Multi-objective design of quantum circuits using genetic programming

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Abstract

Quantum computing is a new way of data processing based on the concept of quantum mechanics. Quantum circuit design is a process of converting a quantum gate to a series of basic gates and is divided into two general categories based on the decomposition and composition. In the second group, using evolutionary algorithms and especially genetic algorithms, multiplication of matrix gates was used to achieve the final characteristic of quantum circuit. Genetic programming is a subfield of evolutionary computing in which computer programs evolve to solve studied problems. In past research that has been done in the field of quantum circuits design, only one cost metrics (usually quantum cost) has been investigated. In this paper for the first time, a multi-objective approach has been provided to design quantum circuits using genetic programming that considers the depth and the cost of nearest neighbor metrics in addition to quantum cost metric. Another innovation of this article is the use of two-step fitness function and taking into account the equivalence of global phase in quantum gates. The results show that the proposed method is able to find a good answer in a short time.

Key words: quantum gates; quantum Cost; genetic programming; multi-objective design; optimization

1. Introduction

Quantum computing [1-3] is resulted by combining quantum mechanics and classical information theory and leads to a strange and powerful events in the field of quantum. Each unitary matrix represents a quantum gate. The synthesis of quantum circuit is a process of converting a quantum gate to a series of basic gates. The issue of design and optimization of quantum circuits is a difficult issue [4], which is divided into two general categories based on the decomposition and composition. In the methods of the first group, the matrix decomposition method is used to design quantum circuits. In the second group, using evolutionary algorithms and especially Genetic Algorithms (GA) [5-7], matrix gates multiplication is used to achieve the final characteristic of quantum circuit.

Genetic programming [8] is a subfield of evolutionary computing in which computer programs evolve to solve the studied problem. This method was formed followed by genetic algorithm with a new presentation method to improve solving disadvantages of genetic algorithm in solving some problems.

Various methods have been proposed for the evolutionary design of quantum circuits. In this methods, the genetic algorithm has been used for synthesis of circuit and the goal has been defined as achieving the desired characteristic fully or with an acceptable percentage of difference. In [9,4,10,11], simple GA has been used to design quantum circuits. Although these methods search the large space of the solutions in problem, but they are very general and do not consider the cost of the circuit. In [12], Genetic Programming (GP) has been used to design. In these algorithms, the main focus is on specific functions. One of the problems that designing the reversible circuits (a special case of quantum circuits) are faced with is the problem of complexity of quantum search space [13,14]. The complexity of the search space include high dimensions of search space, a large number of gates and so on. Of course, in a series of research could design the medium-sized circuits with evolutionary algorithms. However, none of the reviewed articles have not considered a multi-objective fitness function for optimal designing especially with genetic programming.

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In this paper, a multi-objective design method based on GP was proposed for designing quantum circuits. Another innovation of this article is taking into account the equivalence of global phase and the use of two-step fitness function that in the first step, the accuracy of the circuit is evaluated. Then, quantum circuits cost metrics, depth and nearest neighbor have been considered that in the previous articles, only criterion of quantum cost has been considered that is not enough.

The rest of this paper is structured as follows: in Section 2, the required background corresponding to quantum computing, quantum gates and definitions of quantum circuits cost have been proposed. The proposed method has been presented in Section 3. In Section 4, a comparison between results of the proposed method with previous methods has been performed and finally, conclusion has been presented in Section 5.

2. Basic concepts

2.1. Principles of Quantum Computing

Quantum states can be represented by vectors or a more famous notation of bra/Ket. Kets (shown as |x⟩) display column vectors and are generally used to describe quantum states. The bra notation (shown as ⟨x|) display transpose conjugate of x vector (|x⟩). Basic states of |1⟩ and |0⟩ can be stated as vectors of [0 1]^T and [1 0]^T respectively. Any combination of |1⟩ and |0⟩ states (α|0⟩ + β|1⟩) can be showed as [α β]^T ∈ C^2, in which C denote set of complex number.

A qubit is a unit vector in a complex two-dimensional space that the specific basis vectors with the notation of |0⟩ and |1⟩ have been selected for this space. The base vectors of |0⟩ and |1⟩ are quantum counterpart of classic bits of 0 and 1, respectively. Unlike classic bits, qubits can be in any superposition of |0⟩ and |1⟩ like α|0⟩ + β|1⟩ where α and β are the complex numbers that |α|^2 + |β|^2 = 1. If such a combination is measured compare with the base of |0⟩ and |1⟩, then |0⟩ and |1⟩ are seen with probability of |α|^2 and |β|^2, respectively.

2.2. Quantum gates

Quantum operations can be achieved with a network of gates. Each quantum gate is a linear transformation that is defined on the n-qubit space by an effective unitary matrix. The matrix U is unitary, if $U U^\dagger = 1$ where $U^\dagger$ is the transpose conjugate of matrix U. Examples of helpful single-qubit gates are members of π Pauli collection composed of the following four functions:

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

(1)

Matrix I is the identity transformation, X is the bit rotation gate, Z is the phase rotation gate and Y is a combination of both.

The controlled-NOT (CNOT) gate is a two-qubit gate. The first qubit has the role of the control and the second qubit has the role of the target. If the control qubit is |1⟩, CNOT reverses the target qubit and if the control qubit is |0⟩, the target qubit exits with no change. In other words, the second output is XOR qubit of the control and the target. View CNOT gate matrix is as equation (2). Also, Fig. 1 shows the circuit schematic of CNOT gate.

$$CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

(2)

Fig. 1 The circuit schematic of CNOT gate [1].
Fig. 2 illustrate another permutation gate called a Swap gate. As show in this figure, this gate just swaps the wires A and B. The most another used reversible logic gate is Fredkin gate or controlled Swap gate. It is a $3 \times 3$ reversible gate. If $A$, $B$, and $C$ are the inputs then $P$, $Q$, and $R$ will be the outputs such that $P = A$, $Q = A'B + AC$ and $R = A'C + AB$. Fig. 3 shows this gate.

![Fig. 2 implementation of Swap gate with CNOT gate and the its circuit schematic](image)

![Fig. 3 The circuit schematic of Fredkin gate](image)

2.3. Tensor product and matrix multiplication

If there are two assumed matrices with dimensions $a \times b$ and $c \times d$, respectively, tensor product [15] is defined as multiplication of each components of the first matrix in all components of the second matrix that produces a matrix with a dimension of $ac \times bd$. For example, if two matrices $A$ and $B$ are as follows:

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}, \quad B = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}$$

Then the tensor product of these two matrices is equal to:

$$A \otimes B = \begin{bmatrix} a_{11} [b_{11} & b_{12} & a_{12} & b_{12}] \\ a_{21} [b_{11} & b_{12} & a_{12} & b_{12}] \\ a_{11} [b_{21} & b_{22} & a_{12} & b_{12}] \\ a_{21} [b_{21} & b_{22} & a_{12} & b_{12}] \end{bmatrix}$$

(3)

And product matrix of two assumed matrices with dimensions of $a \times b$ and $b \times d$ (number of columns in the first matrix must be equal to the number of rows in the second matrix) is a matrix with dimensions of $a \times d$ that is calculated as follows:

$$AB = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{bmatrix}$$

(4)

2.4. Cost metrics of designing quantum circuit

Cost metrics to evaluate and compare different reversible and quantum designs are as following [16]:

1. Quantum Cost: Quantum cost of a circuit is the number of elementary gates of the circuit. In order to evaluate a designing algorithm based on quantum cost, the quantum cost per gate should be firstly considered and then, the total of these costs is reported as the final cost of the circuit.
2. Depth: The elementary gates in a quantum circuit that can be implemented simultaneously are considered as a logic level. The logic levels of a circuit are called the logic depth of the circuit or simply depth.
3. Nearest Neighbor Cost: In the Linear Nearest Neighbor (LNN) architecture, only adjacent qubits can act on each other. This architecture is so that only the interaction of adjacent qubits is physically desirable for practical implementation of quantum circuits. If a quantum gate is considered on the two qubits, while its target and control bits are located on $c$th and $t$th lines, respectively ($0 \leq c, t < n$, where $n$ is the numbers of input), in this case, NNC of this gate is calculated using this equation: $|c - t - 1|$ that determines the distance between the control and target. NNC criteria of a circuit is the sum of NNC of all its gates. The optimal NNC criteria for a circuit is zero in which, the circuit is composed of single-qubit and two-qubit gates and its two-qubit gates are located on neighbor qubits.
Fig. 4 shows a circuit for a full adder that is simplified in terms of quantum cost and compacted in terms of the depth [17]. The logic levels of this circuit are separated by dotted. The quantum cost of this circuit is 6 and its depth is equal to 4. NNC value of this circuit is equal to the number 3. The number of main output of this circuit is 2, so 2 outputs of x and G are considered as unused output.

![Simplified circuit in terms of cost with compacted logic levels for a full adder](Image)

2.5. Genetic programming

Genetic Programming (GP) [8] plays the role of an evolutionary algorithm distinctively functioning on a varying-sized chromosome, generally in a tree structure. The populations of computer programs are genetically developed through the Darwinian tenet of natural choice and hereditary processes. Individual in a GP population acts as a program in a hierarchical tree structure, comprised of primitives such as functions and terminals defined in the problem field. The functions are able to be made up of the programming operators (e.g. if, for), standard arithmetic operators (e.g. +, -), logical operators (e.g. or, and), mathematical functions (e.g. sin, exp) or any problem-specific function in the field. Terminals are typically represented by constants or variables.

GP commences by means of a preliminary population of programs randomly created in most cases. Each individual in this population is, therefore, assessed via a predefined problem-specific fitness function. Each individual in this population possess a fitness value. The fitness value signifies the competence of the individual to resolve the problem. Selection utilizes the fitness value in order to recognize the individuals which will replicate and pair off to yield the following generation. Mutation and crossover simulate the recombination process. These operators intend to discompose the features of parent individuals to breed distinctive offspring individuals. Crossover stands as is the principal exploration mechanism in GP, capable of adopting diverse configurations. It is possible to employ double-point, n-point, or uniform crossover. Mutation is mostly deemed to be a subordinate search operator. Its utility involves renovating multiplicity which might be vanished from the recurrent usage of selection and crossover. The creative process is reiterated up to when a concluding circumstance is fulfilled. Fig. 5 demonstrates the utilization of crossover and mutation operators.

![Illustration of crossover and mutation operators in tree structure](Image)

2.6. Multi-objective genetic programming

Multi-objective optimization encompasses the progression of optimizing concurrently an assemblage of objective functions. For instance, scheming a circuit acts as a multi-objective problem owing to the numerous objectives that are to be achieved. Devoid of losing generality, all goals are believed to be of maximization type. When the minimization type is concerned, the objective is able to be renewed to a maximization type through multiplying a negative one. A maximization multi-objective decision problem with K objectives can be expressed as follows:
\[
\maximize f(x) = (f_1(X), f_2(X), \ldots, f_k(X)), X \in \Omega \tag{5}
\]

In which \(X = (x_1, x_2, \ldots, x_m)\) represents a variable vector of \(m\) dimensions, \(X\) signifies the possible solution space, and \(f_1(X), f_2(X), \ldots, f_k(X)\) denote \(k\) objective functions. A solution not controlled by any other solution within the solution space is identified as Pareto optimal. A Pareto optimal solution is not capable of being perfected regarding any objective without failing, nonetheless, one other objective \([19,20]\).

Evolutionary algorithms have lately been employed in multi-objective optimization problems, and Genetic Algorithms (GA) and GP in particular are totally appropriate in resolving such problems. The foremost disparity between a single-objective and a multi-objective evolutionary algorithm remains in the fitness calculation. In a single-objective genetic programming, the fitness function is a clear-cut function (for example, identity) of the objective function. Contrarily, in a multi-objective evolutionary algorithm, the fitness function explains the total objectives at the same time.

3. Proposed method

3.1. Coding problem

A quantum circuit cannot directly be modeled as a tree structure due to the following problems:

- Each logic gate is modeled with a matrix and inputs are in the form of vector.
- The logic gates in a column must be multiplied together using tensor product and also the logic gates in a row using matrix multiplication.
- In quantum circuits, some logic gates are as the multiple-input.

The process of solving this problem using genetic programming has been explained in the following:

Instead of defining the tensor product and matrix multiplication as functions and logic gates and inputs as terminals, all of desired logic gates (single-input or multiple-input) in the form of single-input are firstly defined as the function for GP and then, only the main inputs are defined as terminals. Therefore, the made trees are coded as Equation (6):

\[
y' = \text{gate}_1(\text{gate}_2(\ldots(\text{gate}_n(x)))) \tag{6}
\]

Where, \(n\) is the depth defined for the tree, \(X\) is the total input states (\(2^k\) states, \(k\) is the numbers of input) in the form of matrix and \(y'\) is equivalent function obtained by GP. Then, tensor product and matrix multiplication in the number of inputs are defined. For convenience, the braces and inputs are removed at first. Therefore, we have just a combination of logic gates. Then, logic gates are separated based on the number of inputs that in Equation (7), each of them has been marked with group:

\[
y' = \text{gate}_1 \text{gate}_2 \ldots \text{gate}_k \ldots \text{gate}_n \tag{7}
\]

In Equation 7, the number of logic gates in each group is equal to the number of inputs \((k)\), logic gates in each group is multiplied together with tensor product. For example, logic gates of group1 has been multiplied in Equation (8) with tensor product:

\[
\text{group 1} = \text{gate}_1 \otimes \text{gate}_2 \otimes \ldots \otimes \text{gate}_k \tag{8}
\]

Where, \(\otimes\) is symbol of the tensor product. Then, groups are multiplied together with the matrix multiplication, and at the end, they are multiplied in the total inputs \((x)\), which is a matrix. This action has been shown as Equation (9) where \(y'\) is the value of the matrix predicted by the proposed method.

\[
y' = \text{group 1} \times \text{group 2} \times \ldots \times \text{group} k \times x \tag{9}
\]

3.2. Fitness function

In the search process, in order to survey the similarity of a chromosome with the given unitary matrix, which is supposed to be synthesized, the following two-step fitness function can be used:
At first, according to Equation (10), the similarity of the matrix of each chromosome $C$ (which is denoted by $S$) with the target unitary matrix, $(U)$ is calculated as follows:

\[
\text{Fitness}_1(C) = \sum_{i=1}^{2^n} \sum_{j=1}^{2^n} |U_{ij} - S_{ij}|, S, U \in U(2^n)
\]

(10)

Of course, this equation does not consider the equivalency of goal-phase of the target gate and the candidate solution gate.

In order to evaluate the global phase, equivalent circuit matrix of each chromosome is divided by the exponential sentence of displaying polarization of the first non-zero component in its matrix and the corresponding value in the matrix of the quantum gate (to be converted into an identical real number) and then, similarity of two matrices is reviewed. In this paper, instead of above definition of goal phase, is used of Equation (11) according to [21]:

\[
\text{correctness}(C) = \frac{|\text{tr}(U^TS)|}{2^n}
\]

(11)

Where $\text{tr}$ and $U^\dagger$ denote trace matrix and conjugate transpose of $U$ matrix. As shown in Equation (11), If $S$ and $U$ differ only by a complex phase factor, then $C$ is assigned a correctness of 1. Thus, if value of Equation (10) is equaled to zero or value Equation (11) is equaled to one then algorithm is achieved to the solution of problem. In the next step, in the fitness function, other optimization criteria such as the quantum cost, depth and the cost of nearest neighbor are examined. The most common method of calculating the fitness function in the GA or a multi-objective GP is the weighted sum method. Thus, the criteria of quantum cost, depth and nearest neighbor cost (NNC) are evaluated according to Equation (12):

\[
\text{Fitness}_2(C) = 1 + k_1 \times \text{Gates}(C) + k_2 \times \text{Depth}(C) + k \times \text{NNC}(C) \quad 0 < k_1, k_2, k_3 < 1
\]

(12)

In equation (12), the coefficients of $k_1$, $k_2$ and $k_3$ have values between zero and one based on the importance of targets. In the case of parameter QC ($C$), which is the value of quantum cost, based on the logic gate, which is a single-input or multi-input, a coefficient is multiplied in each logic gate that this coefficient is 1 in a single-input logic gate and a numerical value is considered for this coefficient depending on the type of gate in a multi-input logic gate. Since the implementation time of CNOT gate is 10 times more than a single-qubit [16], the cost of quantum gates is calculated as the sum of the number of single-qubit gates and the number of CNOT gates multiplied by 10. Because we usually divide multi-qubit gates to the single or two-qubits gates that if there is CNOT in these gates, we consider 10 for its cost. In Table 1, libraries used in synthesis of function with cost of each gate are shown.

**Table 1** a) representation of library of Pauli, Hadamard and CNOT; b) library of NCV.

<table>
<thead>
<tr>
<th>GATE</th>
<th>COST</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>1</td>
</tr>
<tr>
<td>X</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>1</td>
</tr>
<tr>
<td>Y</td>
<td>1</td>
</tr>
<tr>
<td>Z</td>
<td>1</td>
</tr>
<tr>
<td>CNOT</td>
<td>10</td>
</tr>
</tbody>
</table>

a)

<table>
<thead>
<tr>
<th>GATE</th>
<th>COST</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>1</td>
</tr>
<tr>
<td>NOT</td>
<td>1</td>
</tr>
<tr>
<td>C_V</td>
<td>10</td>
</tr>
<tr>
<td>C_V^\dagger</td>
<td>10</td>
</tr>
<tr>
<td>CNOT</td>
<td>10</td>
</tr>
</tbody>
</table>

b)

To obtain parameter Depth ($C$), according to the coding explained in sub-section coding problem, it can be stated that it is determined, if the length of the desired string is divide by the number of inputs of the issue. For parameter NNC ($C$), two-input functions can be found from obtained function strings, and then NNC value can be determined by difference between the control gate and the target gate for each gate and sum of all obtained NNCs.

In detection of algorithm for selecting optimal fitness, to prevent interfering between the values obtained from Equation (10) and the values obtained from Equation (12), the Equation (10) can be multiplied in a large number (such as 100). In this case, if the circuit obtained by GP has not made the desired gate, it gives a large penalty that causes the very low chances of presenting it in future generations.
4. Experimental results

The proposed method was implemented using MATLAB software and GPLAB toolbox [22] (that have been developed by Sara Silva) on a system with CPU 2 GHz Core Duo and RAM 2 GB. Setting used for GPLAB toolbox are shown in Table 2. As shown in this Table, for creating initial population of trees, is used from Ramped Half-and-Half method introduced in [22,23]. Unlike method introduced in Koza [8], this method use from concept of Dynamic Maximum Tree Depth. Dynamic Maximum Tree Depth introduces a dynamic limit on the depth of the trees allowed into the population, initially set with a low value but increased whenever needed to accommodate a new best individual that would otherwise break the limit.

<table>
<thead>
<tr>
<th>Specification name</th>
<th>Used state</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tree initialization</td>
<td>Ramped Half-and-Half method introduced by Silva [22]</td>
</tr>
<tr>
<td>Genetic operators</td>
<td>Crossover and Mutation</td>
</tr>
<tr>
<td>Selection</td>
<td>Roulette Wheel</td>
</tr>
<tr>
<td>Elitism</td>
<td>Replace</td>
</tr>
</tbody>
</table>

Values of k1, k2 and k3 in Equation (12) are considered as 0.8, 0.6 and 0.4 respectively. Table 3 shows the results of the proposed method on some tested circuits. In this table, NNC is not defined for the circuit whose column corresponding to NNC is empty.

<table>
<thead>
<tr>
<th>Test Circuit</th>
<th>The quantum cost of the proposed method</th>
<th>The quantum depth of the proposed method</th>
<th>NNC of the proposed method</th>
<th>Implication Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CZ gate</td>
<td>12</td>
<td>3</td>
<td>0</td>
<td>0.8</td>
</tr>
<tr>
<td>Half Adder</td>
<td>60</td>
<td>2</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>CNOT gate with negative control</td>
<td>12</td>
<td>3</td>
<td>0</td>
<td>1.2</td>
</tr>
<tr>
<td>[1 0 0 1] [0 1 −1 0] [1 0 0 −1] [0 1 1 0]</td>
<td>21</td>
<td>3</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>Fredkin gate</td>
<td>70</td>
<td>3</td>
<td>-</td>
<td>3.5</td>
</tr>
<tr>
<td>SWAP gate</td>
<td>30</td>
<td>3</td>
<td>0</td>
<td>0.9</td>
</tr>
<tr>
<td>XOR4</td>
<td>30</td>
<td>3</td>
<td>0</td>
<td>4.6</td>
</tr>
</tbody>
</table>

In order to assess, experiments have been conducted on 2 to 5-qubit circuits and the results of this implementation were compared with the results presented in [24, 4, 12] in terms of quantum cost. It is worth noting that because these methods only have considered the quantum cost, in the multi-objective function, coefficient k1 is considered 1 and k2 and k3 coefficients are zero. Table 4 shows this comparison. The method of calculation is so that the quantum cost of several basic circuit presented are subtracted from the quantum cost of the circuit synthesized with the proposed method and has been divided by the minimum one. As shown in this table, the proposed approach leads to better responses compared with the previous methods and by increasing the number of qubits, the improvement percentage is increased.

<table>
<thead>
<tr>
<th>n</th>
<th>The improvement percentage of quantum cost compared to [4]</th>
<th>The improvement percentage of quantum cost compared to [12]</th>
<th>The improvement percentage of quantum cost compared to [23]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>33%</td>
<td>25%</td>
<td>21%</td>
</tr>
<tr>
<td>3</td>
<td>37.1%</td>
<td>34%</td>
<td>29%</td>
</tr>
<tr>
<td>4</td>
<td>39%</td>
<td>32.5%</td>
<td>28.8%</td>
</tr>
<tr>
<td>5</td>
<td>52%</td>
<td>49.5%</td>
<td>39.4%</td>
</tr>
<tr>
<td>average</td>
<td>40.27%</td>
<td>35.25%</td>
<td>29.55%</td>
</tr>
</tbody>
</table>
5. **Conclusion**

In this paper, a multi-objective design method was proposed based on Genetic Programming (GP). Another innovation of this article is taking into account the equivalence of global phase and the use of two-step fitness function that in the first step, the accuracy of the circuit is evaluated. By using a two-step fitness function, it is possible to recognize which solution of GP is a correct answer according to the value of fitness function. The results of running on two till five-qubit circuits showed that the proposed method is able to find an optimal answer in a short time for designing these circuits.

As suggestions for future works, to enhance the scalability of evolutionary method in solving quantum circuit design issues, these methods can be combined efficient methods to simulate such as QuIDD [25]. In addition, other multi-objective methods of genetic programming such as Pareto based methods [6] could also be considered as a future work.

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