Quantum Optimal Control with Pulses

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***Abstract*—The development of large-scale fault-tolerant quantum computers is a challenging problem. In the noisy intermediate scale quantum (NISQ) era, we have small-scale noisy quantum computers available to users. But the errors in the hardware limit the application of useful quantum algorithms and circuits. These errors can be reduced if we have noise robust quantum gates. Quantum optimal control is method where we can manipulate the control Hamiltonian of a system to make a quantum gate having fidelity close to unity even in the presence of noise. In this paper, we demonstrate quantum optimal control scheme for the design of $R_x(\pi/2)$ gate using pulses and gradient optimization method.**

I. Introduction

Quantum computer uses the phenomena of quantum mechanics to perform computation. Quantum computers have the potential to perform very complex computations, which are not possible on the current classical computers [1], [2]. In the past few decades, the field of quantum computing has gained a lot of attention, with scientists and engineers trying to develop a large-scale fault-tolerant quantum computer that can run useful quantum algorithms. Many companies like IBM, Google, Intel, and Xanadu have developed a few small-scale quantum computers with small number of qubits, which fall under the NISQ devices [3]. These quantum computers are imperfect due to errors arising from decoherence, crosstalk, and other quantum noise. Hence, any circuit implemented on them also has errors, making it difficult to extract any beneficial result from them [4]. One way of reducing the effects of noise is to make noise robust quantum gates.

If we can model the dynamics of the quantum system accurately, then using quantum optimal control we can design these gates having fidelity close to unity. Quantum optimal control is an important tool used in science and engineering where the goal is to steer the time evolution of the quantum system to a particulate target state [5]. Given the model of a quantum system, like transmons, ions trapped, and photonic, etc., a cost function can be defined corresponding to a required quantum gate which is then optimized to give a set of control sequences which implements the desired gate [6], [7].

A closed quantum system can be represented by a drift Hamiltonian and a control Hamiltonian. The drift Hamiltonian contains information related to quantum systems architecture and cannot be controlled. Meanwhile, the control Hamiltonian describes the effect of the physical control that is driven by the system. A set of control coefficients modulates this control Hamiltonian which can be also be represented by pulses.

In this paper, we implement quantum optimal control to design a $R_x(\pi/2)$ quantum gate using customized pulses. Using this optimization technique with noise model, we can make high fidelity quantum gates required for fault-tolerant quantum computing.

II. Quantum Optimal Control

Quantum control tries to find an optimal method to steer the time evolution of the quantum system to a particular target state, desirable state-to-state transfer, or unitary operation with good accuracy, minimum time, and minimum energy. Quantum control has many applications in many areas like quantum computing, quantum sensing, quantum metrology, nuclear magnetic resonance, and steering of chemical reactions [8]. The goal is to optimize the cost function corresponding to a set of optimal pulses. The fidelity F of a quantum system is usually taken as the cost function. It is a measure of closeness of two quantum systems and the range can be defined as $0 \leq F \leq 1$, where the fidelity of 1 means that the quantum systems are indistinguishable. But if we use fidelity as a cost function, then we will need to maximize the function. Instead, we use infidelity J as the cost function, which can be written as

$$J = 1 - F = 1 - \frac{1}{d}\left|\mathrm{tr}(U_t^\dagger U_0)\right|^2, \tag{1}$$

where U_0 is the unitary realized by optimal quantum control, U_t is target unitary gate, and d is the dimension of the quantum system.

Gradent based approaches are used to minimize the cost function. A few of the techniques used are GRAPE (Gradient Ascent Pulse Engineering), Krotov, chopped random basis optimization (CRAB), and gradient optimization of analytic controls (GOAT). A modified version of GRAPE called L-BFGS-B is also popular as it uses less memory and converges faster.

A closed quantum system dynamics can be modeled using a Hamiltonian, which represents the energy of a system [9]–[11]. A quantum system will have dynamics that cannot be controlled, such as the interaction between the system elements or J-couplings called the drift Hamiltonian H_0. Meanwhile, there are other externally controllable fields that can be manipulated, such as the time-varying amplitude interacting laser beams called the control Hamiltonian H_j. The combined Hamiltonian of a quantum system can be written as

$$H(t) = H_0 + \sum_{j=1} u_j(t) * H_j, \tag{2}$$

where $u_j(t)$ are time varying amplitude functions or pulses for the specific control.

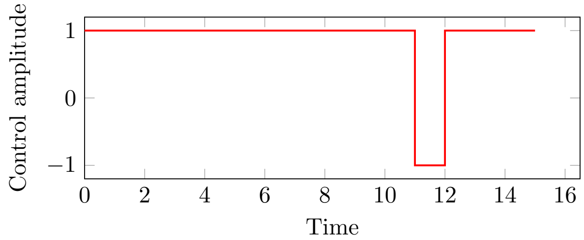

Fig. 1. Initial square pulse

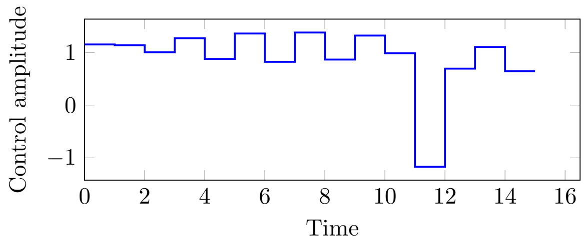

Fig. 2. Optimized control pulse

The quantum systems evolves according to the Schrodinger's equation given as

$$\frac{d\left|\psi\right\rangle}{dt} = -iH(t)\left|\psi\right\rangle. \tag{3}$$

If we assume the control coefficients or pulses in (2) by a piecewise constant approximation, then we can get the solution for (3). Hence, the time evolution operator can be written as

$$U_k = e^{-iH(t_k)\Delta t_k}, \tag{4}$$

where Δt_k is the duration of the single pulse and k is the time slot. If time required for the system to evolve is split into M time slots, then full evolution can be calculated by taking $k = M$ given by

$$U(t_k) = U_k U_{k-1} \ldots U_1 U_0. \tag{5}$$

III. Quantum Optimal Control for Quantum Gate

We demonstrate quantum optimal control working using 'pulseoptim' function in QuTip, which is open-source software for simulating the dynamics of open quantum systems [12]. Suppose we have a single qubit in a constant field in the z direction and a variable field in the x direction. We want to determine control pulses that would apply a $R_x(\pi/2)$ gate on the qubit. The system is governed by the dynamics stated in (2). Here, the drift is the rotation along z, and the control is the rotation along x. The starting point of gate evolution, U_0 is taken as Identity I and target point for gate evolution, U_t is $R_x(\pi/2)$. For our demonstration, we take the number of time slots and time allowed for evolution to be 15. For cost function we chose infidelity defined between U_0 and U_t. We use a simple random square pulse for the initial pulse, as shown in Fig. 1. L-BFGS-B will act act as our optimizer for the cost function.

The algorithm took 6 iterations to converge. The fidelity error was 5.77×10^{-12}. In the Fig. 2, we can see the optimized control pulse given the initial pulse shown in Fig. 1. Using this pulse (control amplitudes), we can produce the target gate evolution within the specified error. Hence, we can drive from U_0 and U_t, effectively implementing the $R_x(\pi/2)$ gate given the defined dynamics of our quantum system.

IV. Conclusion

The development of quantum computers is a challenging task especially making high fidelity quantum gates that work well in the noisy environment. Quantum optimal control is a method that can enable us to design high fidelity gates. In this paper, we demonstrated how quantum optimal control can be used to design the optimal pulses for the control Hamiltonian of a system in order to make a quantum gate that can give us the desired quantum state with high fidelity. This method can be used to design noise robust quantum gates which is crucial in the development of fault-tolerant quantum computers.

Acknowledgments

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2019R1A2C2007037 and 2022R1A4A3033401) and by the MSIT (Ministry of Science and ICT), Korea, under the ITRC (Information Technology Research Center) support program (IITP-2021-0-02046) supervised by the IITP (Institute for Information & Communications Technology Planning & Evaluation).

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