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Detecting Entanglement With Deep Quantum Neural Networks

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ABSTRACT Based on the theoretical basis of quantum computation, entanglement has been further explored as one of the key resources. An outstanding problem in quantum computation is the detecting of entanglement, but no closed-form algorithm exists. According to an advanced matrix rearrangement approach for detecting multipartite quantum states, we give some examples to verify the effectiveness and practicability of this new criterion. Meanwhile, this paper shows how techniques from the quantum neural network can be utilized to detect entanglement. Two models, known as the discrete-variable and the continuous-variable quantum neural network, are applied to solve the separability problem. We demonstrate the utility that such a discrete-variable quantum neural network can be trained to detect the entanglement with great exactness. And the complexity of network and computation is greatly reduced. Besides, the continuous-variable quantum neural network is applied for detecting two-qumode Gaussian state. Compared with the results of the traditional neural network, this deep quantum neural network demonstrates its capability and adaptability as well.

INDEX TERMS Entanglement detecting, matrix rearrangement, multipartite quantum system, deep quantum neural network, discrete variable, continuous variable.

I. INTRODUCTION

As quantum satellite triumphantly launched in August 2016 [1], quantum computing has become a focus and frontier of global research in physics and quantum computer is currently beginning to go out of the laboratory and moving towards industrialization [2], [3]. Based on the theory of quantum mechanics, the superiority of quantum computing lies in quantum parallelism (quantum superposition state) and quantum entanglement. Although researchers can construct a computational setup only exploiting quantum superposition, it cannot realize the full capacity of quantum computing in some case without the use of entanglement.

Entanglement is a valuable quantum resource [4] and plays an important role in many other physical phenomena, such as quantum phase transition [5] and efficient simulation of many body systems [6], [7]. However, it is difficult to determine whether a given quantum state is entangled or separable and to quantify an entangled state [8]. Over the

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years, many criteria have been proposed to detect and quantify entanglement. For instance, the most famous criterion is the Peres-Horodecki criterion or the Positive Partial Transpose (PPT) criterion [9] which is only necessary and sufficient for 2×2 or 2×3 quantum states [10], [11]. Unfortunately, the PPT criteria fail to apply for higher dimensional quantum states, such as bound entangled states (which are a special kind of states that cannot be distilled). Another widely used one is the Computable Cross Norm or Realignment (CCNR) criterion [12], which can detect many bound entangled states. But the criterion is not a real multipartite criterion due to its dividing operation at the beginning. In addition, there are some other criteria for detecting and quantifying entanglement have been proposed, such as the covariance matrix criterion [13] and the concurrence criterion [14]–[16]. However, they all have their own limitations.

Between 2002 and 2003, Chen and Wu presented a generalized partial transposition separability criterion for the density matrix of a multipartite quantum system [17], [18]. Following, the matrix realignment method was further applied and studied. M. Horodecki, *et al.* and S. Q. Shen, *et al.* given

their corresponding multipartite realignment criteria separately [19]–[21]. Despite a great deal of effort in the past years, it is a challenging task and remains an open question to detect whether a given state is entangled or not.

On the other hand, machine learning is the idea in which data is used to train network models without the need for programming a specific algorithm in order to reproduce a desired behavior [22], [23]. What machine learning is best at is to liberate humans from tedious repetitive work. Neural network is a way to realize tasks of machine learning with the structure composed of many simple units, used to simulate the interaction between living things and the natural environment. The most important use of a neural network is to teach machine classification and identification. On quantum computing side, the technology of machine learning, especially neural network, has been applied to many theoretical and experimental studies of quantum physics, such as quantum pattern recognition [24], description of quantum many-body systems [25], and quantum classification problems [26], [27]. These indicate that the neural network provides a new platform for solving problems in quantum information science.

In previous work, E. C. Behrman, *et al.* and J. Wisniewska, *et al.* proposed the use of artificial neural networks to quantify and detect entanglement respectively [28], [29]. Yet they only target the case of the bipartite qubit system. Later, S. Lu, *et al.* built a different separability-entanglement classifier with learning the entanglement feature of arbitrary given quantum states [30]. But only two-qubit and two-qutrit systems were performed. Until 2018, multiple species were extended through transforming Bell's inequalities into state classifiers [31], [32]. Up to now, the methods that quantify and detect entanglement are based on classical neural networks to study problems in quantum information science. There are few descriptions of quantum neural networks. What's more, in our perception, quantum information is encoded not in qubits, but in the quantum states of fields, such as the electromagnetic fields. The quantum computing architecture which is most naturally continuous is the continuous-variable model.

So, in this work, based on an advanced matrix rearrangement criterion, some examples are used to show that the advanced approach can be more efficient and general than previous criteria. Then a discrete-variable quantum neural network model is trained for classifying the separability of multipartite quantum states. In particular, the model is constructed via the supervised learning approach. Furthermore, as a combination with continuous-variable model and neural network model, we employ the continuous-variable quantum neural network [33] to the detecting entanglement of Gaussian states. We simulate the corresponding continuous-variable neural network models using the Strawberry Fields software platform [34], which is equipped with Tensorflow backend [35].

The remainder of this paper is organized as follows. In Section II, we outline preliminaries of realignment

criteria for multipartite quantum states. And the concept of quantum neural networks is also reviewed. How to detect or quantify quantum entanglement with the advanced matrix rearrangement approach is expounded in Section III. In Section IV, the parameters and output results of the discrete-variable quantum neural network are analyzed systematically. In Section V, we simulate the continuous-variable quantum neural network with Gaussian states inputting. Finally, we summarize the paper in Section VI.

II. PRELIMINARIES

In order to better integrate the task of detecting and quantifying quantum entanglement, we briefly introduce quantum entanglement and quantum neural networks in this section.

A. QUANTUM ENTANGLEMENT

E. Schrödinger called quantum entanglement as the essence and a unique property of quantum mechanics in 1935 [36]. Based on quantum entanglement, quantum communication can accomplish many information transmission and processing tasks that cannot be accomplished with classical resources.

The inseparable state is the entangled state, which means that all states cannot be written into the form of separated states. In multipartite quantum system, the entangled state cannot be simply written as the direct product form of some states. Entangled states include entangled pure states and entangled mixed states. The typical entangled state, such as the bipartite entangled Bell states and the tripartite entangled GHZ state, are the maximally entangled state. A pure n-partite state ρ is separable [37] if it can be expressed as

$$\rho = \sum_i p_i \rho_i^1 \otimes \rho_i^2 \otimes \cdots \otimes \rho_i^n, \quad (1)$$

where ρ_i^n denotes pure states of subsystem n , $0 < p_i \leq 1$ and $\sum_i p_i = 1$. A general mixed state is separable if it can be decomposed into

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|, \quad (2)$$

where each $|\psi_i\rangle$ is a separable pure state, $0 < p_i \leq 1$ and $\sum_i p_i = 1$.

Motivated by the Kronecker product approximation technique for a matrix [38]–[40], some kinds of realignment criteria are developed for detecting whether a given state is entangled or not. Next, we shall introduce some of notations and results of various matrix operations. For a quantum state ρ with the $m \times n$ density matrix $A = [a_{ij}]$, a_{ij} is the matrix entry of A , defining the vector $\text{vec}(A)$ as

$$\begin{aligned} \text{vec}(A) = & [a_{11}, a_{21}, \dots, a_{m1}, a_{12}, a_{22}, \dots, a_{m2}, \\ & \dots, a_{1n}, a_{2n}, \dots, a_{mn}]^T, \end{aligned} \quad (3)$$

where T stands for the transpose. Then the realignment matrix $\mathcal{R}(Z)$ can be defined in the following form,

$$\mathcal{R}(Z) \equiv \begin{bmatrix} \text{vec}(Z_{1,1})^T \\ \vdots \\ \text{vec}(Z_{m,1})^T \\ \vdots \\ \text{vec}(Z_{1,m})^T \\ \vdots \\ \text{vec}(Z_{m,m})^T \end{bmatrix}. \quad (4)$$

Here, Z be a $m \times m$ block matrix with block size $n \times n$. Then $\mathcal{R}(Z)$ is used to construct different separability criteria, including the multipartite realignment criteria. Among them, an excellent realignment criterion is proposed by K. Chen, called the generalized partial transposition criterion [17]. The criterion shows that if a n -partite state is separable, it should be satisfied in the following

$$\|\rho^{T_y}\|_1 \leq 1, \quad \forall y \subset \{r_A, c_A, r_B, c_B, \dots, r_Z, c_Z\}. \quad (5)$$

where T_{r_k} or T_{c_k} ($k = A, B, \dots, Z$) means transposition with respect to the row or column for the k th subsystem, and $\|\cdot\|_1$ means Schatten 1-norm [41]. By comparison, other multipartite realignment criteria proposed in [18]–[21] are variants in equation 5.

Through above description, we have a good understanding for the separability of entanglement. In other hand, in order to describe the entanglement degree of entangled states quantitatively, the concept of entanglement measure is used. The entanglement measure should meet features with entanglement of separable state is equal to zero, local unitary transformation will not change entanglement, and entanglement should not be increased under local operations and classical communication (LOCC) [42], [43].

B. DEEP QUANTUM NEURAL NETWORKS

The problem considered in quantum neural network falls under the similar flow chart of classical neural networks, including giving a quantum information task, data preparation, data embedding, training network, optimizing the parameters and best achieving the probability as the result. For calculating entanglement with quantum neural network, the goal should learn to detect and quantify a general measure of entanglement, whether the quantum state is discrete or continuous.

A discrete-variable quantum neural network is a quantum circuit of quantum perceptron organized into hidden layers of unitary operations, acting on input quantum states, and producing corresponding output quantum states. The network uses separate qubit registers for parameterized quantum circuit input and output, and defines the quantum neuron as a completely positive map between the two. According to implementing classical artificial neurons in quantum circuits has been proved to be feasible [44]–[46], the resulting network is universal for quantum computation and can be

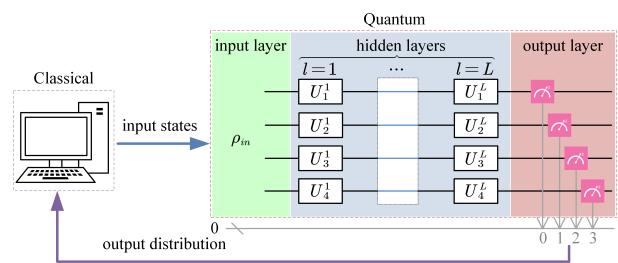


FIGURE 1. The general structure of a discrete-variable quantum neural network. Similar to classical neural networks, the deep quantum neural network has an input, output and L hidden layers. A classical computer sends quantum states to a quantum neural network and samples the output distribution resulted by the quantum neural network. Based on the resulting output, the parameters are updated until the desired output is achieved within the setting error.

trained by an efficient process resembling backpropagation. See Figure 1 for an illustration. The network output can be expressed as the composition of a sequence of completely positive layer-to-layer transition maps [47],

$$\rho^{out} = \xi^{out} \left(\xi^L \left(\dots \xi^2 \left(\xi^1 \left(\rho^{in} \right) \right) \dots \right) \right). \quad (6)$$

where $\xi^l(\rho) \equiv \text{tr}_{l-1} \left(\prod_{j=m_l}^1 U_j^l (\rho \otimes |0\dots0\rangle_l \langle 0\dots0|) \prod_{j=m_l}^1 U_j^{l\dagger} \right)$, U_j^l is the j th quantum neurons and m_l is the total number of quantum neurons acting on layers $l-1$ and l .

Another interesting approach is to use continuous-variable quantum systems to define quantum perceptron [33]. The network architecture is constructed and optimized with the TensorFlow backend of Strawberry Fields [34] by a quantum photonic company Xanadu, which has bringing together exceptional minds from around the world to build practical quantum solutions. Although the quantum continuous-variable neural network is designed to be implemented on a quantum photonic computer, it can also be implemented on classical computers by using Strawberry Fields and Gaussian gate operations. The general continuous-variable quantum neural network is built up as multiple layers \mathcal{L} composed of the sequence of gates,

$$\mathcal{L} := \Phi \circ \mathcal{D} \circ U_2 \circ S \circ U_1, \quad (7)$$

where the right side of the equation represents the single-mode and two-mode combinational rotation gate U_1 , the squeezing transformation gate S , another combinational rotation gate U_2 , the displacement gate \mathcal{D} and the non-Gaussian gate Φ from the right to the left respectively, which all can be defined in Gaussian system. $\mathcal{D} \circ U_2 \circ S \circ U_1$ realizes the weight and bias transformation from classical neural network to continuous-variable quantum neural network that defined as affine transformation. And Φ acts locally on each mode, similar to the nonlinear activation function of a classical neural network. A single layer of continuous-variable quantum neural network model is presented in Figure 2.

To give a better understanding about quantum neural networks for scientists who are not involved with a quantum

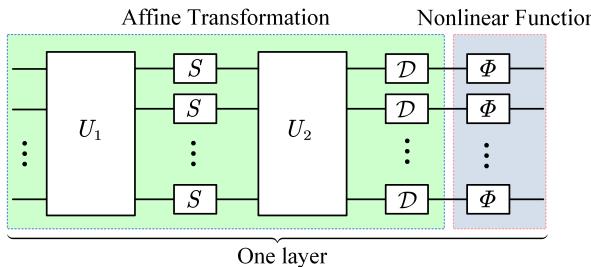


FIGURE 2. The architecture for a single layer of continuous-variable quantum neural network. Analogous to classical signal neural networks, TABLE 1 in Ref. [33] shows the details.

computing area, how to write the input and read the output of neural network are described in detail below.

When deploying machine learning systems to physical circuits, we often fall into a dilemma that how to embed a problem into the qubit network and let qubit interact in the right way. The preparation of quantum states, with loading classical data into quantum states, solve it well. And in practical quantum circuits, measuring quantum state not only returns one random number at a time, but also causes the whole state to collapse. In order to solve this problem, quantum interference is designed to eliminate the wrong answers and consolidate the correct answers. Then when quantum states are measured, the computer will give us the number that we want, not the random number. With the successful implementation of inputting and measuring quantum states, simulating quantum neural networks on classical computers with density matrices is feasible. For the output layer of quantum neural network, the network output is retrieved via measurements on the final quantum state and the measurement results are sent to classical computers. In particular, the Positive Operator Valued Measurement (POVM) operator [48] is used for the discrete-variable quantum neural network, and the Homodyne detection operator [49] is used for the continuous-variable quantum neural network.

III. THE ADVANCED MATRIX REARRANGEMENT CRITERION FOR MULTIPARTITE QUANTUM STATES

For bipartite quantum systems, the density matrix ρ can be expressed as the form of matrix elements,

$$\rho = \sum_{i_1 i_2 j_1 j_2} \rho_{i_1 j_1, i_2 j_2} |i_1 j_1\rangle \langle i_2 j_2|. \quad (8)$$

where subscript i_1, i_2 of matrix element $\rho_{i_1 j_1, i_2 j_2}$ belong to subsystem A and subscript j_1, j_2 belong to subsystem B. Then, the PPT criterion achieves the exchange of the second and fourth subscript, and the realignment criterion achieves the exchange of the second and third subscript. They can be expressed as follows,

$$\rho_{i_1 j_1, i_2 j_2}^{PT} = \rho_{i_1 j_2, i_2 j_1}, \quad (9)$$

$$\rho_{i_1 j_1, i_2 j_2}^R = \rho_{i_1 i_2, j_1 j_2}. \quad (10)$$

Inspired by an advanced matrix rearrangement approach which has been proposed and discussed by Prof. Zhongsheng

Pu from Lanzhou University of Technology [50], we present the advanced criteria in a more concise way. Let \mathcal{T}_{ij}^n denote the transposition between the i th and j th row (or column) element of a tensor-product Hilbert space matrix $H^{\otimes n}$. It means the transformation of \mathcal{T}_{ij}^n is to make partial transpositions of the rows or columns corresponding to some subsystems. Then \mathcal{T}_{ij}^n can be decomposed into tensor products of several operators, such as the row transposition operator \mathcal{T}_R , the column transposition operator \mathcal{T}_C , the transpose operator \mathcal{T}_T and the identity operator \mathcal{T}_I . Consequently, we can get that $\mathcal{T}_{24}^2 \rho_{i_1 j_1, i_2 j_2} = (\mathcal{T}_I \otimes \mathcal{T}_T) \rho_{i_1 j_1, i_2 j_2} = \rho_{i_1 j_1, i_2 j_2}^{PT}$ and $\mathcal{T}_{23}^2 \rho_{i_1 j_1, i_2 j_2} = (\mathcal{T}_C \otimes \mathcal{T}_R) \rho_{i_1 j_1, i_2 j_2} = \rho_{i_1 j_1, i_2 j_2}^R$. Now we arrive at the following advanced matrix rearrangement approach for a bipartite system,

$$\sup_{\mathcal{T}} \|\mathcal{T}_{ij}^2 \rho\|_1 \leq 1, \quad i, j \in \{1, 2, 3, 4\}, \quad (11)$$

here \sup denotes the supremum. Clearly, the PPT criterion and the realignment criterion are special cases of the advanced matrix rearrangement criterion. For a multipartite systems, if all values of i and j are traversed, a multipartite advanced matrix rearrangement approach can be obtained.

Theorem 3.1: If a multipartite quantum state ρ is separable, then,

$$\sup_{\mathcal{T}} \|\mathcal{T}_{ij}^n \rho\|_1 \leq 1, \quad i, j \in \{1, 2, \dots, 2^n\}. \quad (12)$$

Next, two popular examples are used to prove that there exists more rigorous performance in the advanced matrix rearrangement criterion.

Example 3.1: In [10], M. Horodecki, et al. introduced a density matrix of two spin-1/2 states,

$$\rho = p |\varphi_1\rangle \langle \varphi_1| + (1-p) |\varphi_2\rangle \langle \varphi_2|, \quad (13)$$

where $|\varphi_1\rangle = a|00\rangle + b|11\rangle$, $|\varphi_2\rangle = a|10\rangle + b|01\rangle$ with $a^2 + b^2 = 1$ and $a, b \geq 0$. In order to facilitate the analysis, the value of p is fixed at 1/4. It is generally known that the quantum state can only be separable at $a = 0$ or $a = 1$.

To this density matrix, the advanced criterion (Theorem 3.1 with $n = 2$) is used for detecting. We plot the value of $f = \|\mathcal{T}_{ij}^2 \rho\|_1$ in Figure 3 with respect to a . In particular, the matrix rearrangement operators of PPT criterion and realignment criterion are \mathcal{T}_{24}^2 and \mathcal{T}_{23}^2 respectively. Since the PPT criterion is necessary and sufficient condition for 2×2 quantum states, then it can detect the bipartite entanglement completely. Although some of rearrangement operators can also detect entanglement completely, such as \mathcal{T}_{14}^2 , the decision value is smaller than the PPT criterion. This may result in an increase in misjudgment rate when the value of f is close to 1. The supremum of f , which is consistent with the bound of PPT criterion in this example, constitutes the bound of entanglement. In addition, it can be seen from Figure 3 that some entangled states cannot be completely detected by the realignment criterion. We can conclude that the advanced criterion outperforms the realignment criteria in bipartite quantum systems.

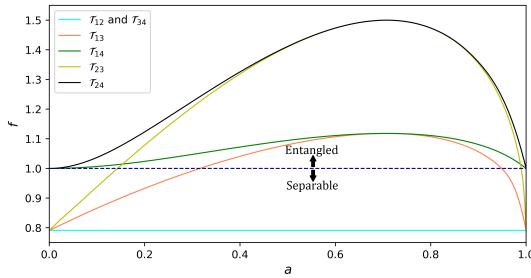


FIGURE 3. The results of each matrix rearrangement operator \mathcal{T}_{ij}^2 for detecting the two spin-1/2 states with variable parameters a . Some redundant operators are ignored. If $f > 1$, the state is determined to be entangled, otherwise to be separable. For brevity, the labels in the figure simplify \mathcal{T}_{ij}^2 to \mathcal{T}_{ij} .

TABLE 1. Entanglement conditions of a tripartite perturbation GHZ state with different ξ from the PPT criterion, the realignment criterion, the S-R criterion and Theorem 3.1.

ξ	PPT	Realignment	S-R	Theorem 3.1
0	$0.2001 \leq p \leq 1$	$0.3334 \leq p \leq 1$	$0.4118 \leq p \leq 1$	$0.2001 \leq p \leq 1$
1	$0.2728 \leq p \leq 1$	$0.3466 \leq p \leq 1$	$0.4256 \leq p \leq 1$	$0.2097 \leq p \leq 1$
10	$0.9273 \leq p \leq 1$	$0.7174 \leq p \leq 1$	$0.7728 \leq p \leq 1$	$0.5594 \leq p \leq 1$
50	$0.9969 \leq p \leq 1$	$0.9261 \leq p \leq 1$	$0.9431 \leq p \leq 1$	$0.8624 \leq p \leq 1$
100	$0.9993 \leq p \leq 1$	$0.9617 \leq p \leq 1$	$0.9707 \leq p \leq 1$	$0.9262 \leq p \leq 1$

Example 3.2: In [21], Y. H. Zhang, *et al.* introduced a tripartite perturbation GHZ state,

$$|\varphi_{PGHZ}\rangle = \frac{1}{\eta} (|000\rangle + \xi |110\rangle + |111\rangle), \quad (14)$$

where η denotes the normalization and ξ denotes the perturbation factor. For comparison, the state should be considered as the mixture with white noise I_8 ,

$$\rho_{WPGHZ} = \frac{1-p}{8} I_8 + p |\varphi_{PGHZ}\rangle \langle \varphi_{PGHZ}|, \quad (15)$$

where p is the probability of the perturbation GHZ state. We apply Theorem 3.1 with $n = 3$ for detecting this quantum state. Table 1 gives the results for different values of ξ . It follows that Theorem 3.1 outperforms the PPT criterion, the realignment criterion and the S-R criterion [21] for different values of ξ . Thus, Theorem 3.1 provides a useful supplement to the multipartite separability criteria based on matrix rearrangement approach.

Moreover, similar to the concept of entanglement negativity [51], Z. S. Pu, *et al.* proposed a corresponding entanglement negativity [50],

$$N_{AR}(\rho) = \frac{\sup_{\mathcal{T}} \|\mathcal{T}_{ij}^n \rho\|_1 - 1}{2}, \quad i, j \in \{1, 2, \dots, 2^n\}. \quad (16)$$

As the entanglement negativity is proved to satisfy features of entanglement measure, $N_{AR}(\rho)$ also satisfies these features. In addition, $N_{AR}(\rho)$ has the advantages of being computable and easy to calculate based on the characteristics of Theorem 3.1.

IV. SEPARABILITY ENTANGLEMENT CLASSIFIER VIA THE DISCRETE-VARIABLE QUANTUM NEURAL NETWORK

Generally, it is a computational complexity problem to detect whether a given multipartite quantum state is an entangled state or not. Although researchers have made a lot of efforts to propose some methods, computational complexity of these methods are very high. Recently, quantum neural network, without the need for programming an algorithm explicitly, is used to train model. This model can solve the separability problem very well. According to the workflow of classical neural network, the discrete-variable quantum neural network is described in a step-by-step way to achieve the task of detecting quantum entanglement.

A. DATA PREPARATION

We employ the quantum machine learning techniques to tackle the multipartite entanglement detection problem by recasting it as a learning task. In particular, the task can be formulated as a supervised binary classification task. Following the standard procedure of supervised learning [52], the feature vector representation of the input states is first created. Any quantum state ρ of $H^{\otimes n}$ can be represented as a density matrix or some probability amplitudes. Next, a datasheet of training examples is produced, with the form

$$\mathcal{D}_{train} = \{(\rho_1, label_1), (\rho_2, label_2), \dots, (\rho_j, label_j)\}, \quad (17)$$

where ρ_i is the input states, $label_i$ is its corresponding label signifying which class it belongs to 0 or 1, and j denotes the size of the set. The task is to analyze these training data and produce an inferred classifier that predicts the unknown class labels for generic new input states. Explicitly, referring to classical machine learning, a cost function is defined to evaluate how well the results of neural network fitting the training labels. Then the corresponding cost function is defined as the match rate,

$$\begin{aligned} \mathcal{M}(\rho, label) \\ = \frac{1}{|\mathcal{D}_{train}|} \sum_{\mathcal{D}_{train}} (Pr(0_{QNN} | 0_{AR}) + Pr(1_{QNN} | 1_{AR})) \\ = 1 - \frac{1}{|\mathcal{D}_{train}|} \sum_{\mathcal{D}_{train}} (Pr(1_{QNN} | 0_{AR}) + Pr(0_{QNN} | 1_{AR})), \end{aligned} \quad (18)$$

where $x_{QNN} \in \{0, 1\}$ labels the output of the quantum neural network predictor, x_{AR} labels the expected output with

$$label = \begin{cases} 0 & \sup_{\mathcal{T}} \|\mathcal{T}_{ij}^n \rho\|_1 \leq 1 \\ 1 & \sup_{\mathcal{T}} \|\mathcal{T}_{ij}^n \rho\|_1 > 1 \end{cases} \quad (19)$$

by the advanced realignment criterion. $0_{QNN}(1_{QNN})$ means separable (entangled), and similarly for x_{AR} .

To evaluate accurately the performance of the network, we trained the neural network in bipartite quantum system first. After the applicability is verified, it can be extended to multipartite quantum systems. Although quantum processing

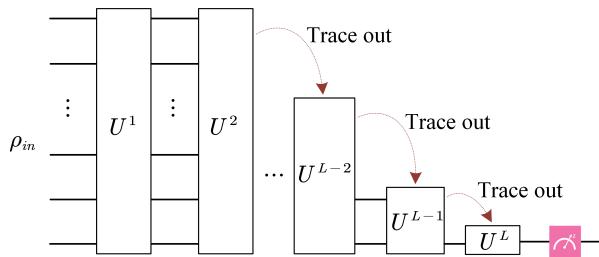


FIGURE 4. A universal deep quantum neural network construction of detecting separability with acting on m input qubits and one output qubit. U^i denotes the hidden layer unitaries, comprised of a product of quantum neural network acting on the qubits in layers $i - 1$ and i . In the structure, the later layers are progressively decreased in size by taking the partial trace over layers. The network output is retrieved via measurements on the final quantum state.

has the unique advantage of parallelism, it is impossible to simulate deep quantum neural networks for a large number of qubits due to the exponential growth of Hilbert space when we run quantum algorithms on classical computers. Firstly, we have carried out pilot simulations for 2×2 and 3×3 quantum states. For 2×2 quantum system, the input states that implemented by using the code of Random Density Matrix [53] are generated and labeled by Theorem 3.1. For 3×3 quantum system, some well-known quantum states are considered, such as the tripartite perturbation GHZ state described in Example 3.2. Secondly, in order to verify the generalization properties of obtained deep quantum neural network, some families of multipartite states are introduced into test of neural network efficiency, such as Cluster states [54], Dicke states [55] and six-partite states [56]. Taking the quadripartite quantum states as an example, we use basis abbreviations to represent multipartite quantum states,

$$|\varphi_{\text{quadr}}\rangle = \sum_{i=0}^{15} a_i |i\rangle, \quad (20)$$

where $\sum_{i=0}^{15} |a_i|^2 = 1$ and $\{|0\rangle, |1\rangle, \dots, |15\rangle\} \equiv \{|0000\rangle, |0001\rangle, \dots, |1111\rangle\}$. Then, the multipartite quantum states labeled by Theorem 3.1 as well.

B. DEEP QUANTUM NEURAL NETWORK ARCHITECTURE

A universal deep quantum neural network construction of detecting separability is outlined in Figure 4. A deep quantum neural network has one input layer, one output layer and many hidden layers. The quantum state output from one layer is used as the input for the next. By adding or removing qubits between layers, different layers can be made to have different widths. Removal can be accomplished by measuring or tracing out the extra qubits. The architecture also can be fitting for classical inputs. We can do this by fixing some of the gate arguments to be set by classical data rather than free parameters. This scheme can be thought of as an embedding of classical data into a quantum feature space [57]. The output of the network can be obtained by performing measurements and (or) computing expectation values.

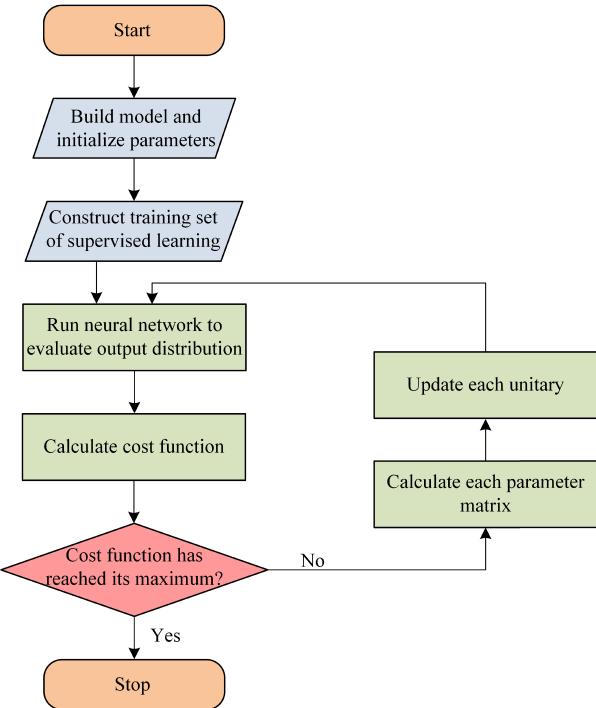


FIGURE 5. Process of quantum machine learning training.

The selection of measurement operators is flexible, and different choices may be more suitable for different situations.

C. TRAINING

Training network then corresponds to finding a path of unitaries $U(s)$ that eventually maximize the cost function. See Figure 5 for the flow chart of training. We should configure the task of quantum neural network as the supervised learning model. Further details about training algorithm can be found in Ref. [47].

D. MODEL PERFORMANCE

In the first place, we test the model on a classical computer using arbitrary density matrix of 2×2 quantum states as inputs. To avoid a bias in training set, the number of entangled states which is set up to 1000 is the same as the number of separable states.

During the training process, some hyperparameters, such as the learning rate and the number of layers and epochs, need to be analyzed. The effect of the number of layers on the final value of the cost function is shown in Figure 6. We can conclude that increasing the number of layers is helpful, but this is at the expense of increasing the computational complexity. In the training experiment, the training time increased more than twice with each additional layer. During the training process, we also observed an interesting result. When the number of epoch is lower than 100, the higher number of layers of the network, the faster loss drops. But with the increase of the number of epoch, the higher number of layers, the slower loss drops. This is because increasing the number

TABLE 2. Exemplary detection rates for the discrete-variable quantum neural networks with different structure of layers. The network with structure [2, 4, 2, 1] means that the number of qubits in each layer is 2, 4, 2, 1, respectively. Other network structures are similar. To avoid a bias in training set, the number of entangled states (subscript e) which can be set up to 1000 is the same as separable states (subscript s).

Deep Networks	Training Data	Test Data	Number of Entangled	Number of Separable	Matching Rate
Part 1: Arbitrary two-qubit state					
[2, 1]			952/1000	919/1000	93.55%
[2, 2, 1]	2000	2000	970/1000	945/1000	95.75%
[2, 4, 2, 1]	(1000 _e , 1000 _s)	(1000 _e , 1000 _s)	971/1000	962/1000	96.65%
[2, 4, 4, 4, 1]			978/1000	964/1000	97.10%
Part 2: Tripartite quantum states in Example 3.2					
[3, 3, 1]		(2500 _e , 1500 _s)	2377/2500	1369/1500	93.65%
[3, 3, 1]	2000	(2000 _e , 2000 _s)	1921/2000	1895/2000	95.40%
[3, 3, 6, 3, 1]	(1000 _e , 1000 _s)	(2000 _e , 2000 _s)	1932/2000	1903/2000	95.88%
Part 3: Arbitrary quadripartite quantum states					
[4, 4, 1]	200	300	138/150	150/150	96.00%
[4, 8, 4, 8, 4, 1]	(100 _e , 100 _s)	(150 _e , 150 _s)	135/150	149/150	94.67%

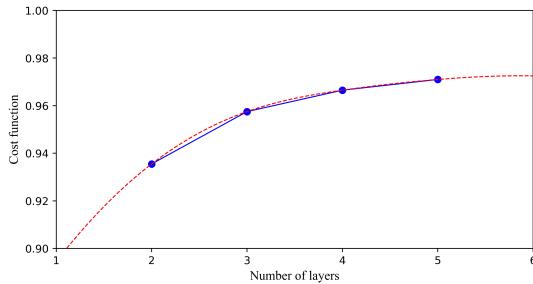


FIGURE 6. Cost function for different number of layers. The solid line represents the output of cost function in deep quantum neural network, the dashed line is the fitting curve.

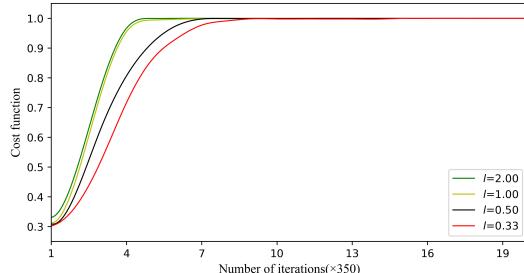


FIGURE 7. Cost function for different values of learning rate l . The lower the learning rate is, the slower the cost function changes. Although using a low learning rate ensures that we do not miss any local minimum (maximum), it also means that we will take longer time to converge.

of layers can reduce network errors, but it also increases the overfitting tendency of the network. So we need to find the optimal value considering these two factors. Another, shown in Figure 7, the cost function is depicted for different values of the learning rate.

Then, we have applied the discrete-variable quantum neural network for detecting entanglement in quantum systems. The match rates (the results of cost function) of both separable and entangled data are listed in Table 2 individually. For 2×2 quantum system, the calculations are run for networks

with different number of layers and quantum neurons. The results are shown in the Part 1 of Table 2. It is possible to reach the efficiency of detecting entanglement exceeding 93.5%. The results demonstrate the capability of our discrete-variable quantum neural network to detect unknown entangled states. Compared with classical neural networks, this quantum neural network only needs a few quantum neurons in hidden layers to achieve good performance. The complexity of network and computation is greatly reduced. Besides, it paves a way to the development of a generic tool for entanglement detection in other intricate, for example, 3×3 quantum states or multipartite systems. As we know, if the qubit number $n \geq 3$, all of traditional methods such as PPT and entanglement witness are not sufficient and necessary conditions of detecting entanglement. Therefore, if the state is labeled by the advanced matrix rearrangement criterion, it only takes us a short time to predict the class of new states after training. The Part 2 and Part 3 in Table 2 also show the results of experiments during which the discrete-variable quantum neural networks are trained to detect multipartite quantum states. The quantum neural network relies on a decision procedure where entanglement is seen as the ability of quantum systems to answer certain “yes-no questions”. We can see that the quantum neural network suffices to detect entanglement with almost 95% confidence and the simulation results preliminarily verify the generalization properties.

To further verify the effectiveness of the network, some bipartite, quadripartite and six-partite quantum states are used as the training and testing data. We choose 1000 randomly generated pure states with basis abbreviations of form,

$$|\varphi\rangle = \sum_{i=0}^{2^n-1} a_i |i\rangle, \quad (21)$$

where n denotes the number of input qubits, a_i is real coefficient. For example, in bipartite case with $n = 2$, the generated

TABLE 3. Some possible states of the multipartite quantum system. For bipartite quantum system, the completely entangled state (the Bell state), the unentangled state (the separable state) and the partially entangled state are included. For quadripartite quantum system, the quadripartite GHZ state, the quadripartite W state, the quadripartite Cluster state and the quadripartite Dicke state are tested. For six-partite quantum system, a six-partite quantum state is considered. The states are all not normalize yet. The network output is the statistical average of 20 identical quantum states input and the RMS errors among all quantum states are essentially zero.

	States	Expression	von Neumann entropy	N_{AR}	Network output
Bipartite	Completely entangled	$ 0\rangle + 3\rangle$	1	1/2	0.5081
	Unentangled	$ 0\rangle + 1\rangle + 2\rangle + 3\rangle$	0	0	0.0005
	Partially entangled	$ 1\rangle + 2\rangle + 3\rangle$	0.32	1/3	0.3372
	States	Expression	Entanglement measure [56]	N_{AR}	Network output
Quadripartite	The GHZ state	$ 0\rangle + 15\rangle$	1.0000	0.5000	0.5016
	The W state	$ 1\rangle + 2\rangle + 4\rangle + 8\rangle$	0.8660	0.4714	0.4689
	A quadripartite state	$2 0\rangle + 3\rangle + 6\rangle + 11\rangle + 2 13\rangle + 14\rangle$	0.9128	0.8119	0.8002
	The Cluster state	$ 0\rangle + 3\rangle + 12\rangle - 15\rangle$	0.9574	1.0000	0.9999
	The Dicker state	$ 3\rangle + 5\rangle + 6\rangle + 9\rangle + 10\rangle + 12\rangle$	0.9428	0.8334	0.8216
Six-partite	A six-partite state	$ 0\rangle + 3\rangle + 5\rangle + 6\rangle + 9\rangle + 10\rangle + 12\rangle + 15\rangle + 17\rangle + 18\rangle + 20\rangle + 23\rangle + 24\rangle + 27\rangle + 29\rangle + 30\rangle + 33\rangle + 34\rangle + 36\rangle + 39\rangle + 40\rangle + 43\rangle + 45\rangle + 46\rangle + 48\rangle + 51\rangle + 53\rangle + 54\rangle + 57\rangle + 58\rangle + 60\rangle + 63\rangle$	0.7559	0.6807	0.6783

pure states are expressed as $|\varphi\rangle = a_0|00\rangle + a_1|01\rangle + a_2|10\rangle + a_3|11\rangle$. The training pair of supervised learning becomes $\{|\varphi\rangle, N_{AR}(\rho_{|\varphi\rangle})\}$. Here, $N_{AR}(\rho_{|\varphi\rangle})$ is the entanglement negativity defined above. Meanwhile, we define the loss function as the mean square error (MSE) between the neural network outputs and the desired function values, namely

$$L = \frac{1}{D_{train}} \sum_{\mathcal{D}_{train}} [N'_{AR} - N_{AR}(\rho_{|\varphi\rangle})]^2, \quad (22)$$

where N'_{AR} denotes the output of neural network. A large number of permutations of possible states have been tested with exactly similar results. The Table 3 shows the details.

Simulation results indicate that the RMS precision loss between the value of entanglement negativity and the output of quantum neural network is very small. Compared with other entanglement measures [56], the trend of entanglement negativity is consistent. For example, the quadripartite GHZ state is more entangled than the quadripartite W state [56], the value of entanglement negativity is correspondingly larger than that of the quadripartite W state. In summary, we can draw a conclusion that the quantum neural network can quantify entanglement effectively by the use of entanglement negativity in pure multipartite quantum states.

V. QUANTUM NEURAL NETWORK FOR CONTINUOUS-VARIABLE SYSTEM

A discrete-variable quantum system can be represented by vectors in the finite Hilbert space and can be described as the density matrix for simplicity and efficiency of computation. However, the density matrix is difficult to describe a continuous-variable quantum system that can only be

represented by vectors in infinite dimensional Hilbert space. The most typical continuous-variable quantum system is a harmonic oscillator. The continuous-variable state, called the Gaussian state, presents a certain probability distribution in the phase space picture, can be uniquely determined by a position coordinate \hat{x} , and a conjugate momentum \hat{p} . Both of them should meet the commute condition $[\hat{x}_j, \hat{p}_k] = i\delta_{jk}$. Thus, the state of a N-qumode Gaussian is encoded with $2N$ real-valued variables $(\hat{x}, \hat{p}) \in R^{2N}$. The above description is consistent with the theory of quantum continuous-variable neural networks [33]. Therefore, it is not necessary to operate on the input information and only put it into the neural work, which simplifying the topology the neural network greatly. The architecture of continuous-variable quantum neural network to detect two-qumode Gaussian states is illustrated in Figure 8.

For continuous-variable quantum system, we overview the condition for detecting whether a two-qumode Gaussian state is entangled state or not [58]–[61]. C. J. Zhang *et al.* proposed a stronger necessary and sufficient condition for two-qumode Gaussian states in 2010 [58],

$$\langle (\Delta\hat{\mu})^2 \rangle + \langle (\Delta\hat{v})^2 \rangle \geq a^2 + \frac{1}{a^2} + M^2, \quad (23)$$

$$\hat{\mu} = |a| \hat{x}_1 + \hat{x}_2/a \quad (24)$$

$$\hat{v} = |a| \hat{p}_1 - \hat{p}_2/a \quad (25)$$

$$M = |a| \sqrt{\langle (\Delta\hat{x}_1)^2 \rangle + \langle (\Delta\hat{p}_1)^2 \rangle - 1} - \sqrt{\langle (\Delta\hat{x}_2)^2 \rangle + \langle (\Delta\hat{p}_2)^2 \rangle - 1/|a|^2}. \quad (26)$$

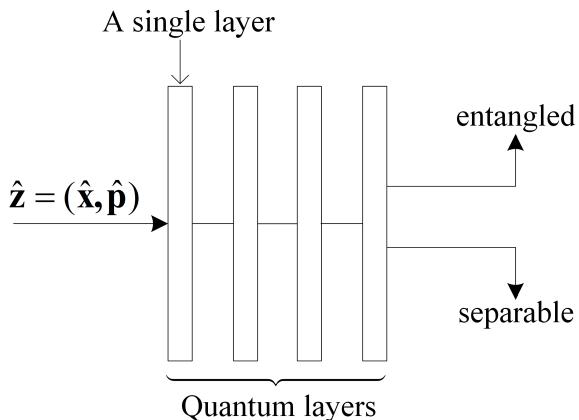


FIGURE 8. The scheme of continuous-variable quantum neural network used to detect whether a two-qumode Gaussian state is entangled or not. The input information are vector forms of position and momentum. The output value will be 0 or 1, representing the two-qumode state is entangled or separable. This kind of neural network can be simplified as a classifier of supervised machine learning.

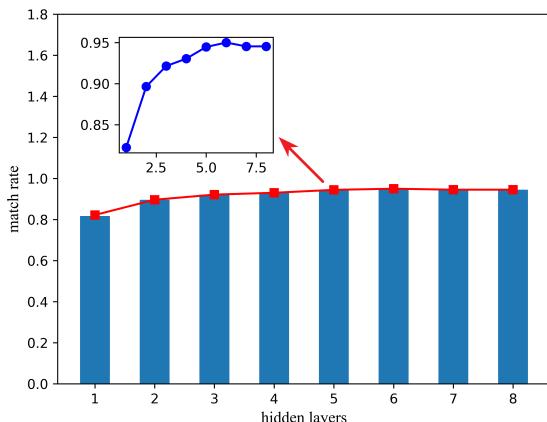


FIGURE 9. The results of the continuous-variable quantum neural network for detecting entanglement of two-qumode Gaussian states.

where $\{|a|\hat{x}_1, |a|\hat{p}_1\}$ and $\{\hat{x}_2/a, \hat{p}_2/a\}$ are local operators set for subsystems A and B respectively, $\langle \cdot \rangle$ represents the expectation value, and a denotes the real parameter.

Comparing results on both sides of the inequality (24), the label value is set to 0 when the value on the left side of the inequality is greater than the right side, which means that the input Gaussian state is separable. Conversely, the label value is set to 1, which means the input state is entangled. This principle is necessary to construct the learning set, where the training and testing data are tuples $((\hat{x}_i, \hat{p}_i), \text{label})$ for input (\hat{x}_i, \hat{p}_i) . Figure 9 presents the results of experiments, showing the increase in the performance of the continuous-variable quantum neural network as the number of layer increases until a saturation point is reached with six layers. After that, the performance is getting worse. For the best case, the error for the testing dataset decreases to about 5%. We can infer that quantum continuous variable neural networks can also be an effective tool for detecting two-qumode Gaussian state.

VI. CONCLUSION

In this paper, through the simulated results of two instances, we have achieved that the advanced matrix rearrangement approach outperforms the PPT criterion, the realignment criterion and the S-R criterion. It provides a useful supplement to the multipartite separability criteria. Next, we have applied two methods of deep machine learning, known as the discrete-variable and the continuous-variable quantum neural network, to solve problems of detecting entanglement in quantum information science. First, the discrete-variable quantum neural network is described by a step-by-step way, with steps of data preparation, network architecture, training process and model performance, to achieve the task of detecting entanglement. The results demonstrate that it is possible to reach the efficiency of detecting entanglement exceeding 93.5%. Compared with classical neural networks, this quantum neural network only needs a few quantum neurons and hidden layers to achieve good performance. Further, the successful application of entanglement negativity proves the availability of quantum neural network. We can say that the discrete-variable quantum neural network paves a way to the development of a generic tool for entanglement detection in multipartite systems. Second, the continuous-variable quantum neural network demonstrates its capability and adaptability as well. With regard to the two-qumode Gaussian state, the work can detect the possibility of entanglement with high accuracy. The weakness that continuous variables are difficult to be described by density matrices can be remedied. It can be stated that the continuous-variable quantum neural network improves the overall framework of the quantum neural network. In the future, it will be interesting that quantum neural networks can be implemented on a quantum computer. Then, more complex quantum states, such as multi-qumode Gaussian or non-Gaussian states, can be detected and quantified.

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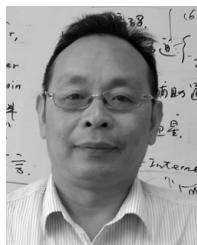


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