Markovian Quantum Neuroevolution for Machine Learning

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Neuroevolution, a field that draws inspiration from the evolution of brains in nature, harnesses evolutionary algorithms to construct artificial neural networks. It bears a number of intriguing capabilities that are typically inaccessible to gradient-based approaches, including optimizing neural-network architectures, hyperparameters, and even learning the training rules. In this paper, we introduce a quantum neuroevolution algorithm that autonomously finds near-optimal quantum neural networks for different machine-learning tasks. In particular, we establish a one-to-one mapping between quantum circuits and directed graphs, and reduce the problem of finding the appropriate gate sequences to a task of searching suitable paths in the corresponding graph as a Markovian process. We benchmark the effectiveness of the introduced algorithm through concrete examples including classifications of real-life images and symmetry-protected topological states. Our results showcase the vast potential of neuroevolution algorithms in quantum architecture search, which would boost the exploration towards quantum-learning advantage with noisy intermediate-scale quantum devices.

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I. INTRODUCTION

Quantum machine learning studies the interplay between machine learning and quantum physics [1–4]. On the one hand, machine learning has achieved dramatic success over the past two decades [5,6] and many problems that were notoriously challenging for artificial intelligence, such as playing the game of Go [7,8] or predicting protein structures [9], have been cracked recently. This gives rise to opportunities for using machine-learning techniques to solve difficult problems in quantum science. Indeed, machine-learning ideas and tools have been invoked in various applications in quantum physics, including representing quantum many-body states [10,11], quantum-state tomography [12,13], nonlocality detection [14], topological quantum compiling [15], and learning phases of matter [16–26], etc. On the other hand, the idea of quantum computing has revolutionized the theories and implementations of computation [27]. Alternative quantum algorithms may offer unprecedented prospects to enhance, speed up, or innovate machine learning as well [28–35]. Without a doubt, the studies of the interplay between machine learning and quantum physics will benefit both fields and the emergent research frontier of quantum machine learning has become one of today's most rapidly growing interdisciplinary fields [1–4].

An intriguing approach widely studied in quantum machine learning is to exploit the hybrid quantum-classical scheme, where parameterized quantum circuits are optimized with classical methods (such as stochastic gradient descent) to satisfy certain objective functions. Notable examples in this category include various quantum classifiers [35–49], variational quantum eigensolvers [50–53], quantum Born machines [54,55], and quantum approximation optimization algorithms [56–58]. In this scenario, one typically chooses a variational ansatz circuit with a fixed structure and then optimizes its tunable parameters to tackle the given problem. Yet, different families of parameterized quantum circuits may bear distinct entangling capabilities and representation power, and thus are suitable for different tasks. For a given learning task, how to obtain a well-performing ansatz circuit as short as possible is extremely useful, especially for quantum learning with noisy intermediate-scale quantum (NISQ) devices [59], where the depth of the quantum circuits would be limited due to undesirable noises carried by such a device. In the classical machine-learning literature, several renowned algorithms have been proposed to search for appropriate neural-network architectures [60–72], including evolutionary or genetic algorithms (such as NeuroEvolution of Augmenting Topologies, NEAT) [62], greedy algorithms [64], reinforcement learning-based algorithms [65–68], and differentiable architecture search [69–72]. Inspired by these algorithms, analogous quantum architecture search algorithms have also been introduced [73–82]. Each of these

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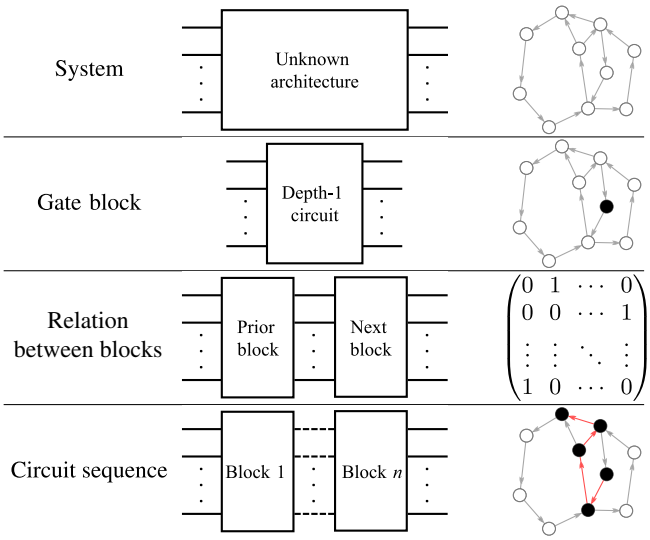
TABLE I. Illustration of the graph-encoding method, based on which the problem of searching the optimal quantum circuits is reduced to a task of finding paths in the corresponding directed graphs. Each node represents one gate block, and each path (red arrows) represents a sequence of gate blocks. The nodes that the path passes through are solid, while other nodes are empty.



algorithms carries its own pros and cons, and the choice depends on the specific problem.

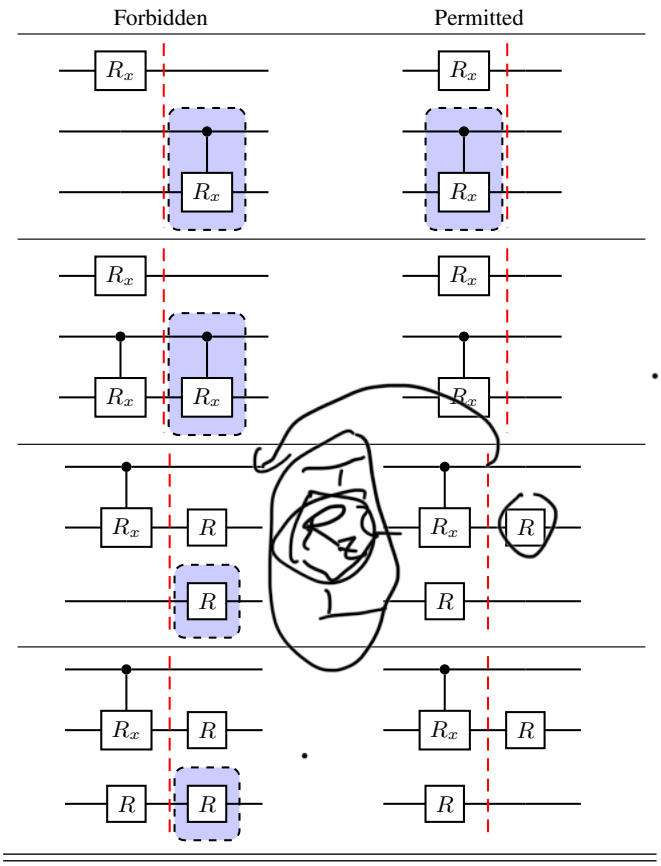
In this paper, we introduce a quantum neuroevolution algorithm, which we call the Markovian quantum neuroevolution (MQNE) algorithm, to search for optimal ansatz quantum circuits for different machine-learning tasks. We propose a graph-encoding method (see Table I), where the nodes of the graph correspond to the elementary gate blocks and the directed edges represent the allowed connection between gate blocks, to injectively map quantum circuits to directed graphs. Consequently, we recast the problem to a task of searching an appropriate directed path of the graph in a Markovian fashion. To illustrate the effectiveness of the MQNE algorithm, we apply it to a variety of quantum-learning tasks, including classifications of real-life images (such as handwritten digit images in the MNIST dataset [83], and the Wisconsin Diagnostic Breast Cancer dataset [84]) and symmetry-protected topological (SPT) states. We find that our algorithm yields ansatz quantum circuits with notably smaller depths, while maintaining a comparable classification accuracy.

II. THE MQNE ALGORITHM

In designing classical neural networks, a renowned neuroevolution algorithm is the NEAT algorithm [62], which exploits concepts (e.g., genome, crossover, speciation, and mutation) from biology to evolve neural-network topologies along with weights. However, straightforward adoption of NEAT in the quantum domain would not work since quantum neural networks differ substantially from classical ones. For instance, the quantum neurons (qubits) are connected by multiqubit unitaries rather than weight parameters. As a result, certain techniques, such as explicit fitness sharing and matching up genomes [62], used in NEAT become invalid or ambiguous in the quantum scenario. Indeed, as shown in the Supplemental Material [86], the simple genetic algorithm for designing quantum classifiers, which uses crossover and mutation directly, performs poorly in classifying images. The ineffectiveness of this algorithm is due to the following: (i) the encoding of the quantum circuits into bit strings is not a bijection, which increases the search space and slows down the searching process; (ii) the performance of the offspring generated from crossover and mutation is not guaranteed to be better than that of their parents, since crossover and mutation of unitaries may result in meaningless structures.

Our MQNE algorithm overcomes these shortcomings. First, we introduce a graph-encoding method, which maps quantum circuits to directed paths in the corresponding graph. Suppose we need to design a k-qubit quantum circuit to solve a given quantum machine-learning problem, and for simplicity we restrict our discussion to the case that the circuits are composed with only single-qubit rotations R and two-qubit controlled-R_x gates. The universal single-qubit rotation gate R is defined as the gate composed of $R_zR_xR_z$, i.e., the Z-X decomposition for a single-qubit rotation, where R_z and R_x denote rotations along z and x axis, respectively [27]. We choose the controlled-R_x gate, rather than the controlled NOT gate typically used in designing quantum neural networks, to guarantee that the circuits from later generations cover these from earlier generations, so as to ensure improved performance of the offsprings. This can be easily deduced from the fact that the controlled-R_x gate reduces to identity when setting the controlled rotation angle to 0. To avoid ambiguity and duplication of successive rotations, we invoke some connection rules for arranging gate blocks (a gate block is a depth-1 quantum circuit) in sequential order to form the desired circuits (see Table II): (i) the latter gate-block should not include any gate which can be operated in parallel with the former one; (ii) the latter gate block should not include the same gates as the former one on the same qubits. Such connection rules restrict the process of searching the optimal circuit structure in a Markovian fashion. We suppose that the qubits are arranged in a one-dimensional geometry and the controlled-R_x gates act only on adjacent qubits. We use a length-$(k+2\lfloor k/2\rfloor)$ vector to represent a quantum gate block. The first $2\lfloor k/2\rfloor$ numbers encode controlled-R_x gates in a gate block. Here, two adjacent nonzero numbers represent a controlled-R_x gate acting on these two qubits labeled by them, and two adjacent 0 numbers mean that there is no controlled-R_x gate acting on the remaining qubits. The next k numbers encode the single-qubit rotation gates in a gate block, where we use

TABLE II. The connection rules for gate blocks (drawn using Quantikz [85]). The left column shows the forbidden connection configurations, which should be replaced by the corresponding permitted ones in the right column. Here, only two-qubit controlled-R_x gate and single-qubit rotation gate R are used in constructing various quantum circuits.



0 to denote the absence of rotation for the corresponding qubit [86].

Without further restrictions, it is straightforward to obtain that the number of possible gate blocks is $f_1(k) = [(1+\sqrt{3})^{k+1} - (1-\sqrt{3})^{k+1}]/2\sqrt{3}$ [86]. These gate blocks form a gate-block library and we use a directed graph to represent this library. Each node of the graph corresponds to a gate block, and each directed edge represents a legitimate connection of gate blocks according to the connection rules: there is an edge pointing from node x to y if and only if the gate block y is allowed to be put next to gate block x. For convenience, we use an adjacency matrix to denote the directed graph as in graph theory [87]. Noting that a quantum circuit is just a sequence of gate blocks in the corresponding library, hence the task of designing a well-performing quantum circuit is reduced to finding an optimal path in the directed graph. This can be solved with the following procedure: (1) Initialization. we start from a fixed node and uniformly sample n_1 paths with length l based on the directed graph, and compute the fitness (classification accuracy) of the corresponding variational quantum circuits. These n_1 paths form the first generation. (2) Iteration in a Markovian fashion. From the ith generation, we choose t_i paths with the largest fitness. For each of the selected paths, we uniformly sample n_{i+1} segments of length l', and then add these segments to the end of the path. Here we remark that one segment refers to a sequence of l' gate blocks. Due to the connection rules, not all possible segments can be added at will to the existed paths. Whether a new segment is allowed to be added depends on the last gate block of the given paths, which is similar to a Markovian process. In this way, we obtain the paths of the $(i+1)$th generation. We then parallel evaluate the fitness of all $(i+1)$th generation quantum circuits. whose running time is independent of the number of paths at each generation. If the fitness of a circuit is larger than a certain given threshold value f_c (or the number of iteration exceeds a given number g_c), we terminate the iteration and output the corresponding path and quantum circuit. If none of the circuits has a fitness larger than f_c, we repeat this step to generate paths and circuits for the next generation. A schematic illustration for our MQNE algorithm is given in Fig. 1, with the pseudocode provided within the Supplemental Material [86].

We note that the number of nodes of the directed graph scales exponentially with the number of qubits involved $f_1(k) = \Theta(2^k)$. For large k, the size of the graph might exceed the capacity of any classical computer, rendering our MQNE algorithm infeasible in practice. To reduce the size of the graph, we can impose some further restrictions on building possible gate blocks. For instance, we may require that for each gate block there are at most c (a cutoff constant number) controlled-R_x gates, and the rest qubits all undergo single-qubit rotations. With these restrictions, the number of possible gate blocks reduces to a polynomial function of k [86]. Accordingly, the size of the directed graph is also reduced. However, it is worthwhile to

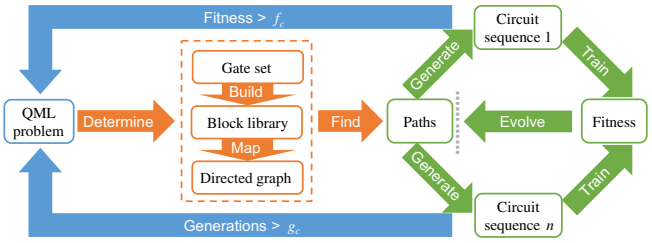


FIG. 1. Schematic illustration of the MQNE algorithm. For a given quantum machine-learning (QML) problem and experimental setup, we first determine the allowed gate blocks and the corresponding directed graph, and iteratively generate quantum circuits in a Markovian fashion. The algorithm terminates when the highest fitness of the generated circuits becomes larger than a certain threshold value f_c or the number of generations exceeds a given number g_c.

mention that the reduction of the graph may also bring up a problem: we may not be able to find the optimal ansatz circuits since the searching space is reduced too much by the restrictions. In the following, we give a couple of concrete examples to benchmark the effectiveness of our MQNE algorithm.

III. CLASSIFICATION OF HANDWRITTEN-DIGIT IMAGES

The first example we consider is the classification of handwritten-digit images in the MNIST dataset. This is a prototypical machine-learning task for benchmarking the effectiveness of various learning approaches. The MNIST dataset consists of gray-scale images for handwritten digits from 0 through 9. Each image is two dimensional, and contains 28×28 pixels. In the Supplemental Material [86], we display four gray-scale images for digits 1, 4, 7, and 9 from the MNIST dataset. For our purpose, we choose only a subset of MNIST consisting of images for digits 1 and 9 and reduce the size of the images to 16×16 pixels, so that we can run our MQNE algorithm and simulate the quantum classifiers generated with moderate classical computational resources. We use amplitude encoding to map the input images into quantum states and define the following loss function based on cross entropy for a single data sample encoded as $|\psi\rangle_{\text{in}}$ (see Ref. [88] for more details):

$$L\left[h\left(|\psi\rangle_{\text{in}};\Theta\right),\mathbf{a}\right]=-a_1\log g_1-a_2\log g_2, \qquad (1)$$

where $\mathbf{a}=(a_1,a_2)=(1,0)$ or $(0,1)$ denotes the one-hot encoding [89] of the label of $|\psi\rangle_{\text{in}}$, $h\left(|\psi\rangle_{\text{in}};\Theta\right)$ represents the output of the quantum classifier with its parameters denoted by Θ collectively, and $g_{1,2}$ denote the output probabilities of digits 1 and 9. For training the quantum classifier, we use a classical optimizer to search the optimal parameters Θ^* that minimize the averaged loss over the training dataset.

For images with 16×16 pixels, we need eight qubits to encode each input sample, and for convenience, we also use an additional qubit to output the results of the binary classification. Thus, the ansatz circuit we aim to design is a nine-qubit variation circuit. Applying the graph-encoding method and supposing that controlled-R_x gates act only on adjacent qubits, we obtain 6688 gate blocks and the corresponding directed graph has 6688 nodes. Based on the connection rules, we compute the adjacency matrix and apply the MQNE algorithm with hyperparameters set as $(n_i,t_i,l,l')=(10,1,5,2)$. Our results are summarized in Fig. 2. In Fig. 2(a), we randomly choose the initial variational parameters for single-qubit rotation gates when training the generated quantum classifiers at each generation. The MQNE algorithm outputs a quantum circuit with fitness (accuracy) 97% at the sixth generation, whose circuit structure

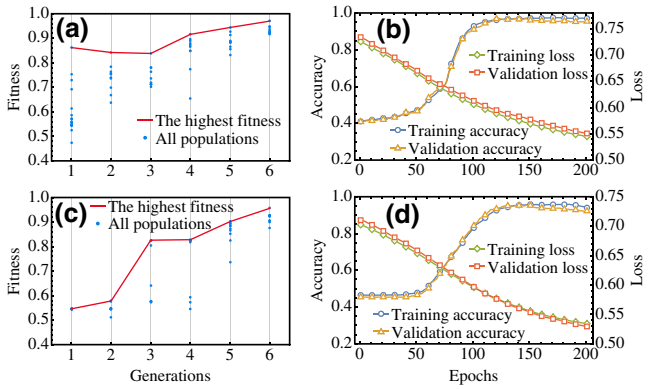


FIG. 2. Numerical results for classification of handwritten-digit images in the MNIST dataset. In (a), the initial variational parameters of single-qubit rotation gates are randomly chosen during the training process. In (b), we plot the loss and accuracy as a function of training epochs for the sixth-generation quantum circuit with the highest fitness. (c) The fitness of generated circuits for each generation with fixed initial variational parameters and (d) plots the loss and accuracy for the sixth-generation circuit that has largest fitness [86].

is explicitly shown within the Supplemental Material [86]. The corresponding path for this circuit on the directed graph reads [6687 → 3969 → 4418 → 1321 → 6319 → 2817 → 5933 → 859 → 2183 → 5160 → 4641 → 4097 → 4388 → 2305 → 4388], where the numbers denote the labels of the nodes of the graph. In Fig. 2(b), we plot the average accuracy and loss for both the training and validation datasets as a function of epochs during the training process. After training, the performance of this quantum classifier is also tested on the testing dataset and an accuracy of 97% is obtained. Figures 2(c) and 2(d) are analogous to Figs. 2(a) and 2(b), respectively, but with fixed initial parameters for single-qubit rotation gates during the training process. We find that fixing the initial parameters would lead to a more stable improvement of the performance for next-generation classifiers.

IV. CLASSIFICATION OF SYMMETRY-PROTECTED TOPOLOGICAL STATES

Unlike classical classifiers, quantum classifiers may also be used to directly classify quantum states produced by quantum devices. To show the power of our MQNE algorithm in this scenario, we consider a quantum machine-learning task of classifying SPT states. For simplicity and concreteness, we consider the following cluster-Ising model, whose Hamiltonian reads [90]

$$H(\lambda)=-\sum_{j=1}^{N}\sigma_{j-1}^{x}\sigma_j^{z}\sigma_{j+1}^{x}+\lambda\sum_{j=1}^{N}\sigma_j^{y}\sigma_{j+1}^{y}, \qquad (2)$$

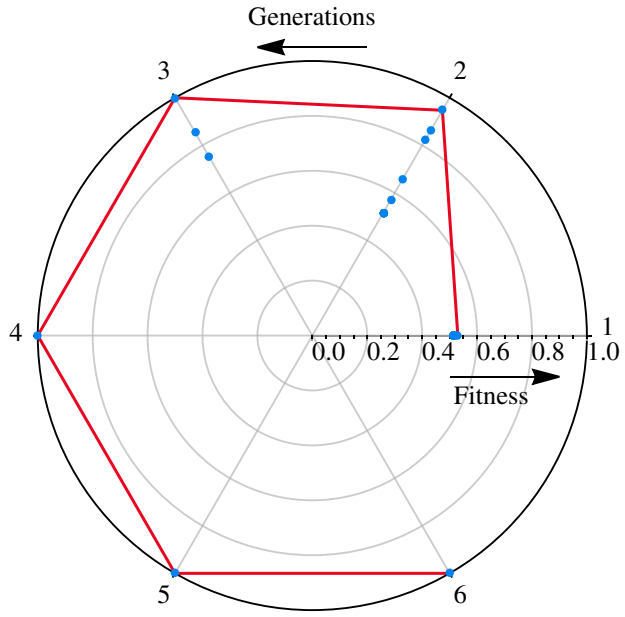


FIG. 3. Performance of the MQNE algorithm in the task of classifying symmetry-protected topological states [86].

where σ_i^α, $\alpha = x, y, z$, are Pauli matrices acting on the ith spin and λ is a parameter describing the strength of the nearest-neighbor interaction, and N denotes the number of spins. This model is exactly solvable and features a well-understood quantum phase transition at $\lambda = 1$, between a $Z_2 \times Z_2$ SPT cluster phase characterized by a string order for $\lambda < 1$ and an antiferromagnetic phase with long-range order for $\lambda > 1$. Here, we apply the MQNE algorithm to obtain an optimal ansatz variational circuit, which serves as a quantum classifier for classifying these two distinct phases. To this end, we set $N = 8$ and uniformly sample 2000 Hamiltonians with varying λ from 0 to 2 under the periodic boundary condition. We compute their corresponding ground states, which are the input data to the classifier, and randomly choose 1600 of them for training and the remaining ones for testing. Our results are plotted in Fig. 3, from which it is evident that the largest fitness increases at the first several generations and then saturates. We find a circuit at the third generation, which involves only 36 single-qubit and 10 two-qubit gates but has a fitness equals 100% [86].

We stress that, in comparison with the typical variational circuits used in previous works [88], the ansatz circuits found by the MQNE algorithm involve much fewer gates and variational parameters, while maintaining a comparable classification accuracy. For instance, for the example of classification of handwritten-digit images, the classifier used in Ref.[88] uses more than 90 single-qubit and 80 two-qubit gates with circuit depth larger than 30 and the number of variational parameters larger than 270, whereas the circuit found by the MQNE algorithm at the sixth generation contains only 28 single-qubit rotation gates and 22 two-qubit gates with 106 variational parameters and circuit depth 15.

This significant reduction of the circuit depth and number of gates (up to a constant factor) is crucial for experimental demonstration of quantum learning with NISQ devices, as the depth of the quantum circuits would be limited due to undesirable noises carried by such devices. It not only simplifies the implementation of quantum classifiers substantially from the practical perspective, but also would mitigate the possible barren plateau problem (i.e., vanishing gradient) [91–93] in training deep networks. We also mention that the performance of the MQNE may be improved further by choosing the hyperparameters judiciously according to different learning problems and experimental setups. In the Supplemental Material, we also tested the MQNE algorithm in the task of classification of images from the Wisconsin Diagnostic Breast Cancer dataset, which may have useful application in medical machine learning [94].

V. DISCUSSION AND CONCLUSION

Recent advances in quantum machine learning have revealed that quantum classifiers are highly vulnerable to adversarial attacks—adding a tiny amount of carefully crafted perturbations into the original legitimate data will cause the quantum classifiers to make incorrect predictions [88,95]. Thus, how to enhance the robustness of quantum classifiers to adversarial perturbations is a problem for practical applications of quantum learning in the future. With the MQNE algorithm, a possible solution to this problem is to design ansatz circuits that are more robust to the given type of adversarial attack. This could be achieved by replacing the original loss function [e.g., Eq. (1)] with a modified one that incorporates the adversarial perturbations [96]. In addition, the graph-encoding method would also be combined with other evolution or genetic algorithms to construct optimal circuit structures for different quantum-learning problems. In the future, it would be interesting to consider some symmetries in the data as prior knowledge to enhance our algorithm by restricting the searching space into a smaller subspace.

In summary, we introduce a quantum neuroevolution algorithm, named the MQNE algorithm, to design optimal variational ansatz quantum circuits for different quantum-learning tasks. Through concrete examples involving classifications of real-life images and SPT quantum states, we demonstrate that the MQNE algorithm performs excellently in searching appropriate quantum classifiers. It finds ansatz circuits with notably smaller depths and number of gates, while maintaining a comparable classification accuracy. Our results provide a valuable guide for experimental implementations of quantum machine learning with NISQ devices.

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