Generalization Study of Quantum Neural Network

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Abstract. Generalization is an important feature of neural network, and there have been many studies on it. Recently, with the development of quantum computing, it brings new opportunities. In this paper, we studied a class of quantum neural network constructed by quantum gate. In this model, we mapped the feature data to a quantum state in Hilbert space firstly, and then implement unitary evolution on it, in the end, we can get the classification result by implement measurement on the quantum state. Since all the operations in quantum neural networks are unitary, the parameters constitute a hypersphere of Hilbert space. Compared with traditional neural network, the parameter space is flatter. Therefore, it is not easy to fall into local optimum, which means the quantum neural networks have better generalization. In order to validate our proposal, we evaluated our model on three public datasets, the results demonstrated that our model has better generalization than the classical neural network with the same structure.

Keywords: Neural network, Quantum neural networks, Generalization, Classification

1 Introduction

Neural network (NN) is an important direction of machine learning, and is also play an important role in the field of deep learning. The NN have strong ability of feature learning, and that can handle complex tasks such as image recognition, object detection or neural language processing. However, because of the nonlinear item of NN, the overfitting effect always occur, and it affect the generalization seriously. There are some method to alleviate the overfitting behavior, such as regularization, dropout and early stopping. Unfortunately, those method can only relieve it but not solve it.

With the development of quantum computing, it bring a new perspective to study the NN with quantum computing [1-4]. The quantum neural network (QNN) is an important outcome, the QNN is constructed by quantum gate based on quantum circuit model [5-8]. Many studies have shown that QNN have more advantage than traditional NN in some areas, such as, pattern recognition and function approximation
multi-class task of Iris data set [10], little parameters network [11], and so on. So, the QNN get more attention recently.

In this paper, we studied the generalization of QNN originally, and the main contribution as described follow.

(1) We proposed a QNN structure which is constructed by single-qubit rotation gate and multi-qubit controlled-NOT gate, the essence of quantum gate is the rotation of vector in the hypersphere of Hilbert space, so we can rotate the vector to the nearby of a orthonormal basis by training the parameters which corresponding to a label, so we can get the classification result after the measurement.

(2) We proposed a new classification method named projection measurement, which project the quantum state (vector of Hilbert space) to the nearest orthonormal basis of Hilbert space. This is a more efficient method than softmax, because we can get the result directly rather than calculate the score of all the classification label, more importantly, we need not introduce the nonlinear item in the model.

We construct a QNN model with unitary evolution and projection measurement based on the above contribution, the parameter space is constrained to the hypersphere. So, if the training dataset and test dataset have same distribution, they have same recognition rate. We experimented with three public datasets, and they all support this view.

The rest of this work is following. Section 2 introduces some quantum concepts in QNN, in order to explain this work more clearly. Our QNN structure is proposed in section 3 in details. Section 4 shows the generalization of NN and QNN with same structure on three public data sets. In the end, section 5 gives a discussion of the results.

2 Background

2.1 Quantum Bit

The quantum bit (qubit) play an important role in quantum computing, and it is the basis of quantum computing as bit in classical computing. However, different from conventional bit, the qubit satisfy quantum entangle and superposition principle. For a single qubit, its state can be described by below formula.

\[ |\psi> = \alpha |0> + \beta |1>\] (1)

The coefficient \( \alpha \) and \( \beta \) are complex numbers which represent the probability amplitude of every state. And the probability amplitude needs to satisfy normalization, so the coefficient satisfy \( |\alpha|^2 + |\beta|^2 = 1 \).

For a more general scenario, we consider n qubit scenario, which represent \( 2^n \) states superposition, as shown in the following formula.

\[ |\psi> = \alpha_0 |00...0> + \alpha_1 |00...1> + ... + \alpha_{2^n} |11...1> \] (2)

Here, each state’s probability amplitude satisfies \( |\alpha_0|^2 + |\alpha_1|^2 + ... + |\alpha_{2^n}|^2 = 1 \).

Through the above discussion, the qubit can store all \( 2^n \) states, but the classical bit can only store one of them. For example, if the n equal 50, that is a 50-qubit quantum
register, which means that the classical computer need 8388608GB memory to store all the states.

2.2 Quantum Gates

In classical computing, information regulation can be realize by several number of logic gates. In quantum computing, Deutsch has proved that every unitary evolution can be realized by limited number single qubit gate and controlled NOT (CNOT) gate. This is the foundation of quantum computing. The commonly used gate include Hadamard gate, X gate, Y gate, Z gate, rotation gate, CNOT gate and so on.

We introduce two gates used in this work in detail, rotation gate and CNOT gate. The rotation gate is an operation that can change target qubit state with given angle. This gate can be described as the unitary matrix form

\[
R(\theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix},
\]

when it operates on a qubit \(|\psi\rangle\), the result of the states will be \(R(\theta)|\psi\rangle\).

Multi-qubit controlled-NOT gate is a generalization of CNOT gate. We have known that CNOT gate is a controlled operation on two qubits that one control bit and one target bit, the multi-qubit CNOT gate is the operation that has more than one control bit. The schematic diagram of CNOT gate and multi-qubit CNOT gate shown in Figure 1. In multi-qubit CNOT gate, only all of control qubits are in \(|1\rangle\) state, the target qubit will flip.

2.3 Quantum Neural Network

Quantum neural network is the combine of quantum computing and neural network, which solve some problem the classical neural network encountered using the advantage of quantum computing. Nowadays, the QNN study mainly focus on designing low algorithm complexity networks by using the parallelism of quantum circuit. In the work, we study the generalization of QNN by the unitarily of quantum gate originally.
3 Our Model

3.1 Model Design

The QNN is an idea that combining the neuron structure with quantum circuit, similar with traditional NN the QNN is the stack of quantum neurons. As shown in Figure 1, it give the structure of classical neural network and quantum neural network. In Figure 2(a), the inputs $x_n$ firstly product with weights $w_n$, which are trainable parameters, then the sum of the product go through a activate function to output the result.

The quantum neural network structure shown in Figure 2 (b). The input qubits $|x_n>$ are adjusted by quantum rotation gates $R(\theta_n)$, which are corresponding to trainable weights $w_n$. And then the aggregation operation in neuron are replaced by multi-qubit controlled gate, which the target qubit which contains all the control qubits information is the output, the same effect as neuron. Basing on this neuron-like quantum structure, we can build more complicated QNN circuit to accomplish some machine learning tasks.

3.2 Data Encoding

A classical data using in neural networks are n dimensional vectors, with form as $\mathbf{X} = (x_1, x_2, ..., x_n)^T$. In order to using quantum computing theory, we need to transform the classical data into quantum state description. In this work, we use tensor product encoding method, each element of vector $\mathbf{X}$ is encoded as a quantum qubit:

$$x_i \rightarrow |x_i> = \cos(\theta_i)|0> + \sin(\theta_i)|1>, i = 1, 2, ..., n \quad (3)$$

And $\theta_i \in [0, 2\pi]$ is defined as:

$$\theta_i = \frac{x_i - \text{min}}{\text{max} - \text{min}} \times 2\pi \quad (4)$$

The min and max represent the minimum and maximum of the whole data set. After that, the $\mathbf{X}$ transforms into quantum state, also a vector in n dimensional Hilbert space as following:

$$\mathbf{X} \rightarrow |\mathbf{X}> = |x_1> \otimes |x_2> \otimes \cdots \otimes |x_n> \quad (5)$$
3.3 Network Structure

The QNN’s structure using in this work is composed of quantum rotation gates and n-bit CNOT gates, showing in Figure 3 [12]. $|x_n\rangle$ represents the input data encoding into quantum states. $R(\theta_{mn})$ represents the quantum rotation gate which updates qubit in the hide layer, and $|h_m\rangle$ is the output of hidden layer. On the basis of quantum theory, it is convenient to set the output of each layer to the probability amplitude of $|1\rangle$.

$$h_m = \prod_n \sin(\theta_n + \theta_{mn})$$ (6)

After computing by several hidden layers, the output of output layer is $|y_i\rangle$, the same setting as $|h_m\rangle$. The amount of parameter $\theta$ and hidden layer depend on the data set and classification.

3.4 Learning Algorithm

In this quantum neural network model, we obtain output state $|0\rangle$ and $|1\rangle$ as the predicted label of input, instead of Softmax method using in traditional neural network. The output state $|y_i\rangle$ owns the probability $P(|0\rangle)$ and $P(|1\rangle)$. We define the label $\bar{y} = 0$, if $P(|0\rangle) = y_i^2 < 0.5, \bar{y} = 1$ otherwise. So we can use binary system to represent classification labels, with $\log_2(c)$ outputs, where $c$ is the number of classes. For instance, a binary classification task needs only one output qubit whose two states are corresponding to the labels. Two output qubits are needed for a three categories problem showing in next simulation section, and the output states 00, 01, 10 are the label codes of the classes. It is reasonable to define the loss function as:

$$L(\theta) = \sum_i(y_i^2 - \text{target label})^2, i = 1, ..., c$$ (7)

When the target label is 0, the training operation—minimizing the loss will make $y_i^2$ approaching 0, then we will get $\bar{y} = 0$ as we wander, and if the target is 1, we will get 1 after training. We optimize the loss function by gradient descent method in training process.
4 Experiments

To compare the QNN and NN’s performance in generalization, we do the simulations on three data sets with these two models in classical computer. According the scale of data set, a model with two hidden layers of 10 and 6 neurons is adopted. In the output layer, QNN uses the classification method mentioned in section 2.3, and for NN situation it is Softmax method as usual. Each data set, we separates the data into training set and test set by 75% and 25%.

4.1 Breast Cancer Data Set

Breast cancer data set has 683 samples with 9 features and two classes. The simulation results are shown in Figure 4, the plots in first row (a) and (b) are NN’s results, (c) and (d) in second row are QNN’s. The plots in left column show the training results and the right column for the test ones. The blue dotted line represents model’s loss, and red solid line for accuracy, both varying with epochs in X axis.

Plot (a) shows a perfect result in the training data, after 1000 epochs the prediction accuracy reaches 100% almost, sometimes 100%, and the loss reaches 0, this model fits the training data wonderfully. However, this doesn’t appear in (b), the accuracy on test data reaches a peak than descends with the training process when they are ascending here on training data. The loss’s results have the opposite trend in two data sets, too. We know this is the typical overfitting phenomenon in neural networks.

But in (c) and (d) we see a similar variation here, the prediction accuracy both increase with the training process and reach peak about 92% after 1000 epochs, the losses become smaller all the time before the model keeps stable. It is obviously that QNN has the same effects on these data sets—an ideal generalization, better than NN.
4.2 Diabetes Data Set

Diabetes is another popular data set of binary classification task with 768 samples and 8 features. The simulation results are in Figure 5 as the same setting of Figure 4. We can see that NN model has a satisfying fitting on training data in plot (a), the accuracy peak can reach 98% after 3000 epochs. But it is terrible on test data, the accuracy keep falling during the whole process. It reaches 63% at 4000 epochs, and there is a huge gap more than 30% between the training results.

![Fig. 5. Simulation results of diabetes dataset with traditional NN and QNN.](image)

QNN model also has the same performance on training and test data sets in (c) and (d). After 3500 epochs training, the accuracy rises to 77% and 73% separately on two parts of data, while the loss descends to about 0.08. It is obvious that the prediction is worse than breast cancer data’s, then we check the data’s difference and find that diabetes data set has a much larger standard deviation than breast cancer data’s. So it is more complex, harder to be fitting, and needs more model optimizing tricks to obtain a better result which will not be studied in this work. By these examples we can suggest that QNN really owns a better generalization ability than NN in binary classification tasks.

4.3 Iris Data Set

Here let’s see QNN’s performance in multiclass classification task. There are three classes and 4 features in Iris data set with 150 samples. The comparison between two models is in Figure 6. The same as showing above, plot (a) gives a good prediction on training data with about 100% accuracy that increasing with epochs by NN. Then the test result in plot (b) shows that the accuracy goes down to 92% after reaching peak value 97%, meanwhile the loss keep increasing. On the other hand, the lines’ shapes
representing QNN’s results in plot (c) and (d) are almost same. We can say that QNN has a good generalization in multiclass task, too.

5 Discussion

We introduce a QNN structure to accomplish classification tasks, and find that it has more powerful generalization ability than traditional NN. But due to the rare resource of quantum computer, our simulations are programed on classical computer with same algorithm. It is ideal to test or apply the model on real quantum computer in the future, however the training process only can be implemented on classical computer right now, calculating and adjusting the model’s parameters. It is an important open question in quantum computing.

This work mainly focuses on comparing two models’ performance of generalization, so the models’ accuracy of data is not concerned firstly here. And then we use the similar basic NN and QNN model structure without optimizing method, causing that the QNN’s performance on diabetes data set are not perfect as other data set because of its larger standard deviation. With the development of machine learning this years, there are many works about optimizing NN model and they propose lots of methods such as different activate function, batch normalization, gradient clip and so on. But this area of QNN is hungrieness, it needs more attention and research. We think different way of input encoding may affect the result of QNN, and may research further in the future.

The most important thing is why QNN owns the perfect generalization. Here we try to understand this phenomenon from the view of Hilbert space. It has been shown that QNN may be regarded as a quantization of classical kernel methods which implicitly embedded data to a high-dimensional Hilbert space which owns a decision hyperplanes that separate the data according to their classes [13-15]. It means that the
data, whether training data or test data, are separated naturally when they are encoding into high dimension Hilbert space, like what is happening in classification with kernel methods. The target classes also can be treated as a vector in the Hilbert space, so the training process adjusts the angle of rotation on input data to approach the target class in order to obtain the correct answer when measuring the output data. And the circuit does the same operation on training data and test data, so they approach the target together and have the same performance during training process. This theory can explain the results of diabetes data set reasonably. Because of the data’s complexity, the encoding step doesn’t separate them as perfect as other data, so after training process the accuracy can’t exceed 80% in the end. In this theory, encoding method is as important as training process, it determines the upper limitation of classification, and how to decide a proper encoding method needs more works in the future.

To a summary, this work introduces a quantum neural network structure consisting of quantum gates. We use this QNN on three data sets including binary and multi classes, then find that this linear structure could accomplish classification task well. Furthermore QNN is superior to NN in generalization, its effect on test data set is almost the same as on training data set.

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