Reinforcement Learning for Quantum State Preparation

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1 Introduction

A central requirement in order to engineer functional quantum computers is the ability to control quantum bits (qubits) robustly, flexibly, and cost-effectively with classical control systems. A fundamental problem in quantum control is quantum state preparation: a dynamical process that involves setting up one or more qubits in a desired configuration. One potential avenue towards improved quantum state preparation is the use of reinforcement learning. Reinforcement learning is a branch of machine learning in which a computer agent learns how best to perform a task using feedback from interactions with its environment. Reinforcement learning has been applied to a variety of quantum physics problems with great success [1] [2] [3] [4] [5]. In 2018 and 2019, M. Bukov et al. and Zheng An and D. L. Zhou established the potential for quantum state preparation using reinforcement learning [6] [7]. In a comparative study on quantum state preparation, X.-M. Zhang et al. demonstrated the advantages of reinforcement learning compared to other machine learning methods in terms of scalability and efficiency [8]. Despite the favourable characteristics of the reinforcement learning approach, performance challenges remain when increasing the set of potential controls and the number of controls applied between the start and end state [8]. Recently, a reinforcement learning framework was developed to incorporate correction for control errors; however, multiple sources of error such as approximation errors and environmental defects were not considered [9]. Moving forward, there are improvements to be made by tailoring reinforcement learning algorithms specifically for quantum state preparation. There is also more work to be done investigating the ability of reinforcement learning to find control solutions that are robust enough to withstand experimental imperfections. The objective of our research is to design and implement a reinforcement learning algorithm which will discover a sequence of discrete controls to bring one qubit from an initial state toward a desired state. The algorithm will maximize fidelity between the final state achieved by the control and the desired state.

2 Background Information

2.1 Quantum States

To discuss quantum state preparation, it is first necessary to define quantum states. In quantum computers, the fundamental unit of information is the quantum bit or qubit. Unlike classical computers, which work in a binary system of 0s and 1s, qubits can exist in a state of superposition. When a property of a qubit, such as spin or momentum, is measured, the state of superposition collapses into one of two possible outcomes. Often these outcomes are labelled as 0 or 1, although the use of 1 and -1 is also common.

Quantum mechanical states are defined in Hilbert spaces. The most convenient way to represent a qubit is in $\mathbb{C}^2$ with orthonormal basis vectors:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The superposition state $|\psi\rangle$ of a qubit can be represented as $|\psi\rangle = a_0 |0\rangle + a_1 |1\rangle$. Here a_0 and a_1 are the complex scalar amplitudes of measuring 0 and 1 respectively. Amplitudes are like probabilities but must be complex to account for quantum effects (superposition and entanglement). $|\psi\rangle$ is a unit vector.

$$\begin{aligned} 1 &= \langle\psi|\psi\rangle \\ &= (\bar{a_0} \langle 0| + \bar{a_1} \langle 1|) \cdot (a_0 |0\rangle + a_1 |1\rangle) \\ &= |a_0|^2 \langle 0|0\rangle + |a_1|^2 \langle 1|1\rangle + \bar{a_0} a_1 \langle 0|1\rangle + \bar{a_1} a_0 \langle 1|0\rangle \\ &= |a_0|^2 + |a_1|^2 \end{aligned}$$

The squares of the absolute values of amplitudes in a quantum system must add to 1. The probability of observing a single state from the superposition is obtained by squaring the absolute value of its amplitude. The state of a qubit $|\psi\rangle = a_0 |0\rangle + a_1 |1\rangle$ can also be represented by points (θ, ϕ) on the unit sphere (also called Bloch sphere) depicted in Figure 1. Here,

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right) |0\rangle + e^{i\phi} \sin\left(\frac{\theta}{2}\right) |1\rangle.$$

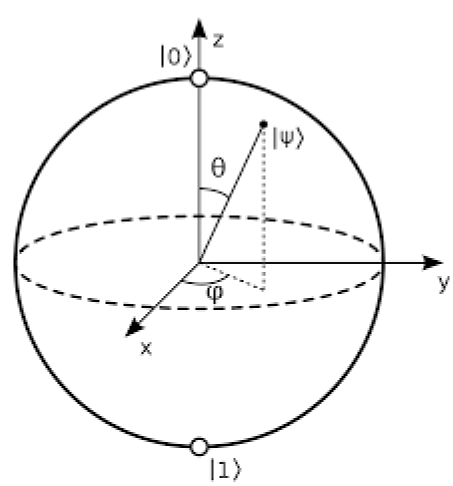

Figure 1: Bloch sphere

2.2 Quantum State Evolution

The basic dynamical assumption of quantum mechanics is that knowing the state at one time, the quantum equations of motion determine what it will be later. The state at time t, denoted $|\psi(t)\rangle$, is given by some operation $U(t)$ acting on the state at time 0. That is, $|\psi(t)\rangle = U(t)|\psi(0)\rangle$. Time evolution in quantum mechanics is linear and unitary. Note that the time evolution of the state-vector is deterministic. Just as in classical physics, incremental change in time leads to a differential equation for the evolution of the state vector:

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = H|\psi\rangle \,. \tag{1}$$

Eqn. 1 is called the generalized Shrödinger equation or the time-dependent Schrödinger equation. $\hbar \approx 1.05457 \times 10^{-34}\ kg\ m^2/s$ is the reduced Planck constant, from now on taken to be 1 for simplicity. H is called the quantum Hamiltonian. It can be represented as a Hermitian matrix and its eigenvalues are the values that would result from measuring the energy of a quantum system. The Hamiltonian differs between quantum systems and is often derived through experimentation. Given an initial state $|\psi_i\rangle$, the solution to Eqn. 1 is easily derived and presented in Eqn. 2.

$$|\psi(t)\rangle = e^{-iHt}|\psi_i\rangle \tag{2}$$

2.3 Spin in a Magnetic Field

Quantum spin is a property, just like position and momentum, that can be attributed to particles (electrons, quarks, neutrinos etc.). The quantum spin is a quantum system in its own right. Just as the Hamiltonian is an operator related to the energy of a system, there are spin operators. Again, these operators are Hermitian matrices whose eigenvalues correspond to the two possible outcomes of measuring the spin component in a specific direction. By convention, the basis states $|0\rangle$ and $|1\rangle$ are taken to be spin up and spin down on the z-axis. The possible outcomes of measurement along the z-axis are spin $+1$ and spin -1. Similarly, the spin can be measured along the x-axis and y-axis. In this case, the orthogonal states are $\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$ and $\frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle$, and $\frac{1}{\sqrt{2}}|0\rangle + \frac{i}{\sqrt{2}}|1\rangle$ and $\frac{1}{\sqrt{2}}|0\rangle - \frac{i}{\sqrt{2}}|1\rangle$ respectively. Altogether, this yields the following spin operators:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

Particles can have a permanent magnetic moment along the direction of their spin, and this magnetic moment gives rise to electromagnetic interactions that depend on the spin. An example Hamiltonian for a two-level spin system controlled by magnetic fields h_t^x and h_t^z applied along the x-axis and z-axis is given in Eqn. 3.

$$H = -h_t^x \sigma_x - h_t^z \sigma_z \tag{3}$$

The Hamiltonian specified in Eqn. 3 and the differential equation in Eqn. 1 together with some initial state $|\psi_i\rangle$ and desired state $|\psi_f\rangle$ provide a control problem.

2.4 Noise

Perhaps the greatest challenge in quantum computing arises from errors broadly known as decoherence. Dephasing is a common source of error which occurs when there is fluctuation in a magnetic field along the z-axis [10]. When some dephasing noise η_t is introduced to the Hamiltonian in Eqn. 3, it becomes a stochastic control problem which can be solved using reinforcement learning. The system is now that shown in Eqn. 4.

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = (\eta_t \sigma_z - h_t^x \sigma_x - h_t^z \sigma_z) |\psi\rangle \tag{4}$$

The noise η_t can be modelled as a Gaussian distribution with zero mean [11].

3 Problem Description

3.1 Model

The previous section has provided the background necessary to present the stochastic control problem we aim to solve using reinforcement learning. Consider the problem of preparing a quantum state $|\psi_f\rangle$ from an initial state $|\psi_i\rangle$ in a finite time τ in n steps. We study the Hamiltonian introduced in Eqn. 3 for spin in a magnetic field. At each time t, a constant magnetic field $h_t = (h_t^x, h_t^z)$ is applied for the time step $\Delta t = \frac{\tau}{n}$ and some dephasing noise η_t drawn from a zero-mean Gaussian distribution is present. Together this yields the Hamiltonion in Eqn. 5.

$$H_t = \eta_t \sigma_z - h_t^x \sigma_x - h_t^z \sigma_z \tag{5}$$

Overall, the state evolves according to the model in Eqn. 6.

$$|\psi_{t+1}\rangle = e^{-iH_t \Delta t} |\psi_t\rangle \tag{6}$$

The set of states is given by

$$\mathbb{X} := \left\{ |\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle : 0 \leq \theta \leq \pi, 0 \leq \phi \leq 2\pi \right\}$$

which correspond to points on the Bloch sphere. In practice, there is a maximum and minumum possible magnetic field strength within which the control can be tuned so the set of controls can be simplified to

$$\mathbb{U} := \{h = (h^x, h^z) : h_i \in \{h_{min}, h_{min} + \Delta, h_{min} + 2\Delta, \ldots, h_{max}\},\ i = x, z\}$$

where $\Delta = (h_{max} - h_{min})/M$, so that each component of the control field can take $M + 1$ values including h_{min} and h_{max} for some $M \in \mathbb{Z}_{>0}$.

The fidelity between the two states $|\psi_0\rangle$ and $|\psi_1\rangle$ is given by in Eqn. 7.

$$F(\psi_0, \psi_1) = |\langle\psi_0|\psi_1\rangle|^2 \tag{7}$$

Consider the cost function in Eqn. 8, which rewards fidelity between the current state $|\psi_t\rangle$ and the target state $|\psi_f\rangle$.

$$c(|\psi_t\rangle, h_t) = \begin{cases} 100F(\psi_t, \psi_f)^3 & 0 \leq F(\psi_t, \psi_f) < 0.99 \\ 5000 & 0.99 \leq F(\psi_t, \psi_f) \leq 1 \end{cases} \tag{8}$$

Altogether, the model in Eqn. 6, the state space $\mathbb{X}$, the action space $\mathbb{U}$, and the cost function in Eqn. 8 constitue a Markov control problem.

3.2 Controllability

Before proceeding with the algorithm design, we first verify the controllability of the system. In many situations, the Schrödinger equation introduced in Section 2 takes the form of the system in Eqn. 9, where $H_0, \ldots, H_m$ are $n \times n$ Hermitian matrices.

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = \left(H_0 + \sum_{i=1}^{m} H_i u_i(t) \right) |\psi\rangle \tag{9}$$

Such a system is (pure state) controllable if for every pair of initial and final states, $|\psi_i\rangle$ and $|\psi_f\rangle$, there exist control functions $u_1(t), \ldots, u_m(t)$ and a time $\tau > 0$ such that the solution of Eqn. 9 at time τ, with initial condition $|\psi_i\rangle$, is $|\psi(\tau)\rangle = |\psi_f\rangle$ [12].

Eqn. 9 can be transformed into the equivalent system given in Eqn. 10.

$$\frac{\partial |\psi\rangle}{\partial t} = A|\psi\rangle + \sum_{i=1}^{m} B_i |\psi\rangle u_i(t) \tag{10}$$

Under the assumption that $u_1, \ldots, u_m$ are piecewsie continuous functions, there is an equivalent characterization of controllability. Namely, the system is controllable if the matrices $B_1, \ldots, B_m$ generate the Lie-algebra of $n \times n$ skew-Hermitian matrices with zero trace [12].

For the specific Hamiltonian introduced in Eqn. 5,

$$A = -i\eta_t\sigma_z \text{ and } B_1 = i\sigma_x = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \text{ and } B_2 = i\sigma_z = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}.$$

Since B_1 and B_2 are skew-Hermitian with zero trace and linearly independent, they form a basis for the Lie-algebra of 2×2 skew-Hermitian matrices with zero trace (for details see [13]). As a result, the overall system in Eqn. 6 is controllable.

References

[1] X.-M. Zhang, Z.-W. Cui, X. Wang, and M.-H. Yung, "Automatic spin-chain learning to explore the quantum speed limit," *Physical Review*, vol. 97, 052333 2018.

[2] T. Fosel, P. Tighineanu, T. Weiss, and F. Marquardt, "Reinforcement learning with neural networks for quantum feedback," *Physical Review*, vol. 8, 031084 2018.

[3] J. Halverson, B. Nelson, and F. Ruehle, "Branes with brains: Exploring string vacua with deep reinforcement learning," *Journal of High Energy Physics*, 6 2019.

[4] N. D. H. P. Nautrup, V. Dunjko, H. J. Briegel, and N. Friis, "Optimizing quantum error correction codes with reinforcement learning," *Quantum*, vol. 3, p. 215, 2019.

[5] A. A. Melnikov, H. P. Nautrup, M. Krenn, V. Dunjko, M. Tiersch, A. Zeilinger, and H. J. Briegel, "Active learning machine learns to create new quantum experiments," *Proceedings of the National Academy of Sciences of the United States of America*, vol. 115, no. 6, pp. 1221–1226, 2018.

[6] M. Bukov, A. G. R. Day, D. Sels, P. Weinberg, A. Polkovnikov, and P. Mehta, "Reinforcement learning in different phases of quantum control," *Physical Review*, no. 3, 2018.

[7] Z. An and D. L. Zhou, "Deep reinforcement learning for quantum gate control," *EPL*, vol. 126, no. 60002, 2019.

[8] X.-M. Zhang, Z.-W. Cui, X. Wang, and M.-H. Yung, "When does reinforcement learning stand out in quantum control? a comparative study on state preparation," *NPJ Quantum Information*, vol. 5, no. 85, 2019.

[9] M. Y. Niu, S. Boixo, V. N. Smelyanskiy, and H. Neven, "Universal quantum control through deep reinforcement learning," *NPJ Quantum Information*, vol. 5, no. 33, 2019.

[10] "Quantum noise and error correction," in *Quantum Computing Explained*. John Wiley & Sons, Ltd, 2007, ch. 12, pp. 251–278.

[11] T. Zaborniak and R. de Sousa, "Benchmarking hamiltonian noise in the d-wave quantum annealer," *IEEE Transactions on Quantum Engineering*, vol. 2, 1–6, 2021.

[12] D. D'Alessandro, *Introduction to Quantum Control and Dynamics*, ser. Chapman & Hall/CRC Applied Mathematics & Nonlinear Science. Taylor & Francis, 2007.

[13] D. D'Alessandro, "Topological properties of reachable sets and the control of quantum bits," *Systems & Control Letters*, vol. 41, 213–221, 2000.