Quantum Approximate Optimization Algorithm

Microsoft Quantum research challenge QRISE 2024:
Resource estimation

Nikhil Londhe

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Quantum Approximate Optimization Algorithm - QAOA

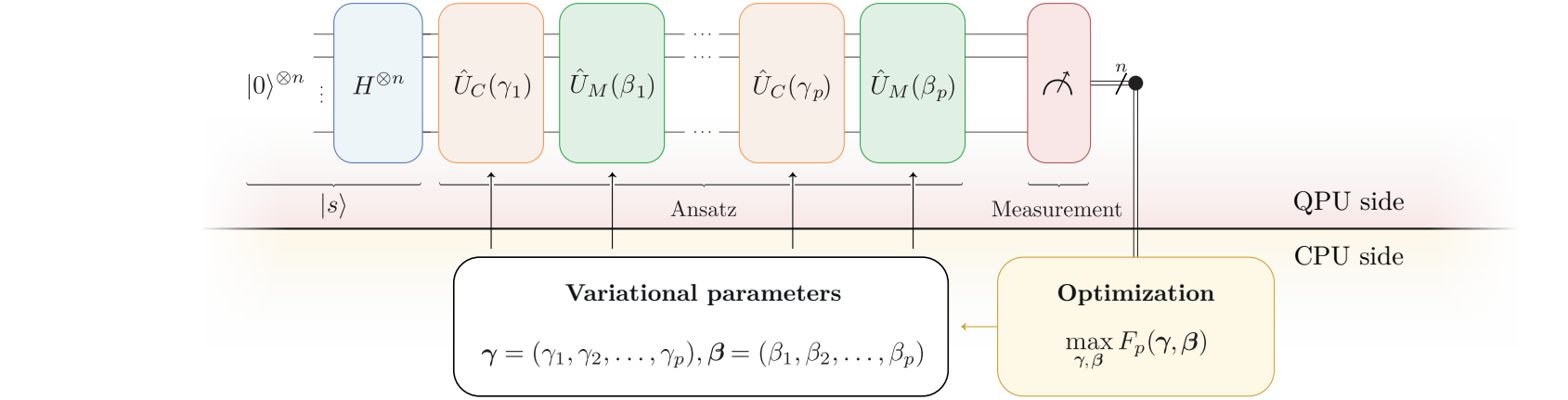

Figure 1: QAOA Overview

1. Algorithm to solve Combinatorial Optimization Problems.
2. Gives approximate solutions.
3. Uses Adiabatic Theorem.

Cost Function

We must pose our optimization problem as a Quantitative Unconstrained Binary Optimization (QUBO) problem. That means we need to define a cost function $C(X)$ for our problem, where $X = (x_1, .., x_n)$ is a binary vector with $x_i \in \{0, 1\}$, and $C(X)$ is of the form,

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

Cost Hamiltonian and Mixer Hamiltonian

Convert $C(X)$ (1) into a Hamiltonian by using a map ($x_i \rightarrow \frac{Z_i - 1}{2}$) that maps the binary variable x_i to a Pauli string, say Z_i. This Hamiltonian is called the cost Hamiltonian H_C because it represents our objective function.

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

And the mixer Hamiltonian H_M,

$$H_M = \sum_{i=1}^{n} X_i. \tag{3}$$

State Preparation

We prepare the state as an eigenstate of the mixer Hamiltonian H_M with the highest energy.

$$|s\rangle = |+\rangle^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{X \in \{0,1\}^n} |X\rangle \tag{4}$$

n is the number of qubits, and it is equal to the length of the binary vector X.

Circuit Ansatz

We must define unitaries representing the Hamiltonian's (H_C and H_M).

$$\hat{U}_C(\gamma) = e^{-i\gamma H_C} \tag{5a}$$
$$\hat{U}_M(\beta) = e^{-i\beta H_M}, \tag{5b}$$

where γ and β are variational parameters of the circuit. We call $\hat{U}_C(\gamma)$ and $\hat{U}_M(\beta)$ the cost and mixer layers, respectively.

$$\hat{U}_M(\beta) = e^{-i\beta_M} = \prod_{i=1}^{n} R_{X_i}(2\beta) \tag{6}$$

$$\hat{U}_C(\gamma) = \prod_{i=1, j<i}^{n} R_{Z_i Z_j}\left(\frac{1}{4} Q_{ij}\gamma\right) \prod_{i=1}^{n} R_{Z_i}\left(\frac{1}{2}\left(c_i + \sum_{j=1}^{n} Q_{ij}\right)\gamma\right) \tag{7}$$

Layers

Define the total number of QAOA layers, $p \geq 1$. Initialize the $2p$ variational parameters $\gamma = (\gamma_1, \gamma_2, \ldots, \gamma_p)$ and $\beta = (\beta_1, \beta_2, \ldots, \beta_p)$ such that $\gamma_k \in [0, 2\pi)$ and $\beta_k \in [0, \pi)$ for $k = 1, \ldots, p$.

The final state output by the circuit is, therefore, given by

$$|\psi_p(\gamma, \beta)\rangle = e^{-i\beta_p H_M} e^{-i\gamma_p H_C} \ldots e^{-i\beta_1 H_M} e^{-i\gamma_1 H_C} |s\rangle . \tag{8}$$

Measurement and Expectation Value

The expectation value of the Hamiltonian H_C with respect to the ansatz state $|\psi_p(\gamma, \beta)\rangle$, which corresponds to the cost obtained by the quantum algorithm for the underlying problem, is calculated through repeated measurements of the final state in the computational basis:

$$F_p(\gamma, \beta) = \langle \psi_p(\gamma, \beta) | H_C | \psi_p(\gamma, \beta) \rangle \tag{9}$$

Optimization

A classical (or quantum) optimization algorithm is employed to iteratively update the parameters γ and β. The goal of the optimizer is to find the optimal set of parameters (γ^*, β^*) such that the expectation value $F_p(\gamma, \beta)$ is maximized:

$$(\gamma^*, \beta^*) = \arg\max_{\gamma,\beta} F_p(\gamma, \beta) \tag{10}$$

Review

1. Prepare the Problem (QUBO Cost Function)
2. Cost Hamiltonian and Mixer Hamiltonian
3. State Preparation
4. Circuit Ansatz
5. Layers
6. Measurements
7. Optimization