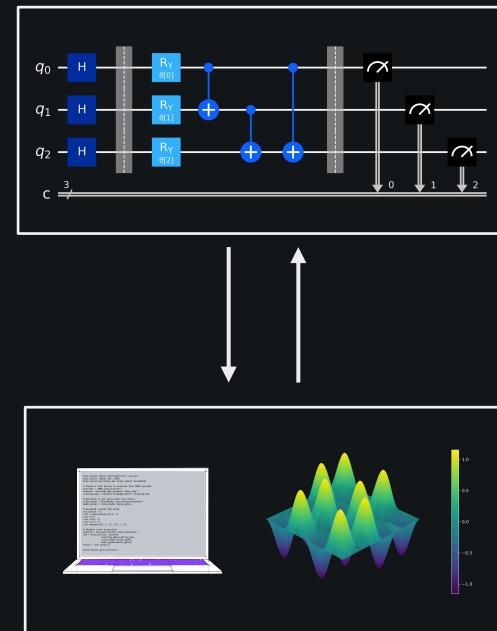
$$\theta_i \rightarrow \theta_{i+1}$$

Classical Optimizer



Variational Quantum Eigensolvers

- Use variational method to approximate ground state of Hamiltonian H_C
- Use classical-quantum hybrid loop to optimize circuit parameters
- Similar in structure to classical neural networks
- Typical architectures: layerized and tensor network circuits
- Applications in chemistry, quantum mechanics, **optimization**



QUBO and MaxCut

Quadratic Programs

- Optimization problems with quadratic objective function and linear and quadratic constraints
- Special case: Quadratic Unconstrained Binary Optimization (**QUBO**)
 - Quadratic objective function
 - No variable constraints
 - Binary optimization variables

$$\text{minimize} \quad x^T Q x + c^T x$$

$$Q \in \mathbb{R}^{n \times n} \quad c \in \mathbb{R}^n$$

$$\text{subject to} \quad Ax \leq b$$

$$x^T Q_i x + a_i^T x \leq r_i$$

$$l_j \leq x_j \leq u_j$$

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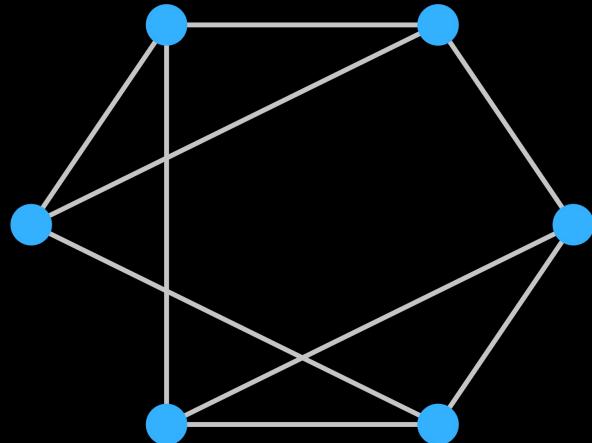
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Graph

Set of vertices or nodes V connected by
(weighted) edges E



Cut

Partition of vertices into two disjoint subsets

The *weight* of a cut is the weight of the edges
connecting vertices from different sets

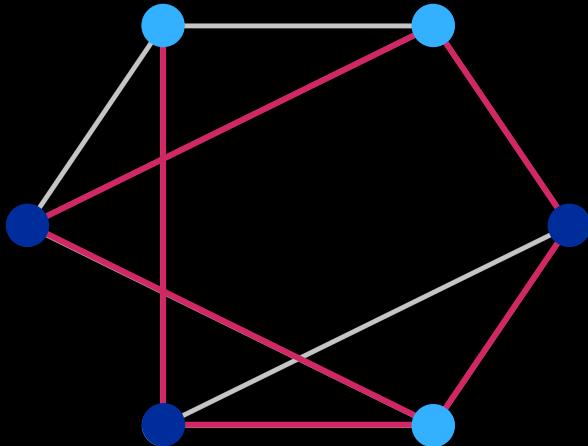
Graph

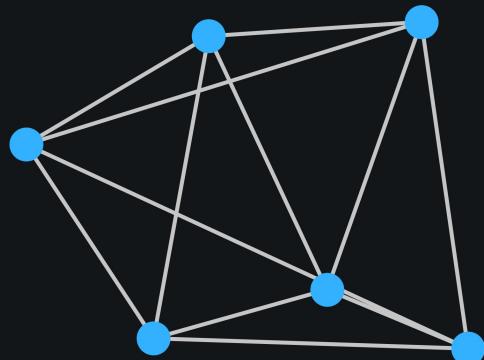
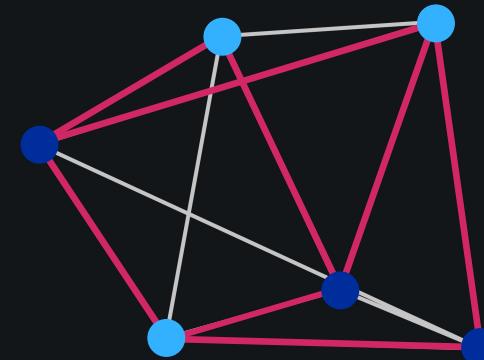
Set of vertices or nodes V connected by
(weighted) edges E

Cut

Partition of vertices into two disjoint subsets

The *weight* of a cut is the weight of the edges
connecting vertices from different sets



Input(Weighted) graph $G = (V, E)$ **Output**Maximal cut $x \in (0,1)^n$ 

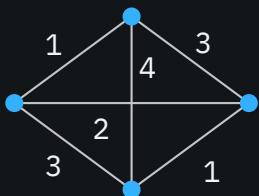
$$x = [1,0,0,0,1,1] \quad \bullet = 0 \quad \textcolor{blue}{\bullet} = 1$$

MaxCut as QUBO

MaxCut

Weight matrix

$$W = \begin{pmatrix} 0 & 1 & 2 & 3 \\ 1 & 0 & 3 & 4 \\ 2 & 3 & 0 & 1 \\ 3 & 4 & 1 & 0 \end{pmatrix}$$



Cost function

$$C(x) = \sum_{i,j=1}^n W_{ij} x_i (1 - x_j)$$

QUBO

QUBO matrix and vector

$$c_i = \sum_{j=1}^n W_{ij} \quad Q_{ij} = -W_{ij}$$

Cost function

$$C(x) = \sum_{i,j=1}^n x_i Q_{ij} x_j + \sum_{i=1}^n c_i x_i = x^T Q x + c^T x$$

MaxCut: Classical Limitations

- Equivalent to general QUBOs by simple transformation
- NP-hard to achieve better approximation ratio than

$$\alpha \sim 0.941^{[1]}$$

- Best classical approximation ratio under *Unique Games Conjecture*

$$\alpha \sim 0.878$$

- Achieved by classical Goemans-Williamson^[2] algorithm

From QUBO To Hamiltonian

Goal: Find Hamiltonian operator H_C that encodes cost function $C(x)$

$$H_C|x\rangle = C(x)|x\rangle$$

QUBO cost function

$$C(x) = \sum_{i,j=1}^n x_i Q_{ij} x_j + \sum_{i=1}^n c_i x_i$$



Hamiltonian operator

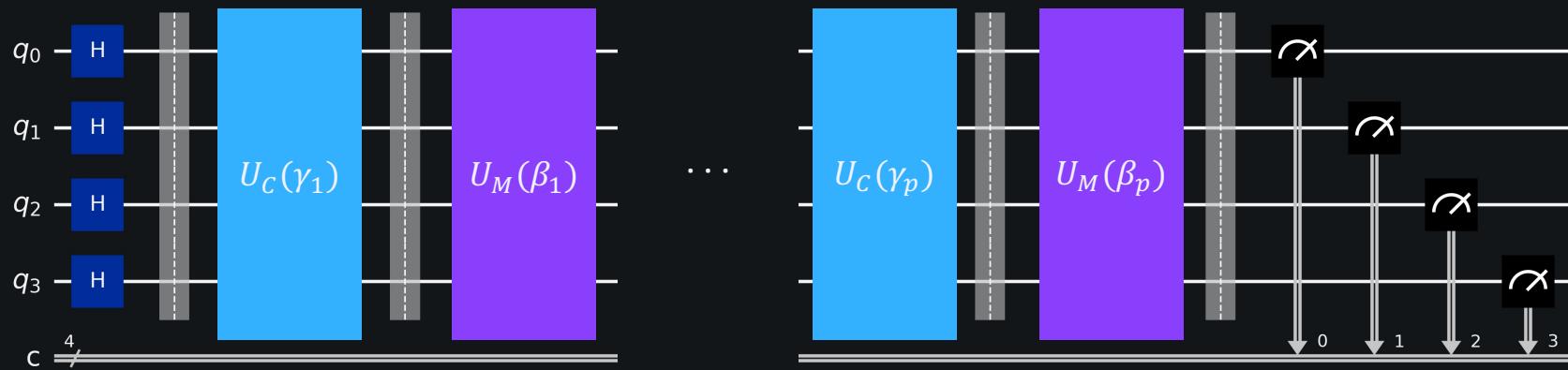
$$H_C = \sum_{i,j=1}^n \frac{1}{4} Q_{ij} Z_i Z_j - \sum_{i=1}^n \frac{1}{2} \left(c_i + \sum_{j=1}^n Q_{ij} \right) Z_i + \left(\sum_{i,j=1}^n \frac{Q_{ij}}{4} + \sum_{i=1}^n \frac{c_i}{2} \right)$$

The QAOA Circuit

Quantum Approximate Optimization Algorithm (QAOA)

- Introduced in 2014 by Farhi, Goldstone and Gutmann^[3]
- Finds approximate solutions for QUBO instances
- Can be regarded as special case of VQE
- Idea: Encode cost function of optimization problem as problem Hamiltonian H_C
- Layerized variational form based on trotterized adiabatic process

QAOA Variational Form



Preparation of equal superposition state

$$|+\rangle^n = \sum_{x \in \{0,1\}^n} \frac{1}{\sqrt{2^n}} |x\rangle$$

p repetitions of alternating cost and mixer layers

$$U_C(\gamma_i) = e^{-i\gamma_i H_C}$$

$$U_M(\beta_i) = e^{-i\beta_i H_M}$$

Measurement in computational basis

Matrix Exponentiation

Matrix exponential

For a matrix M the matrix exponential is defined as the power series

$$e^M = \sum_{k=0}^{\infty} \frac{1}{k!} M^k$$

$$e^{-i\theta X} = R_X(2\theta) = \begin{pmatrix} \cos(\theta) & -i \sin(\theta) \\ -i \sin(\theta) & \cos(\theta) \end{pmatrix}$$

$$e^{-i\theta Y} = R_Y(2\theta) = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}$$

Pauli matrices

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

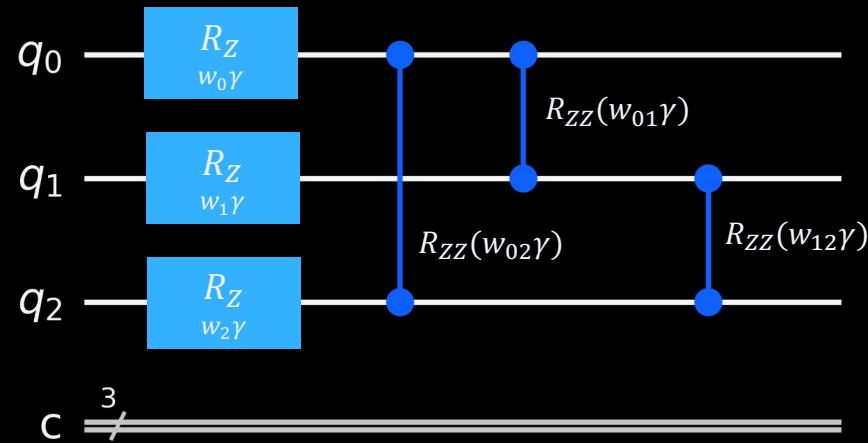
$$e^{-i\theta Z} = R_Z(2\theta) = \begin{pmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{pmatrix}$$

QAOA Cost Layer

$$H_C = \sum_{i,j=1}^n \frac{1}{4} Q_{ij} Z_i Z_j - \sum_{i=1}^n \frac{1}{2} \left(c_i + \sum_{j=1}^n Q_{ij} \right) Z_i$$

$$e^{-i\gamma H_C} = \prod_{i,j=1}^n R_{Z_i Z_j} \left(\frac{1}{2} Q_{ij} \gamma \right)$$

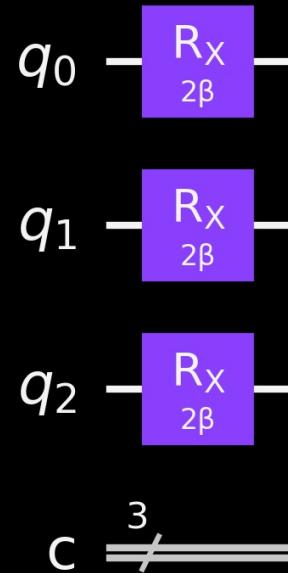
$$\prod_{i=1}^n R_{Z_i} \left(\frac{1}{2} \left(c_i + \sum_{j=1}^n Q_{ij} \right) \gamma \right)$$



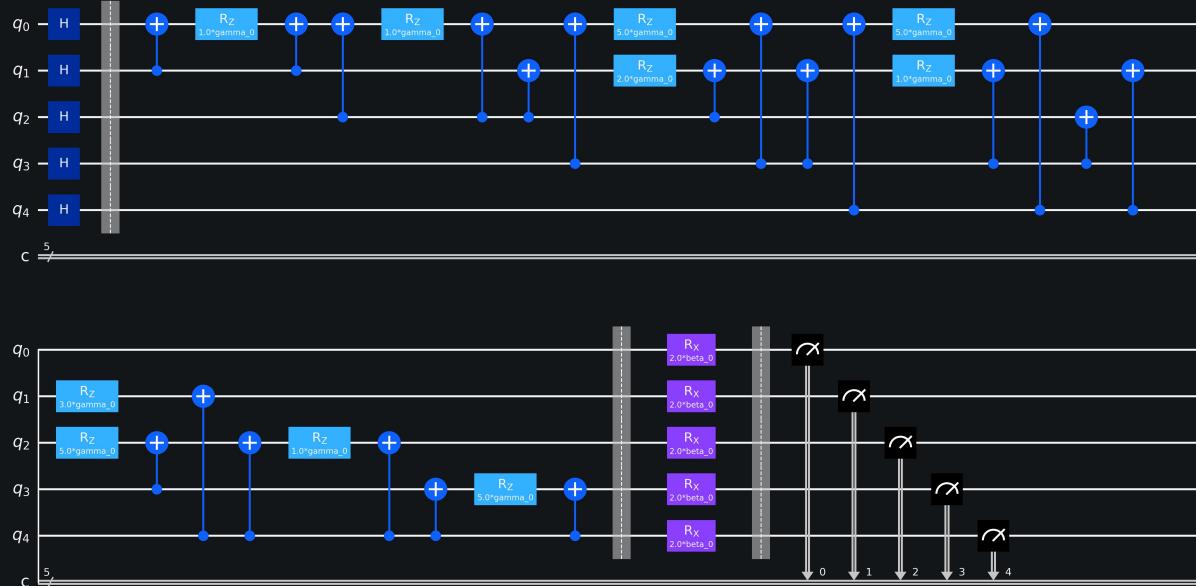
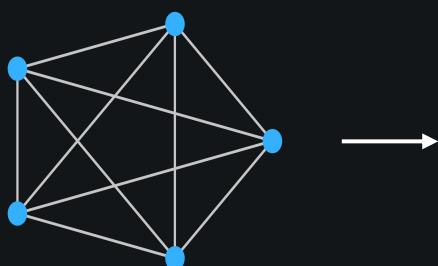
QAOA Mixer Layer

$$H_M = \sum_{i=1}^n X_i \quad X = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

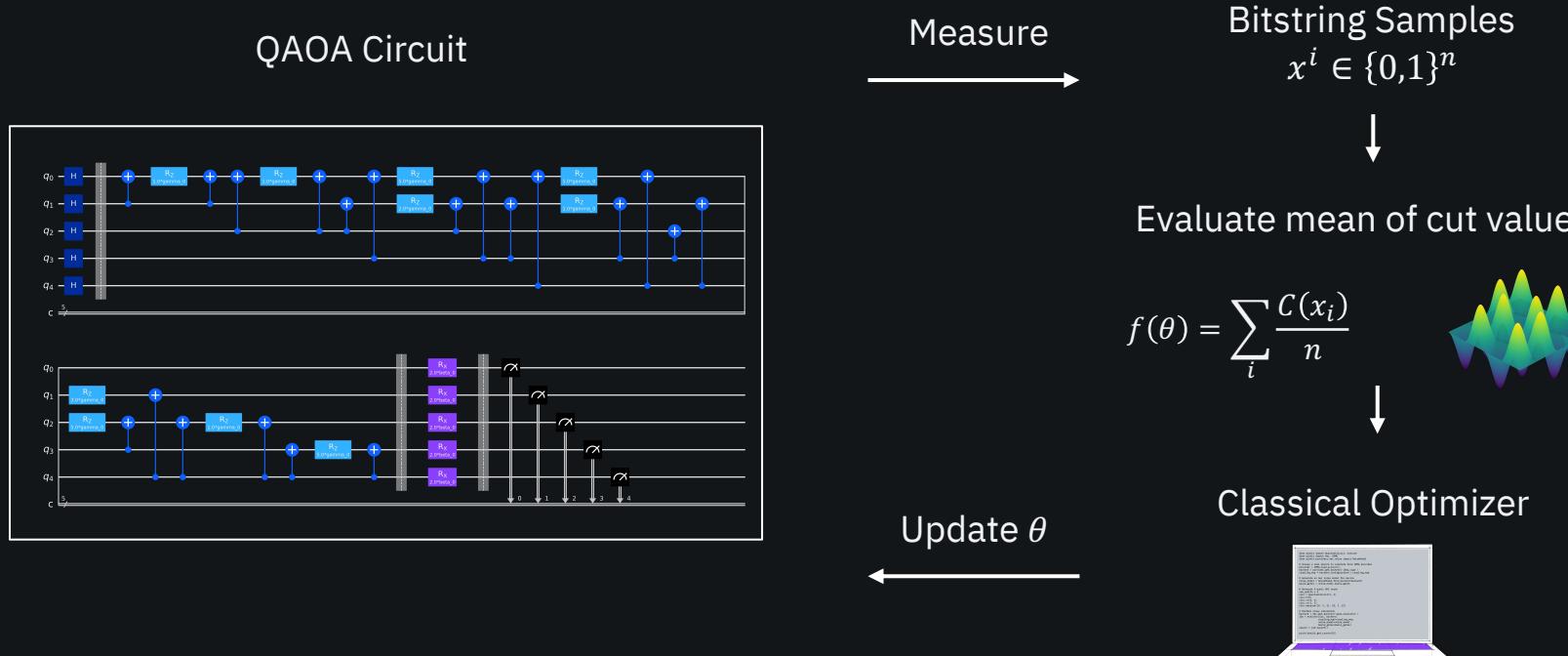
$$e^{-i\beta H_M} = \prod_{i=1}^n R_X(2\beta)$$



QAOA Example

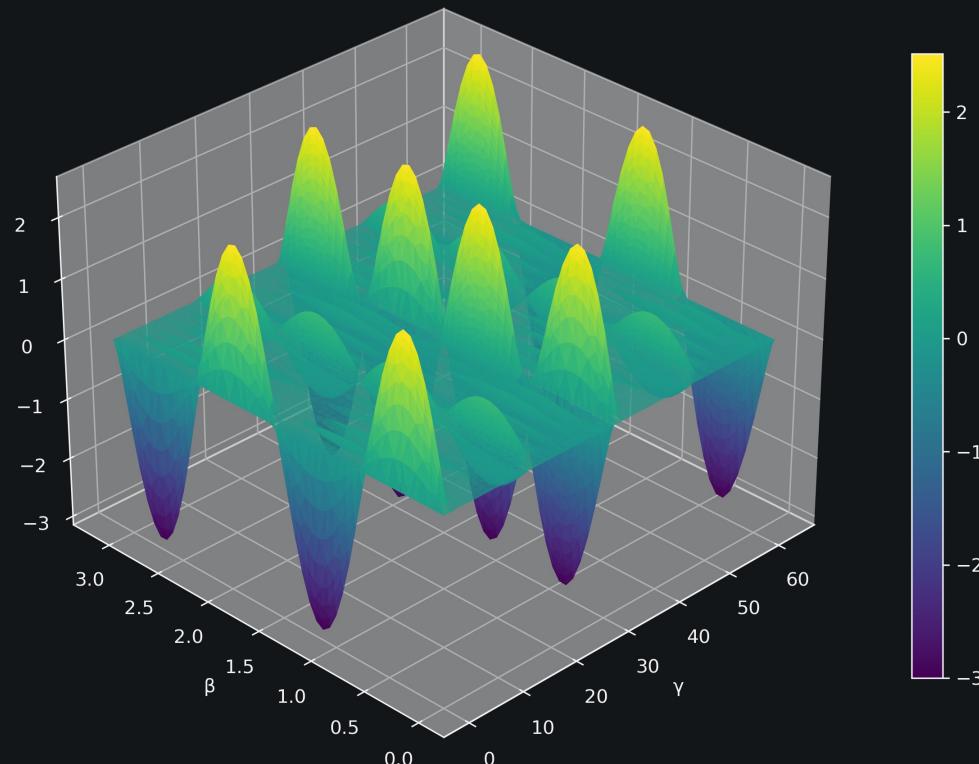


QAOA Overview



QAOA Energy Landscape

- Observe periodicity in both parameters
- Can be smoothed by algorithmic adaptations
- Classical optimizer crucial for QAOA success



Adiabatic Quantum Computing

Hamiltonians and Time Evolution

Schrödinger Equation

Time evolution of a quantum system with Hamiltonian H

$$H|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle$$

For time-independent H :

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle$$

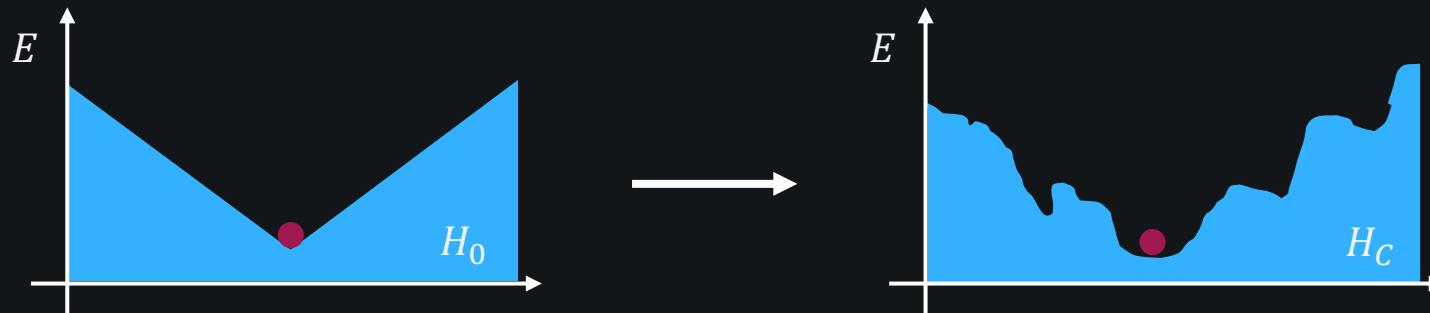
Adiabatic Theorem

If the Hamiltonian of a quantum system in its ground state is perturbed slowly enough, the system remains in its ground state.

Adiabatic Quantum Computing

Form of quantum computing that uses adiabatic theorem

- 1.) Encode problem as Hamiltonian whose ground state is the problem solution
- 2.) Prepare quantum system in ground state of a simple Hamiltonian
- 3.) Adiabatically evolve simple Hamiltonian to problem Hamiltonian



Trotterization

- Consider problem Hamiltonian $H_c = H_1 + H_2$
- Time evolution operator

$$U(t) = e^{-iHt/\hbar} = e^{-i(H_1+H_2)t/\hbar}$$

- For commuting matrices A, B

$$e^{A+B} = e^A e^B$$

Trotter Suzuki Formula

Approximates the exponential of a sum of matrices

$$e^{-i(H_1+H_2)t} \approx (e^{-iH_1 t/r} e^{-iH_2 t/r})^r$$

QAOA as adiabatic schedule

- Consider adiabatic evolution with runtime T

$$H(t) = \frac{t}{T} H_C + \left(1 - \frac{t}{T}\right) H_M$$

- Mixer Hamiltonian

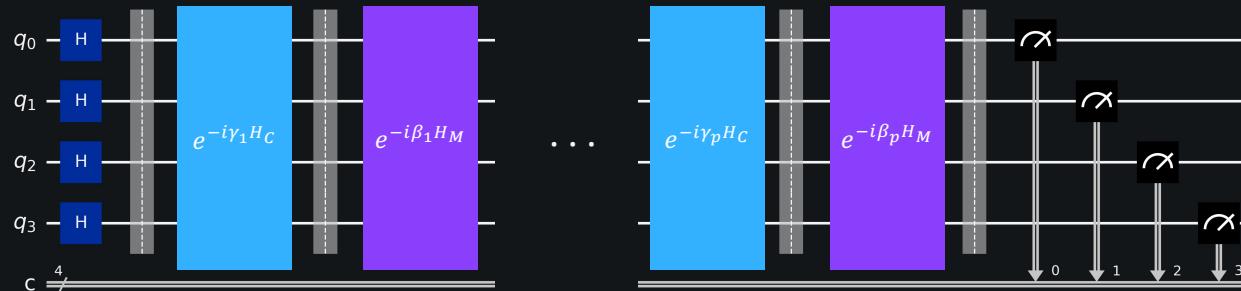
$$H_M = \sum_i X_i$$

Eigenvectors of X :

$$X|+\rangle = |+\rangle \quad X|-\rangle = -|-\rangle \quad \Rightarrow$$

Initial QAOA state is highest energy state of H_M

- Layers of QAOA correspond to trotterized segments of time evolution operator



QAOA as adiabatic schedule

- QAOA = Trotterized quantum adiabatic algorithm
- Yields performance guarantee for $p \rightarrow \infty$

$$M_{p+1} \geq M_p \quad \lim_{p \rightarrow \infty} M_p = C_{max}$$

- Support for why QAOA might produce good results, however adiabatic theorem yields no statement about finite p
- Expect adiabatic schedule reflected in optimal parameters (rising γ and falling β)

Recent Results and Caveats

Caveats

- As variational circuit QAOA has no performance guarantees
- *Bravyi et. al. '19^[4]*: QAOA requires super-logarithmic depth to beat classical GW-algorithm
$$p \leq \mathcal{O}(\log(n)) \Rightarrow \alpha \leq \frac{5}{6} + \mathcal{O}\left(\frac{1}{\sqrt{D}}\right)$$
- *Hastings '19^[5]*: compares QAOA to **local** classical algorithms for MaxCut
 - There exists classical local algorithm that outperforms QAOA for $p = 1$
 - Other contributing factors include
 - limited device connectivity
 - increasing number of shots and iterations for increasing problem size

- Introduced by Barkoutsos et. al. in 2020^[6]
- Idea: Use **Conditional Value-at-Risk (CVaR)** to speed up optimization process
- Only consider fraction α of best measured outcomes c_i

Sample mean

$$f(\theta) = \frac{1}{n} \sum_{i=1}^n c_i$$

CVaR $_{\alpha}$

$$f(\theta) = \frac{1}{\lceil \alpha n \rceil} \sum_{i=1}^{\lceil \alpha n \rceil} c_i$$

- Most extreme case: Consider only best outcome

Warm Starting QAOA

- Proposed by Egger, Marecek and Woerner in 2020^[7]
- Idea: Replace initial state of QAOA with a state obtained by classical optimization procedure

Equal superposition state

$$|+\rangle^{\otimes n} = \sum_{x \in \{0,1\}^n} \frac{1}{\sqrt{2^n}} |x\rangle$$

Warm-starting state

$$|\psi\rangle = \otimes_i R_Y(\theta_i) |0\rangle^n$$

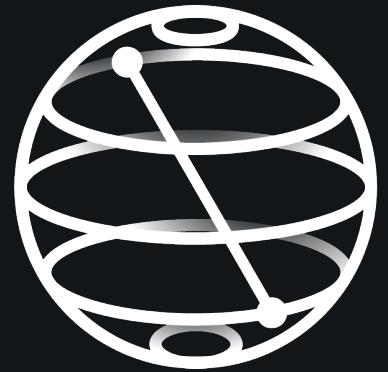
- θ_i correspond to solution of continuous-valued relaxation
- Mixer Hamiltonian H_M replaced, such that $|\psi\rangle$ is corresponding ground state

Parameter concentration

- Optimal QAOA parameters show concentration over different problem instances^{[8][9][10]}
 - *Farhi et. al. '20*^[9]: Full instance independence of parameters for $n \rightarrow \infty$ in SK model
 - *Akshay et. al. '21*^[10]: Parameter concentration across problems of different problem size
- Gives rise to new optimization techniques
 - Use optimal parameters of one instance as starting values for others
 - Find optimal parameters for large problem instance by initially focusing on smaller subproblem

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$$C(x) = x^T Q x + c^T x = \sum_{i,j=1}^n Q_{ij} x_i x_j + \sum_{i=1}^n c_i x_i$$

We want to find Hamiltonian H_C , s.t.

$$\underline{H_C |x\rangle = C(x)|x\rangle}$$

$$Z_i |x\rangle = (-1)^{\sum_i x_i} = 1 - 2x_i \Rightarrow \underbrace{\frac{1-2x_i}{2} |x\rangle}_{=x_i}$$

$$H_C = \sum_{i,j=1}^n Q_{ij} \frac{1-x_i}{2} \frac{1-x_j}{2} + \sum_{i=1}^n c_i \frac{1-x_i}{2}$$

$$= \sum_{i,j=1}^n \frac{Q_{ij}}{4} + \sum_{i=1}^n \frac{c_i}{2}$$

$$- \sum_{i=1}^n \left(\sum_{j=1}^n Q_{ij}/4 \right) z_i - \sum_{j=1}^n \left(\sum_{i=1}^n Q_{ij}/4 \right) z_j$$

$$- \sum_{i=1}^n \frac{c_i}{2} z_i$$

$$+ \sum_{i,j=1}^n Q_{ij}/4 z_i z_j$$