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Artificial Neural Network-inspired Quantum Adiabatic Evolution Algorithm with Energy Dissipation

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Abstract—An ANN(artificial neural network)-inspired quantum adiabatic evolution algorithm, which is a new quantum computation algorithm based on both the ANN-like method and the adiabatic Hamiltonian evolution, has been proposed for solving a combinatorial optimization problem. However, it has been known that the adiabatic evolution algorithm can not be applied to a quantum system with degenerated states during the evolution of a Hamiltonian. In order to remove this limitation, we propose an improved ANN-inspired algorithm with energy dissipation and discuss how to use this algorithm for solving an optimization problem.

1. Introduction

Real parallel computing is possible with a quantum computer which makes use of quantum states [1]. Recently, a few quantum calculation algorithms utilizing features of quantum dynamics have been proposed. However, the scope in which these algorithms are applied has been limited to specific problems such as factorization and database search [2, 3]. Therefore, it is necessary to devise a new general purpose algorithm from the viewpoint of the practical application. More recently, Farhi et al. have proposed a quantum adiabatic evolution(QAE) algorithm that is a new quantum computation algorithm based on the adiabatic evolution for solving one kind of the satisfiability problem, 3-SAT [4]. In addition, Kinjo et al. have proposed an ANN-inspired quantum computation algorithm based on both the QAE algorithm and an ANN-like method for solving a combinatorial optimization problem [5, 6]. However, these QAE algorithm can not be applied to a quantum system with degenerated states during the evolution of a Hamiltonian because of no guarantee according to the adiabatic theorem [7]. Therefore, we propose an application of energy dissipation to the ANN-inspired algorithm in order to remove the above restriction. First, we discuss the energy relation between a neural network and a qubit network. Next, we focus on an algorithm to find the optimal solution by changing the Hamiltonian adiabatically (adiabatic evolution algorithm) proposed by Farhi et al. and propose a new algorithm with energy dissipation. Successful numerical simulation results are shown.

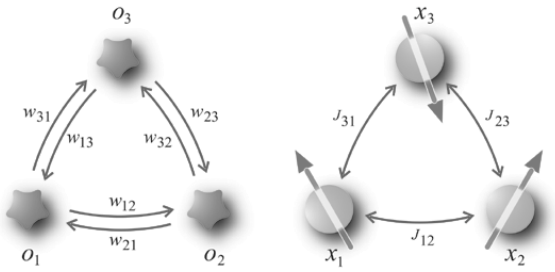

Figure 1: Illustration of 3-neuron network and 3-qubit system

2. ANN-inspired Quantum Computation

2.1. Qubit Neuron

Let us consider a qubit operating like a neuron. The dynamics of a quantum system is defined by Schrödinger equation, and it is important how to design a Hamiltonian. On the other hand, it has been known that the energy function is defined for a Hopfield neural network [8]. Therefore, we consider the N-queen problem as an example in order to study the relation between a Hopfield neural network and a qubit network.

The N-queen problem, which is one of the combinatorial optimization problems, is a placement problem of N queen figures of chess on an $N \times N$ chess board, so that no two queens attack each other according to the rules of the game as shown in Fig. 1. In this paper, we choose $N = 4$ to be a suitable size for the problem by considering the restrictions of numerical simulations. The cost function of the 4-queen problem is given as

$$\begin{aligned} E_{\text{cost}} &= a\sum_{i}^{4}\left(\sum_{j}^{4} o_{ij} - 1\right)^2 + b\sum_{j}^{4}\left(\sum_{i}^{4} o_{ij} - 1\right)^2 \\ &\quad + c\sum_{q=3}^{7}\sum_{i+j=q}\sum_{k+l=q}\sum_{k\neq i}\sum_{l\neq j} o_{ij}o_{kl} \\ &\quad + d\sum_{q=-2}^{2}\sum_{i-j=q}\sum_{k-l=q}\sum_{k\neq i}\sum_{l\neq j} o_{ij}o_{kl}, \end{aligned} \tag{1}$$

where o_{ij} is the output of a neuron, the two suffixes i and j

indicate the position of the neuron on the 4x4 chess board, and a, b, c, d are arbitrary positive constants.

The synaptic weights w_{ijkl}s are given by comparing E_{cost} in (1) and the following energy E_{HN} of a Hopfield network.

$$E_{\text{HN}} = -\frac{1}{2}\sum_{ij}\sum_{kl} w_{ijkl}o_{ij}o_{kl} - \sum_{ij} h_{ij}o_{ij}, \tag{2}$$

where h_{ij} is the external bias for a neuron. The synaptic weights are obtained as

$$\begin{aligned} w_{ijkl} &= -2a\delta_{j,l}(1-\delta_{i,k}) - 2b\delta_{i,k}(1-\delta_{j,l}) \\ &\quad -2c\delta_{i+j,k+l}(1-\delta_{i,k}) - 2d\delta_{i-j,k-l}(1-\delta_{i,k}), \end{aligned} \tag{3}$$

where $\delta_{i,j}$ is the Kronecker delta.

Let us consider that each qubit corresponds to each neuron of a Hopfield Network. The state vector $|\psi\rangle$ of the whole system is given by the product of all qubit states. Let each qubit be realized with a spin-$\frac{1}{2}$ particle, where $|x_i = 0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ corresponds to the i-th spin being up in the z-direction and $|x_i = 1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ corresponds to the i-th spin being down in the z-direction. In order to clarify the relationship between a qubit and a neuron, we give a number in decimal notation for each state where each qubit $|x_i\rangle$ takes $|0\rangle$ or $|1\rangle$ exclusively,

$$|x_{16}\rangle \cdots |x_2\rangle|x_1\rangle \equiv |x_{16}\cdots x_2 x_1\rangle \equiv |n\rangle. \tag{4}$$

The Hamiltonian H_F for the 4-queen problem is obtained as shown in the following equation. The eigenvalue ϵ_n of the state $|n\rangle$ should be obtained from the cost function in (1). Therefore, H_F has ϵ_ns as diagonal elements as

$$H_F = \begin{pmatrix} \epsilon_0 & & & 0 \\ & \epsilon_1 & & \\ & & \ddots & \\ 0 & & & \epsilon_{2^{16}-1} \end{pmatrix} = \sum_{n=0}^{2^{16}-1} \epsilon_n |n\rangle\langle n|. \tag{5}$$

2.2. Adiabatic Evolution Algorithm

It is known that E_{HN} in (2) decreases with time, so that the state of the neural network evolves toward a lower energy state. However, since the state change is driven by local features of the energy surface, the network would often be trapped at local minima. On the other hand, local minima are not considered in the adiabatic evolution algorithm because the system is always in a ground state. It may be possible to solve optimization problems by composing a new H_F considering the w_{ijkl}s.

The quantum computation algorithm utilizing adiabatic Hamiltonian evolution has been proposed by Farhi et al. [4]. Adiabatic Hamiltonian evolution is given as

$$H(t) = \left(1 - \frac{t}{T}\right)H_I + \frac{t}{T}H_F, \tag{6}$$

where H_I and H_F are the initial and final Hamiltonians, respectively. The H_I is chosen so that its ground state is given by the superposition of all states as

$$|\psi(0)\rangle = \frac{1}{\sqrt{2^N}}\sum_{n=0}^{2^N-1} |n\rangle, \tag{7}$$

where N is the number of qubits and $|n\rangle$ is the n-th eigenvector. In consideration with the fact that the ground state of a spin-$\frac{1}{2}$ particle aligned in the x-direction is $|x_i\rangle = \frac{1}{\sqrt{2}}(|x_i = 0\rangle + |x_i = 1\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$, the H_I is given as

$$\begin{aligned} H_I &= \left({\sigma_x}^{(0)} + {\sigma_x}^{(1)} + \cdots + {\sigma_x}^{(2^{16}-1)}\right) \\ &= (\sigma_x \otimes I \otimes \cdots \otimes I + I \otimes \sigma_x \otimes \cdots \otimes I \\ &\quad + \cdots + I \otimes I \otimes \cdots \otimes \sigma_x), \end{aligned} \tag{8}$$

where σ_x is the x-component of the Pauli spin matrix. One can choose any other H_I which satisfies that its ground state is expressed by a linear combination of all states. For example, σ_x can be replaced by σ_y.

The H_F is chosen so that its ground state satisfies the condition of the solution for a target problem as discussed in the previous section. We assume that the quantum system starts at $t = 0$ in the ground state of H_I, so that all possible candidates are set in the initial state $|\psi(0)\rangle$. T denotes the period in which the Hamiltonian evolves and the quantum state changes, and we can control the speed of such changes to be suitable for finding the optimal solution among all candidates set in $|\psi(0)\rangle$. If a sufficiently large T is chosen, the evolution becomes adiabatic. The adiabatic theorem says that the quantum state will remain close to each ground state [7]. Therefore, the optimal solution can be found as the final state $|\psi(T)\rangle$. However, successful operation is not guaranteed in the case that there exists any degeneracy in energy levels or any energy crossing during the evolution [7].

The time evolution of the system is given by the following Schrödinger equation.

$$|\psi(t+1)\rangle = U(1)|\psi(t)\rangle = e^{-\frac{iH(t)}{\hbar}}|\psi(t)\rangle. \tag{9}$$

Here, the operator $U(1)$ is given by the Padé approximation [9].

2.3. ANN-inspired Quantum Computation

Various functions of an ANN are realized by choosing suitable synaptic weights. A full-connection neural network has N^2 synapses, where N is the number of neurons. We consider interactions between qubits and study a new method with a new H_F comprising nondiagonal elements considering its analogy to ANN. For convenience, we assume we have closely coupled 2-spin-$\frac{1}{2}$ qubits. The Hamiltonian of this quantum system is

$$H = J(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) = J_{12}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{10}$$

1. Generate the initial state $|\psi(0)\rangle$ and $H(0)$
2. for $0 \le t \le T$
3. $\quad |\psi(t+1)\rangle := \exp\{-i \cdot \tau \cdot H(t)\}|\psi(t)\rangle$
4. $\quad E(t+1) := \langle\psi(t+1)|H(t)|\psi(t+1)\rangle$
5. $\quad$ for $1 \le k \le k_{max}$
6. $\quad\quad$ Generate ΔH_k at random
7. $\quad\quad |\psi_k(t+1)\rangle := \exp\{-i \cdot \tau \cdot (H(t) + \Delta H_k)\}|\psi(t)\rangle$
8. $\quad\quad E_k(t+1) := \langle\psi_k(t+1)|H(t)|\psi_k(t+1)\rangle$
9. $\quad$ Calculate Boltzmann distribution,
$\quad\quad Z := \sum_k \exp\{-\beta \cdot (E_k(t+1) - E(t+1))\}$,
$\quad\quad P(k) := \frac{1}{Z} \exp\{-\beta \cdot (E_k(t+1) - E(t+1))\}$
10. $\quad$ Pick a state $|\psi_j(t+1)\rangle$ from among k_{max} states according to $P(k)$
11. $\quad |\psi(t+1)\rangle := |\psi_j(t+1)\rangle$
12. $\quad H(t+1) := \left(1 - \frac{t+1}{T}\right) H_I + \frac{t+1}{T} H_F$
13. Observe the final state $|\psi(T)\rangle$

Figure 2: Algorithm for adiabatic evolution with energy dissipation

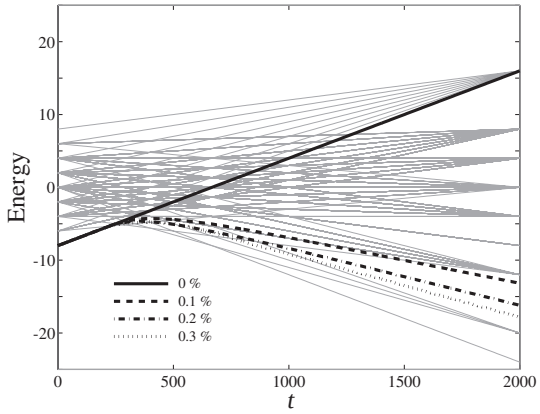

Figure 3: Energy changes of the spin qubit network by using adiabatic evolution with 0%, 0.1%, 0.2%, and 0.3% energy dissipation rate

where J_{12} is the magnitude of the interactions, and $\boldsymbol{\sigma}_i$ is the Pauli spin matrix. The possible states to be measured are $|10\rangle$ or $|01\rangle$ if the system is in the ground state $|01\rangle - |10\rangle$. It can be said that the interaction of two neurons is inhibitory if we consider the analogy with an ANN model. Excitatory interaction is also possible with another Hamiltonian [6].

From the above consideration, we can design a new Hamiltonian by converting the synaptic weights in (3) to the interactions of qubits. Since the synaptic weights of the 4-queen problem are either 0 or -1, we have tested this new method for the 4-queen problem by setting $J_{ij} = 0$ or 1. The parameters used here are $a = b = c = d = \frac{1}{2}$.

3. ANN-inspired Algorithm with Energy Dissipation

Quantum device is always affected by external noise, and quantum coherence disappears gradually as time goes. It is basic requirement that quantum coherence is kept during operation for a conventional quantum computation algorithm. The same holds for using the QAE algorithm. However, such decoherence is worth for the QAE algorithm eventually. This is because the successful execution of a QAE algorithm is not guaranteed for a quantum system with degenerated states during the evolution of a Hamiltonian, and then decoherence can be helpful for the state transition from a degenerated state to a lower energy state. Thus, we evaluate performance enhancement of a QAE algorithm after introducing decoherence. We suppose a quantum system obeying Boltzmann distribution as the simplest case and use Monte Carlo method in numerical simulations. The decoherence effect is incorporated as fluctuation of a Hamiltonian. An amplitude of the fluctuation is set to λ. A parameter $\beta = 1/k_B T_s$ of Boltzmann distribution, where k_B and T_s are Boltzmann factor and temperature, respectively, has same amplitude as $1/\lambda$. The proposed algorithm has two time constants for system and Hamiltonian evolutions. The former is sufficientry small compared to the later following the requirement of adiabatic evolution. Figure 2 shows the proposed algorithm for adiabatic evolution with decoherence. At first, $H(0)$ and the initial state are set to H_I in (8) and the ground state $|\psi(0)\rangle$, respectively. Next, the state evolves from $|\psi(t)\rangle$ to $|\psi(t+1)\rangle$ adiabatically, and the energy $E(t+1)$ is calculated. Then, ΔH_k which is introduced in order to simulate energy dissipation is generated at random ($(\Delta h_{ij})_k \in \Delta H_k$, $-\lambda \le (\Delta h_{ij})_k \le \lambda$). $|\psi_k(t+1)\rangle$ evolves from $|\psi(t)\rangle$ depending on $H(t) + \Delta H_k$. We calculate a probability $P(k)$ for $|\psi_k(t+1)\rangle$ based on Boltzmann distribution. We pick a state $|\psi_j(t+1)\rangle$ from among k_{max} states according to $P(k)$ and thus get $|\psi(t+1)\rangle = |\psi_j(t+1)\rangle$. Repeating the procedure T times results in $|\psi(T)\rangle = |\psi_{0_F}\rangle$ where $|\psi_{0_F}\rangle$ is the ground state of H_F. Finally we get a result for a target problem by observing the system.

For example, we apply this algorithm to the 4-queen problem, and Fig. 3 shows the results of energy changes. In this case, $\tau = 10000$ and $T = 2000$. The thin gray lines denote eigen-energy changes, and there are some degenerated points. The thick solid line represents the energy change of the system without energy dissipation, and it finally reaches the maximum energy level of the final Hamiltonian. Three other energy changes with decoherence for different λs are shown as the other thick lines. The energies are kept near the lowest energy before $t \approx 220$. Then the system meets the first degenerated point and its energy change related to the amplitude of decoherence has been seen. The energy of the final state decreases with increasing λ. We calculate the averages of successful probability of obtaining a solution as a function of λ. The statistical results for each λ are obtained with 20 samples of randomly generated ΔH_k. The results are shown in Fig. 4. The ground state of H_F is given as the combination of two solution states and others, and the probability for observing solutions is 40%. As λ in-

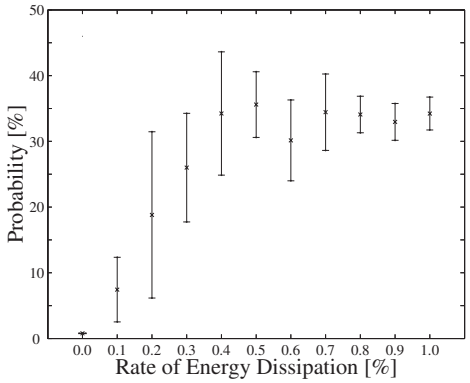

Figure 4: Successful probabilities of the final state after adiabatic evolution with the energy dissipation

creases, the successful probability increases toward 40%. Please note that the successful probability doesn't reach 40% exactly with any λ since the finite error rises from the fluctuation of a Hamiltonian in this simulation. However, the successful probability is vastly improved as compared with 0% in the case without energy dissipation.

4. Discussion

Here, we discuss about calculation cost of a final Hamiltonian in comparison with the original QAE algorithm. Farhi et al. have presented the QAE algorithm for the satisfiability problem (SAT) [4]. SAT consists of a Boolean formula in N variables and requires that one finds a value (true or false) for each variable that makes the formula true. This problem has 2^N assignments. For k-SAT, the formula consists of a conjunction of M clauses and each clause is a disjunction of k variables, any of which may be negated. Farhi et al. define a H_F that an energy of a quantum system is a minimum only if a state of the system satisfies all M clauses. In this case, the calculation cost of the H_F is less than $O(2^N)$ because a H_F can be gotten by calculating for M clauses with 3 variables. However, in order to solve a general combinatorial optimization problem, the calculation of such H_F is equal to calculating for diagonal elements of a H_F. Therefore, the cost of the H_F is $O(2^N)$ in general case. On the contrary, although the requirement that a cost function is given in a quadratic form is imposed, the cost of the proposed algorithm is extremely small $O(N^2)$. The proposed algorithm can be executed practically for solving the large scale optimization problem, though the proposed algorithm has the matter that a successful probability is small. For the 4-queen problem, the probability is at most 40%. However, 40% is enough large to obtain the solutions for the N-queen problem since an obtained state can be confirmed simply whether it corresponds to a solution or not in polynomial time order. Additionally, its physical implementation is easy since the H_F is realized only by the interactions between qubits. Spin qubits are the most likely candidates for implementing the proposed algorithm [10].

5. Conclusion

We suggest a quantum adiabatic evolution algorithm with energy dissipation as the decoherence effect. The proposed algorithm is applicable to a quantum system with degenerated states during the evolution of a Hamiltonian. We apply the improved algorithm to one of the combinatorial optimization problem, the 4-queen problem and show its successful results. A study on some other procedure in order to improve the probability observed for the desired state is future work.

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