Variational Quantum Algorithm and Its Application on Non-Linear Equations

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Abstract. Quantum algorithms of factoring problem have been paid more and more attention since Shor's algorithm was proposed. Combining the current quantum computer hardware level and integer factorization quantum algorithms, this paper proposes a "classical + quantum" hybrid solution. This scheme first adopts classical methods and corresponding rules in the preprocessing step to simplify the nonlinear equations, which is used to reduce the number of qubits needed for the cost Hamiltonian. Then the variational quantum algorithm is used to find the approximate ground state of the cost Hamiltonian, which encodes the solution of the nonlinear equations. The program was verified on the IBM QX4 quantum machine, and the results showed that this hybrid solution can effectively reduce the quantum resources required to solve the nonlinear equations.

1. Introduction
While quantum computing systems have demonstrated quantum supremacy over classical computing when dealing with some specific problems [1, 2], they are limited in the number of physical qubits, circuit depth, and fiderity to be applied to practical applications [3]. Hybrid quantum-classical algorithms hold great promise for achieving a meaningful quantum advantage in the NISQ (Noisy Intermediate Scale Quantum) era [4, 5] by combining the quantum resources and classical processors. Variational quantum algorithm (VQA) is a quantum-classical hybrid algorithm aiming at solving combinatorial optimization problems. Understanding how quantum and classical computing resources could be leveraged together is significant for extracting maximal utility from quantum computers.

The security of RSA relies on the practical difficulty of factoring the product of two large prime numbers, the “factoring problem”. Moreover, “factoring problem” can be transformed into a combinatorial optimization problem, which is further equivalent to solving a set of non-linear equations. VQA is a typical case and can be used to tackle an NP problem with a tunable trade off between classical and quantum computing resources, which is feasible for NISQ devices. VQA has the additional advantage of maintaining the depth of quantum circuits and reducing noise compared with quantum algorithms developed for the fault-tolerant era.

2. Variational quantum algorithm in solving equations
In this section, we propose a "classical + quantum" hybrid solution based on the variable quantum algorithm (see Figure 1). First, classical methods and corresponding rules in the preprocessing part to
simplify the non-linear equations are used to reduce the need of the number of qubits for the cost Hamiltonian. Then it seeks an approximate ground state of the cost Hamiltonian by training variational circuits using the variational quantum algorithm.

2.1. Optimization of equations
The equations are used to derive a complex Hamiltonian in the process of solving equations, which encodes the solution of the ground state. However, too many variables will occupy too many quantum resources. In order to reduce the number of qubits required by eliminating enough variables to make the sorting unique, we introduce a classic method to reduce the variables in the equation. One of the simplification methods is to directly find a subset of the binary variables. This simplification can reduce the required variables and operate polynomial operations in the best case.

2.2. Constructing the cost Hamiltonian
A key aspect of the variational quantum algorithm is to construct simplified nonlinear equations into the cost Hamiltonian. The Hamiltonian is an operator corresponding to the total energy of the system, which is mathematically expressed as a matrix with real eigenvalues. The eigenvector of the Hamiltonian corresponds to each eigenstate of the physical system, and the eigenvalue is the energy corresponding to the eigenstate of the physical system. For a problem, finding its Hamiltonian and obtaining its eigenstate and eigenenergy based on this Hamiltonian is equivalent to solving the problem.

After classical preprocessing, the solution of simplified equations \( C'_i = 0 \) correspond to the minimization of the classical energy function:

\[
E = \sum_{i=0}^{n} C'^2_i
\]  

simplified equations are derived as a complex Hamiltonian, i.e., the problem Hamiltonian:

\[
H_p = \sum_{i=0}^{n} \hat{C}^2_i
\]  

Each term \( \hat{C}^2_i \) is obtained by mapping the variables \( x, y, \) and \( z \) in the clause \( C'_i \) to qubit operators. \( x, y \) and \( z \) consist of \( \sum_{i=0}^{l-1} 2^i \left( \frac{1-\sigma_z}{2} \right) \), \( \sum_{i=0}^{l-1} 2^i \left( \frac{1-\sigma_y}{2} \right) \) and \( \sum_{i=0}^{l-1} 2^i \left( \frac{1-\sigma_z}{2} \right) \). Where \( \sigma_z \) represents the quantum operation of pauli-z gate in the i-th bit of variables \( x, y \) and \( z \).

2.3. Quantum initial state
For some Hamiltonians that are not easy to directly prepare the ground state, an initial Hamiltonian can be prepared first, and carries out adiabatic evolution by controlling the parameters to evolve the initial Hamiltonian into the cost Hamiltonian.
The remaining variables after the simplification of the equations correspond to n qubits which is used to record the index of each data in the database. It can represent a total of $2^n$ data, which is recorded as N:

$$|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_n |n\rangle$$  \hspace{1cm} (3)

The quantum processor in the uniform superposition state $|\psi_0\rangle=|+\rangle^\otimes N$ of the bit string is prepared by adding a Hadamard gate to each qubit in the zero state:

$$H_{\beta} = \sum_{n=0}^{N-1} \sigma^n_x$$  \hspace{1cm} (4)

2.4. Quantum circuit generation
A set of angle sums (i=1,2,...,p) with any p is selected as parameters to construct a quantum circuit. Alternate application of p-layer $U\left(H_p, \gamma_i\right)$ and $U\left(H_B, \beta_i\right)$. Please note that conjugating $U\left(H_p, \gamma_i\right)$ with a single qubit operator will produce an operator involving only that qubit and the interacting qubit. $U\left(H_B, \beta_i\right)$ conjugates a single qubit to rotate the qubit without affecting other qubits.

$$U\left(\beta, \gamma\right) = \prod_{i=1}^{p} U\left(H_B, \beta_i\right) U\left(H_p, \gamma_i\right)$$  \hspace{1cm} (5)

Where p represents the number of evolutionary steps. The quantum circuit corresponding to each step is the product of two unitary transformations, and both correspond to the sum of two parameters.

Two unitary transformations repeatedly act on the initial ground state, and eventually evolve into the ground state $|\psi_1\rangle$ of the cost Hamiltonian:

$$|\psi_1\rangle = |\gamma, \beta\rangle = U\left(\beta, \gamma\right)|\psi_0\rangle = e^{-i\beta_p \tilde{r}_x} e^{-i\gamma_p \tilde{r}_z} \cdots e^{-i\beta_1 \tilde{r}_x} e^{-i\gamma_1 \tilde{r}_z} |+\rangle^\otimes n$$  \hspace{1cm} (6)

For the unitary transformation with $H_B$ as the generator and the parameter $\beta$, we bring the value of $H_B$ in, and then deduced a set of RX gate operations as follows:

$$U\left(H_B, \beta\right) = e^{-iH_B/\beta} = e^{-i\sum_{i=0}^{N-1} \sigma^i_x \beta_i} = \prod_{n=0}^{N-1} e^{-i\sigma^i_x \beta_i} = \prod_{n=0}^{N-1} RX(n, 2\beta_i)$$  \hspace{1cm} (7)

Similarly, the unitary transformation with $H_p$ as the generator and $\gamma$ as the parameter takes the cost Hamiltonian into consideration and deduces it. Finally, it can be deduced that it is a combination operation of CNOT gate and RZ gate. Take $H_p = \sum_{ij} \frac{1}{2} \left(I - \sigma^i_z \sigma^j_z\right)$ as an example:

$$U\left(H_p, \gamma_i\right) = e^{-iH_p/\gamma_i} = e^{-i\sum_{j} \frac{1}{2} (I-\sigma^j_z \otimes \sigma^j_z) \gamma_i} = \prod_{j} e^{-i\gamma_i} \cdot \prod_{j} e^{i\gamma_i}$$  \hspace{1cm} (8)
2.5. Quantum expectation estimation

Ideally, on the basis of calculation, use the optimizer of the classical computer to repeatedly measure the ground state $|\psi_1\rangle$, and obtain the weighted sum of the average value of the cost Hamiltonian $pH$ on the corresponding ground state $|\psi_1\rangle$, i.e., the expectation value. This function $F_p(\tilde{\gamma}, \tilde{\beta})$ defined by the cost Hamiltonian is called the cost function of the variational quantum algorithm.

$$F_p(\tilde{\gamma}, \tilde{\beta}) = \langle \gamma, \beta | H_p | \gamma, \beta \rangle$$

By repeatedly running QPU, we use quantum expectation estimation program to estimate the expectation value of Hamiltonian $H_p$. After that, the estimated expectation value is passed to the CPU, and the classical optimizer running on the CPU suggests a new set of parameters for subsequent iterations until the parameters $\gamma$ and $\beta$ corresponding to the minimum expectation value are found, and the quantum state containing the final solution of the problem is obtained, as shown in Figure 2. The number of iterations of the loop is a key factor in the runtime of VQA. A higher circuit depth VQA implementation has better performance, but more parameters may lead to more loop iterations.

![Figure 2. Quantum expectation estimation](image-url)
2.6. Quantum optimization
The next step is to train the parameters $\gamma$ and $\beta$ to find the minimum of the cost function once the cost Hamiltonian and ansatz are defined. In order to optimize the parameters $\gamma$ and $\beta$ of the variational quantum algorithm, a layer-by-layer iterative grid search method is carried out on each pair $(\gamma_i, \beta_i)$, with the output fed into a BFGS global optimization algorithm [42]. For a fixed quantum circuit depth $p$, you can run the quantum computer at an angle $(\gamma, \beta)$ selected in the fine grid formed by the tight set $[0, 2\pi]^p \times [0, \pi]^p$, and move in the grid to find the maximum value. More precisely, each dimension of the expectation grid should be $O(n^2 n^4)$.

3. Numerical simulations
This chapter uses the following equations to carry out experimental simulations in order to verify the practicability and reliability of the variable quantum algorithm for solving equations. The experimental results and simulation results are as follows.

3.1. Instance
Take the following equations as input:

\[
\begin{align*}
p_1 + q_1 &= 1 + 2 C_0 \\
p_2 + p_1 q_1 + q_2 + C_0 &= 1 + 2 C_1 + 4 C_2 \\
1 + p_2 q_1 + p_3 q_2 + 1 + C_2 &= 1 + 2 C_3 + 4 C_4 \\
p_1 + p_2 q_2 + q_1 + C_2 + C_3 &= 0 + 2 C_5 + 4 C_6 \\
p_2 + q_2 + C_4 + C_5 &= 0 + 2 C_7 + 4 C_8 \\
1 + C_6 + C_7 &= 0 + 2 C_9 \\
C_8 + C_9 &= 1
\end{align*}
\]

In order to reduce the qubits needed to solve the equations in this scheme, the equations are optimized by citing the classical rules. This simplification can reduce all carry variables and the required polynomial operations in the best case.

\[
\begin{align*}
p_1 + q_1 &= 1 & (11) \\
p_2 + q_2 &= 1 & (12) \\
p_2 q_1 + p_2 q_2 &= 1 & (13)
\end{align*}
\]

Establishing the cost Hamiltonian is an essential step in the adiabatic quantum algorithm. The simple form of the Hamiltonian is the square of each equation. The cost Hamiltonian is obtained by summing all the Hamiltonian in Eq.(11-13):

\[
H_p = \left(\hat{p}_1 + \hat{q}_1 - 1\right)^2 + \left(\hat{p}_2 + \hat{q}_2 - 1\right)^2 + 2 \left[\frac{1}{2} \left(\hat{p}_1 + \hat{q}_2 - \frac{1}{2}\right) + \hat{p}_2 \hat{q}_1 - 1\right]^2
\]

\[
= 5 - 3 \hat{p}_1 - \hat{p}_2 - \hat{q}_1 + 2 \hat{p}_1 \hat{q}_1 - 3 \hat{p}_2 \hat{q}_1 + 2 \hat{p}_1 \hat{p}_2 \hat{q}_1 - 3 \hat{q}_2 + \hat{p}_1 \hat{q}_2 + 2 \hat{p}_2 \hat{q}_2 + 2 \hat{p}_1 \hat{q}_2 + \hat{q}_2
\]

The variable $\hat{p}_1, \hat{q}_1, \hat{q}_2, \hat{p}_2$ is mapped to the operator $a_1, a_2, a_3, a_4$, and the selection method is the same as described above. Therefore, the four-qubit problem Hamiltonian obtained as follows:
3.2. Simulations

This experiment has been performed on an open access 5-qubit quantum processor placed on cloud by IBM corporation. In particular, we have used the architecture of IBM’s QX4 (IBM Q 5 Tenerife)\cite{6}, which consists of superconducting Transmon qubits \cite{7}.

![Circuit diagram of variable quantum algorithm for solving equations](image1)

The quantum circuit diagram of the variational quantum algorithm to solve the equations is shown in Figure 3. The basic gate library for single-qubit gates is $H$, Pauli operator $X$, $Y$, $Z$. The variational quantum algorithm selects qubits $q[0]q[1]q[2]q[3]$ to realize the quantum adiabatic evolution of the ground state search. By applying $X$ gate ($\sigma_x$) to the qubits $q[0]q[1]q[2]q[3]$, the system is initialized to the ground state of the initial Hamiltonian. Then through a series of $RZ$, $RX$ and $CNOT$ gate operations, the quantum circuit of the target problem is obtained.

![Circuit diagram of variable quantum algorithm for solving equations](image2)

The experimental results are shown in Figure 4. We find the corresponding measurement operator in the Clifford library to measure the final state. The ground state of the cost Hamiltonian provides a solution to the problem. In this case. After 8192 experiments (the maximum number of runs that can be selected from the interface provided by IBM QE), the probabilities of the status $|0\rangle$ and $|1\rangle$ of $p_1$, $p_2$, $q_1$ and $q_2$ will be obtained respectively. The results show that after complete adiabatic evolution, the system is in the ground state of the cost Hamiltonian. Since the Hamiltonian at this time is degenerate, solution of the problem Hamiltonian are any of the two states $|0101\rangle$ and $|1010\rangle$. If we

\[
\hat{H}_p = \frac{1}{8}[13I_4 + 5\sigma_z^0 \otimes \sigma_z^1 + 5\sigma_z^3 \otimes \sigma_z^2 + \sigma_z^0 \otimes \sigma_z^2 - \sigma_z^0 \otimes \sigma_z^0 + \sigma_z^1 \\
+ \sigma_z^0 \otimes \sigma_z^1 - \sigma_z^0 \otimes \sigma_z^0 + \sigma_z^1 \otimes \sigma_z^0 - \sigma_z^0 \otimes \sigma_z^1 + \sigma_z^1 \otimes \sigma_z^0 \\
- \sigma_z^0 \otimes \sigma_z^0 - \sigma_z^0 \otimes \sigma_z^1 + \sigma_z^1 \otimes \sigma_z^0 - \sigma_z^0 \otimes \sigma_z^1 + \sigma_z^1 \otimes \sigma_z^0]
\]
consider $|0101\rangle$ as the solution, then the corresponding classical bit value will be $p_1=0$, $p_2=1$, $q_1=1$, $q_2=0$, leading to the first solution of equations in the binary system as $1 p, p_1=1011$, and therefore in the decimal system as $P = \sum_k 2^k p_k = 11$ and $Q = \sum_k 2^k q_k = 13$.

![Computational basis state](image)

Figure 4. Probability distribution in depth $p = 2$

In order to further study the performance of the variational quantum algorithm for solving equations, on the basis of the previous experiment, BFGS optimization is performed for different depths until the global minimum is reached, and the final state is obtained. The experimental results are shown in Table 1:

| Circuit depth | Number of iterations | Sq_overlap(%) |
|---------------|----------------------|---------------|
| P=1           | 136                  | 43.2          |
| P=2           | 157                  | 57.7          |
| P=3           | 223                  | 64.8          |
| P=4           | 295                  | 68.1          |
| P=5           | 377                  | 71.5          |

Table 1. Comparison of results in different depths

From the Table 1 that as the circuit depth continues to increase, the accuracy of the experimental results also gradually increases. It is further proved that the deeper the circuit, the better the effect of the variable quantum algorithm in solving equations. In addition, it can be seen that the number of loop iterations in the process of finding the best parameters by the optimizer is also increasing,
indicating that the running time is increasing.

4. Conclusions
This paper introduces the principle of variable quantum algorithm and the realization process of solving equations in detail. This is a hybrid solution of quantum and classical, which uses classical optimization techniques and variational quantum optimization techniques. Its advantage is that compared with pure quantum solutions designed for the same purpose, it can use fewer quantum resources (currently these resources are fragile and expensive) to solve the problem. In short, the proposed scheme has the ability to solve equations using less quantum resources. To illustrate this point, we used the smallest quantum machine available on the cloud (that is, a 5-qubit quantum machine named IBM QX4) to explicitly perform the process of solving the above equations.

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