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Quantum artificial neural networks with applications ☆

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ABSTRACT

Since simulations of classical artificial neural networks (CANNs) run on classical computers, the massive parallel processing speed advantage of a neural network is lost. A quantum computer is a computation device that makes direct use of quantum–mechanical phenomena while large-scale quantum computers will be able to solve certain problems much quicker than any classical computer using the best currently known algorithms. Combining the advantages of quantum computers and the idea of CANNs, we propose in this paper a new type of neural networks, named a quantum artificial neural network (QANN), which is presented as a system of interconnected "quantum neurons" which can compute quantum states from input-quantum states by feeding information through the network and can be simulated on quantum computers. To show the ability of approximation of a QANN, we prove a universal approximation theorem (UAT) which reads every continuous mapping that transforms n quantum states as a non-normalized quantum state can be uniformly approximated by a QANN. The UAT implies that QANNs would suggest a potential computing tool for dealing with quantum information. For instance, we prove that the state of a quantum system driven by a time-dependent Hamiltonian can be approximated uniformly by a QANN. This provides a possible way for finding approximate solution to a Schrödinger equation with a time-dependent Hamiltonian.

1. Introduction

In computer science and related fields, classical artificial neural networks (CANNs) are computational models and capable of machine learning and pattern recognition. A CANN is usually presented as a system of interconnected "neurons" which can compute values from inputs by feeding information through the network. Since simulations of artificial neural networks run on classical computers, the massive parallel processing speed advantage of a neural network is lost [22]. Clearly, it would be better to utilize the intrinsic physics of a physical system to perform the computation. Many efforts have been expended in this direction, using systems ranging from nonlinear optical materials to proteins [15]. At the same time, many other researchers have been exploring the possibility of building quantum computers [2,1,6]. By using arrays of coupled quantum dot molecules, a quantum cellular automata has been posed in [11], which provides a valuable concrete example of quantum computation in which a number of fundamental issues come to light. An architecture for a quantum neural computer has

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been proposed in [14] in light of the real time evolution of quantum dot molecules, and simulations have proved that such an architecture can perform any classical logic gate, which can be used to calculate a purely quantum gate (a unitary matrix).

In this paper, we propose an analog of a CANN, named a quantum artificial neural network (QANN), and prove that every continuous mapping that maps n quantum states as a non-normalized quantum state can be uniformly approximated by a QANN. As an application, we show that the state of a quantum system driven by a time-dependent Hamiltonian can be approximated uniformly by a QANN.

2. Construction of a quantum artificial neural network

Let $\mathbb{C}^d = \{(z_1, z_2, \ldots, z_d)^T : z_k \in \mathbb{C}(k = 1, 2, \ldots, d)\}$ be the d-dimensional complex Hilbert space with the inner product

$$\langle x|y\rangle = \sum_{k=1}^{d} \overline{x_k} y_k \tag{2.1}$$

for all elements $|x\rangle = (x_1, x_2, \ldots, x_d)^T$ and $|y\rangle = (y_1, y_2, \ldots, y_d)^T$, where $\overline{x_k}$ denotes the conjugate of the complex number x_k and

$$\langle x| = |x\rangle^\dagger = (\overline{x_1}, \overline{x_2}, \ldots, \overline{x_d}). \tag{2.2}$$

The norm induced by the inner product above reads

$$\||x\rangle\| = \langle x|x\rangle^{1/2} = \left(\sum_{k=1}^{d} |x_k|^2\right)^{1/2}. \tag{2.3}$$

In quantum mechanics, a d-dimensional quantum system is described by the Hilbert space $\mathbb{C}^d$ and quantum states of the system are described by unit vectors in $\mathbb{C}^d$. Let $S_d(\mathbb{C})$ be the set of all quantum states of the quantum system $\mathbb{C}^d$ and define

$$S_d^n(\mathbb{C}) = \{(|x_1\rangle, |x_2\rangle, \ldots, |x_n\rangle)^T : |x_k\rangle \in S_d(\mathbb{C})(k = 1, 2, \ldots, n)\}, \tag{2.4}$$

which is clearly a closed bounded subset of the Hilbert space

$$(\mathbb{C}^d)^n = \{(|x_1\rangle, |x_2\rangle, \ldots, |x_n\rangle)^T : |x_k\rangle \in \mathbb{C}^d(k = 1, 2, \ldots, n)\} \equiv \mathbb{C}^{nd}. \tag{2.5}$$

First, we define a mapping $\mathcal{T} : S_d^n(\mathbb{C}) \to \mathbb{R}^{2nd}$ as

$$\mathcal{T}|x\rangle = (\mathrm{Re}|x_1\rangle, \mathrm{Im}|x_1\rangle, \mathrm{Re}|x_2\rangle, \mathrm{Im}|x_2\rangle, \ldots, \mathrm{Re}|x_n\rangle, \mathrm{Im}|x_n\rangle)^T \tag{2.6}$$

for all $|x\rangle = (|x_1\rangle, |x_2\rangle, \ldots, |x_n\rangle)^T \in S_d^n(\mathbb{C})$. We call $\mathcal{T}$ the *realization mapping*. Clearly, $\|\mathcal{T}|x\rangle\| = \sqrt{n}$ for all $|x\rangle \in S_d^n(\mathbb{C})$. Put

$$\Delta_{2d}^n(\mathbb{R}) = \mathcal{T}(S_d^n(\mathbb{C})) \subset \{|y\rangle \in \mathbb{R}^{2nd} : \||y\rangle\| = \sqrt{n}\}.$$

Then $\Delta_{2d}^n(\mathbb{R})$ is a compact subset of $\mathbb{R}^{2nd}$, and $\mathcal{T} : S_d^n(\mathbb{C}) \to \Delta_{2d}^n(\mathbb{R})$ becomes a homeomorphism.

Next, we let $\sigma_k : \mathbb{R} \to \mathbb{R}(k = 1, 2, \ldots, M)$ be M real-valued functions. For real numbers $\alpha_{j,k}^{(i)}, \theta_{j,k}^{(i)} (i = 1, 2; j = 1, 2, \ldots, N; k = 1, 2, \ldots, M)$ and vectors $|w_{j,k}^{(i)}\rangle (i = 1, 2; j = 1, 2, \ldots, N; k = 1, 2, \ldots, M)$ in $\mathbb{R}^{2nd}$, we define a mapping $\mathcal{Q}_k : S_d^n(\mathbb{C}) \to \mathbb{C}$ as follows:

$$\mathcal{Q}_k(|x\rangle) = \sum_{j=1}^{N} \left(\alpha_{j,k}^{(1)} \sigma_k(\langle w_{j,k}^{(1)}|\mathcal{T}|x\rangle + \theta_{j,k}^{(1)}) + \mathrm{i}\alpha_{j,k}^{(2)} \sigma_k(\langle w_{j,k}^{(2)}|\mathcal{T}|x\rangle + \theta_{j,k}^{(2)})\right) \tag{2.7}$$

for all $|x\rangle \in S_d^n(\mathbb{C})$ where $\langle w_j^{(i)}|\mathcal{T}|x\rangle$ denotes the inner product of $|w_j^{(i)}\rangle$ and $\mathcal{T}|x\rangle$.

Last, we define $\mathcal{Q} : S_d^n(\mathbb{C}) \to \mathbb{C}^M$ as

$$\mathcal{Q}(|x\rangle) = (\mathcal{Q}_1(|x\rangle), \mathcal{Q}_2(|x\rangle), \ldots, \mathcal{Q}_M(|x\rangle))^T \tag{2.8}$$

for all $|x\rangle \in S_d^n(\mathbb{C})$. We call such a mapping $\mathcal{Q}$ a *quantum artificial neural network* (QANN).

If we use $\{|e_1\rangle, |e_2\rangle, \ldots, |e_M\rangle\}$ to denote the canonical basis for $\mathbb{C}^M$, then the QANN above can be rewritten as

$$\mathcal{Q}(|x\rangle) = \sum_{k=1}^{M}\sum_{j=1}^{N} \left(\alpha_{j,k}^{(1)} \sigma_k(\langle w_{j,k}^{(1)}|\mathcal{T}|x\rangle + \theta_{j,k}^{(1)}) + \mathrm{i}\alpha_{j,k}^{(2)} \sigma_k(\langle w_{j,k}^{(2)}|\mathcal{T}|x\rangle + \theta_{j,k}^{(2)})\right)|e_k\rangle. \tag{2.9}$$

Put

$$y_{j,k}^{(i)} = \sigma_k\left(\sum_{t=1}^{n} \langle w_{j,k}^{(i)}(t)|\mathcal{T}|x_t\rangle + \theta_{j,k}^{(i)}\right), \ |a_k^{(i)}\rangle = \sum_{j=1}^{N} \alpha_{j,k}^{(i)} y_{j,k}^{(i)} |e_k\rangle.$$

Then a QANN can be illustrated by Figs. 1 and 2 below.