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Uniqueness theorem for quaternionic neural networks

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ABSTRACT

Quaternion algebra is a four-dimensional extension of the complex number field. The construction of artificial neural networks using complex numbers has recently been extended to that using quaternions. However, there have been few theoretical results for quaternionic neural networks. In the present work, we prove the applicability of the uniqueness theorem to quaternionic neural networks. Uniqueness theorems are important theories related to the singularities of neural networks. We provide the quaternionic versions of several important ideas, such as reducibility and equivalence, for proof of the uniqueness theorem. We can determine all the irreducible quaternionic neural networks that are I/O-equivalent to a given irreducible quaternionic neural network due to the uniqueness theorem.

1. Introduction

Quaternion algebra is a four-dimensional extension of the complex number field. The use of complex numbers to represent neural networks has recently been extended to quaternions [1–4]. For example, several models of quaternionic Hopfield neural networks have been proposed. Isokawa et al. proposed quaternionic Hopfield neural networks with a split activation function [5]. Moreover, they extended the use of quaternions to neural networks with multistate activation function [6]. Kobayashi proposed hybrid quaternion Hopfield neural networks utilizing the non-commutativity property of quaternions and improved the noise tolerance [7]. Nitta applied a single quaternionic neuron to a 4-bit parity problem [8]. Moreover, quaternions have been utilized in signal processing [9–11].

Several quaternionic feed-forward neural networks have also been proposed and widely applied. Nitta proposed three-layered quaternionic neural networks and showed that their learning speed was faster than that of real-valued neural networks by computer simulations [12]. Kobayashi and Nakajima proposed quaternionic neural networks utilizing the non-commutativity property of quaternions and improved the learning speed [13]. Kobayashi et al. provided a matrix representation of quaternionic neural networks [14]. Matsui et al. applied quaternionic neural networks to various field, such as color-image compression, counting pedestrians and night-vision [15–17]. Shang and Hirose applied quaternionic neural networks to land classification [18]. Arena et al. applied three-dimensional models of quaternionic neural networks to control in robotics [4]. Although many applications of quaternionic neural networks have been studied, there have been few theoretical results on quaternionic neural networks [19].

Sussmann proved the uniqueness theorem for real-valued feedforward neural networks. His theory has been tightly related to singularities of neural networks. Singularity is an important problem, because it causes stagnation in the learning process. Nitta extended limited versions of the uniqueness theorem to complex-valued neural networks [21–24]. Kobayashi found exceptional reducibility of complex-valued neural networks and proved the full version of the uniqueness theorem for complex-valued neural networks [25]. Kobayashi also proved a limited version of the uniqueness theorem for complex-valued neural networks represented in polar variables [26]. Fukumizu and Amari showed the relations between singularity and stagnation in the learning process based on the uniqueness theorem [27]. Nitta extended their theory to complex-valued neural networks [28]. Nitta also studied the singularity of a single complex-valued neuron with polar variables [29]. Satoh and Nakano improved the learning process using singular regions [30–32]. In the present work, we prove a limited version of the uniqueness theorem for quaternionic neural networks. To prove the uniqueness theorem, we define the quaternionic versions of some necessary concepts, such as reducibility and equivalence. They are important ideas related to singularity. Since quaternions are much more complicated than real and complex numbers, the proof of the uniqueness theorem for quaternionic neural networks is more difficult than those for real-valued and complex-valued neural networks.

The rest of this paper is organized as follows. Section 2 describes the real-valued version of the present work. Section 3 prepares the necessary ideas for quaternionic neural networks. In Section 4, we prove the uniqueness theorem for quaternionic neural networks. We finish with conclusions in Section 5.

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2. Real-valued neural networks

In this section, we briefly describe real-valued neural networks. In this work, only three-layered feedforward neural networks with one output neuron will be considered. We also suppose that hidden neurons do not have bias terms. The number of input neurons is fixed to m. We denote the connection weight from input neuron b to hidden neuron a as w_{ab}. Let $\mathbf{w}_a = (w_{a1}, w_{a2}, \ldots, w_{am})$ and $\mathbf{x} = (x_1, x_2, \ldots, x_m)$ be the connection weight vector to hidden neuron a and an input vector, respectively. The vector $\mathbf{w}_a = (w_{a1}, w_{a2}, \ldots, w_{am})$ is referred to as the connection weight vector to neuron a. Then, the weighted sum input $\nu_a(\mathbf{x})$ to hidden neuron a is defined as follows:

$$\nu_a(\mathbf{x}) = \mathbf{w}_a \cdot \mathbf{x} = \sum_{b=1}^{m} w_{ab} x_b. \tag{1}$$

The activation function of hidden neurons is $\tanh(\cdot)$. For the input vector $\mathbf{x}$, the output of hidden neuron a is $\tanh(\nu_a(\mathbf{x}))$. Let c_a be the connection weight from hidden neuron a to the output neuron. In addition, let c_0 be the bias term of the output neuron. The output $\mu(\mathbf{x})$ of the output neuron is given as follows:

$$\mu(\mathbf{x}) = c_0 + \sum_{a=1}^{n} c_a \tanh(\nu_a(\mathbf{x})), \tag{2}$$

where n is the number of hidden neurons.

We define several important concepts for the uniqueness theorem.

Definition 1. If two neural networks have the same I/O map, then they are said to be I/O-equivalent.

Definition 2. If a neural network is not I/O-equivalent to any neural networks having fewer hidden neurons, the neural network is said to be minimal.

The above definitions are not limited to real-valued neural networks.

We consider two non-zero vectors $\mathbf{g}_a = (g_{a1}, g_{a2}, \ldots, g_{am})$ $(a = 1, 2)$ and two linear functions $g_a(\mathbf{x}) = \mathbf{g}_a \cdot \mathbf{x} = \sum_{b=1}^{m} g_{ab} x_b$ with m variables.

Definition 3. If $\mathbf{g}_1 = \pm \mathbf{g}_2$, then two linear functions $g_1(\mathbf{x})$ and $g_2(\mathbf{x})$ are said to be sign-equivalent.

We define reducibility and irreducibility for real-valued neural networks. Later, these definitions will be extended to quaternionic versions.

Definition 4. If a neural network satisfies one of the following conditions, it is said to be reducible.

1. There exists c_a such that $c_a = 0$ and $a > 0$.
2. There exists $\mathbf{w}_a$ such that $\mathbf{w}_a = \mathbf{0}$.
3. There exist $a \neq \hat{a}$ such that $\mathbf{w}_a = \pm \mathbf{w}_{\hat{a}}$.

The third condition implies that two linear functions $\mathbf{w}_a \cdot \mathbf{x}$ and $\mathbf{w}_{\hat{a}} \cdot \mathbf{x}$ are sign-equivalent.

Definition 5. If a neural network is not reducible, then it is said to be irreducible.

Proposition 1. *A reducible neural network is not minimal.*

Proof. In the case of $c_a = 0$ or $\mathbf{w}_a = \mathbf{0}$, the neural network without hidden neuron a is I/O-equivalent to the original one. Suppose $\mathbf{w}_{\hat{a}} = \rho \mathbf{w}_a$ and $\rho = \pm 1$, then the following equality holds:

$$c_a \tanh(\mathbf{w_a} \cdot \mathbf{x}) + c_{\hat{a}} \tanh(\mathbf{w}_{\hat{a}} \cdot \mathbf{x}) = c_a \tanh(\mathbf{w_a} \cdot \mathbf{x}) + c_{\hat{a}} \tanh(\rho \mathbf{w_a} \cdot \mathbf{x}) \tag{3}$$

$$c_a \tanh(\mathbf{w_a} \cdot \mathbf{x}) + c_{\hat{a}} \tanh(\mathbf{w}_{\hat{a}} \cdot \mathbf{x}) = c_a \tanh(\mathbf{w_a} \cdot \mathbf{x}) + \rho c_{\hat{a}} \tanh(\mathbf{w_a} \cdot \mathbf{x}) \tag{4}$$

$$c_a \tanh(\mathbf{w_a} \cdot \mathbf{x}) + c_{\hat{a}} \tanh(\mathbf{w}_{\hat{a}} \cdot \mathbf{x}) = (c_a + \rho c_{\hat{a}}) \tanh(\mathbf{w_a} \cdot \mathbf{x}). \tag{5}$$

We obtain an I/O-equivalent neural network with fewer hidden neurons by eliminating hidden neuron $\hat{a}$ and replacing c_a by $c_a + \rho c_{\hat{a}}$. Therefore, a reducible neural network is not minimal.□

The inverse of Proposition 1 is also true [20].

Theorem 1. *A neural network is minimal if and only if it is irreducible.*

The following helpful lemma was proven by Sussmann [20].

Lemma 1. *Consider non-constant linear functions, $\nu_1(\mathbf{x}), \nu_2(\mathbf{x}), \ldots, \nu_n(\mathbf{x})$. If no two of them are sign-equivalent, then $\tanh(\nu_1(\mathbf{x}))$, $\tanh(\nu_2(\mathbf{x}))$, …, $\tanh(\nu_n(\mathbf{x}))$ and the constant function 1 are linearly independent of* $\mathbf{R}$.

Moreover, Sussmann proved the uniqueness theorem for real-valued neural networks. The following definition is necessary for the description of the uniqueness theorem.

Definition 6. We define the following translations of the neural networks with n hidden neurons.

1. Select $0 < a \le n$ and replace c_a and $\mathbf{w}_a$ by $-c_a$ and $-\mathbf{w}_a$, respectively. We denote this translation as g_a.
2. Exchange two different hidden neurons a and $\hat{a}$. We denote this translation as $g_{a\hat{a}}$.

These translations maintain the I/O map. We denote the finite group generated by $\{g_a\} \bigcup \{g_{a\hat{a}}\}$ as G_R. The order of G_R is $2^n n!$. For $g \in G_r$ and a neural network N with n hidden neurons, N and $g(N)$ are I/O-equivalent.

Definition 7. For two neural networks N_1 and N_2 with n hidden neurons, if there exists $g \in G_R$ such that $N_1 = g(N_2)$, N_1 and N_2 are said to be equivalent.

The following theorem is referred to as the uniqueness theorem.

Theorem 2. *Let N_1 and N_2 be irreducible neural networks with n_1 and n_2 hidden neurons, respectively. If they are I/O-equivalent, they are equivalent and $n_1 = n_2$ holds.*

The above-described uniqueness theorem is a limited version of the uniqueness theorem proven by Sussmann. Theorem 1 was obtained as a corollary of Theorem 2. Nitta proved the complex-valued version of Theorem 2 [22]. The full version proof was very complicated, because there existed exceptional reducibility, which is irreducible but not minimal [25]. In the present work, we prove the quaternionic version of Theorem 2.

3. Quaternionic neural networks

3.1. Quaternion

Quaternions form a non-commutative field and are extensions of complex numbers. Quaternions have three imaginary units i, j and k, defined as follows:

$$i^2 = j^2 = k^2 = -1, \tag{6}$$

$$ij = -ji = k, \tag{7}$$

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