The Useful Quantum Computing Techniques for Artificial Intelligence Engineers

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***Abstract*—The hottest topics for many researchers in the past five years were Artificial Intelligence (AI) and machine learning. With many kinds of researches using machine learning, numerous AI engineers are still emerging. If the center of current research trends is on AI and machine learning, the center of near-future research trends will be on quantum computing techniques. The qubit implementation via superconductivity, diamond Nitrogen-Vacancy (NV) center, ion-trap, and etc. has made quantum computers really exist. And cloud computing has made it possible for researchers around the world to use quantum computers remotely to their researches. The universalization of quantum computing techniques is no longer a story of the distant future, even more so for numerous AI engineers. This paper introduces some useful quantum computing techniques for AI engineers such as Quadratic Unconstrained Binary Optimization (QUBO), Variational Quantum Eigensolver (VQE), Quantum Approximate Optimization Algorithm (QAOA), and Harrow-Hassidim-Lloyd (HHL) algorithm.**

***Index Terms*—QUBO, VQE, QAOA, HHL**

I. Introduction

We live in the Artificial Intelligence (AI) era. The keywords such as AI, machine learning, and deep learning are always included in almost research topics. Many non-researchers are also interested in these keywords. The budgets of countries and enterprises funded on AI-related research and development topics are enormous. Only about a decade ago, AI did not receive the explosive interest of mankind as it is now. So, what is the research topic that will monopolize the interest of mankind in the next decade? Our answer is quantum computing.

The expectations for quantum computing have been around for a long time, and many people expect huge speed-up on quantum computers. However, at present, quantum computers only bring huge speed-up in quantum research areas which are highly impacted by superposition and entanglement. We remember that deep learning, the hottest topic in AI, was also a boring topic, before the development of useful overfitting handling methods and the development of hardware, such as Graphics Processing Unit (GPU) parallel processing. At present, quantum computers have some limits. But, as we saw in the deep learning case, we are confident that there is a solution to these limits in future-oriented research.

As one of the great steps in future-oriented research on quantum computing, we are now entering the Noisy Intermediate-Scale Quantum (NISQ) era [1]. Rather than quantum algorithms for a distant future, the NISQ algorithms such as the Variational Quantum Eigensolver (VQE) [2], and the Quantum Approximate Optimization Algorithm (QAOA) [3], at the border of classical computers and quantum computers, are really practical. VQE and QAOA are also related to machine learning as an optimizer.

This paper first discusses the Quadratic Unconstrained Binary Optimization (QUBO) modeling for adiabatic quantum computation and QAOA [4]. Next, this paper discusses VQE and QAOA. Finally, this paper discusses the Harrow-Hassidim-Lloyd (HHL) algorithm, also known as the Quantum Linear System Algorithm (QLSA), which shows an exponential speed-up improvement over the best classical algorithm [5].

II. Quadratic Unconstrained Binary Optimization

The Quadratic Unconstrained Binary Optimization (QUBO) model is a useful model for expressing combinatorial optimization problems. Because of its relevance to the Ising model in physics [6], [7], QUBO model became the basis of quantum annealing and the subject of the study of neuromorphic computing [4], [8]–[10].

QUBO model has the following objective function:

$$f(x) = x^T Q x, \tag{1}$$

where x is a vector of binary variables and Q is a square matrix with real weights which can be an upper-triangular form or a symmetric form. In the following paragraph, we will see details about QUBO modeling with a simple example.

Suppose that we have an objective function for an optimization problem as follows:

$$\begin{aligned} y = x_1 + 2x_2 + 3x_3 + 4x_4 + 5x_1x_2 + 6x_1x_3 \\ +7x_1x_4 + 8x_2x_3 + 9x_2x_4 + 10x_3x_4, \end{aligned} \tag{2}$$

where $x_n = 0$ or 1, $n \in \{1, 2, 3, 4\}$. Since $x_n = {x_n}^2$, the objective function (2) can be expressed as follows:

$$\begin{aligned} y = x_1^2 + 2x_2^2 + 3x_3^2 + 4x_4^2 + 5x_1x_2 + 6x_1x_3 \\ +7x_1x_4 + 8x_2x_3 + 9x_2x_4 + 10x_3x_4. \end{aligned} \tag{3}$$

The equation (3) can be re-expressed as follows:

$$y = \begin{pmatrix} x_1 & x_2 & x_3 & x_4 \end{pmatrix} \begin{pmatrix} 1 & 2.5 & 3 & 3.5 \\ 2.5 & 2 & 4 & 4.5 \\ 3 & 4 & 3 & 5 \\ 3.5 & 4.5 & 5 & 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}. \quad (4)$$

The equation (4) is QUBO model, the same form as the equation (1). Q matrix of QUBO model (4) is a symmetric form and $q_{i,j}$, the component of Q matrix, satisfies the following conditions:

$$q_{i,j} = q_{j,i} = \begin{cases} \frac{C_{x_i x_j}}{2}, & \text{if } i \neq j \\ C_{x_i x_j}, & \text{if } i = j \end{cases}, \quad (5)$$

where $C_{x_i x_j}$ is the coefficient of $x_i x_j$ term in the equation (3).

We have studied QUBO modeling method with a basic example. Q matrix of QUBO model contains all the data in the problem. In other words, QUBO model is an unconstrained model other than the restrict of binary decision, limited to 0 or 1 [4], [9]. Due to these characteristics and relevance to the Ising problem, QUBO model is considered to be at the core concept of the near-term quantum computing area dealing with the combinatorial optimization problem [11].

III. Variational Quantum Eigensolver (VQE)

The Variational Quantum Eigensolver (VQE) is a hybrid quantum-classical algorithm that can efficiently find the lowest eigenvalue κ_1 of the Hermitian matrix E. In VQE, the quantum process is executed within the classical optimization process [2]. The quantum process consists of two main steps. The first step is to prepare the quantum state $|\psi(\theta)\rangle$, where θ is a parameter. The second step is to measure the expectation value of E in the quantum state $|\psi(\theta)\rangle$ as follows:

$$\langle E \rangle := \langle \psi(\theta) | E | \psi(\theta) \rangle . \quad (6)$$

By the variational principle, expectation value $\langle E \rangle$ is always greater than or equal to the lowest eigenvalue κ_1:

$$\langle E \rangle \geq \kappa_1. \quad (7)$$

Thus, we can get the approximate value of the lowest eigenvalue by finding the parameter that minimizes the expectation value in the classical optimization process.

Actually, VQE is used to find the energy state of the molecule and applied to various quantum simulation systems [2], [12], [13].

IV. Quantum Approximate Optimization Algorithm (QAOA)

The Quantum Approximate Optimization Algorithm (QAOA) belongs to the category of the hybrid quantum-classical algorithm, like VQE. QAOA is an algorithm designed to solve many known combinatorial optimization problems using quantum systems. In some combinatorial optimization problems, the N binary string x and the objective function $f(x) : \{0,1\}^n \to R$ are given. The goal in these problems is to find the optimal solution x^* that maximizes or minimizes

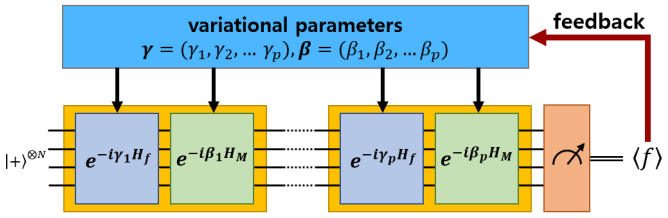

Fig. 1. p-level Quantum Approximate Optimization Algorithm [3], [14].

the objective function $f(x)$. QAOA maps this information to the quantum system by defining a phase Hamiltonian H_f as follows:

$$H_f |x\rangle = f(x) |x\rangle , \quad (8)$$

where $|x\rangle$ is the state corresponding to x. In addition, the mixing Hamiltonian H_M commonly used in QAOA is defined as:

$$H_M = \sum_{j=1}^{n} X_j, \quad (9)$$

where X_j is the Pauli-X operator.

In p-level QAOA, as shown in Fig. 1, $|+\rangle^{\otimes N}$ is given as the initial state, and the two Hamiltonians are applied alternately p times. At this time, the variables β and γ are applied to each Hamiltonian, creating a new state as follows:

$$|\boldsymbol{\beta}\ \boldsymbol{\gamma}\rangle = e^{-i\beta_p H_M} e^{-i\gamma_p H_f} \ldots e^{-i\beta_1 H_M} e^{-i\gamma_1 H_f} |+\rangle^{\otimes N} . \quad (10)$$

If we measure this state with H_f, we will get the expectation value of f. In other words, it can be expressed as:

$$\langle f \rangle = \langle \boldsymbol{\beta}\ \boldsymbol{\gamma} | H_f | \boldsymbol{\beta}\ \boldsymbol{\gamma} \rangle . \quad (11)$$

At this point, we can adjust the $2p$ variables to make $\langle f \rangle$ closer to $f(x^*)$. This optimization process can be used to learn β and γ through feedback based on measurement results. From this learning process, a good approximate solution can be obtained.

In the recently proposed Quantum Alternating Operator Ansatz [15], the mixing operator encodes the structure or constraints of the problem. This algorithm searches only within the state that meets the condition, not all states. This method can be used as a more generalized combinatorial optimization problem-solving model.

V. Harrow-Hassidim-Lloyd (HHL) algorithm

The Harrow-Hassidim-Lloyd (HHL) algorithm is a quantum algorithm for estimating the sample solution of a set of linear equations [5], [16]. Most of the problems in mathematics, science, and engineering can be formulated by solving the following linear system:

$$Ax = b, \quad (12)$$

where given $A \in \mathbb{R}^{N \times N}$ is a matrix, given $b \in \mathbb{R}^N$ is a vector, and x is the solution we need to find. These problems are usually solved in time polynomial in N by simple linear-algebra methods such as Gaussian elimination [16]. HHL algorithm can solve these problems faster than the classical

methods using superposition principle [17], Hamiltonian simulation [18], [19], and phase estimation [20]. In the following paragraph, we will see the brief procedure of HHL algorithm.

HHL algorithm finds the solution vector x in equation (12) when A is a Hermitian matrix and b is a unit vector. The first step of HHL algorithm is to prepare the quantum state for b as follows:

$$|b\rangle = \sum_{i=1}^{N} \zeta_i |\nu_i\rangle, \tag{13}$$

where $\nu_1 \cdots \nu_N$ are eigenvectors of A. And the state of the system is as follows:

$$\sum_{i=1}^{N} \zeta_i |\nu_i\rangle |\lambda_i\rangle, \tag{14}$$

where $\lambda_1 \cdots \lambda_N$ are eigenvalues of A. The next step is to map $|\lambda_i\rangle$ to $C\lambda_i^{-1} |\lambda_i\rangle$, where C is a normalizing constant. We have to repeat the mapping process until it succeeds. After the mapping succeeds, finally we can get $|x\rangle$ as follow:

$$|x\rangle = A^{-1} |b\rangle = \sum_{i=1}^{N} \zeta_i \lambda_i^{-1} |\nu_i\rangle. \tag{15}$$

In equation (15), We can see that applying A^{-1} corresponds to multiplying λ^{-1}.

To find out all the components of x, we must run the above procedure at least N times. But often, some problems require only a few features of x. In this case, we can get a following estimation of the expectation value by quantum measurements corresponding to some linear operator M:

$$\langle M \rangle := \langle x|M|x\rangle = x^T M x. \tag{16}$$

We can get various features of the vector x (e.g., normalization, weights in different parts of the state space, moments) via this value [5].

HHL algorithm, we have studied in this section, has an exponential speed-up improvement compared to classical algorithms [5], [21]. This speed-up makes HHL algorithm a key concept in quantum machine learning along with the Singular Value Estimation (SVE) algorithm [22].

VI. Concluding Remarks and Future Work

In summary, we have studied QUBO, VQE, QAOA, and HHL algorithm. QUBO model is valuable in both quantum computing and AI areas, also important because it is the basic model for QAOA mapping. Both VQE and QAOA are hybrid quantum-classical optimizers on the NISQ era, so there are various fields of their applications. The importance of optimizer cannot be ignored, especially in machine learning applications. This raises expectations for future machine learning researches using the hybrid quantum-classical optimizer. HHL algorithm is a kind of solvers that guarantees definite speed-up in linear systems of equations, which is one of the key techniques of quantum machine learning. We recommend that AI engineers seeking future machine learning research such as quantum machine learning should understand details of HHL algorithm.

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