Generating efficient quantum circuits for preparing maximally multipartite entangled states

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In this work we provide a method for generating quantum circuits preparing maximally multipartite entangled states using genetic programming. The presented method is faster than known realisations thanks to the applied fitness function and several modifications to the genetic programming schema. Moreover, we enrich the described method by the unique possibility to define an arbitrary structure of a system. We use the developed method to find new quantum circuits, which are simpler from known results. We also analyse the efficiency of generating entanglement in the spin chain system and in the system of complete connections.

I. INTRODUCTION

One of the key resources in the quantum information theory is entanglement [1, 2]. It is an inherent part to many branches of research in the field of quantum information computing. One of the most perspective applications of quantum computing, the quantum key distribution, utilizes the entanglement of parts of the key possessed by a sender and a receiver. Similarly, the experimental implementation of quantum teleportation requires sharing of maximally entangled states between the communicating parties. Entanglement is also necessary in applications such as dense coding and quantum direct communication protocols. It is considered that entanglement plays a crucial role in the exponential speedup of quantum algorithms [3].

The above applications are based on harnessing bipartite maximally entangled states. This suggests searching for new quantum algorithms that would make use of maximally multipartite entangled states. However, searching for maximally entangled states itself is a known problem [10, 11, 19].

The main goal of this work is to provide an efficient method of searching for circuits preparing maximally multipartite entangled states. The algorithm described in this work is based on genetic programming (GP). We take advantage of efficient fitness function and introduce the modifications to the genetic programming engine that result in shorter runtime of the process. We also introduce the method of representing quantum circuits allowing for the reduction of the search space. Additionally we use narrowed sets of universal quantum gates in order to increase computational efficiency. Apart from improving performance of the algorithm we also take the structure of a system into consideration.

This paper is organized as follows. In section II we describe the proposed method, focusing mainly on the circuits representation and the fitness function. Then, in section III we present the obtained results.

II. DESCRIPTION OF THE METHOD

Genetic programming is the numerical method based on evolutionary mechanisms. We decided to use such a method because of the two main reasons. First of all it enables to perform numerical search in complicated, mathematically untraceable space. On the other hand, we assume that entanglement in a quantum circuits increases in particular segments quite independently. Genetic programming enables to exchange segments between different circuits generating high entanglement by the use of evolution mechanisms.

A. General GP algorithm

Genetic programming belongs to the family of search heuristics inspired by the mechanism of natural evolution (in genetic algorithms each element of a search space being candidate for a solution is encoded as a representative of a population). Every member of a population has its unique genetic code, which is its representation in optimization algorithm. In most of the cases the genetic code is a sequence of values from a finite set \( \Sigma \) of possible values of all the features that characterize a potential solution \( x \in \Sigma^n \) in the search space. Searching for the optimal solution is done by the modification of genetic code due according to the rules of the evolution such as mutation, selection, crossover and inheritance.

Mutators are the functions that change single elements of a genetic code of a population member randomly. A basic example of a mutator is a function that randomly changes values of a representative \( x \) at all positions with some non-zero probability.
\[ M(x)_i = \begin{cases} x_i, & \text{probability } p \\ \text{rand}(\Sigma), & \text{probability } 1 - p \end{cases} \]  

(1)

Crossovers implement the mechanism of inheritance. This function divides parental genetic codes and create a new genetic code. Commonly two new codes are created at the same time from two parental codes. An example of such crossover is so called two point cut, where both parental codes \((x, y)\) are cut into three regions and the middle segments are interchanged

\[
\begin{align*}
\begin{cases}
x'_i = x_i \quad & i \leq c_1 \lor c_2 \leq i, \\
y'_i = y_i \quad & c_1 < i < c_2,
\end{cases}
\end{align*}
\]

where \(c_1 < c_2\) are randomly chosen indices. In every iteration of the algorithm all members of the population are evaluated using fitness function \(f : \Sigma^n \rightarrow \mathbb{R}\) which enables ordering elements. Then, using the selector function, the set of the best members is obtained and used to create a new generation of a population using mutation and crossover functions. There is a number of strategies for defining the selector function – from completely random choices to the deterministic choice of best representatives.

In this work we use a solution which places somewhere in between. During every selection we begin with establishing a random set \(R_S \subset S\) of elements from population \(S\):

\[
R_S = \text{rand}\{U \subset S : |U| = n\},
\]

where \(n\) is a fixed number of elements in every set. Then we apply the fitness function to choose a maximally well fitted one from this narrowed set (a random element from a set of maximally well fitted ones)

\[
\text{Selector}(S) = \text{rand}\{x \in R_S : f(x) = \max_{x \in R_S} f(x)\},
\]

(3)

where \(f(x)\) is the fitness function.

The strategy based on evolution mechanism makes genetic programming especially usable when parts of genetic code represent the features of elements of search space and can be interchanged between elements independently. In such case GA is expected to find the features that occur in well fitted representatives and mix them in order to find the best possible combination. Pseudo code representing this approach is presented in Listing 1.

```
population = RandomPopulation()
for( generationsNumber ){
    newPopulation = []
    for(i = 0; i<population.size()/2; i++){  
        mom = Selector(population)  
        dad = Selector(population)  
        (sister, brother) = CrossOver(mom, dad)
        Mutator(sister)
        Mutator(brother)
        newPopulation.append(sister)
        newPopulation.append(brother)
    }
    population = newPopulation
}
```

Listing 1: Pseudo code representing the algorithm of genetic programming. Functions Selector, Mutator and CrossOver work as defined in Section II.

While the customization of population representation and fitness function unavoidably relies on the optimization problem, other parameters of genetic programming such as crossover and mutation methods are universal. When treating quantum circuits as the strings of integers representing quantum gates one can use various, already developed methods [16].
B. Circuits representation - population

In order to apply the Genetic Algorithm it is necessary to define a population, a fitness function, the methods of crossing-over, mutation and selection. In the case of the optimization of quantum circuits generating entanglement the population consists of quantum circuits. The most convenient way to represent a computation in a quantum circuit is a sequence of quantum gates. Every quantum gate can be approximated using the gates from a set of universal quantum gates. In this work we use a set containing the Hadamard gate $H$, the $R(\pi/4)$ (called $\pi/8$) gate and the controlled-NOT gate $CNOT$.

\[
H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad R(\pi/4) = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{2} \end{pmatrix}.
\] (4)

However, initial experiments suggest that the $R(\pi/4)$ gate is not necessary for generating maximally entangled states in small systems (i.e. with less than 7 qubits). Thus, in order to simplify the resultant state, we consider a set containing only $H$ and $CNOT$ gates when the obtained entanglement is maximal.

One should note that using a general representation of circuits, we treat circuits that are equivalent with respect to permutations of qubits as completely different. In our scheme to decrease the number of equivalent circuits in the search space we reduce the number of available gates on a few first positions to the ones operating on first 2 qubits, where $p$ is the number of a gate. Such simplification does not influence the space of feasible solutions, because it is not possible to act on more than 2$q$ qubits using $p$ gates which all act on maximum 2 qubits.

C. Multipartite entanglement potential - fitness function

As our goal is to find a circuit which prepares maximally multipartite entangled state, our fitness function must determine how entangled the resultant state is. In this case computing fitness score of a quantum circuit requires obtaining the output state and then the estimation of its entanglement. One should note that we do not necessarily need an entanglement measure to perform a successful numerical optimization. We only need a function for some kind of estimation of multipartite entanglement that reaches its maximum only for maximally entangled states, which can be characterized by a number of criteria.

Definition 1 State $\rho \in D(\mathcal{X} \otimes \mathcal{Y})$, $\dim(\mathcal{X}) \geq \dim(\mathcal{Y}) = n$ is maximally entangled if and only if the reduced state is maximally mixed: $\text{Tr}_\mathcal{X}(\rho) = \mathbb{I}/n$ i.e. $S(\text{Tr}_\mathcal{X}(\rho)) = n$.

As we do not have a good measure of multipartite entanglement that we can use in our computation, we try to find a function that estimates the entanglement quantitatively. In this work we rely on the definition of maximally multipartite entangled states introduced by Facchi et al. [8].

Definition 2 State $|\psi\rangle \in \mathbb{C}^{2^n}$ is called maximally multipartite entangled state if it is maximally entangled according to every bipartition.

That definition induces a construction for multipartite entanglement potential, which is based on the algebraic sum of the purity of all possible bipartitions of a system. Such an approach guarantees that the maximally entangled states are classified correctly. However, the purity function does not distinguish some states with different values of entanglement measures such as negativity or von Neumann entropy. For this reason in this work we use analogous algebraic sum of bipartite entanglement measure defined as

\[
E^{(n)}_{\mathcal{V}\mathcal{N}}(|\psi\rangle\langle\psi|) = \sum_{(\mathcal{X},\mathcal{Y})} E_{\mathcal{V}\mathcal{N}}(\text{Tr}_\mathcal{X}(|\psi\rangle\langle\psi|)),
\] (5)

where $(\mathcal{X},\mathcal{Y})$ is a bipartition of a system, and $\dim(\mathcal{X}) \geq \dim(\mathcal{Y})$. For pure states it holds that $\text{Tr}_\mathcal{Y}(|\psi\rangle\langle\psi|) = AA^\dagger$, where $A$ is the coefficients matrix of a state $|\psi\rangle$ (i.e. $|\psi\rangle = \text{vec}(A)$). Thus we have:

\[
E_{\mathcal{V}\mathcal{N}}(|\psi\rangle\langle\psi|) = E_d(|\psi\rangle\langle\psi|) = S(\text{Tr}_\mathcal{Y}(|\psi\rangle\langle\psi|)) = S(AA^\dagger) = -\sum \lambda_i \log_2 \lambda_i,
\] (6)

where $S$ is the von Neumann entropy, and $\lambda_i$ are of the matrix $A$. 

| System   | qubits | 3 | 4 | 5 | 6 | 7 | 8 |
|----------|--------|---|---|---|---|---|---|
| Spin chain |       | 2 | 3 | 5 | 8 | 11| 16|
| Complete |       | 2 | 3 | 7 | 11| 18| 23|

TABLE II: The minimal number of CNOT gates necessary to generate maximum multipartite entanglement in spin chain and system of complete connections

Although we considered a number of functions, only proper bipartite measures of entanglement have met our restrictions. In order to select one for further computation we performed computational speed comparison (see Figure 1). Finally we decided to use algebraic sum of a measure using von Neumann Entropy over all possible bipartitions of a system.

III. GENERATION OF MULTIPARTITE ENTANGLEMENT

As an example of an application of the described method we find the minimal circuits preparing the maximally multipartite entangled states. We perform search both for spin chain and complete connection systems. Finally we compare the obtained results. The method developed in this paper is probabilistic. This makes the optimization of additional parameters a tedious task. In order to obtain a minimal circuit we execute an algorithm with increasing number of gates. We stop when a maximally entangled state is prepared in a circuit of a fixed size. When the hypothetical maximum of the fitness function is unreachable, we search for the maximal value of the entanglement potential and then optimize the size of a circuit. In this work we restrict ourselves to 8 qubits. This is caused by the long runtimes of the algorithm.

The optimization is performed simultaneously for the spin chain and the system of complete connections. By a completely connected system we mean a system in which we are able to act on every pair of qubits. It is equivalent to defining the set of all available CNOT gates as \{CNOT(i; j) : i \neq j\}, where CNOT(i, j) is a controlled NOT gate acting on i-th and j-th qubit (4). The sets of Hadamard gates and phase gates are independent of changes of possible qubit connections as this gate acts on one qubit only. By the spin chain system we mean a system where we are able to act on pairs of the nearest neighbors in a chain. In such a case the set of available CNOT gates is \{CNOT(i; j) : |i - j| = 1\}. In each complete system we additionally analyze the minimum topology of necessary connections by investigating the connections graph where the vertices represent qubits of a system, and the edges represent connections, that is CNOT gates of a circuit connecting two qubits.

A. Resultant states and circuits

The upper bound of the potential of entanglement can be given explicitly if the number of all possible bipartitions is known. However, it is not always possible to find a pure state with the maximum value of the entanglement potential.

We have managed to reach the hypothetical maximum in the case of 3, 5 and 6 qubits. These are the most important cases, because there are no concerns about the correctness of their classification by the fitness function. 3- and 5-qubit states obtained by us are analogous to the states presented in [20]. In the 6 qubit case the best known state was
TABLE III: The maximum value of the entanglement potential obtained for $d = 1, \ldots, 8$ qubits and hypothetical upper bound

| Value       | 3  | 4  | 5  | 6  | 7  | 8  |
|-------------|----|----|----|----|----|----|
| Number of qubits | 3  | 10 | 25 | 66 | 154| 372|

FIG. 1: Average computational time (log scale) required to calculate negativity and von Neumann entropy. For each dimension $d = 1, \ldots, 8$ the results were obtained for a sample of $10^4$ random states.

presented in work [20]. However, that state consists of 32 non-zero coefficients. We have managed to find a state with 16 non-zero coefficients

$$|\psi_6\rangle = \frac{1}{4}((|0000\rangle - |1111\rangle)|\psi^+\rangle + (|0011\rangle + |1100\rangle)|\psi^-\rangle + (|0101\rangle + |1010\rangle)|\phi^+\rangle + (|0110\rangle - |1001\rangle)|\phi^-\rangle),$$

where $|\psi^\pm\rangle = |00\rangle \pm |11\rangle$ and $|\phi^\pm\rangle = |01\rangle \pm |10\rangle$.

In the case of 4 and 7 qubits it is not known whether there is any state with hypothetical maximum of the potential of entanglement and in 8-qubit case it is definitely not possible. Thus we can only search for circuits that generate the amount of entanglement that we consider maximally possible. The values obtained in our research are gathered in Table III.

B. Systems comparison

The main feature of a quantum circuit that gives us some information about the generated state is its size. In our work we put the main interest in the minimal number of quantum gates needed to obtain a circuit which manages to generate a maximally entangled state. The number of basic gates needed to generate maximum entanglement provide insight into the difficulty of this process.

All obtained data are gathered in Tables I and II. The computation performed by us shows that the size of the circuit grows exponentially with the size of a system (see Figure 2). If we treat the gates used in our work as the elementary operations, we find out that the complexity of all quantum algorithms that harness the generation of
 multiparticle entanglement is exponential. It means that all hypothetical quantum algorithms which are supposed to bring essential computational speed-up by utilising multiparticle entanglement may be practically inefficient.

Additionally, considering both complete systems and spin chains, the obtained results show that the simulation of dynamics of a complete system using spin chain system brings an exponential growth of the number of quantum gates needed. That may suggest that quantum systems of informatics based on spin chains may be exponentially less efficient than the systems where the interactions between all pairs of qubits are possible.

C. Optimal structures

In our work we additionally analyse the structure of quantum systems for the presented circuits. While spin chain systems seem to be inefficient in the context of generating MME we find it interesting to find a structure that guarantees maximum efficiency without complete connections. The results shown in Figure 3 represent the structures of systems allowing the generation of maximum entanglement in an optimal time. These examples show that it is not necessary to allow the interaction between all qubits to obtain maximum efficiency. We can get an essential reduction of qubit connections without increasing the number of gates necessary to generate maximum entanglement. The evolution of the structure seems to be regular.

IV. CONCLUDING REMARKS

In this paper we have presented the method of applying the genetic algorithm to generate quantum circuits preparing maximally entangled states. The algorithm provided in this work can be applied to optimize the size of a circuit preparing maximally multipartite entangled states. We have provided an analysis of minimum number of quantum gates necessary for generating MMES. The size of a circuit is interesting both in the context of minimal complexity of a circuit generating the maximum entanglement and in obtaining maximally entangled states itself, because the complexity of the algebraic representation of a resulting state increases with the number of gates in a circuit. The circuit we have obtained for a 6-qubit system that contains 12 quantum gates and generates a maximally entangled state with 16 non-zero coefficients is an example. The best result known so far included a 13-gate circuit generating a state with 32 coefficients [20].

Moreover, the described method allows taking into account the topology of connections between the particles in the system. Developed method enables one to ensure that the resultant circuit will be possible to implement in a system with arbitrarily defined connections between particles. This gives us the possibility of analysis the process of generation of the multiparticle entanglement. We exploit this possibility and provide the comparison of efficiency of generating maximally multipartite entangled states in the spin chain system and in the system of complete connections. We

FIG. 2: The minimum number of gates (log scale) necessary for generating maximally (highly) entangled states.
have shown that in the case of generation the multipartite entanglement a spin chain is essentially less efficient than the system of complete connections. Moreover, we have presented some topologies with relatively sparse connections between qubits that enable the generation of maximum entanglement with the same efficiency as the systems of complete connections.

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