Evolving Quantum Oracles with Hybrid Quantum-inspired Evolutionary Algorithm

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Abstract. Quantum oracles play key roles in the studies of quantum computation and quantum information. But implementing quantum oracles efficiently with universal quantum gates is a hard work. Motivated by genetic programming, this paper proposes a novel approach to evolve quantum oracles with a hybrid quantum-inspired evolutionary algorithm. The approach codes quantum circuits with numerical values and combines the cost and correctness of quantum circuits into the fitness function. To speed up the calculation of matrix multiplication in the evaluation of individuals, a fast algorithm of matrix multiplication with Kronecker product is also presented. The experiments show the validity and the effects of some parameters of the presented approach. And some characteristics of the novel approach are discussed too.

1 Introduction

Quantum computation is a flourishing research area and it has been believed that quantum computers hold a computational advantage over classical ones \cite{1}. Generally, for simplification in the studies of quantum computation, a transformation or even a quantum gate which isn’t directly implemented physically, is treated as a black box, i.e. quantum oracle. However, one of the challenges implementing practical quantum computers is to design the quantum oracle with quantum circuits made of available quantum gates \cite{2}. Mathematically, designing a quantum oracle can be formulated as decomposing the expected unitary matrix to some smaller matrices which correspond to the primary quantum gates. But the best known mathematic algorithms are not very efficient \cite{1}. Moreover, the potential mechanics of quantum computation is not well understood yet. So it’s very difficult to develop heuristic approaches designing quantum circuits at

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present. Finally, the designed quantum circuit may be inefficient. Appropriate optimization techniques are required to reduce its cost, such as rewriting rules based [3] or templates based [4] techniques.

However, we could get some surprised results with genetic programming [5]. Genetic programming is a sort of robust optimization algorithm, which mimics natural evolution that encodes the solution with chromosome, crossovers the old individuals according to the fitness, mutates them with probability and obtains the new individuals each generation over and over again. It is used to figure out complex optimization problems and requires little prior knowledge of the problems. All the advantages of genetic programming smooth out the above mentioned difficulties in designing quantum oracles, thus it has been used to automatic designing quantum circuits [6,7,8,9,10,11,12].

In this paper we develop a novel approach to evolve quantum oracle with a Hybrid Quantum-inspired Evolutionary Algorithm (HQEA) which has been successfully applied in numerical optimization and 0-1 knapsack problems (see [13] for detail introduction of HQEA). Taking the matrix corresponding to an oracle as input, the presented approach can achieve designing and optimizing the quantum circuits at the same time. This paper is organized as follows. In Section 2 the novel approach evolving quantum oracles is presented. To speed up the evaluation of individuals, a fast algorithm for matrix multiplication with Kronecker product is presented in Section 3 too. The validity of the presented approach is shown and the effects of some parameters of the approach are discussed in Section 4. In the last section, some conclusions are drawn.

2 Novel approach evolving quantum oracles

The novel approach takes HQEA as optimization algorithm. To take advantage of HQEA, it is necessary to encode quantum circuit with numerical value, which is different to the symbol notations in the previous works. Here, the different quantum gates or the same gates operating on different qubits are treated as different cases, which correspond to different number. Although it is possible that several quantum gates are operated parallelly, for simplification, it is assumed that only one quantum gate is applied on some qubits each time.

In the previous works [3,6,7,8,9,10,11,12], the quantum gates operating on non-adjacent or multiple qubits are taken as primitive gates. The commonly used non-adjacent quantum gates, for example, are generalized CNOT in which a NOT operation on a qubit is controlled by a non-adjacent one. In fact it’s difficult to implement the quantum operations on distant qubits. It’s more reasonable to take some one-qubit and adjacent two-qubit operations as primitive gates. One might argue that a realizable circuit could be obtained by replacing the generalized CNOT with the equivalent circuit composed by adjacent CNOT. But it is likely to generate redundances, see Fig. 1 as an illustration. In this paper, the available primitive gates include Phase(S), π/8(T), Hadamard(H) and CNOT [1]. But our approach is not confined to these gates. Generally speaking, if \( n_1 \) one-qubit gates and \( n_2 \) adjacent two-qubit gates are available, there are
\( N = n_1m + 2n_2(m - 1) + 1 \) different cases on \( m \) qubits (including the quantum wire). So \( k = \lceil \log_2 N \rceil \) bits are required to encode one case. And if a codon is decoded as integer \( s \), it corresponds to the case indexed by \( \left\lfloor \frac{sN}{2^k} \right\rfloor \). An individual representing a quantum circuit is consisted of \( gk \) qubits where \( g \) is the maximal number of allowable gates for the circuit.

Since even the same primitive gates have different costs depending on realization technologies of quantum computers, the cost of the designed quantum circuits should be considered. However, our approach is independent to the used cost function. In our work we just assign the one-qubit gate costs one, two-qubit gate costs two, and the quantum wire costs nothing. The cost of a circuit, \( \text{allcost} \), is the total cost of the gates presented in the circuit.

Let \( C \) be the implemented circuit which corresponds to the matrix \( \lambda(C) = (I_{2^{m_g}} \otimes A_g \otimes I_{2^{n_g}}) \times \cdots \times (I_{2^{m_1}} \otimes A_1 \otimes I_{2^{n_1}}) \), where \( m_i \) and \( n_i \) are respectively the numbers of qubits before and after the gate \( A_i \). If \( G \) be the goal matrix the circuit should implement, the correctness of \( C \) is defined by \( \text{correctness}(C) = \left| \text{tr}(G^\dagger \lambda(C)) \right|^2 \) such as

\[
\text{correctness}(C) = \frac{|\text{tr}(G^\dagger \lambda(C))|}{2^m} \quad (1)
\]

The fitness function takes \( \text{allcost} \) into account as well as the correctness of the circuit. Evolving quantum oracles is time-consuming when the scale of problem is very big. Sometimes we could be satisfied with a non-optimal circuit whose cost is less than some value. Such a value is called the satisfying cost (\( \text{satcost} \)). But it’s more important to obtain a correct quantum circuit. So a tradeoff between the cost and correctness should be taken. We take two thresholds \( \text{award} \) and \( \text{punish} \), and then the fitness function is defined as

\[
\text{fitness}(C) = \text{award} \times (\text{allcost} - \text{satcost}) + \text{punish} \times (1 - \text{correctness}(C)) \quad (2)
\]

As an evolutionary algorithm, the termination condition of the proposed approach is meeting the satisfying cost as well as fulfilling the correctness, or evolving allowable generation.
3 Fast matrix multiplication with Kronecker product

Lots of matrix multiplications are required in the process of evaluating individuals. It is well known that we should perform $O(n^3)$ multiplications when two $n \times n$ matrices are multiplied naively. Although the best algorithm currently known has an asymptotic complexity of $O(n^{2.376})$ [14], some improvement is still possible for the matrix multiplication with Kronecker product which is required in this paper. Firstly, we put up some conventions.

- Kronecker product, matrix multiplication and scalar product are denoted as $\otimes$, $\times$ and $\cdot$ respectively. The priority of $\cdot$ is higher than others and $\times$ takes on the lowest priority.
- $A_n^{(k)}$ denotes arbitrary $n \times n$ matrix $A$ treated as $k \times k$ blocks, each of which is a $\frac{n}{k} \times \frac{n}{k}$ matrix. Specially, $A_n$ means $A_n^{(1)}$ and $1_n$ denotes the $n \times n$ identity matrix.
- $B_{(i,j)}^{(m)}$ denotes the block located at the $i$-th row and the $j$-th column in $B_{mnk}^{(m)}$. In particular, $A_{(i,j)}$ denotes an element of $A$, for short, $a_{ij}$.

The trick is based on the block multiplication and the calculation is shown as follows.

\[
F = (1_m \otimes A_n \otimes 1_k) \times B_{mnk} \\
= \left( \begin{array}{c}
A_n \\
\vdots \\
A_n
\end{array} \right) \otimes 1_k \times B_{mnk} \\
= \left( \begin{array}{c}
A_n \otimes 1_k \\
\vdots \\
A_n \otimes 1_k
\end{array} \right) \times \left( \begin{array}{c}
\vdots \\
B_{(i,j)}^{(m)} \\
\vdots \\
\vdots \\
\vdots
\end{array} \right)_{mnk} \\
= \left( \begin{array}{c}
\vdots \\
A_n \otimes 1_k \times B_{(i,j)}^{(m)} \\
\vdots \\
\vdots \\
\vdots
\end{array} \right)_{mnk} \\
\tag{3}
\]

Let $A_n \otimes 1_k \times B_{(i,j)}^{(m)} = D = F(i,j)_{mnk}$, $(i, j = 1 \ldots m)$, then

\[
F(i,j)_{mnk} = \left( \begin{array}{c}
\vdots \\
\vdots \\
\vdots \\
\vdots \\
\vdots
\end{array} \right)_{nk} \times \left( \begin{array}{c}
\vdots \\
\vdots \\
\vdots \\
\vdots \\
\vdots
\end{array} \right)_{nk}^{(n)} \\
\tag{4}
\]

\[
D(p,q)_k = \sum_{l=1}^{n} (a_{pl} \cdot B(i,j)_{mnk}(l,q)_k) (p,q = 1 \ldots n) \\
\tag{5}
\]

It’s very clear that obtaining $D(p,q)$ requires $O(nk^2)$ multiplications, and then $O(n^3k^2)$ multiplications to obtain $D$ and lastly $O(m^2n^3k^2)$ multiplications to obtain $F$. So the fast algorithm speeds up $O_{\frac{(mnk)^{2.376}}{m^2n^3k^2}} = (mk)^{0.376}/n^{0.624}$ to the
original best algorithm. Simple algebra shows that our fast algorithm exceeds the best traditional algorithm when the number of qubits before the gate, $M = \log_2 m$, the number of qubits after the gate, $K = \log_2 k$, and the number of qubits the gate processes, $N = \log_2 n$, satisfy $M + K > 1.66N$.

4 Experiments and discussions

The presented approach is not confined to circuit design or circuit optimization, and the key factor is the satisfying cost. When this constraint is loose corresponding to a bigger satisfying cost, the algorithm performs mainly as an automatic designer which aims to discover a circuit implementing the desirable unitary transformation, and regardless whether the result is optimal. If this constraint is tight corresponding to a smaller satisfying cost, the algorithm not only tries to dig out a circuit functioning as desired, but also to reduce the cost of the circuit. As an instance, the optimal circuit of oracle SWAP is CNOT * CNOT2 * CNOT (CNOT2 denotes the CNOT taking the latter qubit as control bit and the former qubit as controlled bit) such as Fig. 2(a) which costs 6, but if we assign satcost as 8, another circuit could be obtained by our approach, such as Fig. 2(b).

![Optimal circuit](image1)

![Non-optimal circuit](image2)

(a) Optimal circuit  
(b) Non-optimal circuit

Fig. 2. Equivalent circuits of SWAP

| Goal oracle | Optimal cost | Satisfying cost | Maximal number of allowable gates | Maximal generation | AS | ST | OT |
|-------------|--------------|----------------|----------------------------------|-------------------|----|----|----|
| entangle2   | 3            | 4              | 6                                | 100               | 86.1 | 20 | 4  |
|             | 6            | 6              | 100                              | 14.8              | 20  | 0  |    |
| entangle3   | 5            | 6              | 6                                | 200               | 141.7 | 20 | 10 |
|             | 8            | 8              | 8                                | 200               | 48.65 | 20 | 1  |
| controlled-S| 7            | 8              | 8                                | 500               | 111.5 | 20 | 3  |
|             | 10           | 8              | 8                                | 500               | 62.5  | 20 | 1  |

*AS = average generation of success, ST = times of success in all tests, OT = times of getting optimal results in all tests.*

To study the affection of satisfying cost on evolving results, we apply novel algorithm on the oracle entangling two qubits, denoted by entangle2 as Fig. 3.
the oracle entangling three qubits, denoted by \textit{entangle3} as Fig. 4 and the oracle implementing controlled-phase, denoted by \textit{controlled-S} as Fig. 5. Each case is tested 20 times and in all the test, the number of quantum chromosome is 20, measurement times of each quantum chromosome is 10. The comparison results are shown in Table 1. In the experiment, all the tests obtain the circuits satisfying condition successfully. However, obtaining the circuits meeting more rigorous constraints needs more evolving time. Additionally, it can be found that there are many equivalent circuits implementing the same oracle, although some of them cost differently. Some of these circuits are illustrated in Fig. 3-5.

![Circuits entangling two qubits](image)

(a) Optimal one(cost 3)  
(b) One of non-optimal circuits(cost 5)

**Fig. 3.** Circuits entangling two qubits

![Circuits entangling three qubits](image)

(a) Optimal one(cost 5)  
(b) One of non-optimal circuits(cost 7)

**Fig. 4.** Circuits entangling three qubits

![Circuits implementing controlled-phase](image)

(a) Optimal one(cost 7)  
(b) One of non-optimal circuits(cost 8)  
(c) One of non-optimal circuits(cost 9)

**Fig. 5.** Circuits implementing controlled-phase

To effectively discover desired quantum circuits for different cases, it is useful to adopt the appropriate reward-punish factor in the fitness function. Table 2 shows the evolutionary results of oracle \textit{entangle2} with different reward-punish factors, where each case is tested 20 times. It is found that bigger punishment...
to the error of circuits is required to get the correct circuits, with the same satcost, \( g \) and other parameters. Another fact is that with the same \( g \) and other parameters, to get the correct circuits bigger punish is required for bigger satcost.

| Satisfying cost | Maximal number of allowable gates | Maximal generation | ST | AS
|----------------|----------------------------------|--------------------|----|-----|
| 6              | 6                                | 100                | 0  | 0   | 1   |
|                |                                  | 100                | 20 | 16.9| 5   |
|                |                                  | 100                | 20 | 10.65| 20   |
|                |                                  | 100                | 20 | 12.8| 100  |
|                |                                  | 100                | 20 | 15.55| 1000 |
| 8              | 8                                | 200                | 0  | 0   | 1   |
|                |                                  | 200                | 0  | 0   | 5   |
|                |                                  | 200                | 20 | 32  | 20   |
|                |                                  | 200                | 20 | 94  | 100  |
|                |                                  | 200                | 20 | 62.55| 1000 |
| 10             | 8                                | 500                | 0  | 0   | 1   |
|                |                                  | 500                | 0  | 0   | 5   |
|                |                                  | 500                | 0  | 0   | 20   |
|                |                                  | 500                | 20 | 40.45| 100  |
|                |                                  | 500                | 20 | 31.1| 1000 |

*ST = times of success in all tests, AS = average generation of success.

Table 2. Comparison with different reward-punish factors (reward = 1)

When comparing our work with others [3,4,6,7,8,9,10,11,12], we observe the following aspects:

1. Problems considered: Our approach evolves quantum circuits taking the desired unitary matrix as input, while some other works are based on the description of an oracle and evolve quantum circuits by comparing the outputs of the quantum oracle on random inputs with desirable ones [8]. In addition, the simplification of known quantum circuits are considered by [3,4]. Notably, only reversible quantum oracles are considered in our work. Thus measurements, not like the cases in [7,8], are not permitted.

2. Primary gates set: As has been stated, only two-qubit gates on adjacent qubits are available in our work while non-adjacent two-qubit or even multi-qubit gates are taken as primary gates in other works, although it can simplify the problem of quantum circuit design. Of course, our approach is not confined to any special quantum gates set.

3. Circuit representations: While all the previous works use symbolic representations, our approach encodes the quantum circuits with numerical values. In despite of the apparent difference within them, all of them are equivalent. But it is more natural to apply evolutionary operators on the individuals coded by our means.
4. Fitness function: The cost of designed quantum circuits is ignored in [6,7,8,9]. Moreover, the cost and correctness are individually considered in [12]. To reflect the fitness of evolved quantum circuits more accurately and expediently, our approach combines them together by simple reward-punish factors.

5. Application: Our approach can be adapted to both circuit designing and circuit optimization. When applied to the later, more rigorous conditions should be assigned, such as the smaller satisfying cost and maximal gates number.

6. Common challenge: The bottleneck in designing quantum circuits with evolutionary algorithms is the individual evaluation, i.e. the matrix multiplications in the computing of fitness which have potentially exponential space increment and speed slow down. The intractable problem results from the argument that the quantum system can not be effectively classically simulated.

5 Conclusions

Genetic programming appears to be useful in designing quantum circuits. We propose how to evolve quantum oracle with a hybrid quantum-inspired evolutionary algorithm. With our approach no additional knowledge is required to design an optimized quantum oracle as expected. Especially, we design a novel approach to represent quantum circuits with numerical values in the evolutionary algorithm. A faster algorithm for matrix multiplication with Kronecker product is presented too. It speeds up the evaluation of individuals very much. Obviously, the numerical representation and fast algorithm of matrix multiplication are not unique to our approach, but adaptable to other evolutionary quantum programming algorithms or hierarchical approaches. By assigning different parameters, the novel approach could be inclined to designing a quantum circuit or optimizing it. Our approach provides insights into quickly evolving quantum oracles. A possible improvement to the approach may be encoding the quantum circuits with variable length.

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