A simple approach to design quantum neural networks and its applications to kernel-learning methods

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Abstract

We give an explicit simple method to build quantum neural networks (QNNs) to solve classification problems. Besides the input (state preparation) and output (amplitude estimation), it has one hidden layer which uses a tensor product of $\log M$ two-dimensional rotations to introduce $\log M$ weights. Here $M$ is the number of training samples. We also have an efficient method to prepare the quantum states of the training samples. By the quantum-classical hybrid method or the variational method, the training algorithm of this QNN is easy to accomplish in a quantum computer. The idea is inspired by the kernel methods and the radial basis function (RBF) networks. In turn, the construction of QNN provides new findings in the design of RBF networks. As an application, we introduce a quantum-inspired RBF network, in which the number of weight parameters is $\log M$. Numerical tests indicate that the performance of this neural network in solving classification problems improves when $M$ increases. Since using exponentially fewer parameters, more advanced optimization methods (e.g. Newton’s method) can be used to train this network. Finally, about the convex optimization problem to train support vector machines, we use a similar idea to reduce the number of variables, which equals $M$, to $\log M$.

Keywords: Quantum neural network, quantum computing, kernel method, radial basis function network, support vector machine.

1 Introduction

Artificial neural networks (ANNs) are powerful methods to solve problems in machine learning [1, 2]. Quantum computer, on the other hand, is a new computing device that can solve some problems much faster than the classical computers [3, 4]. In the past decades, many ideas were proposed to integrate the powers of neural networks and quantum computing, which lead to the concept of quantum neural networks (QNNs) [5–8]. In the context of near-term quantum technology, the proposal of Farhi and Neven [5] seems more attractive. Comparing the structures between feed-forward neural networks and quantum circuits, Farhi and Neven’s idea seems a natural way to design QNNs. Their basic idea is roughly described by figure 1, where $|x\rangle$ is the input, $\vec{\theta} = (\theta_1, \ldots, \theta_k)$ is a series of parameters, and the unitary $U(\vec{\theta})$ plays the role of weights. Perform measurements on the Pauli-$Y$ operator, the probability

$$\varphi(\vec{\theta}, |x\rangle) = \langle x, 1| U(\vec{\theta})^\dagger Y_{n+1} U(\vec{\theta}) |x, 1\rangle$$

defines the output of their QNN.

The idea of figure 1 is an initial step to design near term QNNs. When compared with the structure of ANNs, it induces some problems that deserve further study. For instance, the input-output relationship is usually nonlinear for an ANN. Even though the output $\varphi(\vec{\theta}, |x\rangle)$ defined in equation (1) quadratically depends on the input $|x\rangle$, this kind of non-linear relationship is not stronger enough. Since we can find some states $|u_1(\vec{\theta})\rangle, \ldots, |u_l(\vec{\theta})\rangle, |v_1(\vec{\theta})\rangle, \ldots, |v_l(\vec{\theta})\rangle$ such that $\varphi(\vec{\theta}, |x\rangle) = \sum_{j=1}^l \text{Im}\langle u_j(\vec{\theta}) |x\rangle \langle x | v_j(\vec{\theta})\rangle$. This
value is determined by linear forms $\langle u_j(\tilde{\theta})|x \rangle$ and $\langle v_j(\tilde{\theta})|x \rangle$ for all $j$. Also in the construction of ANN, the number of neurons (which can be viewed as dimensions of the data) in different layers may different; however, this is impossible for QNN constructed in figure 1 because of the unitary property. Finally, when considering about solving practical machine learning problems, such as binary classification, one technical problem we need to solve in figure 1 is how to choose the unitary $U(\tilde{\theta})$. There are too many choices of this unitary, we hope to find a simple one such that the QNN can solve as many problems as possible. Some suggestions were proposed in [5].

Based on the problems (especially the last one) addressed above, in this paper we will give an explicit simple way to construct a type of QNNs. The basic idea is shown in figure 2. The unitary $U_x$ is used to prepare the quantum states of the inputs. We will focus on an explicit special construction of this unitary, which is given in equation (6) in section 3. As for the weight unitary, we just choose $U(\tilde{\theta}) = \otimes_{j=1}^{m} \exp(iY\theta_j)$ as the tensor product of rotations, where $Y$ is the Pauli-Y matrix. One obvious feature is that this QNN only uses $m$ weight parameters. If we use it to solve the classification problems, then we can choose $m$ as the logarithm of the number of training samples. As a result, the complexity to train these parameters by the variational method [9, 10] in a quantum computer should be low. The output of this QNN is defined as the amplitude of $|0\rangle\otimes^m$ of the final state $U(\tilde{\theta})U_x|0\rangle\otimes^m$.

The underlying mathematical theory of our construction is the kernel method and the radial basis function network (RBF network). The kernel method applies the idea that complex pattern-classification problems often become linearly separable when transform the data into a high dimensional space. So when using the kernel method, such as in the RBF network or support vector machine, we first apply a non-linear map (called feature map) to embed the data into a high dimensional space (called feature space), then solve a linear problem in the feature space. It turns out that this kind of idea is pretty useful in solving machine learning problems [11]. Recently, the kernel method has been introduced in quantum computing to study quantum machine learning [12, 13]. The QNN model shown in figure 2 also follows this idea. The unitary $U_x$ plays the role of feature map. The linear property in the feature space is a reason why we use the tensor products to define the weight unitary.

RBF network is a special type of neural network with one hidden layer. For any input vector $x$, we use the radial basis function as the feature map to generate a high dimensional vector $y$, then define the output as $y \cdot w$ for some weight vector $w$. In the RBF network, the number of weights can as large as the number of training samples. This is one big obstacle to use it classically. The definitions of our QNN
and RBF network are close to each other. Due to this closeness, we can modify the definition of RBF network by changing the weight vector into the one we used in the QNN model. We call this network the quantum-inspired RBF network. This is an unusual way to define feed-forward neural networks as usually the weight is introduced independently between two neurons. Actually, this unusual property is verified by the numerical tests, which show that the quantum-inspired RBF network can solve classification problems with great accuracy, but it is not good at solving regression problems. In comparison the classical RBF network is a universal approximator that can approximate smooth input-output mappings with high precision [14]. However, if we only interested in the classification problems, then the quantum-inspired RBF network is much easier to be trained especially in a quantum computer because of the simple choice of the weights.

On the other hand, support vector machines (SVMs) [15, 16] are elegant kernel-learning methods to solve classification and regression problems. The training of the SVM needs us to solve a convex optimization problem. However, the number of variables in the convex optimization problem equals the number of training samples. As a result, SVM becomes time and space consuming when the number of training samples is large. Following the idea of quantum-inspired RBF network and the connection between RBF network and SVM [1], we can modify the model of the convex optimization problem by changing the vector of the variables into the one used in the QNN model. The advantage is that the number of variables reduces to the logarithm of the number of training samples. This can improve the efficiency of training SVM. While this method cannot find the support vectors.

The rest of this paper is organized as follows: In section 2, we briefly introduce the kernel method and the radial basis function networks. In section 3, we present more details about the construction of our QNN model, including the implementation of the unitary $U_x$, and the training algorithm. In section 4, we discuss the structure of quantum-inspired RBF network and its advantages in training. Section 5 devotes to present the results of the numerical tests. In section 6, we state some related ideas to the design of support vector machines.

## 2 Kernel method and radial basis function networks

In machine learning, kernel method is a type of algorithm that solves problems by first non-linearly mapping the data into a high dimensional space, where the problems are often much easier to solve. The underlying mathematical theory is the Cover’s theorem [17], which states that “a complex pattern-classification problem, cast in a high-dimensional space non-linearly, is more likely to be linearly separable than in a low-dimensional space, provided that the space is not densely populated.” The non-linear map used in kernel method is called feature map, and the higher dimensional space is called the feature space.

![RBF network](image)

Figure 3: The structure of RBF network.

Radial basis function network (RBF network) is a type of feed-forward neural networks which has only one hidden layer. Its construction is based on the kernel method, see figure 3. The feature maps used in the RBF network are radial basis functions, which are real-valued functions whose value only depend on the distance between the input vector and a fixed vector. A typical example is the Gaussian
function \( \varphi(x) = \exp(-\|x - c\|^2/2\sigma^2) \), where \( c \) is a fixed vector and \( \sigma \) is a fixed real parameter. One advantage in designing RBF network is that different choices of the radial basis functions used in the hidden layer have little influence on the performance [18], so we can just focus on the Gauss function. It is a commonly used feature map.

In a RBF network, the input is an \( n \)-dimensional real vector \( x = (x_1, \ldots, x_n)^T \). In the hidden layer, \( y_i = \varphi_i(x) \) is determined by a radial basis function \( \varphi_i \). Finally, the output is defined by the linear form \( z = \sum y_i w_i \) for some weights \( w_1, \ldots, w_M \). Generally, a bias \( b \) should be introduced such that the output becomes \( b + \sum y_i w_i \). However, in this paper, we will not consider the bias. The training of RBF network contains two steps. First, determine the parameters used in the radial basis functions. For example, if we use the Gaussian function \( \varphi_i(x) = \exp(-\|x - c_i\|^2/2\sigma^2) \) in the hidden layer, then we should determine the centers \( c_i \) and the width \( \sigma \). Usually, we use the same width \( \sigma \) for all the Gaussian functions. A simple choice of the centers are the training samples. More practically, we can use the \( K \)-means algorithm to find the centers. In this case, the number of weights can be much smaller than the number of training samples. Since this paper is not devoted to study the performance of RBF networks, in the following when talking about RBF networks, we always assume that the centers are the training samples.

For instance, we can apply the RBF network to solve the binary classification problems. Suppose we need to solve the binary classification problem discussed above. Classically, we can use neural network to solve this problem. In the quantum case, we will design a quantum neural network to solve the problem. Our basic idea is already depicted in figure 2. For convenience, we assume that \( M = 2^m \). In figure 2, \( |x \rangle \) is the input of the QNN. It is a quantum state of dimension \( n \). The unitary \( U_x \) is used to generate a high dimensional state. It plays the role of feature map in the kernel method. In this paper we choose \( U_x \) such that

\[
|f(x)\rangle := U_x |0\rangle^\otimes m \propto \sum_{t=1}^M \exp(-\|x - x^{(t)}\|^2/2\sigma^2) |t\rangle.
\]

After that, we apply \( m \) rotations to \( |f(x)\rangle \) to generate an output state. The \( m \) arguments used in the rotations are the parameters we need to train in this QNN. They are close to the roles of weights used in the RBF network. The difference is that here we just use \( m = \log M \) parameters instead of \( M \) parameters in the RBF network. If we denote the tensor product of the \( m \) rotations as \( U(\vec{\theta}) \), then

\[
U(\vec{\theta}) = \bigotimes_{j=1}^m \exp(iY \theta_j) = \bigotimes_{j=1}^m \begin{pmatrix} \cos \theta_j & \sin \theta_j \\ -\sin \theta_j & \cos \theta_j \end{pmatrix}.
\]

3 An explicit way to construct quantum neural networks

In this section, we will provide an explicit way to design quantum neural networks. Suppose we need to solve the binary classification problem discussed above. Classically, we can use neural network to solve this problem. In the quantum case, we will design a quantum neural network to solve the problem. Our basic idea is already depicted in figure 2. For convenience, we assume that \( M = 2^m \). In figure 2, \( |x \rangle \) is the input of the QNN. It is a quantum state of dimension \( n \). The unitary \( U_x \) is used to generate a high dimensional state. It plays the role of feature map in the kernel method. In this paper we choose \( U_x \) such that

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\[
U(\vec{\theta}) = \bigotimes_{j=1}^m \exp(iY \theta_j) = \bigotimes_{j=1}^m \begin{pmatrix} \cos \theta_j & \sin \theta_j \\ -\sin \theta_j & \cos \theta_j \end{pmatrix}.
\]
As a result, the output state is
\[ |z \rangle := U(\vec{\theta})|f(x)\rangle = |w(\vec{\theta})\rangle |0\rangle^\otimes m + |0^\perp\rangle^\otimes m, \] (8)
where \(|0^\perp\rangle^\otimes m\) refers to the state that is orthogonal to the first term, and
\[ |w(\vec{\theta})\rangle = U^\dagger(\vec{\theta})|0\rangle^\otimes m = \bigotimes_{j=1}^m \left( \cos \theta_j |0\rangle + \sin \theta_j |1\rangle \right). \] (9)

Finally, we define the output of the QNN as the amplitude \( \langle w(\vec{\theta}) |f(x)\rangle \) of \(|0\rangle^\otimes m\) of \(|z\rangle\). It can be estimated by swap test in a quantum computer.

**Remark 1** Usually, for any two real unit vectors \(x, y\), swap test can only help us detect the information of \(\langle x | y \rangle\). However, by considering \((1, x)\) and \((1, y)\), then we can extract \(\langle x | y \rangle\) in a quantum computer by swap test. For more information, we refer to the book [20].

By comparing figure 2 and figure 3, it is not hard to see that the design of QNN is similar to the design of the RBF network. The only difference is the weights used to define the output. The choices of the weights in the RBF network is a common method to define neural networks; that is each arrow between two neurons of adjacent layers has a weight. In the quantum case, we use a similar idea to introduce the weights, so each circuit is being given a weight. However, this kind of neural network is more suitable for a quantum computer due to its structure. Moreover, in a quantum computer we can design efficient quantum algorithms to train the neural network. We will discuss this in the following two subsections.

### 3.1 The implementation of the unitary \(U_x\)

In this subsection, we will use the idea of coherent state and quantum linear algebraic technique to implement the unitary \(U_x\) in a quantum computer. Coherent states are known in the area of quantum optics as a description of the light model. They are defined in the Fock states \(\{|0\rangle, |1\rangle, \ldots\}\), which is a basis of the infinitely dimensional Hilbert space. Let \(r \in \mathbb{R}\) be a real number, its coherent state is defined by
\[ |\psi_r\rangle = e^{-r^2/2\sigma^2} \sum_{k=0}^{\infty} \frac{(r/\sigma)^k}{\sqrt{k!}} |k\rangle. \] (10)

Generally, the coherent state of a real vector \(x = (x_1, \ldots, x_n)^T\) is defined by
\[ |\psi_x\rangle = |\psi_{x_1}\rangle \otimes \cdots \otimes |\psi_{x_n}\rangle. \] (11)

A simple fact is that \(\langle \psi_x | \psi_y \rangle = \exp(-||x - y||^2/2\sigma^2)\) for any two real vectors \(x, y\).

Now consider the following superposition of coherent states of the training samples:
\[ |\Psi\rangle = \frac{1}{\sqrt{M}} \sum_{t=1}^M |t\rangle |\psi_{x(t)}\rangle. \] (12)

Taking the partial trace on the second register of \(|\Psi\rangle\langle \Psi|\) gives the density operator of the kernel matrix
\[ \rho := \text{Tr}_2 |\Psi\rangle\langle \Psi| = \frac{1}{M} \sum_{s,t=1}^M \langle \psi_{x(s)} | \psi_{x(t)} \rangle |s\rangle\langle t|. \] (13)

As a result,
\[ \rho |s\rangle = \frac{1}{M} \sum_{t=1}^M \exp(-||x(s) - x(t)||^2/2\sigma^2) |s\rangle, \] (14)
from which we can get the quantum state of $|f(x^{(t)})\rangle$ defined in equation (6). The matrix-vector multiplication (14) can be accomplished by the basic quantum linear algebraic techniques, such as the HHL algorithm [21].

To apply the HHL algorithm, we need to implement the Hamiltonian simulation of $\rho$. Since $\rho$ is a density operator, by quantum principal component analysis [22], we can implement $e^{-i\rho t}$ to precision $\epsilon$ by using $O(t^2/\epsilon)$ copies of $\rho$. This derives from the following simple identity:

$$\text{Tr}\{e^{-iS\Delta t}\rho \otimes e^{i\tau S\Delta t}\} = \tau - i [\rho, \tau] \Delta t + O((\Delta t)^2) = e^{-i\rho\Delta t} e^{i\tau S\Delta t} + O((\Delta t)^2),$$

(15)

where $S$ is the swap operator and $\tau$ is a given density operator. Equation (15) provides a method to simulate $e^{-i\rho \Delta t}$. If we denote the error $(\Delta t)^2$ as $\epsilon_0$, then after $k$ steps of applying equation (15), the error to simulate $e^{-i\rho k\Delta t}$ becomes $k\epsilon_0$. Setting $t = k\Delta t$, then the error can be rewritten as $k\epsilon_0 = t^2/k$. Thus we need $O(t^2/\epsilon)$ copies of $\rho$ to implement $e^{-i\rho t}$ to precision $\epsilon$.

Denote the eigenvalues and eigenvectors of $\rho$ as $\{\sigma_1, \ldots, \sigma_M\}$ and $\{|u_1\rangle, \ldots, |u_M\rangle\}$ respectively. Formally rewrite $|t\rangle = \sum_{j=1}^{M} \beta_j |u_j\rangle$, then by quantum phase estimation, we can prepare

$$\sum_{j=1}^{M} \beta_j |u_j\rangle |\tilde{\sigma}_j\rangle$$

(16)

in cost $O((\log M)/\epsilon^3)$, where $|\sigma_j - \tilde{\sigma}_j| \leq \epsilon$. This is because $\sigma_j \leq 1$, so we can choose $t = 1/\epsilon$. Next, apply control rotation to generate

$$\sum_{j=1}^{M} \beta_j |u_j\rangle |\tilde{\sigma}_j\rangle \left( |\tilde{\sigma}_j\rangle |0\rangle + \sqrt{1 - \tilde{\sigma}_j^2} |1\rangle \right).$$

(17)

Finally, undo the quantum phase estimation algorithm, then we obtain

$$\sum_{j=1}^{M} \beta_j |u_j\rangle \left( |\tilde{\sigma}_j\rangle |0\rangle + \sqrt{1 - \tilde{\sigma}_j^2} |1\rangle \right) \approx \rho |t\rangle |0\rangle + (\cdots) |1\rangle.$$  

(18)

We can perform measurements on the state (18) to get the state $|f(x^{(t)})\rangle$. The complexity is influenced by the norm of $f(x^{(t)})$ and $M$. However, we can also choose (18) as the result of $U_x$ since we need to do the measurements in the end of the quantum circuit in figure 2. The error of the first term to $\rho|t\rangle$ is smaller than $\epsilon$, and the complexity to get the state (18) is $O((\log M)/\epsilon^3)$. However, any classical algorithm to get the vector $f(x^{(t)})$ has complexity at least linear at $M$. This is an advantage of using quantum computer to train the QNN designed in figure 2.

### 3.2 The training algorithm

Following the idea of variational eigensolver [9], the training of the QNN is accomplished by using the variational method to train the parameters $\vec{\theta}$. The loss function is

$$L(\vec{\theta}) = \frac{1}{2M} \sum_{t=1}^{M} \left( \langle w(\vec{\theta})|f(x^{(t)})\rangle - r^{(t)} \right)^2.$$  

(19)

We can use the stochastic gradient method to minimize the loss function. At each step of iteration, we randomly choose a sample $(x^{(t)}, r^{(t)})$. It defines an instantaneous loss function $L_t(\vec{\theta}) = \frac{1}{2} (\langle w(\vec{\theta})|f(x^{(t)})\rangle - r^{(t)})^2$. Then we update $\vec{\theta}$ via

$$\theta_j = \theta_j - \eta \left( \langle w(\vec{\theta})|f(x^{(t)})\rangle - r^{(t)} \right) \frac{\partial w(\vec{\theta})}{\partial \theta_j} |f(x^{(t)})\rangle,$$

(20)

where $j = 1, 2, \ldots, m$. Since the weight state is generated by a tensor product of rotations, equation (20) implies that the updating of the weight state is finished by a unitary operator.
Consequently, to estimate network, the weight becomes (9). In vector form of RBF network the quantum-inspired RBF network. Its basic structure is the same as the usual RBF network, where \( f \) is not high. This is another advantage of using quantum computer to train the QNN.

\[
\frac{\partial w(\hat{\theta})}{\partial \theta_j} = \langle 0 \rangle^\otimes M \sum_{i=1}^{j-1} \exp(iY \theta_i) \otimes \exp(iY(\theta_j + \frac{\pi}{2})) \otimes \bigotimes_{l=j+1}^{M} \exp(iY \theta_l). \tag{21}
\]

Consequently, to estimate \( \frac{\partial w(\hat{\theta})}{\partial \theta_j} \) \(|f(x^{(t)})|\), we only need to change the parameter \( \theta_j \) into \( \theta_j + \frac{\pi}{2} \) in the \( j \)-th ancilla qubit in figure 2, then use the amplitude estimate to estimate the amplitude of \(|0\rangle^\otimes M\). Since we only have \( m = \log M \) parameters, the calculation complexity at each step by the variational method is not high. This is another advantage of using quantum computer to train the QNN.

4 Quantum-inspired RBF network

Because of the similarity between RBF network and the QNN defined in figure 2, as an inspiration, we can use the idea of QNN to modify the choices of the weights of the RBF network. We call this new type of RBF network the quantum-inspired RBF network. Its basic structure is the same as the usual RBF network, that is figure 3, except the weights used in the hidden layer. In the quantum-inspired RBF network, the weight becomes (9). In vector form

\[
w(\hat{\theta}) = \prod_{j=1}^{m} \left( \frac{\cos \theta_j}{\sin \theta_j} \right), \tag{22}
\]

where \( m = \log M \) and \( M \) is the number of training samples. More precisely, let \( t = t_1 + t_2 2 + \cdots + t_m 2^{m-1} \) be the binary expanding of integer \( t \), then it is easy to verify from equation (22) that the \( t \)-th weight equals

\[
\cos(\theta_{t_1} - \frac{t_1 \pi}{2}) \cos(\theta_{t_2} - \frac{t_2 \pi}{2}) \cdots \cos(\theta_{t_m} - \frac{t_m \pi}{2}). \tag{23}
\]

When using neural networks, its training is really important. For the quantum-inspired RBF network, we need to solve the following minimization problem (19). Now the neural networks are in the classical sense, so we change the notations of quantum states into vectors in the following. The loss function (19) becomes

\[
L(\hat{\theta}) = \frac{1}{2M} \sum_{t=1}^{M} \left( w(\hat{\theta}) \cdot f(x^{(t)}) - r^{(t)} \right)^2, \tag{24}
\]

where \( f(x^{(t)}) \) is the \( M \)-dimensional vector generated by \( \exp(-\frac{\|x^{(s)} - x^{(t)}\|^2}{2\sigma^2}) \) for all \( s = 1, \ldots, M \). For comparison, we denote the loss function of the usual RBF network as

\[
\tilde{L}(\tilde{w}) = \frac{1}{2M} \sum_{t=1}^{M} \left( \tilde{w} \cdot f(x^{(t)}) - r^{(t)} \right)^2, \tag{25}
\]

where \( \tilde{w} = (\tilde{w}_1, \ldots, \tilde{w}_M) \) is an \( M \) dimensional vector.

Typically, we use the gradient descent or stochastic gradient descent to minimize \( L \) and \( \tilde{L} \). Assume that the gradient descent method is used. Set the standard basis of \( \mathbb{R}^m \) as \( \{e_1, \ldots, e_m\} \); i.e., the basis \( e_j \) is the \( \{0, 1\} \) vector such that only the \( j \)-th entry equals 1. Then the gradients of them satisfy

\[
\nabla L = \frac{1}{M} \sum_{j=1}^{m} \left( \sum_{t=1}^{M} \left( w(\hat{\theta}) \cdot f(x^{(t)}) - r^{(t)} \right) \frac{\partial w(\hat{\theta})}{\partial \theta_j} \cdot f(x^{(t)}) \right) e_j, \tag{26}
\]

\[
\nabla \tilde{L} = \frac{1}{M} \sum_{t=1}^{M} \left( \tilde{w} \cdot f(x^{(t)}) - r^{(t)} \right) f(x^{(t)}), \tag{27}
\]
By equation (23), the $t$-th entry of the vector $\partial w(\tilde{\theta})/\partial \theta_j$ is easy to obtain, which equals

$$\cos(\theta_1 - \frac{(t_1 - \delta_j^1)\pi}{2}) \cos(\theta_2 - \frac{(t_2 - \delta_j^2)\pi}{2}) \cdots \cos(\theta_m - \frac{(t_m - \delta_j^m)\pi}{2}),$$

(28)

where $\delta_j^i$ is the Kronecker symbol.

Since $f(x^{(t)})$ are the same for both of them, we will not count the complexity to obtain all $f(x^{(t)})$ into the complexity comparison of these two methods below. By equations (23) and (28), the complexity to compute all the entries of $w(\tilde{\theta}), \partial w(\tilde{\theta})/\partial \theta_1, \ldots, \partial w(\tilde{\theta})/\partial \theta_m$ is $O(M^2 M)$. They only need to be computed once. So the costs to compute $\sum_{j=1}^m \partial w(\tilde{\theta})/\partial \theta_j$ is $O(mM)$. The $M$ inner products in equation (26) costs $O(M^2)$. Thus, the total cost to compute $\nabla L$ is $O(m^2 M + M^2) = O(M^2)$. On the other hand, it is easy to see that the complexity to use the gradient descent method to minimize $L$ and $\tilde{L}$ are the same at each step of iteration.

More advanced methods, such as the Newton’s method, are rarely used in machine learning due to the high cost to compute the inverse of the Hessian matrix. However, the Hessian matrix $\nabla^2 L$ of $L$ is $m$-by-$m$. So the complexity of Newton’s method may not so high for quantum-inspired RBF network. The $(j, k)$-th entry of $\nabla^2 L$ equals

$$\frac{1}{M} \sum_{t=1}^M \left( w(\tilde{\theta}) \cdot f(x^{(t)}) - r^{(t)} \right) \frac{\partial^2 w(\tilde{\theta})}{\partial \theta_j \partial \theta_k} \cdot f(x^{(t)}) + \frac{1}{M} \sum_{t=1}^M \left( \frac{\partial w(\tilde{\theta})}{\partial \theta_j} \cdot f(x^{(t)}) \right) \left( \frac{\partial w(\tilde{\theta})}{\partial \theta_k} \cdot f(x^{(t)}) \right).$$

(29)

Similar to the analysis of computing $\nabla L$, the complexity to accomplish the calculation of equation (29) is $O(M^2)$. Since there are $m^2$ entries, the cost to get the Hessian matrix of $L$ is $O(m^2 M^2)$. The complexity to compute the inversion of $\nabla^2 L$ is $O(m^3)$. Thus the complexity of each iteration of the Newton’s method to minimize $L$ is $O(m^2 M^2 + m^3)$. Finally, we summarize the above results into the following theorem.

**Theorem 1** To minimize $L(\tilde{\theta})$, if we use the gradient descent method, then the cost of each step of iteration is $O(M^2)$. If we use the Newton’s method, then the cost of each step of iteration is $O(M^2 (\log M)^2)$.

### 5 Numerical tests

To test the performance of the QNN or the quantum-inspired RBF network, we use it to solve the classification problems. However, we only do the experiments for the quantum-inspired RBF network in the classical computer since currently we do not have a universal quantum computer. Due to the same definition of QNN and the quantum-inspired RBF network, the testing results should be true for QNN when we have a large-scale quantum computer.

We use the quantum-inspired RBF network to solve binary classification problems in dimension 2. Figure 4 lists eight testing results with different types of classification patterns. They indicate that the quantum-inspired RBF network can solve the binary classification problems with high precision.

In figure 5, we consider the influence of the number of training samples on the performance of the neural network. Note that for classification problems, we concern more about the ratio of correct prediction (RCP), which is defined as

$$\text{RCP} := 1 - \frac{1}{4M} \sum_{t=1}^M \left( \text{sign}(w(\tilde{\theta}) \cdot f(x^{(t)})) - r^{(t)} \right)^2.$$

(30)

It computes the ratio of training samples that being given the correct labels by the neural network after training. For a classifier, we hope its RCP is large. However, the training procedure of the quantum-inspired RBF network is accomplished by minimizing the mean square error (MSE) defined by equation (19). If MSE is small, then it means that this classifier can also be used to approximate functions, that is it can solve regression problems as well.
Figure 4: Use quantum-inspired RBF network to solve binary classification problems: figure (a)-(c) use 256 training samples, 8 weight parameters; figure (d) uses 512 training samples, 9 weight parameters; figure (e)-(h) use 1024 training samples, 10 weight parameters.

Figure 5: The influence of the number of training samples on the performance of the quantum-inspired RBF network.

In figure 5, we tested all the 8 patterns of figure 4. In each situation, we randomly test 10 examples, then compute the average values of the RCPs and MSEs. As we can see from figure 5, the overall trend of RCP is increasing. When using 1024 training samples, the RCPs are all larger than 0.9. This means quantum-inspired RBF network can solve classification problems with high accuracy when the number of training samples is large enough. The advantage here is that the number of weights is logarithmic at the number of training samples. Even though many samples are used, the number of weights is still not too large. On the other hand, the overall trend of MSE is decreasing. However, in some patterns, the MSEs are still pretty large (≥ 0.4) even if we use 1024 training samples. As a result, this kind of neural network is not a good method to solve regression problems.
6 Some related ideas toward the support vector machines

Support vector machine (SVM) [15, 16] is an important kernel learning method. Consider the binary classification problem discussed in equation (2). Let \( f \) be a feature map, then the kernel-based SVM is a method aims to find a hyperplane \( f(x) \cdot w - b = 0 \) that can separate the two classes with maximal margin. Points on the boundaries \( (f(x^{(t)}) \cdot w - b)r^{(t)} = 1 \) are called support vectors. The distance from support vectors to the hyperplane \( f(x) \cdot w - b = 0 \) equals \( 1/\|w\| \). Thus SVM reduces to solve the following optimization problem:

Minimize \( \frac{1}{2} \|w\|^2 \) subject to \( (f(x^{(t)}) \cdot w - b)r^{(t)} \geq 1 \) for \( t = 1, 2, \ldots, M \). \hspace{1cm} (31)

Introduce the Lagrangian function

\[
L = \frac{1}{2} \|w\|^2 - \sum_{t=1}^{M} v_t \left( (f(x^{(t)}) \cdot w - b)r^{(t)} - 1 \right). \hspace{1cm} (32)
\]

Setting the partial derivatives \( \partial L/\partial w \) and \( \partial L/\partial b \) to zero leads to

\[
w = \sum_{t=1}^{M} v_tr^{(t)}f(x^{(t)}), \quad \sum_{t=1}^{M} v_tr^{(t)} = 0. \hspace{1cm} (33)
\]

Substituting them into equation (32), then we get the Lagrangian dual problem of (31)

Maximize \( Q(v) = \sum_{t=1}^{M} v_t - \frac{1}{2} \sum_{s,t=1}^{M} v_sw_tr(s)r(t)f(x^{(s)}) \cdot f(x^{(t)}) \),

Subject to \( \sum_{t=1}^{M} v_tr^{(t)} = 0, \quad v_t \geq 0 \) for \( t = 1, 2, \ldots, M \). \hspace{1cm} (34)

The solution of the problem (34) is usually sparse, that is \( v_t \neq 0 \) if \( x^{(t)} \) is a support vector. As a result, \( w \) is a linear combinations of the support vector by equation (33). The decision boundary is

\[
\sum_{\text{support vectors}} v_tr^{(t)}f(x^{(t)}) \cdot f(x) - b = 0. \hspace{1cm} (35)
\]

This can be described in the language of RBF network, the support vectors are the centers used in the hidden layer, and \( b \) is the partial bias. Since we do not know the support vectors in advance, if we simply use all the training samples in equation (35), then the decision boundary is the same as that defined in the RBF network. However, the methods to find the weights are different in these two methods.

Figure 6: The black curve is the decision boundary discovered by the SVM with the usual choice of the weight; the red one is obtained by choosing the weight as (9). The circles are the support vectors.
The advantage of SVM is the convex optimization theory it relies on. This perhaps make it the most elegant of all kernel-based learning methods. The major limitation of SVM is the fast increase in the computing and storage requirements with respect to the number of training examples. These requirements tend to leave many large-scale problems beyond the reach of SVM. Based on the idea of quantum-inspired RBF network, we can change the weight \( v = (v_1, \ldots, v_M) \) into the tensor product (22). The advantage of doing so is that we can use variational method to solve the optimization problem (34) in a quantum computer, which should be more efficient. However this will change the nature of SVM. Moreover, the convex property is removed. Numerical tests show that this method can solve classification problems with high precision (see figure 6 for two examples), while it cannot find the support vectors. The solution found by this method is not sparse.

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