A Tutorial on Quantum Graph Recurrent Neural Network (QGRNN)

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***Abstract*—Over the past decades, various neural networks have been proposed with the rapid development of the machine learning field. In particular, graph neural networks using feature-vectors assigned to nodes and edges have been attracting attention in various fields. The usefulness of graph neural networks also affected the field of quantum computing, which led to the birth of quantum graph neural networks composed of parameterized quantum circuits. The quantum graph neural networks have many possibilities as applications from the simulation perspective of quantum dynamics. Among the application models of various quantum graph neural networks, the quantum graph recurrent neural network (QGRNN) is proven to be effective in training the Ising model Hamiltonian. Thus, this paper introduces the concepts of the Ising model, variational quantum eigensolver (VQE) for preparing quantum data, and QGRNN from a software engineer's point of view.**

***Index Terms*—QGRNN, VQE, Ising Model**

I. Introduction

Machine learning has made human life more convenient and enriching in various fields. With the development of the graphics processing unit (GPU), deep learning research has gained momentum, and machine learning research has entered a new era. In this era, various learning models have proposed and applied to many fields such as physics, robotics, industry, and medical science.

However, machine learning research will once again enter a new era by quantum computers. Various researches for more powerful quantum processing unit (QPU) and quantum random access memory (QRAM) have been made, and the noisy intermediate-scale quantum (NISQ) level devices have already developed [1]–[3]. Leading companies and academics have already started working on quantum algorithms and applications that can take full advantage of quantum devices. A new research field named quantum machine learning was also born [4], [5]. The quantum machine learning aims to propose a new perspective of learning methodology or to find cases that can be proved quantum supremacy by tuning classical machine learning structures or models to the quantum device environment. It is very encouraging that remarkable results have been recently announced in the field of quantum machine learning, including quantum approximate optimization algorithm (QAOA), quantum convolutional neural network (QCNN), and quantum graph recurrent neural network (QGRNN) [6]–[8]. In the field of quantum machine learning, researchers in various fields such as mathematics, physics, electronic engineering, statistics, and software engineering are co-working, so more breakthrough achievements will be expected in the future.

However, various researches of quantum machine learning centered on software need more software engineers. Thus, this paper easily introduces QGRNN, one of the major achievements of the quantum machine learning field, to make it easier for software engineers to join the quantum machine learning world. It also introduces the Ising model and variational quantum eigensolver (VQE) which are the backgrounds and components of QGRNN. The high potential of QGRNN, inspired by classical graph neural networks, is verified on the time-evolution Ising model Hamiltonian training example [8]–[10]. This paper hopes that many software engineers catch the potential of QGRNN, and many types of researches will be derived.

II. Ising Model

The Ising model is the simplest magnetic model considering only the interactions between nearby particles. In other words, it is a model in which only the magnetic interactions and external magnetic fields between adjacent particles with magnetic dipoles are considered, and all other interactions are excluded. The Ising model Hamiltonian $\mathcal{H}_I$ is defined as follows:

$$\begin{aligned}\mathcal{H}_I &= -J\sum_{(j,k)}\sigma_j\sigma_k - \mu\sum_j h_j\sigma_j \text{ where} \\ &\qquad \sigma_j \in \{-1,+1\} \text{ and } \sigma_k \in \{-1,+1\}. \qquad (1)\end{aligned}$$

Here, J indicates the interaction between adjacent j and k; μ is the magnetic moment, and h_j is the external magnetic field interacting with j. In the field of theoretical computing, the Ising model Hamiltonian is also used to solve graph-based combinatorial optimization problems [11]. In particular, the Ising Hamiltonian with $h_j = 0$ in (1) can be equivalently formulated as a maximum cut problem [6].

The quantum version of the Ising model is the transverse-field Ising model (TIM) [12], [13]. TIM is a prototypical example that captures the essence of the quantum phase transition [14]. The TIM Hamiltonian $\mathcal{H}_{TIM}$ that cannot be explained by classical statistical mechanics is defined as follows:

$$\mathcal{H}_{TIM} = J\sum_{(j,k)} \sigma_j^z \sigma_k^z - \mu \sum_j h_j \sigma_j^z - \mu \sum_j g_j \sigma_j^x. \quad (2)$$

Here, J, μ, and h_j are as defined in (1); σ_j^z, σ_j^x, and g_j are Pauli-Z operator at j, Pauli-X operator at j, and longitudinal magnetic field, respectively. And (2) can be simplified by adjusting the coefficients as follows:

$$\mathcal{H}_{TIM}(\theta) = \theta_1 \sum_{(j,k)} \sigma_j^z \sigma_k^z + \theta_2 \sum_j \sigma_j^z + \sum_j \sigma_j^x, \quad (3)$$

where $\theta = \{\theta_1, \theta_2\}$. In particular, in the graph using qubits as nodes, θ_1 and θ_2 correspond to edge weights and node weights, respectively. Therefore, the following time-evolution operator which has features of the graph can be constructed:

$$\begin{aligned} U &= e^{-it\mathcal{H}_{TIM}(\theta)} \\ &= e^{-it\left(\theta_1 \sum_{(j,k)} \sigma_j^z \sigma_k^z + \theta_2 \sum_j \sigma_j^z + \sum_j \sigma_j^x\right)} \\ &\approx \prod_{j=1}^{t/\delta} \left(\prod_{k=1}^{K} e^{-i\delta \mathcal{H}_{TIM}^k(\theta)} \right), \end{aligned} \quad (4)$$

where $\delta \ll 1$ is a small number and K is the number of Hamiltonians; and the approximation is performed by Suzuki-Trotter decomposition [8], [15]–[17]. Through unitary operators constructed in this way, it is possible to construct a parameterized quantum circuit representing a graph.

III. Variational Quantum Eigensolver (VQE)

VQE is a hybrid quantum-classical optimizer using near-term quantum devices [18]–[21]. VQE can find the minimum eigenvalue of the Hermitian matrix [22]. The Hamiltonian is Hermitian, so the near ground-state energy of the system can be found via VQE.

VQE is largely divided into the quantum process and classical process. The quantum process which runs within the classical process is as follows:

- Prepare for the initial eigenstate $|\psi_0(\eta)\rangle$.
- Measure the expectation value $\langle\psi_0(\eta)|H|\psi_0(\eta)\rangle$ of the Hermitian matrix H in this state.
- Repeat the measurement of the expectation value, changing the state little by little.
- Get the minimum value $\langle\psi_{min}(\eta)|H|\psi_{min}(\eta)\rangle$ of among the measured expectation values.

The parameter η is controlled in the classical process. By the variational principle, the expectation value $\langle\psi(\eta)|H|\psi(\eta)\rangle$ is always greater than or equal to the minimum eigenvalue. Thus, $\langle\psi_{min}(\eta)|H|\psi_{min}(\eta)\rangle$ approximates the minimum eigenvalue.

VQE is suitable for the NISQ systems because of its low circuit depth [3], [21]. Actually, due to the light and simple structure of VQE, related research is actively underway in various fields [23]–[26].

IV. Quantum Graph Recurrent Neural Network (QGRNN)

The quantum neural network, a kind of variational quantum algorithms, consists of parameterized circuits similar to the parameterized transformations that occurs in deep learning [8]. Among Trotter-based quantum neural networks, quantum graph neural networks that utilize data geometry show some remarkable results in application area of deep learning [27], [28]. QGRNN, proposed by *Verdon et al.* [8], has similarity to the classical recurrent neural network in which parameters are shared over sequential applications of a recurrent neural network map. Therefore, QGRNN shows great performance in training effective real-time quantum Hamiltonian dynamics for graph systems.

A. Definition of QGRNN

QGRNN, a parameterized quantum circuit of a network consisting of Q different Hamiltonian evolution sequences with the entire sequence repeated P times, is generally defined as follows:

$$U_H(\delta, \theta) = \prod_{p=1}^{P} \left(\prod_{q=1}^{Q} e^{-i\delta_q \mathcal{H}_q(\theta)} \right), \quad (5)$$

where δ is the time parameter of parameterized Hamiltonian $\mathcal{H}_q(\theta)$. Note that (4) and (5) have a similar form because the origin of QGRNN is the time-evolution operator of TIM.

B. Process of QGRNN

The general training process via QGRNN is as follows:

1) Prepare TIM Hamiltonian data via VQE.
2) Construct QGRNN layers.
3) Construct fidelity $|\langle\psi_t|U_H(\delta,\theta)|\psi_0\rangle|^2$ with swap test.
4) Calculate the average infidelity loss function $\mathcal{L}(\delta, \theta)$.
5) Train the parameters.

Here, the average infidelity loss function $\mathcal{L}(\delta, \theta)$ is as follows [8]:

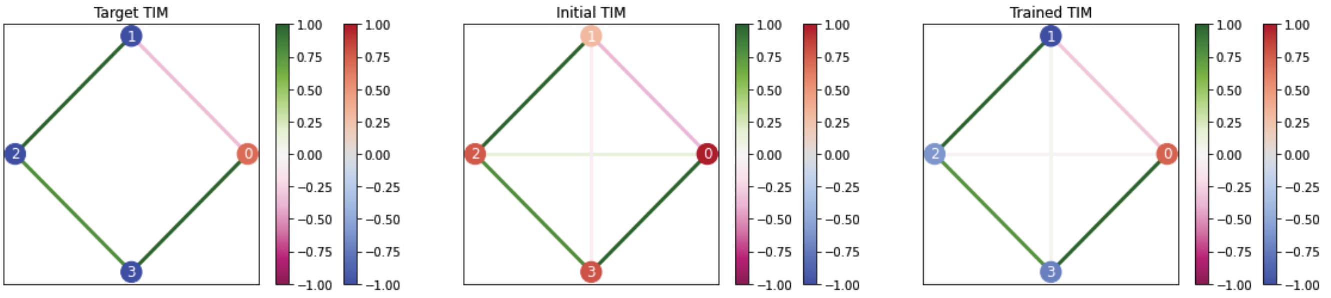
$$\mathcal{L}(\delta, \theta) = 1 - \frac{1}{N} \sum_{j=1}^{N} |\langle\psi_t|U_H(\delta,\theta)|\psi_0\rangle|^2, \quad (6)$$

where N is the number of quantum data that are used for each step, i.e., batch size. The training process of Hamiltonian time-evolution via QGRNN has different features from classical learning methods, e.g., VQE, swap test, and average infidelity loss function. This is because QGRNN handles quantum data.

C. Training Ising Model Hamiltonian via QGRNN

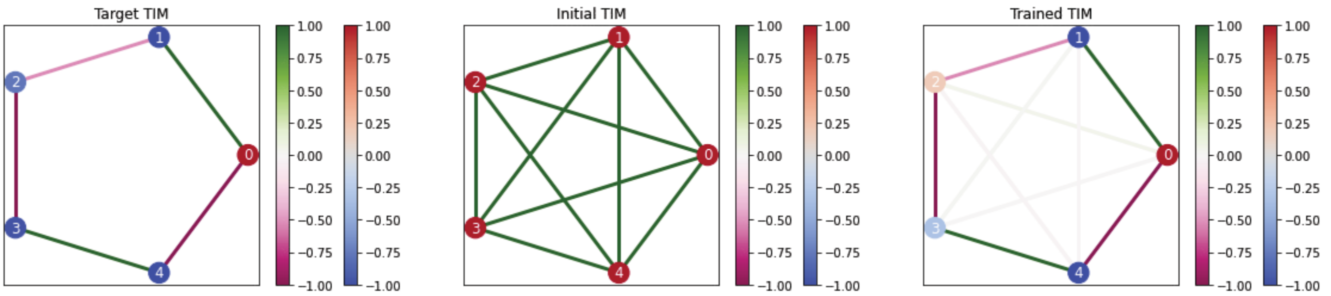
In this section, the arbitrary TIM Hamiltonian is trained via QGRNN using TensorFlow Quantum [10].

The target Hamiltonian is randomly generated in the form of the TIM Hamiltonian of (3) in the n-qubit (n-node) cycle graph. The initial target TIM Hamiltonian on the near ground-state is obtained using VQE. The time-evolution states are simply constructed by multiplying the time-evolution unitary on the initial state (near ground-state). The training is performed



(a) Target TIM with 4-qubit.
(b) Initial TIM with 4-qubit.
(c) Trained TIM with 4-qubit.

Fig. 1: Training result via QGRNN on the 4-qubit graph. The pink-green and blue-red colormaps represent θ_1 and θ_2 in (3), respectively. It is confirmed that training quantum time-evolution dynamics about the transverse-field Ising model (TIM) Hamiltonian via QGRNN is well done because the target and trained models are very similar [8], [10].



(a) Target TIM with 5-qubit.
(b) Initial TIM with 5-qubit.
(c) Trained TIM with 5-qubit.

Fig. 2: Training result via QGRNN on the 5-qubit graph. The description of the colormaps is as same as in Fig. 1. The training result of θ_1 on the 5-qubit graph is as perfect as that of the 4-qubit graph [8], [10].

via the QGRNN model initialized with an n-qubit (n-node) complete graph using time-evolution TIM Hamiltonians.

The training results at $n = 4, 5$ are shown in Fig. 1 and Fig. 2, respectively. Considering a slight error, the target TIM and the trained TIM are almost the same in both cases. Therefore, it is proven that the Ising model Hamiltonian can be trained well via QGRNN. The Ising model emulates quadratic unconstrained binary optimization (QUBO) problem that is effective in modeling non-deterministic polynomial (NP) problems, so the potential of QGRNN will be great implications for software engineers [29], [30].

V. Conclusion

In this paper, we briefly studied the definition, process, and advantages of QGRNN from the perspective of a software engineer. To help understand the components of QGRNN, we also studied the Ising model and VQE. We confirmed that QGRNN shows good performance for Ising model Hamiltonian training. The Ising model Hamiltonian and QUBO are closely related, so the future expansion researches of QGRNN are expected. We hope that this paper can be a booster of interest to quantum machine learning, including QGRNN, for many software engineers.

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