Quantum Approximate Optimization Algorithm

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1. Steps of QAOA

The Quantum Approximate Optimization Algorithm (QAOA) is an algorithm for solving combinatorial optimization problems; unfortunately, QAOA only provides an approximate solution. I used [1] to create the steps.

1.1. Preparing the Cost Function

Before implementing QAOA, we need to 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,

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

Our objective is to maximize the Cost function, but QUBO can also be defined as minimization problems instead of maximization ones by simply inverting the sign of the cost function $C(X)$.

1.2. Cost Hamiltonian and Mixer Hamiltonian

Now we can convert this into a Hamiltonian by using a map ($x_i \to \frac{Z_i - 1}{2}$) that maps the binary variable x_i to a Pauli string Z_i. This Hamiltonian is called the cost Hamiltonian H_C because it represents our objective function.

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

We also need to define the mixer Hamiltonian H_M,

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

1.3. 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.

1.4. 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. A single QAOA layer comprises one cost and one mixer layer, which can be further stacked to build a deeper circuit with more layers. Each element in the mixer layer can be implemented with a single rotation gate R_X.

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

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

(7) and (6) is the gate decomposition of the unitaries in (5).

1.5. Layers

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

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

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

1.6. Measurement and Expectation Value

The expectation value of the Hamiltonian h_C with respect to the ansatz state $\left|\psi_p(\gamma, \beta)\right\rangle$, 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:

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

1.7. Optimizer

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

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

An example of a QAOA circuit instance is shown in Figure 1.

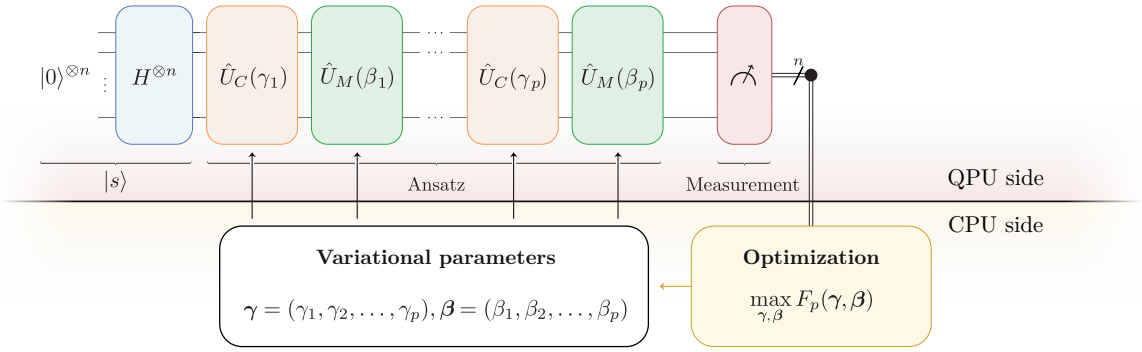

Figure 1. *Schematic of the hybrid workflow of QAOA with p layers.*

References

[1] K. Blekos, D. Brand, A. Ceschini, *et al.*, "A review on quantum approximate optimization algorithm and its variants", *Physics Reports*, vol. 1068, pp. 1–66, Jun. 2024, ISSN: 0370-1573. DOI: 10.1016/j.physrep.2024.03.002. [Online]. Available: http://dx.doi.org/10.1016/j.physrep.2024.03.002.