Evolutionary Computing to Solve Optimal Entangle States in Quantum Circuits

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***Abstract*—This study investigates the efficacy of bio-inspired evolutionary algorithms for designing quantum circuits that proficiently generate highly entangled quantum states, a crucial prerequisite for quantum computing. By employing an evolutionary algorithm, quantum circuits are optimized for entanglement generation, with the Meyer-Wallach entanglement measure serving as the fitness function. The research highlights that an optimal mutation rate, balancing exploration and exploitation, can effectively augment the entanglement capabilities of three-, four-, and five-qubit quantum circuits. Additionally, the study unveils that increasing the number of gates in the quantum circuit inversely affects its entanglement capability. These findings offer valuable insights into the trade-off between circuit complexity and performance, bearing significant implications for the design of quantum circuits in various quantum computing applications. The outcomes of this study hold the potential to substantially contribute to the advancement of quantum computing technology.**

***Index Terms*—Quantum circuits, Quantum Gates, Entanglement, Evolutionary Algorithms**

I. Scope and Motivation

Quantum computing is an innovative field of computer science that utilizes the principles of quantum mechanics to perform certain computations faster and more efficiently than classical computers [1]. The use of quantum bits, or qubits, which can exist in multiple states simultaneously, is a key aspect of quantum computing that enables it to solve complex computational problems [1]. The intersection of quantum computing and artificial intelligence is an area of research that has the potential to revolutionize various industries and scientific fields. Quantum machine learning algorithms and evolutionary computation using evolutionary algorithms are emerging technologies that are being actively explored [2]–[5]. These technologies have the potential to accelerate the optimization process and improve the overall performance of computational algorithms. Further research in these areas is expected to drive the development of more efficient and effective computing technologies, with potential applications in various industries and scientific fields.

Evolutionary quantum computation (EQC) is an emerging paradigm that merges evolutionary algorithms with quantum computing to solve complex optimization problems. EQC has shown great potential in a variety of applications, including entanglement measurement and quantum circuit optimization [6]–[8]. The main goal of this work is to provide a comprehensive review of recent developments in EQC with addressing the problem of maximal entanglement. This work will discuss the key concepts of quantum entanglement and evolutionary algorithms, and how they are integrated to develop EQC-based evolutionary algorithms for entanglement measurement. The work concludes with a discussion of the future prospects of Evolutionary Quantum Computing (EQC) in entanglement measurement and other quantum information processing applications.

Entanglement, a concept in quantum computing, plays a crucial role in quantum information processing. Quantum entanglement, first coined by Erwin Schrödinger in 1935, is a mechanical phenomenon at the quantum level in which the quantum states of two (or more) particles are intrinsically correlated, even though these particles may be spatially separated from each other [9]. An entangled state refers to a quantum state that is intrinsically correlated between two or more particles, even if they are spatially separated [10]. In quantum entanglement, changes in the state of one qubit can affect the state of the other entangled qubit simultaneously meaning that qubits are entangled if the amplitudes of an n-

qubit configuration define a correlation between the individual qubits. Highly entangled quantum systems are more difficult to simulate on classical computers [11], [12]. Therefore, the concept of entanglement has significant implications for the development of quantum information processing technologies. If a quantum system is not highly entangled, it can often be simulated efficiently on a classical computer [12], [13].

Consider a system with two-qubit configurations, where the wave function is given by

$$|\psi\rangle = \frac{1}{2}\sqrt{2}|00\rangle + |11\rangle. \tag{1}$$

Upon measurement of the first two qubits, the wave function will collapse to one of the two possible states. The second bit's value is thus determined by the result of the measurement of the first bit, indicating a correlation between the bits. Entanglement is important because it represents the effects of a measurement on the system and is common in quantum mechanical systems. It also allows interference in a quantum computer, which is the main difference between probabilistic and quantum computers. Any state of the two-qubit system is a superposition of the four basis states, namely

$$|\psi\rangle = \alpha_{00}\,|00\rangle + \alpha_{01}\,|01\rangle + \alpha_{10}\,|10\rangle - \alpha_{11}\,|11\rangle \ , \tag{2}$$

where α_{00}, α_{01}, α_{10}, and α_{11} are amplitudes of the corresponding basis states. The normalization of the basis state is given by

$$|\alpha_{00}|^2 + |\alpha_{01}|^2 + |\alpha_{10}|^2 + |\alpha_{11}|^2 = 1 = \sum_{X\in\{0,1\}^2} |ax|^2 \, ,$$

where $X \in \{0,1\}^2$ means all binary combinations of length 2. When both qubits are measured simultaneously, there are four possible outcomes. Consider an example:

$$|\psi\rangle = \frac{1}{2}\,|00\rangle + \frac{1}{2}\,|01\rangle + \frac{1}{2}\,|10\rangle + \frac{1}{2}\,|11\rangle \ .$$

If we measure the first qubit, the outcome of "0" has probability $\frac{1}{2}$. And if the outcome of first qubit is 0, the probability for the second to be 0 or 1 is $1/2$ each. So, the qubits are not entangled.

The exponential growth of possible values for a system of three or more qubits underlies the power of quantum computing [1]. The outcome of entanglement leads to a large number of possible states, making it expensive to run a quantum program in a classical computer simulation. For instance, the simulation of a 15-qubit quantum computer requires 2^{15} floating-point numbers to store the program state at any instant. As a result, testing and debugging quantum programs in simulation is only feasible for toy-sized programs.

One of the most well-known examples of the use of entanglement in quantum computing is quantum teleportation [14]. In quantum teleportation, the quantum state of a particle is transmitted from one location to another using entanglement, without the need for the actual particle to travel. This process relies on the fact that two entangled particles can share the same quantum state, even when separated by large distances. Therefore, entanglement is a valuable resource in quantum computing, and it is essential for the development of many quantum technologies. Researchers are actively exploring ways to better understand and utilize entanglement to advance the field of quantum computing.

The descriptors, expressibility, and entangling capability has been used to study the capabilities of the parametrized quantum circuit by quantifying its deviation from random circuits to approach the research question of how much generalization is effective enough in a quantum circuit for a given task [15]. The expressibility of a quantum circuit is the ability to generate pure states that are well representative of the Hilbert space. In a single qubit, the expressibility corresponds to the circuit's ability to explore the Bloch sphere. Sim et al. [15] propose to quantify the ability of the quantum circuit to generate a pure state as a representative of Hilbert space by comparing the true distribution of the fidelities corresponding to the parameterized quantum circuit (PQC), to the distribution of fidelities from the ensemble of Haar random states. For example, they propose to approximate the distribution of the fidelities, the overlapped state which is defined as $F = |\langle\psi_\theta|\psi_\theta\rangle|^2$, of the PQC. The ensemble of the Haar random state can be calculated analytically as $P_{Haar} = (N-1)(1-F)^{N-2}$, where N is the dimension of the Hilbert space [16].

Here we focus on the entangling capability and use the the Meyer-Wallach entanglement measure (Meyer and Wallach 2002 [17]) defined as

$$Q(|\psi\rangle) = \frac{4}{n}\sum_{j=1}^{n} D(l_j(0)|\psi\rangle, l_j(1)|\psi\rangle)\, , \tag{3}$$

where $l_j(b)$ represents a linear mapping for a system of n qubits that act on a computational basis with $b_j \in \{0,1\}$: $l_j(b)|b_1....b_n$ Sim et al. [15] approximated the measure of the PQC by sampling and defined the estimate of the entangling capability of the quantum circuit as follows:

$$\text{Ent} = \frac{1}{|S|}\sum_{\theta_i\in S} Q(|\psi_{\theta_i}\rangle)\, , \tag{4}$$

where S is the set of sample circuit parameter vectors θ.

For more than two systems, most entanglement measures require knowledge of the state itself, which involves performing quantum state tomography. For a pure state of n qubits, Equation 3 [18] can be simplified as ,

$$Q(|\psi\rangle) = \frac{4}{n}\sum_{j=1}^{n} D(|\hat{u}^k\rangle\,, |\hat{v}^k\rangle)\, , \tag{5}$$

where $|\hat{u}^k\rangle$ and $|\hat{v}^k\rangle$ are vectors in $\mathbf{C^{2n-2}}$ which are non-normalized (indicated by the $\hat{}$) and obtained by projecting on state $|\psi\rangle$ with local projectors on the k^{th} qubit,

$$|\psi\rangle = |0\rangle_k \otimes |\hat{u}^k\rangle + |1\rangle_k \otimes |\hat{v}^k\rangle\, . \tag{6}$$

The function $D(|\hat{u}^k\rangle\,, |\hat{v}^k\rangle)$ measures a distance between the two vectors $|\hat{u}^k\rangle$ and $|\hat{v}^k\rangle$. It is obtained by taking the generalized cross-product:

$$D(|\hat{u}^k\rangle, |\hat{v}^k\rangle) = \sum_{i<j} |\hat{u}_i^k \hat{v}_j^k - \hat{u}_j^k \hat{v}_i^k|^2. \tag{7}$$

Also, the state $|\psi\rangle$ can be written in the form of Schmidt decomposition over the bipartite division of the k and the other qubits as:

$$|\psi\rangle = |\bar{0}\rangle_k \otimes |\hat{x}^k\rangle + |\bar{1}\rangle_k \otimes |\hat{y}^k\rangle, \tag{8}$$

where $\langle \hat{x}^k | \hat{y}^k \rangle = 0$, and $||\bar{0}\rangle_k, |\bar{1}\rangle_k$ are related to $||0\rangle_k, |1\rangle_k$ by a logical unitary operator $\mathcal{U}_k$. The purity of the state of qubit k is therefore $Tr[\rho_k^2] = \langle \hat{x}^k | \hat{x}^k \rangle^2 + \langle \hat{y}^k | \hat{y}^k \rangle^2$. The generalized cross product under logical unitaries, $D(|\hat{u}^k\rangle, |\hat{v}^k\rangle) = D(|\hat{x}^k\rangle, |\hat{y}^k\rangle)$ in relation to the norm of an anti-symmetric tensor $M_k = |\hat{x}^k\rangle \langle \hat{y}^{*k}| - |\hat{y}^k\rangle \langle \hat{x}^{*k}|$ is written as [18]

$$\begin{aligned} D(|\hat{x}^k\rangle, |\hat{y}^k\rangle) &= \sum_{i<j} |\hat{u}_i^k \hat{v}_j^k - \hat{u}_j^k \hat{v}_i^k|^2 \\ &= \frac{1}{2} \sum_{i,j} (M_k^\dagger)_{ij} (M_k^\dagger)_{ji} \\ &= \frac{1}{2} Tr[M_k^\dagger M_k] \\ &= \langle \hat{x}^k | \hat{x}^k \rangle \langle \hat{y}^k | \hat{y}^k \rangle \\ &= \frac{1}{2}(1 - Tr[\rho_k^2]). \end{aligned}$$

Therefore,

$$Q(|\psi\rangle) = 2(1 - \frac{1}{n} \sum_{k=0}^{n-1} Tr[\rho_k^2]). \tag{9}$$

This equation of the entanglement measure Q simplified the physical meaning of the multi-particle entanglement as an average over the entanglements of each qubit with the rest of the system.

The given equation is an expression for the quantum purity of a state $|\psi\rangle$, denoted by $Q(|\psi\rangle)$. The purity is a measure of how pure or mixed a quantum state is, and it is defined as the trace of the square of the density matrix ρ that represents the state. Here, n is the number of times the state is measured or prepared, and ρ_k is the density matrix of the state after the k^{th} measurement or preparation. To understand how this equation relates to the purity of the state, we can start by considering the purity of a pure state. If the state $|\psi\rangle$ is pure, then its density matrix is given by $\rho = |\psi\rangle \langle\psi|$, and its purity is:

$$\begin{aligned} \mathrm{Tr}[\rho^2] &= \mathrm{Tr}[(|\psi\rangle \langle\psi|)(|\psi\rangle \langle\psi|)] \\ &= \mathrm{Tr}[|\psi\rangle \langle\psi|\psi\rangle \langle\psi|] = \mathrm{Tr}[|\psi\rangle \langle\psi|] = 1 \end{aligned}$$

Therefore, for a pure state, the expression $1 - \frac{1}{n} \sum_{k=0}^{n-1} Tr[\rho_k^2]$ is equal to zero.

For a mixed state, the density matrix can be written as a convex combination of pure states, $\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|$, where p_i are probabilities and $\sum_i p_i = 1$. The purity of this mixed state is:

$$\begin{aligned} \mathrm{Tr}[\rho^2] &= \mathrm{Tr}\left[\left(\sum_i p_i |\psi_i\rangle \langle\psi_i|\right)\left(\sum_j p_j |\psi_j\rangle \langle\psi_j|\right)\right] \\ &= \sum_i p_i^2 \,\mathrm{Tr}[|\psi_i\rangle \langle\psi_i|] + \sum_{i\neq j} p_i p_j \,\mathrm{Tr}[|\psi_i\rangle \langle\psi_j| \, |\psi_j\rangle \langle\psi_i|] \\ &= \sum_i p_i^2 + \sum_{i\neq j} p_i p_j |\langle\psi_i|\psi_j\rangle|^2 \\ &\leq \sum_i p_i^2 + \sum_{i\neq j} p_i p_j = \left(\sum_i p_i\right)^2 = 1 \end{aligned}$$

Therefore, the purity of a mixed state is always less than or equal to one. Using this result, we can see that the expression $1 - \frac{1}{n} \sum_{k=0}^{n-1} Tr[\rho_k^2]$ is a measure of how mixed the state is. If the state is pure, then this expression is zero, and if the state is entangled/mixed, then this expression is positive.

II. Implementing the Evolutionary Algorithm: A Step-by-Step Guide

The use of evolutionary algorithms to generate quantum circuits has become increasingly popular. In this approach, an algorithm optimizes the types of quantum gates and their connectivity by generating a list of integers representing the gates and their connections. The fitness function evaluates each chromosome and identifies the current best solution, which is then used to perform operations such as entangling qubits and computing mutations. This creates a quantum evolutionary circuit that performs genetic evolution on a quantum device and identifies a new best solution. We evaluated the performance of our proposed approach using a simulator provided by Qiskit and created a string representation of the circuits, gates, and connections. Our results show the potential of this approach for solving optimization problems in quantum computing. The implementation was initially done for evolving quantum circuits to determine stochastic and deterministic cellular automata rules, and this work has already been published [19]. The implementation code is available at GitHub repository https://github.com/Overskott/Quevo. In this study, we modified the same algorithm used for evolving stochastic and deterministic cellular automata rules to include the Mayor Wallach entanglement measure as a fitness function for quantum circuit design with the measure of entanglement of thus generated circuits. Specifically, the algorithm aims to maximize entanglement in three, four, and five-qubit quantum circuits.

A. Main Ingredients of Implementation

The implementation of our approach was carried out in Python and resulted in a Python module called **QUEVO**. This module consists of three classes: `Chromosome`, `Generation`, and `Circuit`. The `Chromosome` and the `Generation` classes are part of the genetic algorithm, while the `Circuit` class is responsible for generating and simulating quantum circuits.

1) The Chromosome: The `Chromosome` class is the core of the genetic algorithm used for generating quantum circuits. It handles the integer representation of the gates and their connections. The class contains a list of integers and functions for generating and mutating the list. It also handles the initialization of the population and the evolution of the population into a new one. Mutations in the `Chromosome` class can occur in two different ways: replacing gates from the pool of gates in the chromosome with a randomly generated new one or replacing the chromosome to generate the four best parents. The class is also responsible for checking the chromosome for gates that connect multiple qubits. If the gate has an invalid connection, meaning that it is connected to itself through the randomly generated integers, the class generates a valid configuration randomly. Overall, the `Chromosome` class handles the creation of random series, the list of angles needed by some of the gates, mutation of the series, and other list-related functions. It takes a list of the desired gate types as a parameter on construction and automatically creates the tables needed for parsing.

2) The Generation: The `Generation` class is another important class in the QUEVO module, responsible for managing the population of chromosomes. It is a collection of chromosomes that undergo evolution for a specified number of generations. After each evolution step, changes in the chromosomes in the generation occur by selecting a fixed number of chromosomes as elite and allowing the rest of them to evolve further. In each evolution step, the chromosomes are evaluated with the fitness function, and the fittest chromosomes become the parents for the next generation. The rest of the chromosomes are reset for the initial chromosomes. The `Generation` class stores a generation of chromosomes, the fitness associated with each chromosome, methods for running and retrieving fitness for two different fitness functions, and functions for printing. It provides methods for performing selection, crossover, and mutation to generate a new population of chromosomes. The class also provides methods for evaluating the fitness of the chromosomes, a crucial step in determining the parents for the next generation.

3) The Circuit Class: The `Circuit` class in the QUEVO module is responsible for generating a Qiskit quantum circuit from a string representation, simulating the circuit, performing measurements, and visualizing the circuit. The class is run on the Qiskit AER simulator and returns the results as a dictionary. The class can be configured to mimic an IBMQ backend using the *aer_sim = Aer.get_backend('aer_simulator')* method, which configures the simulator to use the user's quantum gates for that backend, as well as the same basis gates and coupling map.

The `Circuit` class is a crucial component of the QUEVO module because it enables the implementation of the genetic algorithm to generate, simulate, and measure quantum circuits. The class interfaces with Qiskit to create and simulate circuits using the gates specified in the chromosomes. The results of the simulations are used to evaluate the fitness of each chromosome and guide the search for an optimal solution. The performance of the algorithm depends on the quality of the simulations and the accuracy of the measurements. The accuracy of the simulations is affected by the number of qubits in the circuit, the complexity of the gates used, and the noise and other sources of errors associated with the quantum circuits.

B. Mayor Wallach Entanglement measures as fitness functions

The `compute_MW_entanglement` method is an implementation of the Mayer-Wallach measure of entanglement, which is a commonly used entanglement measure in quantum information theory. The method takes in a state vector as an input, which represents the quantum state of the circuit. The state vector is reshaped into a tensor of dimensions 2^n x 2^n, where n is the number of qubits in the circuit. The Mayer-Wallach measure of entanglement is then calculated by computing the reduced density matrix of each qubit and summing over the squared eigenvalues of the reduced density matrix. Specifically, for each qubit k, the reduced density matrix is obtained by tracing out all the other qubits from the quantum state. The squared eigenvalues of the reduced density matrix are then computed and summed over all qubits to obtain the entanglement value. The entanglement value is then scaled by a factor of $1 - \frac{1}{n}$ to ensure that it lies between 0 and 1. The Mayer-Wallach measure of entanglement provides a useful fitness function for evolutionary algorithms because it quantifies the degree of entanglement in a quantum circuit. Maximizing the Mayer-Wallach measure of entanglement can lead to the generation of highly entangled quantum circuits, which may have practical applications in quantum communication and quantum computing. For more information about the module and instructions on how to use it, please visit the Github repository https://github.com/shailendrabhandari/QUEVO1.

III. Simulations and Results

This section presents the results of an evolutionary algorithm for quantum circuit design that employs the Mayor-Wallach entanglement measure as a fitness function. Our experiments involved 3, 4, and 5 qubit circuits, and the algorithm's performance was evaluated using varying mutation probabilities and numbers of gates. We conducted 50 iterations over 500 generations and present the results as the mean fitness with standard error of the mean and the best fitness with its standard error. The results are elaborated separately for the 3, 4, and 5 qubit circuits.

Quantum entanglement is a fundamental aspect of quantum computing that enables the generation of correlations between quantum systems. However, designing efficient quantum circuits with maximum entanglement can be challenging due to the exponential increase in the number of parameters with the problem size. Recently, evolutionary algorithms (EAs) have emerged as a promising tool for quantum circuit design [7], [8], [20]. In this chapter, we present our implementation of EAs for quantum circuit design, which aims to maximize entanglement. Our QUEVO framework employs an evolutionary algorithm to automatically generate quantum circuits that satisfy defined properties specified through a fitness function. The evolution properties can be controlled by tuning parameters such as initial population, number of generations, probability of mutation operator, number of gates in the circuit, and the chosen fitness function.

A. Evolutionary algorithm for three-qubit quantum circuit design

Figure 1 displays the average and best fitness scores of a three-qubit quantum circuit generated by an evolutionary algorithm over 500 generations. This study investigated the effectiveness of different mutation rates (5%, 10%, and 15%) in generating a quantum circuit having different numbers of gates(3, 5, 8, 10, and 12) with maximum entanglement. The best fitness scores obtained for all mutation rates approached unity, indicating that the generated circuits had a high degree of entanglement between the qubits. The fitness function used in the study was the Mayor-Wallach entanglement measure [18], which is based on the largest eigenvalue of the partial transpose of a quantum system's density matrix and has been widely used to quantify entanglement in various quantum systems.

The results of the experiment suggest that evolutionary algorithms can be an effective method for designing three-qubit quantum circuits with a desired degree of entanglement. The optimal mutation rate was found to be 10%, which struck a balance between exploring different solutions in the search space and exploiting the best solutions. A mutation probability of 1/9 (11.11%) is needed to replace at least one individual population consisting of nine integer lists (three lists of integer gates for each qubit). Therefore, 10% which can at least replace one individual population in each generation can be considered an optimal probability for the mutation rate. Figure 2 (Top) supports the finding that a lower mutation rate is able to strike a balance between exploration and exploitation, leading to a higher average fitness score across all runs. However, a mutation rate of 10% can be more effective in discovering the best-performing circuit in each run due to the higher degree of exploration it allows.

However, Figure 2 (Top) shows, the best fitness score obtained for each run over 50 runs is highest for a mutation rate of 10%. This indicates that a lower mutation rate is able to strike a balance between exploration and exploitation, leading to a higher average fitness score across all runs. On the other hand, a mutation rate of 10% may be more effective in discovering the best-performing circuit in each run due to the higher degree of exploration it allows.

In the experiment where the number of gates in the quantum circuit varied from 3 to 12 while the mutation rate was fixed at 10%, it was observed that the fitness score decreased as the number of gates in the circuit increased as shown in Figure 2 (Bottom). This suggests that as the circuit becomes more complex with an increasing number of gates, the fitness score reduces, indicating that the circuit is less efficient at performing the desired task. There may be a trade-off between circuit

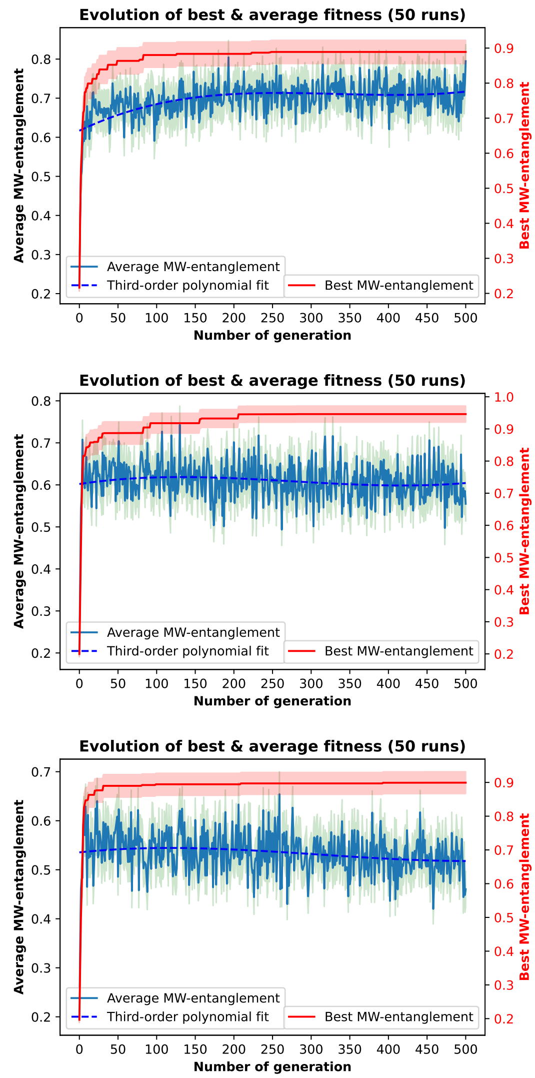

Fig. 1. Evolutionary optimization of three-qubit quantum circuits with 3 gates using the Meyer-Wallach entanglement measure as the fitness function. The plot shows the mean fitness (green line) and its shaded standard error, as well as the mean of the best fitness (red line) and its shaded standard error, against the number of generations for different mutation percentages in the evolutionary algorithm: Top (Top) 5%, Top (Middle) 10%, and (Bottom) 15%. The blue dashed line represents the third-order polynomial fit to the mean fitness.

complexity and performance, and there may be an optimal number of gates that provides the best balance between the two.

The visualization of the best-generated three-qubit quantum circuit with three gates, as shown in Figure 3(Top) with a fitness score of 0.9999999999999996, provides a concrete example of the potential of evolutionary algorithms for designing highly entangled quantum circuits. Figure 3(Bottom) shows another example of a three-qubit quantum circuit with 12 gates having a fitness value of 0.999999887999999. These three-qubit circuits appear to be relatively simple, yet they achieve a very high degree of entanglement between the qubits.

However, it is important to consider the robustness of the

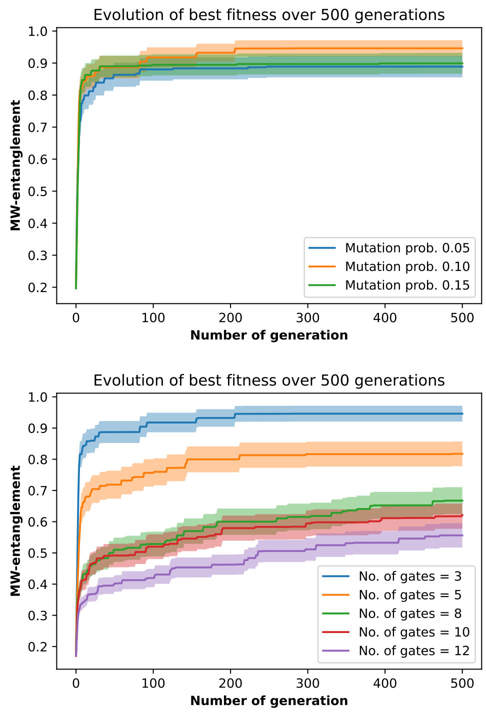

Fig. 2. Comparison of best fitness generated for (Top) different mutation rates for 3 gates and (Bottom) different numbers of gates for a constant mutation probability of 10%. The results are averaged over 50 runs and the error bars represent the standard error of the mean best fitness.

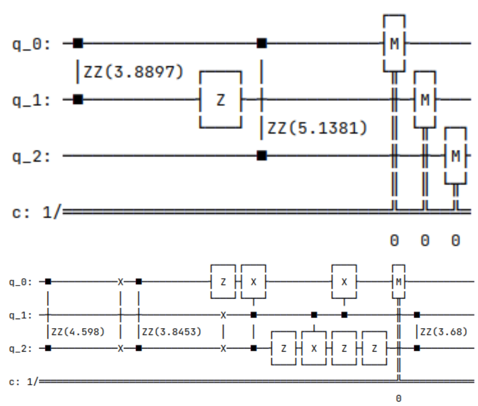

Fig. 3. Two examples of three-qubit circuits evolved with a 10% mutation probability and optimized for MW-entanglement fitness scores. (Top) A circuit with only 3 gates achieved a high fitness score of 0.9999999999999996. (Bottom) A more complex circuit with 12 gates achieved a slightly lower fitness score of 0.999999887999999.

generated circuits to noise and other sources of interference, as this is a critical factor in the practical applications of quantum circuits. Further research will be needed to investigate the robustness of circuits generated using evolutionary algorithms and to identify methods for improving their resilience to noise.

It is worth noting that the choice of gate set used in the study could impact the results. Different gate sets may have different levels of expressivity and may lead to different results in terms of the entanglement and fitness scores of the generated circuits. Further studies may consider exploring the effectiveness of different gate sets in generating highly entangled circuits.

The reduced density matrices for a three-qubit system are calculated by tracing over the other two qubits in a three-qubit system. The use of reduced density matrices as a tool for analyzing the properties of entangled states in complex quantum systems. After calculating the reduced density matrix for all qubits, the code computes the entanglement of the circuit using the Mayor Wallach entanglement measure. The reduced density matrix of a subsystem can reveal the degree of entanglement between the qubits in that subsystem, but not necessarily the degree of entanglement of the entire system. Therefore, calculating the entanglement measure of a quantum circuit by tracing out all qubits is necessary to obtain an accurate assessment of the entanglement of the circuit.

Overall, the effectiveness of evolutionary algorithms in designing three-qubit quantum circuits with a desired level of entanglement has been investigated. Our findings indicate that the choice of mutation rate and the number of gates is crucial in achieving the desired level of entanglement. We found that a mutation rate of 10% struck a balance between exploration and exploitation, leading to a higher average fitness score across all runs. Furthermore, we observed that as the number of gates in the circuit increased, the fitness score decreased, suggesting a trade-off between circuit complexity and performance. By carefully balancing exploration and exploitation through the selection of an appropriate fitness function, initial population, and mutation rate, it may be possible to generate circuits with even higher degrees of entanglement. These findings could have significant implications for the development of quantum computing and could lead to the design of new and more powerful quantum circuits.

B. Evolutionary algorithm for four-qubit quantum circuit design

In addition to studying the evolution of three-qubit and five-qubit quantum circuits, the evolution of four-qubit quantum circuits will be examined. Specifically, the results for the evolution of quantum circuits with four gates and a 10% mutation probability generate the fitness of the circuit. By examining the evolution of quantum circuits with varying numbers of qubits and gates, and with different mutation rates, insights into the impact of these factors on the evolution of quantum circuits and the degree of entanglement that can be achieved.

Figure 4 shows the evolutionary algorithm optimization of four-qubit quantum circuits with four gates and a 10% mutation probability, using the Meyer-Wallach entanglement measure as the fitness function. The plot shows the mean fitness (green line) and its shaded standard error, as well as the mean of the best fitness (red line) and its shaded standard error, against the number of generations. The blue dashed line represents the third-order polynomial fit to the mean fitness. It can be seen from the figure that the mean fitness score is near 0.5, while the mean of the best fitness score is close to 0.9. This indicates that circuits generated with the best fitness score

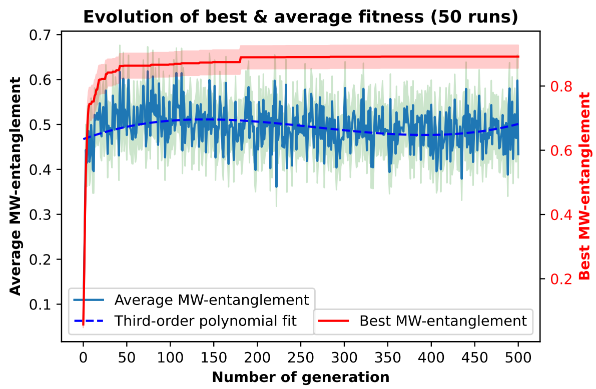

Fig. 4. Evolutionary algorithm optimization of four-qubit quantum circuits with four gates and 10% mutation probability, using the Meyer-Wallach entanglement measure as the fitness function. The plot shows the mean fitness (green line) and its shaded standard error, as well as the mean of the best fitness (red line) and its shaded standard error, against the number of generations. The blue dashed line represents the third-order polynomial fit to the mean fitness.

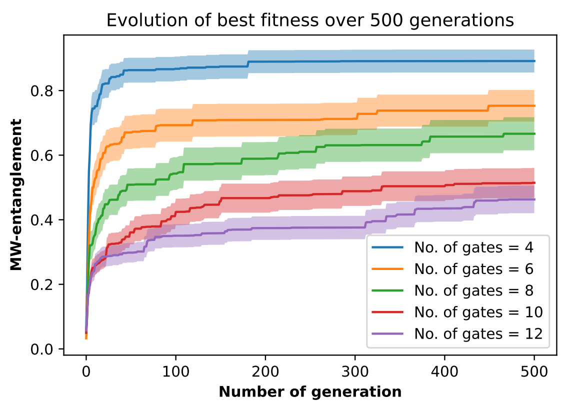

Fig. 5. Comparison of the best fitness generated for five different numbers of gate sets in a four-qubit circuit using 10% mutation, 20 chromosomes. The results are averaged with 50 runs over 500 generations and the error bars represent the standard error of the mean best fitness.

in each generation have a very high degree of entanglement among the qubits.

The experiment with a 10% mutation probability for four-qubit circuits was repeated for circuits with varying numbers of gates. Figure 5 displays the best fitness scores for circuits with 4 to 12 gates. The figure shows that as the number of gates increases, the circuit becomes more complex and the fitness score decreases, indicating lower entanglement. This finding is consistent with the results obtained for three-qubit and five-qubit circuits, suggesting a potential trade-off between circuit complexity and entanglement capability.

Figure 6 represents an example of a four-qubit circuit that was generated using an evolutionary algorithm, consisting of four gates and having a fitness score of 0.999957846. This demonstrates that evolutionary algorithms hold promise as a tool for designing quantum circuits that exhibit high levels of entanglement between qubits.

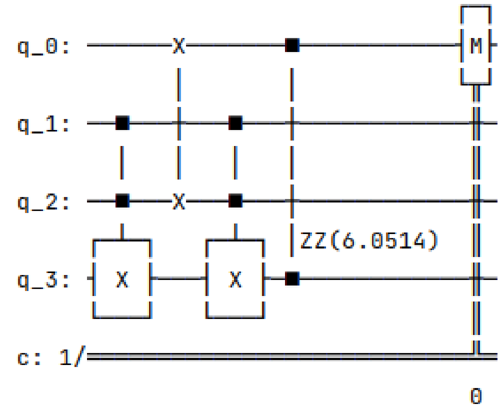

Fig. 6. Evolutionary generation of four-gate four-qubit circuits with MW-entanglement fitness scores using a 10% mutation probability with a fitness score of 0.999957846.

C. Evolutionary algorithm for five-qubit quantum circuit design

Figure 7 displays the results of a study that investigated the effectiveness of an evolutionary algorithm in generating a five-qubit quantum circuit with five gates. The figure includes the average fitness, third-order polynomial fit to the average fitness, and the best fitness values. The study explored the impact of different mutation rates (3%, 5%, and 15%) on the generated circuits' average and best fitness scores over 500 generations. The best fitness scores obtained for all mutation rates were close to 0.8, with an expected target fitness value of one, indicating a high degree of entanglement between the qubits. The third-order polynomial fit to the average fitness shows a smooth curve that approximates the general trend of the data.

The results of the study indicate that a mutation rate of 3% was the most effective in optimizing the quantum circuit, as shown in Figure 7, which displays the best and average fitness values obtained. The study also found that increasing the mutation rate beyond 5% resulted in a decrease in the average fitness value, indicating that excessive randomness in the optimization process can have a negative impact on circuit performance. However, it was observed that the average of the best fitness value was not affected by a higher mutation rate. The results of this study highlight the importance of selecting an appropriate mutation rate for optimizing quantum circuits. To determine the optimal mutation rate, we calculated the probability of replacing at least one individual population, which consisted of 15 integer lists (three lists of integer gates for each of the 5 qubits). Our analysis found that the probability of this occurring was 6.67%. Based on this finding, we determined that a mutation rate of 5% (close to 6.67%) would be an optimal probability for the mutation rate, as it would be sufficient to replace at least one individual population in each generation.

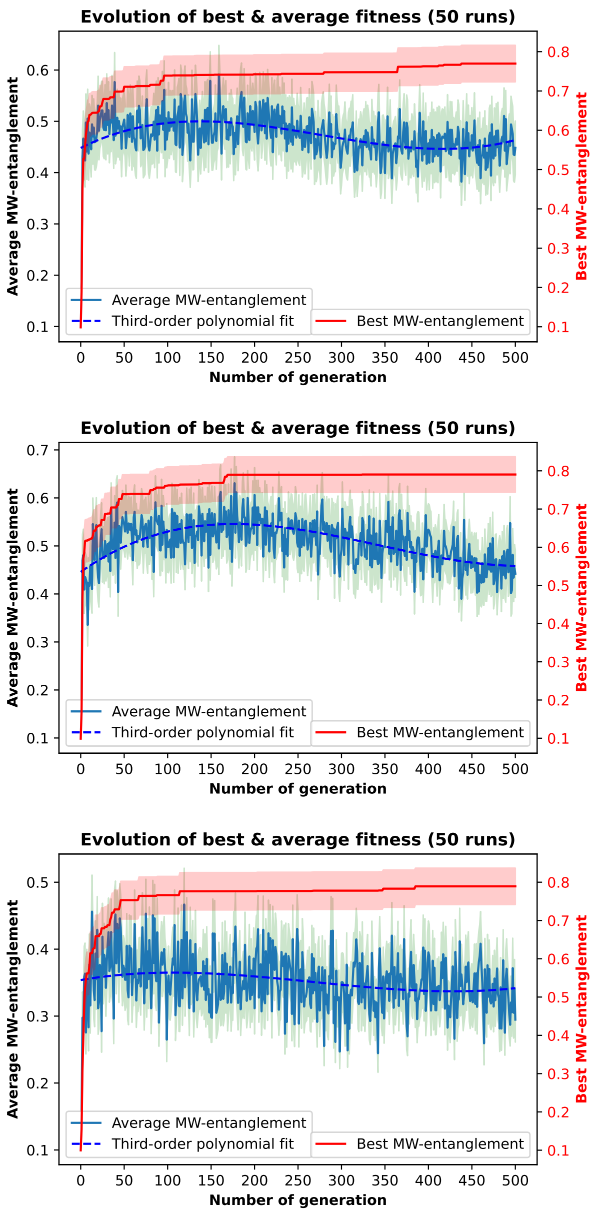

Fig. 7. Evolutionary optimization of five-qubit quantum circuits with five gates using the Meyer-Wallach entanglement measure as the fitness function. The plot shows the mean fitness (green line) and its shaded standard error, as well as the mean of the best fitness (red line) and its shaded standard error, against the number of generations for different mutation percentages in the evolutionary algorithm: Top (Left) 3%, Top (Right) 5%, and Bottom 15%. The blue dashed line represents the third-order polynomial fit to the mean fitness.

In the second step of our investigation, we kept the mutation rate constant at 5% (optimal to replace at least one individual in each generation) and varied the number of gates to explore the entanglement capacity of the generated quantum circuit. The results, as shown in Figure 8, indicates that the fitness score is maximum or close to 1 for the 3-gate 5-qubit circuit. However, as the number of gates increases, the fitness scores decrease continuously. This finding suggests that increasing

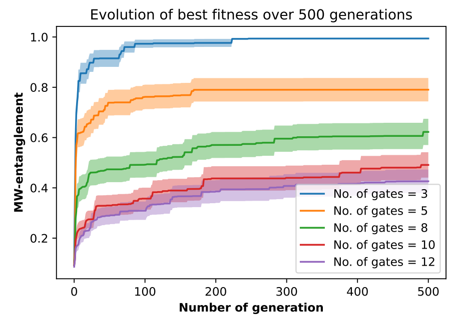

Fig. 8. Comparison of the best fitness generated for five different numbers of gate sets in a 5-qubit circuit using 5% mutation, 20 chromosomes, and 50 runs over 500 generations.

the number of gates in the quantum circuit (i.e., increasing the circuit depth) reduces the entanglement capability of the generated quantum circuits. Overall, the study suggests that a simpler quantum circuit with fewer gates may have better entanglement capability than a more complex circuit with more gates. These findings could be useful for researchers and practitioners who are interested in optimizing the design of five-qubit quantum circuits using evolutionary algorithms.

The best-generated five-qubit quantum circuit with five gates, shown in Figure 9(Top) with a fitness score of 0.999656736, provides a concrete example of the potential of evolutionary algorithms for designing highly entangled quantum circuits. Despite its simplicity, with only 5 gates, the circuit achieves a remarkably high degree of entanglement between the qubits. This high degree of entanglement makes it useful for various applications in quantum information processing such as quantum teleportation, quantum cryptography, and quantum error correction. This visualization highlights the power of evolutionary algorithms in optimizing quantum circuits for specific tasks, such as generating high-entanglement states. Increasing the circuit depth, i.e., the number of gates in a circuit increases the complexity of the quantum circuit and hence decreases the entanglement capability of the circuit as shown in Figure 8. The lower fitness score of the 12-gate circuit is evidence of this fact. However, a deeper circuit can still be useful for specific quantum algorithms that require a specific gate sequence.

IV. Discussion and Conclusions

In this work, we have demonstrated the effectiveness of evolutionary algorithms in generating highly entangled quantum circuits and calculating their reduced density matrices. The circuits we generated for three, four, and five-qubit systems exhibited a high degree of entanglement, as measured by the Mayor-Wallach entanglement measure. By tracing out all other qubits, we showed how the reduced density matrices could be used to extract information about the entanglement of the circuit. Our results highlight the importance of circuit depth in determining the entanglement capability of a quantum circuit, and we found that increasing the circuit depth decreases its

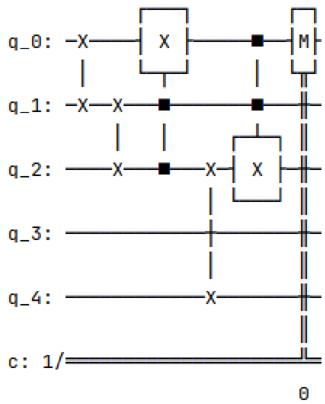

Fig. 9. Evolutionary generation of five-qubit circuits with MW-entanglement fitness scores using a 5% mutation probability with a five-gate having a fitness score of 0.999656736.

entanglement capability. Our study also found that an optimal mutation rate can effectively optimize quantum circuits for entanglement generation, with different numbers of qubits and gates. For example, the optimal mutation rate was found to be 10% for three-qubit circuits and 5% for five-qubit circuits.

Our findings demonstrate the potential of evolutionary algorithms as a useful tool for quantum circuit design and optimization and provide insights that could guide future research. Future research could explore the use of other fitness functions (the Von Neumann entropy [21], and Schmidt [22], [23]) and hybrid optimization methods to maximize the entanglement capacity of quantum circuits. Additionally, more complex quantum circuits with a higher number of qubits and gates could be investigated using more advanced evolutionary algorithms. Overall, the results presented in this study demonstrate the potential of evolutionary algorithms for quantum circuit design and provide a foundation for further research in this field.

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