Finding efficient observable operators in entanglement detection via convolutional neural network

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In quantum information, it is of high importance to efficiently detect entanglement. Generally, it needs quantum tomography to obtain state density matrix. However, it would consume a lot of measurement resources, and the key is how to reduce the consumption. In this work, we successfully applied CNN to detect entanglement. CNN is one of the most representative neural networks which is considered more efficient than FC [51]. At present, CNN has been used to express quantum state of multi-particle system [7,10], estimate entanglement entropy of quantum many-particle system [23], and fully connected neural network (FC) can be used to predict the multipartite entanglement structure of states composed by random subsystems [34] or find semi-optimal measurements for entanglement detection [50].

In this work, we successfully applied CNN to detect entanglement. CNN is one of the most representative neural networks which is considered more efficient than FC [51]. At present, CNN has been used to express quantum state of multi-particle system [7,10], estimate entanglement entropy of quantum many-particle system [23], and the parameters of multi-particle Hamiltonian [52]. Here, we first show why the observable operator of quantum system with discrete energy levels can be regarded as a special convolution kernel and how to use a convolution kernel to represent an observable operator and get the parameters of multi-particle Hamiltonian [52].

Then, we devised branching convolutional neural network (BCNN) (depicted in Fig. 3(c)) which has a number of independent convolutional paths. Every convolutional path accurately calculates average value of observable operators in inputted quantum state. According to the features of quantum state, the structures of convolutional paths, it can automatically find appropriate observable operators which can extract information required by training goal. Because of that, it can decrease resource consumption in practice. We detected the entanglement of 2-qubits state and research the influence of the number of observable operators on the accuracy of our model.
RESULTS

Regard observable operator as a kernel

CNN extract features from input data by the kernels, which are composed of trainable parameters. Every kernel scans the input data according to a certain step size. In each step, its parameters are multiplied with the corresponding input data and all are added as output. We can see a simple example of convolution without bias and activation function in Fig. 1(a).

As we know, quantum states can completely describe a system. Observable operators can extract features such as momentum, spin, position, etc. from quantum states. From the point of feature extraction, we prove that the observable operator of discrete level system is a special convolution kernel. In Fig. 1(b), we show how the convolutional layer can accurately calculate the average value of observable operator. We take state density matrix $\rho$ as the input of the neural network and the transpose of observable operator $M^T$ as the kernel, and the output of convolution without activation function and bias is

$$\rho * M^T = \sum_{ij} \langle i | \left( \sum_{kl} \rho_{kl} M_{lk} | l \rangle \langle l | \right) | j \rangle$$

$$= \sum_{ij} \rho_{ij} M_{ji}$$

$$= \langle M \rangle,$$

where $*$ means the convolution in the artificial neural network. If there are 2 subsystem with the dimension $d^{(1)}$ and $d^{(2)}$, its state density matrix can be written as $\rho = \sum_{ijkl} \rho_{ijkl} | i \rangle \langle j | \otimes | k \rangle \langle l |$ and the observable operator $M$ can be written as $M = M^{(1)} \otimes M^{(2)}$. In the same way, we take $M^{(2)T}$ and $M^{(1)T}$ as the kernels of the first and the second convolutional layers, and their step sizes are exactly equal to their own dimensions. The output of the first convolutional layer is

$$O^{[1]} = \rho * M^{(2)T} = \left( \sum_{ijkl} \rho_{ijkl} | i \rangle \langle j | \otimes | k \rangle \langle l | \right) * M^{(2)T}$$

$$= \sum_{ijkl} \rho_{ijkl} | i \rangle \langle j | \otimes \left( | k \rangle \langle l | * M^{(2)T} \right)$$

$$= \sum_{ijkl} \rho_{ijkl} | i \rangle \langle j | \otimes \left( | [M^{(2)}] k \rangle l \rangle \right)$$

$$= tr(2) \left( \rho \cdot I^{(1)} \otimes M^{(2)} \right).$$

i.e., the first convolutional layer calculate the partial trace for the subsystem (2) of $\rho \cdot I^{(1)} \otimes M^{(2)}$, thus $O^{[1]}$ is Hermitian and its dimension is $d^{(1)}$. Then, the output of the second convolutional layer can be got as

$$O^{[2]} = O^{[1]} \ast M^{(1)T}$$

$$= \left( \rho \ast M^{(2)T} \right) \ast M^{(1)T}$$

$$= tr(2) \left( \rho \cdot I^{(1)} \otimes M^{(2)} \right) \ast M^{(1)T}$$

$$= tr \left[ \rho \cdot \left( M^{(1)} \otimes M^{(2)} \right) \right]$$

$$= \langle M^{(1)} \otimes M^{(2)} \rangle.$$

Similarly, suppose that there are $N$ subsystems with dimension $d^{(1)}, d^{(2)}, \ldots, d^{(N)}$, and the observable operator $M$ can be written as $M = M^{(1)} \otimes M^{(2)} \otimes \cdots \otimes M^{(N)}$, it is possible to caculate its average via the convolutional path with $N$ convolutional layers. For $\forall n \leq N$, the kernel of the $n$-th convolutional layer is $M^{(N-n+1)T}$, and the step size equal to its dimensions. Therefore, for $\forall n < N$, the output $O^{[n]}$ is

$$O^{[n]} = O^{[n-1]} \ast M^{(N-n+1)T}$$

$$= tr_{(N-n+1)} \left( O^{[n-1]} \otimes I^{(1)} \otimes \cdots \otimes I^{(N-n)} \otimes M^{(N-n+1)} \right)$$

$$= tr_{(N-n+1, \ldots, N)} \rho I^{(1)} \otimes \cdots \otimes I^{(N-n)} \otimes M^{(N-n+1)} \otimes \cdots \otimes M^{(N)}.$$

Likewise, it can be prove that $O^{[n]}$ is also Hermitian, and its dimension is $d^{(O)} = d^{(1)} \cdot d^{(2)} \cdots d^{(N-n)} = d^{(O')} \cdot d^{(M')}$, where $d^{(O')}$ and $d^{(M')}$ are the dimensions of the output $O^{(n+1)}$ and kernel $M^{(N-n)T}$ of next layer. In the same
way, the output of the last layer also can be obtained
\[
O^{[N]} = \left( \left( \rho \ast M^{[N]T} \right) \ast M^{[N-1]T} \ast \cdots \right) \ast M^{[1]T} = \langle M^{[1]} \otimes M^{[2]} \otimes \cdots \otimes M^{[N]} \rangle.
\]

Furthermore, considering that artificial neural networks are usually trained based on gradient descent, we prove that if the input and kernel of the convolutional layer are initialized as Hermitian matrixes, the gradient of the kernel will also be Hermitian. The calculation of kernel’s gradient depends on the neural network error matrix from back propagation and the input of convolutional layer. We let \( \delta^{[n]} \) be the error matrix which is propagated into the \( n \)-th convolutional layer. Its dimension always equal to dimension of \( O^{[n]} \). Since the step size of the kernels here are equal to their dimensions, for \( \forall n < N \), \( \delta^{[n]} \) can be expressed as
\[
\delta^{[n]} = \delta^{[n+1]} \otimes M^{(N-n)T}.
\]

Because of the Hermitianity of \( O^{[N]} \), the error \( \delta^{[N]} \), which is propagated from the fully connected layer, must be a real number too. It means for \( \forall n < N \), \( \delta^{[n]} \) is Hermitian. Considering that, for \( \forall n < N \), \( d^{(O')} = d^{(O')} \cdot d^{(M')} \), so \( O^{[n]} \) can be written as
\[
\sum_{ij, kl} O_{ij, kl}^{[n]} \langle i | \otimes | j \rangle \langle j | \otimes | k \rangle \langle l |.
\]

Then according to the neural network back propagation theory, for \( \forall n \leq N \), the kernel gradient is
\[
\delta M^{(N-n+1)T} = \sum_{ij, kl} d^{(O')} \cdot d^{(M')} O_{ij, kl}^{[n-1]} \langle i | \otimes | j \rangle \langle j | \otimes | k \rangle \langle l |.
\]

Since \( O^{[n-1]} \) and \( \delta^{[n]} \) are Hermitian, so
\[
\sum_{ij} O_{ij, kl}^{[n-1]} \langle j | \delta^{[n]}T \rangle \langle i | = \langle \sum_{ij} O_{ij, kl}^{[n-1]} \langle j | \delta^{[n]}T \rangle \rangle^*,
\]

as well as, \( \delta M^{(N-n+1)T} \) is also Hermitian. Therefore, in the process of updating based on gradient descent, the
Hermitianity of the kernel will not change.

So far, we prove that the observable operator of the discrete level system can indeed be regarded as a special convolution kernel, the convolutional layer can be used to calculate the average of observable operators, and these convolutional layers can naturally keep Hermitianity when trained by gradient-based optimization methods.

**Entanglement detection for 2-qubits state**

Based on the content we introduced above, we devise the BCNN (depicted in Fig. 2) to classify the entanglement of 2-qubits state. BCNN consists of several convolution paths and the following fully connected layers. It can automatically find proper observable operators which can extract information needed for the training goal. Here, we use \( (m; n_1, n_2) \) to describe the structure of convolutional paths, where \( m \) means how many convolutional paths the network has, \( n_1 \) and \( n_2 \) means there are two layers of convolutional layer in a convolutional path and they have \( n_1 \) and \( n_2 \) kernels respectively. After training, the trained observable operators can be obtained from these kernels. More details of BCNN is introduced in the section Methods. Our dataset consists of state density matrices and corresponding entanglement labels. The labels are determined by PPT criterion, which is necessary and sufficient for entanglement classification of \( 2 \times 2 \) and \( 2 \times 3 \) system \([5,3]\). Next, we will briefly introduce the quantum states we tested. The Werner state is

\[
\rho = p|\psi\rangle\langle \psi| + \frac{(1-p)I}{4}, \quad (8)
\]

where, \( |\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \) \( p \in (0, 1) \). It has only one free parameter \( p \), when \( p > \frac{1}{2} \) it is entangled \([5,4]\).

The first generalized Werner state which we called GI-Werner state is

\[
\rho(\theta) = p|\psi_\theta\rangle\langle \psi_\theta| + \frac{(1-p)I_A}{2} \otimes \rho_B, \quad (9)
\]

where, \( |\psi_\theta\rangle = \cos \theta|00\rangle + \sin \theta|11\rangle \), \( p \in (0, 1), \) \( \theta \in (0, 2\pi) \), and \( \rho_B = tr_A(|\psi_\theta\rangle\langle \psi_\theta|) \) is the reduced density matrix of the B system. The GI-Werner state has two free parameters \( \theta \) and \( p \), however its entanglement information only related to \( p \). Like the Werner state, when \( p > \frac{1}{3} \) it is entangled \([28]\).

The second generalized Werner state, which we call the GII-Werner state, is

\[
\rho(\theta, \phi) = p|\psi_{\theta,\phi}\rangle\langle \psi_{\theta,\phi}| + \frac{(1-p)I}{4}, \quad (10)
\]

where, \( |\psi_{\theta,\phi}\rangle = \cos \theta|00\rangle + e^{i\phi}\sin \theta|11\rangle \), \( p \in (0, 1), \) \( \theta \in (0, \pi), \) \( \phi \in (0, 2\pi) \). The GII-Werner state has three free parameters \( \theta \), \( p \), and \( \phi \), but its entanglement information is only related to \( \theta \) and \( p \). It is entangled when \( p > \frac{1}{1+2\sin \theta} \) \([20]\).

Normally, it needs 15 observable operators to reconstruct a 2-qubits state density matrix. However, the number of free parameters of above three quantum states is less than 15, and that of parameters related to entanglement may be even less. In principle, if we can effectively extract and process the entanglement information, we can classify the entanglement of quantum states with the least resource consumption.

We use the BCNN consisting of convolutional paths \((m \in \{1, 2, 3, 4\}; n_1 = 1, n_2 = 1)\) and three fully connected layers to classify the entanglement of Werner state, GI-Werner state and GII-Werner state. The convolutional path used here has two convolutional layer, and each layer has just one kernel. It can train a observable operator and calculate its average. In practice, based on few observable operators, the BCNN can predict the entanglement of the these quantum states with high accuracy, which shown in Fig. 2a. When classifying the entanglement of the Werner state, the accuracy of the BCNN achieve 99.7% with only one observable operator \((m = 1)\). For the GI-Werner state, FC has achieved 97% accuracy with two selected observable operators \([25]\) and BCNN can achieve 99.8% with only one observable operator \((m = 1)\). For the GII-Werner state, BCNN can achieve 98.4% with two observable operators \((m = 2)\) and 99.6% with three observable operators \((m = 3)\), which is at the same level with the performance of FC with four selected observable operators \([20]\). (Compared with using a FC with four selected observable operators \([20]\), our results are about the same.) The error distributions of the BCNN are shown in Fig. 2b-d. As we can see, the errors are concentrated on the boundary of entanglement and separability. Especially for GII-Werner state, the errors also occur when \( \theta = 0 \) and \( \pi \), which there are only separable states. The trained observable operators which used to extract the entanglement information can be acquired from the kernels. We show them in TABLE II and only keep two decimal places.

Finally, we apply BCNN to classify the entanglement of general 2-qubits state. For the state generation, we adopt the method of \( \rho = \sigma \otimes \sigma \), where \( \sigma \) is a random complex matrix and keep the proportion of entangled states and separable states at 1:1. We show the performance of BCNN with three different convolutional path \((m = 1; n_1 = 4, n_2 = 4), (m \in [6, 15]; n_1 = 2, n_2 = 2)\) and \((m \in [6, 15]; n_1 = 1, n_2 = 1)\) in Fig 5. Since the general state is more complicated, we use five fully connected layers in BCNN. For the structure \((m = 1; n_1 = 4, n_2 = 4)\), we fix one kernel in each convolutional layer as the identity matrix, and other kernels are still trainable. The outputs of the convolutional path are the averages of 15 observable operators and a constant 1. In this case, the accuracy of BCNN can achieve 97.5%. For \((m \in [6, 15]; n_1 = 2, n_2 = 2)\), we also fix one kernel in each convolutional layer as the identity matrix. Each convolutional path outputs 3 observable operator averages and a constant 1. When \( m \geq 9 \), the convolutional paths are able to get all the information about the quantum state, and the accuracy of BCNN can be higher than 96.0%. For the structure \((m \in [6, 15]; n_1 = 1, n_2 = 1)\),
FIG. 3. Branching convolutional neural network (BCNN). The input of the network is the density matrix $\rho$, and it goes through several independent convolutional paths (shaded in red dotted box). Every convolutional path has two convolutional layers and each convolutional layer has several kernels. Every convolutional path outputs the average of all combinations of the kernels of its two convolutional layers. Then, we take the outputs of these convolutional paths as the input of fully connected layer to classify the entanglement of states. For Werner, GI-Werner and GII-Werner states, we use three fully connected layers. For general 2-qubits state, we add two fully connected layers in the former structure.

TABLE I. Trained observable operators

| state        | operator number | $X^{(1)}$ | $Y^{(1)}$ | $Z^{(1)}$ | $I^{(1)}$ | $X^{(2)}$ | $Y^{(2)}$ | $Z^{(2)}$ | $I^{(2)}$ |
|--------------|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| Werner       | 1               | -1.26     | -0.97     | -1.40     | 0.61      | 0.49      | -0.18     | 1.63      | 0.62      |
| GI-Werner    | 1               | -0.37     | 0.17      | -1.57     | 0.19      | -0.18     | 0.39      | 0.95      | -0.51     |
| GII-Werner   | 2               | 0.04      | 1.08      | 0.19      | 0.18      | 0.39      | 0.95      | 0.11      | 0.02      |
|              | 3               | -0.20     | -1.23     | -1.33     | 0.10      | 0.38      | 0.29      | -0.25     | -0.08     |

each convolutional path computes the average of just one observable operator. Therefore, with the increase of $m$, the accuracy of this structure raises lowest. And the BCNN still need 15 convolutional paths to extract all quantum state information and its accuracy can achieve 97.2%. In Fig 5(b), we show the error distribution of BCNN with three above convolutional paths when they are just able to extract all the information about quantum state. There only a few errors occur symmetrically around the boundary of entanglement and separability. As long as the structure of the convolutional paths allows all information to be extracted, the BCNN can train appropriate observable operators and detect the entanglement of a general quantum state with high accuracy, which is comparable to the results in article [20].

**DISCUSSION**

In this work, we prove the observable operator of discrete-level systems is a convolution kernel, which means that the convolutional layer of artificial neural network can accurately calculate the average value of observable operator in quantum state, and that the Hermiticity of the convolutional layer can be maintained with the optimization algorithm based on gradient descent. With the foundation of above, we propose a BCNN, which can obtain well-trained observable operators to efficiently extract entanglement information and classify entanglement. We classify the entanglement of 2-qubits states, and studied the accuracy and the error distribution of BCNN.

We believe that CNN will be a promising tool for quantum physics. In our work, for Werner state, GI-Werner state and GII-Werner state, it can achieve 99.7%, 99.8%, and 98.4% respectively when the numbers of observable operators are same with that of parameters related to entanglement. It is superior to previous work in reducing resource consumption. For general 2-qubits state, our model still needs 15 observable operators to achieve the accuracy of 97.2%. In addition, we can extract the
FIG. 4. (a), The performance of BCNN for entanglement detection of Werner state, GI-Werner state and GII-Werner state. The accuracy increases with the number of observable operators. (b), The error distribution of the BCNN with 1 observable operators, when entanglement classification is performed on GI-Werner state. When $p > \frac{1}{3}$, the state is entangled. And the errors concentrate on the boundary of entanglement and separability. (c)(d), The error distribution of the BCNN with 2 and 3 observable operators, when entanglement classification is performed on GII-Werner state. We only drew the distribution when $\theta = 0, 0.1\pi, \cdots, \pi$ for more clear view. The boundary of entanglement and separability is $p = \frac{1}{(1+2\sin^2\theta)}$. And the errors concentrate on the boundary and the area $\theta = 0$ and $\pi$.

trained observable operators from kernels. These observable operators can be rewritten as the sum of the orthogonal normalization operators. We only keep two decimal places of the coefficient and input them into neural network to test again, and find that the accuracy of the BCNN almost keep the original level.

Since the convolutional layer can accurately calculate the average value of observable operator in quantum state, and this property applies to any dimension discrete-level system. It may be a powerful tool for solving measurement direction of the maximum violation of Bell inequality. We believe this property is likely to be used in other research and can bring new inspiration to the understanding of the relationship between quantum physics and artificial neural networks.

**METHODS**

The BCNN has several independent convolutional paths and fully connected layers. A convolutional path has several convolutional layers. The kernel of each convolutional layer represents the transpose of a observable operator acting on the system or subsystem. Therefore their convolutional layers should not have activation functions and biases. Each convolutional layer outputs all the averages of all combinations of the kernels of its convolutional layers. Then, we take the outputs of the convolutional paths as the input of fully connected layers for entanglement detection. And the structure of convolutional paths and fully connected layers should be adjusted according to the task. In this work, we use the BCNN consists of the convolutional paths $(m; n_1 = 1, n_2 = 1)$ and three fully connected layers with the structure $(\alpha, 1024, 1)$ to detect the entanglement of Werner state, GI-Werner state...
FIG. 5. (a) The performance of BCNN for entanglement detection of 2-qubits general state. The accuracy almost increases linearly with the number of observable operators. (b) The error distribution of the BCNN with 15 observable operators, when entanglement classification is performed on 2-qubits general state. The horizontal axis is the minimum eigenvalue $\lambda_{\text{min}}$. The error concentrates on the boundary of entanglement and separability. The error distribution is symmetric about the boundary, so our prediction is unbiased.

### TABLE II. Adam parameters

| state   | operates number | $\beta_1$ | $\beta_2$ | batch size | epoches |
|---------|-----------------|-----------|-----------|------------|---------|
| Werer   | 1-15            | 0.001     | 0.9       | 0.99       | 10      | 10      |
| GI-Werner | 1-15            | 0.001     | 0.35      | 0.99       | 10      | 10      |
| GII-Werner | 1              | 0.001     | 0.35      | 0.9        | 10      | 10      |
|         | 2               | 0.001     | 0.9       | 0.99       | 200     | 30      |
|         | 3-15            | 0.001     | 0.375     | 0.99       | 10      | 10      |
| General | 8               | 0.0003    | 0.325     | 0.825      | 400     | 20      |
|         | 9               | 0.0003    | 0.325     | 0.85       | 400     | 20      |
|         | 10              | 0.0003    | 0.325     | 0.87       | 400     | 20      |
|         | 11              | 0.0003    | 0.325     | 0.9        | 400     | 20      |
|         | 12              | 0.0003    | 0.325     | 0.95       | 400     | 20      |
|         | 13              | 0.0003    | 0.325     | 0.925      | 400     | 20      |
|         | 14              | 0.0003    | 0.325     | 0.925      | 400     | 20      |
|         | 15              | 0.0003    | 0.325     | 0.975      | 400     | 20      |

and GII-Werner state. For general 2-qubits state, we test the BCNN consists of one of three different convolutional paths ($m; n_1 = 4, n_2 = 4$), ($m; n_1 = 2, n_2 = 2$) or ($m; n_1 = 1, n_2 = 1$), and five fully connected layers ($\alpha_1024, 1024, 1024, 1)$. The $\alpha$ is the number of the input nodes of the first fully connected layer, which is related to the structure of convolutional paths. The first layer has no activation functions and bias. The final layer’s activation function is sigmoid and the loss function is cross entropy $^{55}$. For other layers, we take ReLu $^{54}$ as the activation function. We use Adam $^{54}$ as our optimizer to make it more likely to cross the saddle point and local minimum. We did not use the default recommended parameters of Adam, but adjust them according to the quantum state and the number of convolutional paths.

Our adam parameter settings are listed in TABLE II for reference.

In training process, we takes state density matrix as the input, and the kernels are initialized to a random Hermitian matrix. According to the features of the quantum state and the structure of convolutional paths, BCNN can automatically find appropriate observable operators for training task. In test process, we can directly calculate the average value of these trained observable operators, and input them into the following fully connected layers to detect entanglement. Of course, based on Eq. (1), single convolutional layer can be used to find global observable operators for entanglement detection, but the same task can already be completed by FC $^{50}$. Therefore, in this article, we will focus on using two convolutional layers to express the product observable operator.
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