# Quantum Logic Gate Synthesis as a Markov Decision Process

M. Sohaib Alam email: sohaib@rigetti.com<sup>1</sup>

<sup>1</sup>Rigetti Computing, 2919 Seventh Street, Berkeley, CA, 94710-2704 USA (Dated: December 30, 2019)

Reinforcement learning has witnessed recent applications to a variety of tasks in quantum programming. The underlying assumption is that those tasks could be modeled as Markov Decision Processes (MDPs). Here, we investigate the feasibility of this assumption by exploring its consequences for two of the simplest tasks in quantum programming: state preparation and gate compilation. By forming discrete MDPs, focusing exclusively on the single-qubit case, we solve for the optimal policy exactly through policy iteration. We find optimal paths that correspond to the shortest possible sequence of gates to prepare a state, or compile a gate, up to some target accuracy. As an example, we find sequences of H and T gates with length as small as 11 producing  $\sim 99\%$  fidelity for states of the form  $(HT)^n|0\rangle$  with values as large as  $n=10^{10}$ . This work provides strong evidence that reinforcement learning can be used for optimal state preparation and gate compilation for larger qubit spaces.

#### INTRODUCTION

Recent years have seen dramatic advances in the field of artificial intelligence [14] and machine learning [9, 17]. A long term goal is to create agents that can carry out complicated tasks in an autonomous manner, relatively free of human input. One of the approaches that has gained popularity in this regard is reinforcement learning. This could be thought of as referring to a rather broad set of techniques that aim to solve some task based on a reward-based mechanism [19]. Formally, reinforcement learning models the interaction of an agent with its environment as a Markov Decision Process (MDP). In many practical situations, the agent may have limited access to the environment, whose dynamics can be quite complicated. In all such situations, the goal of reinforcement learning is to learn or estimate the optimal policy, which specifies the (conditional) probabilities of performing actions given that the agent finds itself in some particular state.

On the other hand, in fairly simple environments such as the textbook grid-world scenario [19], the dynamics can be fairly simple to learn. Moreover, the state and action spaces are finite and small, allowing for simple tabular methods instead of more complicated methods that would, for example, necessitate the use of artificial neural networks [9]. In particular, one could use the dynamic programming method of policy iteration to solve for the optimal policy exactly [4].

In recent times, reinforcement learning has met with success in a variety of quantum programming tasks, such as error correction [8], combinatorial optimization problems [12], as well as state preparation [1, 3, 5, 6, 21] and gate design [2, 13] in the context of noisy control. Here, we investigate the question of state preparation and gate compilation in the context of abstract logic gates, and

ask whether reinforcement learning could be successfully applied to learn the optimal gate sequences to prepare some given quantum state, or compile a specified quantum gate. Instead of exploring the efficacy of any one particular reinforcement method, we investigate whether it is even feasible to model these tasks as MDPs. By discretizing state and action spaces in this context, we circumvent questions and challenges involving convergence rates, reward sparsity, and hyper-paremeter optimization that typically show up in reinforcement learning scenarios. Instead, the discretization allows us to exactly solve for and study quite explicitly the properties of the optimal policy itself. This allows us to test whether we can recover optimally short programs using reinforcement learning techniques in quantum programming situations where we already have well-established notions of what those optimally short programs, or circuits, should look

There have been numerous previous studies in the general problem of quantum compilation, including but not limited to, the Solovay-Kitaev algorithm [7], quantum Shannon decomposition [18], approximate compilation [10, 15], as well as optimal circuit synthesis [11, 16, 20]. Here, we aim to show that optimally short circuits could be found through solving discrete MDPs, and that these circuits agree with independently calculated shortest possible gate sequences for the same tasks.

The organization of this paper is as follows. We first briefly review the formalism of MDPs. We then investigate the problem of single-qubit state preparation using a discretized version of the continuous  $\{RZ,RY\}$  gates, as well as the discrete gateset  $\{I,H,S,T\}$ , followed by the investigation of the problem of single-qubit compilation into the  $\{H,T\}$  gateset.

#### **Brief Review of MDPs**

Markov Decision Processes (MDPs) provide a convenient framing of problems involving an agent interacting with an environment. At discrete time steps t, an agent receives a representation of the environment's state  $s_t \in \mathcal{S}$ , takes an action  $a_t \in \mathcal{A}$ , and then receives a scalar reward  $r_{t+1} \in \mathcal{R}$ . The policy of the agent, describing the conditional probability  $\pi(a|s)$  of taking action a given the state s, is independent of the environment's state at previous time steps and therefore satisfies the Markov property. The discounted return that an agent receives from the environment after time step t is defined as  $G_t = \sum_{k=0}^{\infty} \gamma^k r_{t+k+1}$  where  $\gamma \in [0,1]$  is the discount factor. The goal of the agent is then to find the optimal policy  $\pi^*(a|s)$  that maximizes the state-value function (henceforth, "value function" for brevity), defined as the expectation value of the discounted return received from starting in state  $s_t \in \mathcal{S}$  and thereafter following the policy  $\pi(a|s)$ , and expressed as  $V_{\pi}(s) = \mathbb{E}_{\pi}[G_t|S_t = s]$ . More formally then, the optimal policy  $\pi^*$  satisfies the inequality  $V_{\pi^*}(s) \geq V_{\pi}(s)$  for all  $s \in \mathcal{S}$  and all policies  $\pi$ . For finite MDPs, there always exists a deterministic The value function for the optimal optimal policy. policy is then defined as the optimal value function  $V^*(s) = V_{\pi^*}(s) = \max_{\pi} V_{\pi}(s) \text{ for all } s \in \mathcal{S}.$ 

The value function satisfies a recursive relationship known as the  $Bellman\ equation$ 

$$V_{\pi}(s) = \sum_{a} \pi(a|s) \sum_{s',r} p(s',r|s,a) [r + \gamma V_{\pi}(s')]$$
 (1)

relating the value of the current state to that of its possible successor states following the policy  $\pi$ . Note that the conditional probability of finding state s' and receiving reward r having performed action a in state s specifies the environment dynamics, and also satisfies the Markovian property. This equation can be turned into an iterative procedure known as iterative policy evaluation

$$V_{k+1}(s) = \sum_{a} \pi(a|s) \sum_{s',r} p(s',r|s,a) [r + \gamma V_k(s')]$$
 (2)

which converges to the fixed point  $V_k = V_\pi$  in the  $k \to \infty$  limit, and can be used to obtain the value function corresponding to the given policy  $\pi$ . In practice, we define convergence as  $|V_{k+1} - V_k| < \epsilon$  for some sufficiently small  $\epsilon$ .

Having found the value function, we could then ask if the policy that produced this value function could be further improved. To do so, we need the state action value function  $Q_{\pi}(s, a)$ , defined as the expected return by carrying out action a in state s and thereafter following the policy  $\pi$ , i.e.  $Q_{\pi}(s, a) = \mathbb{E}_{\pi} [G_t | S_t = s, A_t = a]$ . According to the policy improvement theorem, given deterministic policies  $\pi$  and  $\pi'$ , the inequality  $Q_{\pi}(s, \pi'(s)) \geq V_{\pi}(s)$ 

implies  $V_{\pi'}(s) \geq V_{\pi}(s)$  where  $\pi'(s) = a$ , and in general  $\pi'(s) \neq \pi(s)$ , for all  $s \in \mathcal{S}$ . In other words, having found the value function corresponding to some policy, we can then improve upon that policy by iterating through the action space  $\mathcal{A}$  while maintaining the next-step value functions on the right hand side of Eq. (2) to find a better policy than the current one.

We can then alternate between policy evaluation and policy improvement in a process known as policy iteration to obtain the optimal policy. Schematically, this process involves evaluating the value function for some given policy up to some small convergence factor, followed by the improvement of the policy that produced this value function. The process terminates when the improved policy stops differing from the policy in the previous iteration. Of course, this procedure to identify the optimal policy for an MDP relies on the finiteness of the state and action spaces. As we will see below, by discretizing the space of pure 1-qubit states, as well as identifying a finite gate set, we create an MDP with the goal of state preparation for which optimal policies in the form of optimal quantum circuits may be found through this method.

One could view state evolution under unitary operations or left multiplication of unitaries by other unitaries as deterministic processes. These could be thought of as trivially forming a Markov Decision Process where the probabilities p(s'|s,a) have a  $\delta$ -function support on some (point-like) state s'. Once we impose discretization, this underlying determinism implies that the dynamics of the discrete states are strictly speaking non-Markovian, i.e. the conditional probability of landing in some discrete state s' depends not just on the previous discrete state and action, but also on all the previous states and actions, since the underlying continuous/point-like state evolves deterministically. However, we shall see below that with sufficient care, both the tasks of state preparation and gate compilation can be modeled and solved as MDPs.

# PREPARATION OF SINGLE-QUBIT STATES

In this section, we will discuss the preparation of singlequbit states as an MDP. In particular, we will focus on preparing a discrete version of the  $|1\rangle$  state. We will do so using two different gate sets, a discretized version of the continuous RZ and RY gates, and the set of naturally discrete gates I, H, S and T, and describe probabilistic shuffling within discrete states to arrive at optimal quantum programs via optimal policies. We will also consider states of the form  $(HT)^n|0\rangle$ .

### State and Action Spaces

We apply a fairly simple scheme for the discretization of the space of pure 1-qubit states. As is well known, this space has a one-to-one correspondence with points on a 2-sphere, commonly known as the Bloch sphere. With  $\theta \in [0,\pi]$  denoting the polar angle and  $\phi \in [0,2\pi]$  denoting the azimuthal angle, an arbitrary pure 1-qubit state can be represented as

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$
 (3)

The discretization we adopt here is as follows. First, we fix some small number  $\epsilon = \pi/k$  for some positive integer k. Next, we identify polar caps around the north  $(\theta = 0)$  and south  $(\theta = \pi)$  pole. The northern polar cap is identified as the set of all 1-qubit (pure) states for which  $\theta < \epsilon$  for some fixed  $\epsilon$ , regardless of the value of  $\phi$ . Similarly, the southern polar cap is identified as the set of all 1-qubit (pure) states for which  $\theta > \pi - \epsilon$ , independent of  $\phi$ . Apart from these special regions, the set of points  $n\epsilon \leq \theta \leq (n+1)\epsilon$  and  $m\epsilon \leq \phi \leq (m+1)\epsilon$  for some positive integers  $n, m \leq k$  are identified as the same region.

We identify every region as a "state" in the MDP. As a result of this identification, elements of the space of 1-qubit pure states are mapped onto a discrete set of states such that the 1-qubit states can now only be identified up to some threshold fidelity. For instance, the  $|0\rangle$  state is identified as the northern polar cap with fidelity  $\cos^2\left(\frac{\pi}{2k}\right)$ . Similarly, the  $|1\rangle$  state is identified with the southern polar cap with fidelity  $\sin^2\left(\frac{(k-1)\pi}{2k}\right) = \cos^2\left(\frac{\pi}{2k}\right)$ . In other words, if we were to try and obtain these states using this scheme, we would only be able to obtain them up to these fidelities.

Having identified a finite state space  $\mathcal S$  composed of discrete regions of the Bloch sphere, we next identify single-qubit unitary operations, or gates, as the action space  $\mathcal A$ . There are some natural single-qubit gate sets that are already discrete, such as  $\{H,T\}$ . Others, such as the continuous rotation gates  $\{RZ,RY\}$ , require discretization similar to that of the continuous state space of the Bloch sphere. We discretize the continuous gates  $RZ(\beta)$  and  $RY(\gamma)$  by discretizing the angles  $\beta,\gamma\in[0,2\pi]$ . The resolution  $\delta=\pi/l$  must be sufficiently smaller than that of the state space  $\epsilon=\pi/k$  so that all states  $s\in\mathcal S$  are accessible from all others via the discretized gateset  $a\in\mathcal A$ . In practice, a ratio of  $\epsilon/\delta\sim O(10)$  is usually sufficient, although the larger this ratio, the better the optimal circuits we would find.

Without loss of generality, and for illustrative purposes, we identify the discrete state corresponding to

the  $|1\rangle$  state (hereafter referred to as the "discrete  $|1\rangle$  state") as the target state of our MDP. To prepare the  $|1\rangle$  state starting from any pure 1-qubit state using the gates RZ and RY, it is well-known that we require at most a single RZ rotation followed by a single RY rotation. For states lying along the great circle through the x and z axes, we need only a single RY rotation. As a test of this discretized procedure, we investigate whether solving this MDP would be able to reproduce such optimally short gate sequences. We also consider the gateset  $\{I, H, T\}$ , where we include the identity gate to allow for the goal state to "do nothing" and remain in its state. For simplicity and illustrative purposes, we also include the  $S=T^2$  gate in the case of single-qubit state preparation.

### Reward Structure and Environment Dynamics

An obvious guess for a reward would be the fidelity between the target stated  $|\psi\rangle$  and the prepared state  $|\phi\rangle$ , i.e.  $|\langle\phi|\psi\rangle|^2$ . However, here we consider an even simpler reward structure of assigning +1 to the target state, and 0 to all other states. This allows us to relate the length of optimal programs to the value function corresponding to the optimal policy, as we'll see below. To finish our specification of the MDP, we also estimate the environment dynamics p(s', r|s, a). Since our reward structure specifies a unique reward r to every state  $s' \in \mathcal{S}$ , these conditional probabilities reduce to simply p(s'|s,a). A simple way to estimate these probabilities is to uniformly sample points on the 2-sphere, determine which discrete state they land in, then perform each of the actions to determine the state resulting from this action. Although other means of estimating these probabilities also exist, we find that this simple method works quite well in practice for the particular problem of single-qubit state preparation.

Note that for the target state  $|1\rangle$ , the optimal policy is to just apply the identity, i.e. RZ(0) or RY(0). This action will continue to keep this state in the target state, while yielding +1 reward at every time step. This yields an infinite series  $V_{\pi^{\star}}(s_{target}) = \sum_{k=0}^{\infty} \gamma^k$ , which we can trivially sum to obtain  $(1-\gamma)^{-1}$ . This is the highest value of any state on the discretized Bloch sphere. For  $\gamma=0.8$ , we obtain  $V_{\pi^{\star}}(s_{target})=5.0$ . Using the Bellman equation for states that are removed by a single non-identity instruction from the target state  $s_{one} \in \mathcal{S}$ , we have

$$V_{\pi^*}(s_{one}) = p_t(1 - \gamma)^{-1} + \sum_{s'} p_{s'} \gamma V_{\pi^*}(s')$$
 (4)

where  $p_k$  denotes the probability of obtaining state k upon taking the action  $\pi^*(s)$ . Since the states

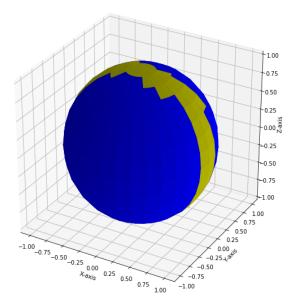


FIG. 1. Optimal values for various states on the Bloch sphere using the discrete RZ and RY gates, with a discount factor  $\gamma=0.8$ . States colored in yellow are those for which  $V_{\pi'}>=4.0$ , while those colored in blue are those for which  $V_{\pi'}<4.0$ . Those colored in yellow are also exactly the states whose optimal circuits to prepare the discrete  $|1\rangle$  state consist of a single RY rotation, while those in blue are also exactly the ones whose optimal circuits consist of an RZ rotation followed by an RY rotation.

s' are by definition non-target states, we have that  $V_{\pi^{\star}}(s') \leq \sum_{k=1}^{\infty} \gamma^k r_{t+k+1} = \gamma/(1-\gamma)$ . Since we have  $p_t + \sum_{s'} p_{s'} = 1$ , and  $0 \leq \gamma \leq 1$ , we have  $p_t + \sum_{s'} \gamma^2 p_{s'} \leq 1$ . From this, it follows that the expression in Eq. 4 is bounded above by  $V_{\pi^{\star}}(s_{target}) = (1-\gamma)^{-1}$ . Thus, the optimal value function for states removed by a single program instruction from the target state will have less than the optimal value for the target state. For states that are removed by two program instructions from the target state,  $s_{two} \in \mathcal{S}$ , we have  $V_{\pi^{\star}}(s_{two}) \leq \gamma \sum_{s_{one}} V_{\pi^{\star}}(s_{one})$ , and so (for  $|\gamma| < 1$ ), will have even less of an optimal value than those removed by a single program instruction from the target state. This intimately relates the length of the optimal program with the optimal value function.

The optimal value landscape for the two gatesets are shown in Figs. (1) and (2). Note that while in the case of the discretized  $\{RZ,RY\}$  gates we have a distinguished ring of states along the x-axis that are only a single gate application away from the target state, we have no such special region for the  $\{I,H,S,T\}$  gateset, using which states that are nearby on the Bloch sphere need not share similar optimal policies or optimal paths to the target state.

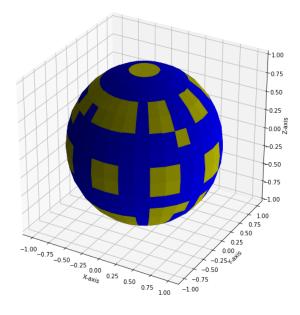


FIG. 2. Optimal value landscape across the Bloch sphere using the gates I, H, S, and T, with a discount factor  $\gamma = 0.95$ . States colored in yellow are those for which  $V_{\pi'} >= 1.0$ , while those colored in blue are those for which  $V_{\pi'} < 1.0$ . There is no clear region of the Bloch sphere that is especially advantageous to start from in order to reach the target  $|1\rangle$  state.

# **Optimal State Preparation Sequences**

Using policy iteration allows us to solve for the optimal policy in an MDP. The optimal policy dictates the best action to perform in a given state. We can chain the actions drawn from the optimal policy together to find an optimal sequence of actions, or gates, to reach the target state. In our case, the actions are composed of unitary operations, which deterministically evolve a quantum state. However, due to the discretization, this is no longer true in our MDP, where the states evolve according to the non-trivial probabilities p(s'|s,a). The optimal policy is learned with respect to these stochastic dynamics, and not with respect to the underlying deterministic dynamics. Therefore, as an example, if we simply start with some specific quantum state, and apply a sequence of actions drawn from the optimal policy of the discrete states that the evolving quantum states belong to, we might not necessarily find ourselves in the target (discrete) state. Instead, to mimic the stochastic dynamics, we must allow room to shuffle our quantum states within the discrete states. Moreover, we sample several paths that lead from the starting state and terminate in the goal (discrete) state, and report the one with the smallest length as the optimal program we're interested in. Schematically, this can be described in pseudo-code as follows.

# Algorithm 1 Optimal State Preparation Sequence

```
1: Initialize empty array Optimal-Programs
2: for s \in \mathcal{S} do
       Initialize empty list Convergent-Programs
3:
       for i = 1 to K do
 4:
            Converged \leftarrow False
 5:
            while not Converged
 6:
                 State \leftarrow s
 7:
                 Prog \leftarrow Empty Program list
8:
9:
                 Counter \leftarrow 0
10:
                 while Counter < MaxCounter
                      Action \leftarrow Optimal-Policy[State]
11:
                      Prog.append(Action)
12:
                      Next-State \leftarrow Env.Step(Action)
13:
                      State \leftarrow Next-State
14:
15:
                      Counter \leftarrow Counter + 1
16:
                      if STATE = TARGET-STATE
17:
                           Converged \leftarrow True
18:
                           Convergent-
    Programs.append(Prog)
19:
       end for
       Optimal-Prog 

Program with Min length in
20:
    Convergent-Programs
       Optimal-Programs[s] \leftarrow Optimal-Prog
21:
22: end for
```

In the above, when we assign s to some state, we are implicitly choosing some random quantum state within the discrete state s. Likewise, when we perform the environment step, we may shuffle the quantum state within the same discrete state before evolving it under the applied action. If we can obtain convergent sequences without this shuffling in the environment steps, we would preferentially avoid it and restrict the shuffling only to the starting state, since the fidelities in the target states from sequences that only differ in their starting states is the same as the fidelities of the starting states, i.e.  $\langle \psi_i' | \psi_i \rangle = \langle \psi_i' | U^{\dagger} U | \psi_i \rangle = \langle \psi_f' | \psi_f \rangle$ , where  $|\psi_i\rangle$  and  $|\psi_i'\rangle$  are two different initial pure states that belong to the same initial discrete state. the other hand, if we allow shuffling of pure states within discrete states during the environment step, then we have  $\langle \psi_f' | \psi_f \rangle = \langle \psi_i' | U_1^{\dagger} U_s^{(1)} ... U_s^{(n-1)} U_n^{\dagger} \rangle$  $U_nU_s^{(n)}...U_s^{(2n-2)}U_1|\psi_i\rangle \neq \langle \psi_i'|\psi_i\rangle$ , in general. Therefore, we would like to avoid shuffling as much as possible, making it necessary only when we are unable to find convergent paths otherwise.

This algorithm described above can used to generate optimal programs for any given (approximately universal) single-qubit gateset. In the case of discrete RZ and RY gates, we find what we would expect—at most, a single RZ rotation followed by a single RY rotation to get from anywhere on the Bloch sphere to the (discrete)  $|1\rangle$  state. For (discrete) states lying along the X-axis, we need only apply a single RY rotation. Empirically,

we chose a state resolution of  $\epsilon=\pi/16$  so that we would find sequences generating the pure  $|1\rangle$  state from various discrete states across the Bloch sphere with  $\cos^2\left(\frac{\pi}{32}\right)\sim 99\%$  fidelity. The optimal programs we find via the preceding procedure for this gateset are composed of programs with lengths either 1 or 2. Using the  $\{I,H,S,T\}$  gateset, as examples, we find the optimal gate sequence HSSH=HZH=X for the discrete state  $|0\rangle$ , while for the discrete state containing the  $|+\rangle$  state, we find the optimal gate sequence SSH=ZH.

We can also use the procedure described above to obtain approximations to the states  $(HT)^n |0\rangle$  for integers  $n \geq 1$ . The unitary HT can be thought of as a rotation by an angle  $\theta = 2\arccos\left(\frac{\cos(7\pi/8)}{\sqrt{2}}\right)$  about an axis  $\vec{n} = (n_x, n_y, n_z) = \sqrt{\frac{1}{17}} \left(5 - 2\sqrt{2}, 7 + 4\sqrt{2}, 5 - 2\sqrt{2}\right)$ . The angle  $\theta$  has the continued fraction representation

$$\theta = \pi + \frac{\cos\left(\frac{\pi}{8}\right)\sqrt{2 - \cos^2\left(\frac{\pi}{8}\right)}}{1 + K_{k=1}^{\infty} \frac{-\cos^2\left(\frac{\pi}{8}\right)\lfloor\frac{1+k}{2}\rfloor\left(-1+2\lfloor\frac{1+k}{2}\rfloor\right)}{1+2k}}$$
(5)

which is infinite, and thus the angle  $\theta$  is irrational. The states  $(HT)^n|0\rangle$  lie along an equatorial ring about the axis  $\vec{n}$ , and no two states  $(HT)^n|0\rangle$  and  $(HT)^m|0\rangle$  are equal for  $n \neq m$ . Although as their form makes explicit, these states can be reproduced exactly using the gates H and T, using our procedure, they can only be obtained up to some fidelity controlled by the discretization as described above. The advantage is that we can obtain good approximations to these states with a very few gates. This is illustrated in the table below where short gate sequences can reproduce states of the form  $(HT)^n|0\rangle$  for very large values of n. In principle, we may keep on increasing the value of n, and would only be preparing some state from among a finite set of states that span the equatorial ring about the axis of rotation. Empirically, we choose to investigate till  $n=10^{10}$ . The sequences in Table (I) are to be read right to left.

TABLE I. Gate sequences to produce states  $(HT)^n|0\rangle$  up to  $\sim 99\%$  fidelity.

Gate sequence
TTHTHTHTH
TTTHTHTTTH
HTH
HTH
HTTTTHTH
HTTTTTHTHTHTHTTTTH
I
I
HTTTHTHTHTH

As we noted earlier, the resolution of the discretization

sets the fidelity bound. However, we also noted that initializing a discrete state amounts to initializing to some arbitrary point on the Bloch sphere lying within that discrete state. This means that when we set our starting state to the discrete  $|0\rangle$  state, we are really initializing our quantum state to some state that is close but not necessarily equal to  $|0\rangle$ . Although it remains true that for some quantum state within the discrete northern polar cap, the gate sequences shown above result in their respective states with at least 99% fidelity using a discrete resolution of  $\pi/16$ , it is not a priori necessary that the same holds true if our starting state is truly the  $|0\rangle$ . We find in practice that the lower bound of 99% is therefore not always respected, but that the gate sequences above nevertheless still converge to their target states with approximately 99% fidelity.

### COMPILATION OF SINGLE-QUBIT GATES

In the previous section, we considered an agentenvironment interaction in which we identified Hilbert space as the state space, and the space of SU(2) gates as the action space. Shifting our attention to the problem of quantum gate compilation, we now identify both the state and action spaces with the space of SU(2) matrices, where for convenience we ignore an overall U(1)phase from the true group of single-qubit gates U(2). We first consider an appropriate coordinate system to use, and discuss why the quaternions are better suited to this task than Euler angles. We focus exclusively on the gateset  $\{I, H, T\}$ , and modify the reward structure slightly so that we now have to work with the probabilities p(s', r|s, a) instead of the simpler p(s'|s, a) as in the previous section. We present empirical results for a few randomly chosen (special) unitaries.

### Coordinate system

We consider the gateset  $\{I, H, T\}$ . We include the identity in our gate set since we would like the target state to possess the highest value, and have the agent do nothing in the target state under the optimal policy. Because we would like to remain in the space of SU(2) matrices, we define  $H = RY(\pi/2)RZ(\pi)$ , which differs from the usual definition by an overall factor of i, and  $T = RZ(\pi/4)$ . Note that owing to our alternative gate definitions, we have that  $H^2 = T^8 = -1 \neq 1$  so that we may obtain up to 3 and 15 consecutive applications of H and T respectively in the optimal program. Next, we choose an appropriate coordinate system. One choice is to parametrize an arbitrary  $U \in SU(2)$  using the ZYZ-Euler angle decomposition. Under this parametrization,

given some  $U \in SU(2)$ 

$$U = U(a, b, c, d) = \begin{pmatrix} a + ib & c + id \\ -c + id & a - ib \end{pmatrix}$$
 (6)

such that  $a^2 + b^2 + c^2 + d^2 = 1$ , we can write  $U = RZ(\alpha)RY(\beta)RZ(\gamma)$  with

$$\alpha = \alpha(a, b, c, d) = \arctan(-b/a) + \arctan(-d/c)$$

$$\beta = \beta(a, b, c, d) = 2\arccos(\sqrt{a^2 + b^2})$$

$$\gamma = \gamma(a, b, c, d) = \arctan(-b/a) - \arctan(-d/c)$$
(7)

for some angles  $\alpha$ ,  $\beta$  and  $\gamma$ . Note that for  $\beta = 0$ , we have a continuous degeneracy of choices in  $\alpha$  and  $\gamma$  to specify some  $RZ(\delta)$  with  $\alpha + \gamma = \delta$ . However, the transformations above will conventionally fix this to  $\alpha = \gamma = \delta/2$ .

Under the action of T, i.e.  $T:U\to U'=TU=RZ(\alpha')RY(\beta')RZ(\gamma')$ , or equivalently  $T:(\alpha,\beta,\gamma)\to(\alpha',\beta',\gamma')$ , the ZYZ-coordinates transform rather simply as  $\alpha'=\alpha+\pi/4$ ,  $\beta'=\beta$ ,  $\gamma'=\gamma$ . Under a similar action of H however, the coordinates transform non-trivially. The matrix entries, on which these parameters depend, transform as

$$a' = \frac{1}{\sqrt{2}} \left[ \sin\left(\frac{\alpha - \gamma}{2}\right) \sin\left(\frac{\beta}{2}\right) - \sin\left(\frac{\alpha + \gamma}{2}\right) \cos\left(\frac{\beta}{2}\right) \right]$$

$$b' = \frac{-1}{\sqrt{2}} \left[ \cos\left(\frac{\alpha - \gamma}{2}\right) \sin\left(\frac{\beta}{2}\right) + \cos\left(\frac{\alpha + \gamma}{2}\right) \cos\left(\frac{\beta}{2}\right) \right]$$

$$c' = \frac{1}{\sqrt{2}} \left[ \sin\left(\frac{\alpha - \gamma}{2}\right) \sin\left(\frac{\beta}{2}\right) + \sin\left(\frac{\alpha + \gamma}{2}\right) \cos\left(\frac{\beta}{2}\right) \right]$$

$$d' = \frac{1}{\sqrt{2}} \left[ \cos\left(\frac{\alpha - \gamma}{2}\right) \sin\left(\frac{\beta}{2}\right) - \cos\left(\frac{\alpha + \gamma}{2}\right) \cos\left(\frac{\beta}{2}\right) \right]$$
(8)

This is a non-volume preserving operation for which

$$\det(J) = \frac{\sin(\beta)}{\sqrt{1 - \cos^2(\alpha)\sin^2(\beta)}} \tag{9}$$

where J denotes the Jacobian of the transformation from  $(\alpha, \beta, \gamma)$  to  $(\alpha', \beta', \gamma')$  under the action of H, and which diverges for values of  $\alpha$  and  $\beta$  such that  $\cos(\alpha)\sin(\beta) = \pm 1$ . This implies that for such pathological values, a unit hypercube in the discretized  $(\alpha, \beta, \gamma)$ space gets mapped to a region that covers indefinitely many unit hypercubes in the discretized  $(\alpha', \beta', \gamma')$ space. In turn, this means that a single state s gets mapped to an unbounded number of possible states s', causing p(s'|s, a = H) to be arbitrary small. This may prevent the agent from recognizing an optimal path to valuable states, since even if the quantity  $(r + \gamma V_{\pi}(s'))$ is particularly large for some states s', this quantity gets multiplied by the negligible factor p(s'|s, a = H), and therefore has a very small contribution in an update rule such as Eq (2).

These problems can be overcome by switching to using quaternions as our coordinate system. Unlike the ZYZ-Euler angles, the space of quaternions is in a one-to-one correspondence with SU(2). Given some  $U \in SU(2)$  as in Eq (6), the corresponding quaternion is given simply as q = (a, b, c, d). Under the action of T, its components transform as

$$a' = a\cos\left(\frac{\pi}{8}\right) + b\sin\left(\frac{\pi}{8}\right)$$

$$b' = b\cos\left(\frac{\pi}{8}\right) - a\sin\left(\frac{\pi}{8}\right)$$

$$c' = c\cos\left(\frac{\pi}{8}\right) + d\sin\left(\frac{\pi}{8}\right)$$

$$d' = d\cos\left(\frac{\pi}{8}\right) - c\sin\left(\frac{\pi}{8}\right)$$
(10)

while under the action of H, its components transform as

$$a' = \frac{b+d}{\sqrt{2}}$$

$$b' = \frac{c-a}{\sqrt{2}}$$

$$c' = \frac{d-b}{\sqrt{2}}$$

$$d' = -\frac{a+c}{\sqrt{2}}$$
(11)

and  $\det(J_{(T)}) = \det(J_{(H)}) = 1$  for the Jacobians associated with both transformations, so that these operations are volume-preserving on this coordinate system. In turn, this implies that a hypercube with unit volume in the discretized quaternionic space gets mapped to a region with unit volume.

For the purposes of the learning agent, this means that the total number of states that can result from acting with either T or H is bounded above. Suppose we choose our discretization such that the grid spacing along each of the 4 axes of the quaternionic space is the same. Then, since a d-dimensional hypercube can intersect with at most  $2^d$  equal-volume hypercubes, a state s can be mapped to at most 16 possible states s'. While this is certainly better than the pathological case we noted previously using the ZYZ-Euler angles, one could ask if it is possible to do better and design a coordinate system such that a state gets mapped to at most one other state.

One possible approach to make the environment dynamics completely deterministic is to consider a discretization  $q=(n_1\Delta,n_2\Delta,n_3\Delta,n_4\Delta)$  where  $n_1,n_2,n_3,n_4\in\mathbb{Z}$ , and choose  $\Delta$  such that the transformed quaternion can also be described similarly as  $q'=(n'_1\Delta,n'_2\Delta,n'_3\Delta,n'_4\Delta)$ , and try to ensure that  $n'_1,n'_2,n'_3,n'_4$  are also integers. Essentially this would mean that corners of hypercubes map to corners of hypercubes, so that discretized states map uniquely to other discretized states. However, consider the transformation

under H, Eq. (11). For this transformation, requiring  $a' = (b+d)/\sqrt{2} = (n_2+n_4)\Delta/\sqrt{2}$  to equal  $n_1'\Delta$  in turn requires that  $n_1' = k/\sqrt{2}$ , for some  $k \in \mathbb{Z}$  (and similarly for the other components). This implies that  $n_1'$  cannot be an integer, and so the map given with this gateset over this discretized coordinate system cannot be made deterministic in this manner. Nevertheless, we find that our construction is sufficient to solve the MDP that we have set up.

#### Reward Structure and Environment Dynamics

Some natural measures of overlap between two unitaries include the Hilbert-Schmidt inner product  $tr(U^{\dagger}V)$ , and since we work with quaternions, the quaternion distance |q - q'|. However, neither does the Hilbert-Schmidt inner product monotonically increase, nor does the quaternion distance monotonically decrease, along the shortest  $\{H, T\}$ gate sequence. As an example, consider the target quaternion  $q^* = [-0.52514, -0.38217, 0.72416, 0.23187]$ from Table (II) with shortest compilation sequence HTTTTHTHHH (read right to left) satisfying  $|q-q^{\star}| < 0.3$ , where q is the prepared quaternion via the sequence. After the first H application,  $|q-q^{\star}| \sim 1.34$ , which drops after the second H application to  $|q-q^{\star}| \sim 0.97$ , and then rises again after the third H application to  $|q-q^{\star}| \sim 1.49$ , before eventually falling below the threshold error. Similarly, the Hilbert-Schmidt inner product starts at  $\sim 0.21$ , rises to  $\sim 1.05$ , then falls to  $\sim -0.21$  before eventually becoming  $\sim 1.96$ . On the other hand, we showed previously how assigning a reward structure of +1 to some target state, and 0 to all other states, made it possible to relate the optimal value function to the length of the optimal path.

Instead of specifying a reward of +1 in some target state and 0 in every other state however, we now assign a reward of +1 whenever the underlying unitary has evolved to within an  $\epsilon$ -net approximation of the target unitary. Since we work with quaternions, we specify this as obtaining a reward of +1 whenever the evolved quaternion q satisfies  $|q - q^*| < \epsilon$ , for some  $\epsilon > 0$  and  $q^*$ is the target quaternion, and 0 otherwise. We note that the Euclidean distance between two vectors (a, b, c, d)and  $(a + \Delta_{bin}, b + \Delta_{bin}, c + \Delta_{bin}, d + \Delta_{bin})$  equals  $2\Delta_{bin}$ , however both those vectors cannot represent quaternions, since only either one of them can have unit norm. Nevertheless, this sets a size of discrete states, and we require that  $\epsilon$  be comparable to this scale, setting  $\epsilon = 2\Delta_{bin}$  in practice. This requirement comes from the fact that in general, the  $\epsilon$ -net could cover more than one state, so that we now need to estimate the probabilities p(s', r|s, a), in contrast to the scenario where a state uniquely specifies the reward. Demanding that  $\epsilon \sim \Delta_{hin}$ 

ensures that p(s', r = 1|s, a) does not become negligibly small.

We could estimate the dynamics by uniformly randomly sampling quaternions, track which discrete state the sampled quaternions belong to, evolve them under the actions and track the resultant discrete state and reward obtained as a result, just as we did in the previous section. However, here we now estimate the environment dynamics by simply rolling out gate sequences. Each rollout is defined as starting from the identity gate, then successively applying either an H or T gate with equal probability until some fixed number K of actions have been performed. The probabilities for the identity action p(s', r|s, a = I) are simply estimated by recording that (s', a = I) led to (s', r) at each step that we sample (s', r)when performing some other action  $a \neq I$  in some other state  $s \neq s'$ . The number of actions per rollout K is set by the desired accuracy, which the Solovay-Kitaev theorem informs us is  $O(\text{polylog}(1/\epsilon))$  [7]. Estimating the environment dynamics in this manner is similar in spirit to off-policy learning in typical reinforcement learning algorithms, such as Q-learning [19].

#### **Optimal Gate Compilation Sequences**

Solving the constructed MDP through policy iteration, we arrive at the optimal policy just as before. We now chain the optimal policies together to form optimal gate compilation sequences, accounting for the fact that while the dynamics of our constructed MDP are stochastic, the underlying evolution of the unitary states are deterministic. The procedure we use for starting with the identity gate and terminating, with some accuracy, at the target state is outlined in pseudo-code below.

# Algorithm 2 Optimal Gate Compilation Sequence

```
1: Initialize empty list Action-Rollouts
 2: Specify number of rollouts
3: for each rollout do
      Initialize empty list Action-Sequence
 4:
5:
       Initialize State to Identity gate
       Counter \leftarrow 0
6:
       while Counter < some large number
 7:
 8:
           Action \leftarrow Optimal-Policy[State]
9:
           ACTION-SEQUENCE.append(ACTION)
10:
           Sample (Next-State, Reward) from estimated
   p(s',r|s,a)
11:
           STATE \leftarrow NEXT-STATE
           if Reward = 1
12:
13:
               break
14:
       if Action-Sequence is not empty
15:
           ACTION-ROLLOUTS.append(ACTION-SEQUENCE)
16: end for
17: Optimal-Sequence ← Minimum length Action-
   SEQUENCE in ACTION-ROLLOUTS that satisfies precision
   bound
```

The accuracy with which we would obtain the minimum length action sequence in Algorithm (2) need not necessarily satisfy the bound  $\epsilon$  set by the reward criterion, r=1 for  $|q-q^{\star}|<\epsilon$ , for reasoning similar to the shuffling discussed in the context of state preparation above. This is why we require Algorithm (2) to report the minimum length action sequence that also satisfies the precision bound. In practice, we found that this was typically an unnecessary requirement and even when the precision bound was not satisfied, the precision did not stray too far from the bound. It should be emphasized that due to the shuffling effect, there is no a priori guarantee that optimal-sequence returned by Algorithm (2) need even exist, since the precision bound is not guaranteed to exist, and the only bound we can safely set is  $|q-q^{\star}| \lesssim \Delta_{bin}k$ , where k is the number of actions in the sequence that prepares q. In practice however, we find the algorithm to work quite well in producing optimal sequences that correspond to the shortest possible gate sequences to prepare the target quaternions  $q^*$ .

To benchmark the compilation sequences found by this procedure, we find shortest gate sequences for compilation to some specified precision using a brute-force search that yields the smallest gate sequence that satisfies  $|q-q^\star| < \epsilon$  for some  $\epsilon > 0$  with the smallest value of  $|q-q^\star|$ , where q is the prepared quaternion and  $q^\star$  is the target quaternion. This brute-force procedure can be described in pseudo-code as follows.

# Algorithm 3 Shortest Gate Compilation Sequence

```
1: Found = False
 2: Specify target accuracy \epsilon
3: n = 1
4: while not FOUND
5:
        Initialize empty list Quaternion-Distances
        SEQUENCES \leftarrow 2^n sequences of \{H, T\}
 6:
 7:
        for Seq in Sequences
8:
             Evolve quaternion according to SEQ
9:
             Quaternion-Distances.append(|q - q^{\star}|)
10:
        if Min(Quaternion-Distances) < \epsilon
11:
             Found \leftarrow True
12:
             SHORTEST-SEQUENCE
                                                 Seq
                                                           with
    MIN(QUATERNION-DISTANCES)
13:
        else
14:
             n \leftarrow n + 1
```

As an experiment, we drew 30 (Haar) random SU(2) matrices, and found their compilation sequences from Algorithms (2) and (3). We set  $\epsilon = 2\Delta_{bin} = 0.3$ , estimated the environment dynamics using 1000 rollouts, each rollout being 50 actions long, and each action being a uniform draw between H and T. The findings are presented in Table (II), where the sequences are to be read right to left. We find that although the two approaches sometimes yield different sequences, the two sequences agree in their length and produce quaternions that fall within  $\epsilon$  of the target quaternion. We expect in general that the two approaches will produce comparable length sequences and target fidelities, though not necessarily equal.

# CONCLUSIONS

We have shown that the tasks of single-qubit state preparation and gate compilation can be modeled as finite MDPs yielding optimally short gate sequences to prepare states or compile gates up to some desired accuracy. These optimal sequences were found to be comparable with independently calculated shortest gate sequences for the same tasks, often agreeing with them exactly. This work therefore provides strong evidence that more complicated quantum programming tasks can also be successfully modeled as MDPs. In scenarios where the state or action spaces grow too large for dynamic programming to be applicable, or where the environment dynamics cannot be accurately learned in the simple manner described above, it could therefore make sense to apply reinforcement learning to find optimally short circuits for particular tasks.

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TABLE II. Compilation Gate Sequences from MDP and Brute-Force (BF) using  $\epsilon = 0.3$ . Note the definitions of  $H = RY(\pi/2)RZ(\pi)$  and  $T = RZ(\pi/4)$ , as described in the main text.

		$T = T(Z(\pi/4))$ , as described in		
$q^{\star}$		Brute-Force Gate Sequence		
[-0.54981 0.35852 0.41549 0.62972]	THTTH	THTTH	0.19996	0.19996
[-0.76688 0.32823 -0.37129 0.4078]	HTHT	HTHT	0.2483	0.2483
[-0.52514 -0.38217 0.72416 0.23187]	HTTTTHHHTH	НТТТТНТННН	0.18812	0.18812
[-0.94809 0.13988 0.25424 -0.13006]	HTTHTHHHTT	ТНТТНННТНТ	0.23144	0.20043
[-0.66457 -0.47827 0.45341 0.35218]	НТТТТНННТН	НТТННТНТТН	0.29977	0.26614
[-0.93392 -0.04759 -0.14279 -0.32426]	THHHTHTHT	ТТНННТНТН	0.25982	0.24801
[-0.06813 -0.20031 0.97526 -0.06406]	TTTTHTTTTH	TTTTHTTTTH	0.22244	0.22244
[-0.52828 0.65335 -0.26856 0.47109]	HTHTT	HTHTT	0.23627	0.23627
[-0.62701 0.42767 -0.1176 0.64041]	HTTHT	HTTHT	0.22121	0.22121
[-0.27418 0.40672 -0.46718 0.73563]	HTTTHTT	HTTTHTT	0.24486	0.24486
[-0.09875 0.75277 0.50256 -0.41354]	TTHTTTTT	TTHTTTTT	0.28736	0.28736
[-0.04894 -0.00402 -0.83205 0.55252]	HTTTTHTT	HTTTTHTT	0.20474	0.20474
[-0.68691 0.36726 0.04274 -0.62566]	TTHTTT	TTHTTT	0.25131	0.25131
[-0.06072 0.76411 -0.12676 -0.62959]	TTTTHTTT	TTTTHTTT	0.27854	0.27854
[-0.62191 -0.0639 -0.76511 0.1541]	TTTTH	TTTTH	0.19609	0.19609
[-0.98674 0.06886 -0.1264 0.07503]	HH	HH	0.16286	0.16286
[-0.86814 0.26898 0.38056 0.17075]	НТТТНТНННТТ	HTHHTHTHTTT	0.22221	0.09319
[-0.2836 -0.03982 0.95045 -0.12098]	HTTTHTHTHTTT	HTTTHTHTHTTT	0.07442	0.07442
[-0.45815 -0.60513 -0.62792 0.17215]	TTTTTHHHTTH	TTTTHTHTHTH	0.2187	0.19569
[-0.60091 -0.54151 0.58106 0.08967]	НТННТТНТН	НТТННТНТН	0.16617	0.16617
[-0.3671 -0.15162 -0.40285 0.8246]	НТНТНТТТТТН	HTHTHTHTTTTH	0.15013	0.15013
[-0.33288 0.42797 0.28725 0.78963]	THTTTH	THTTTH	0.29693	0.29693
[-0.84802 -0.1492 0.02132 0.50808]	HTH	HTH	0.21022	0.21022
[-0.88329 -0.28327 -0.28398 0.2427]	ТНТНТННТТН	ТНТНННТТТН	0.21036	0.21036
[-0.3926 -0.75829 0.34643 -0.38838]	THTHHHTTTT	TTHTHTTTHH	0.26302	0.22761
[-0.85775 0.2746 0.42074 -0.10883]	НТНТНТНТТ	НТНТНТНТТ	0.12494	0.12494
[-0.27497 0.25412 0.69666 0.61195]	TTHTTTH	TTHTTTH	0.0623	0.0623
[-0.47217 0.0121 0.23258 0.85018]	HTTTH	HTTTH	0.26015	0.26015
[-0.67911 -0.46404 -0.35643 0.4432]	НТТНТННТТН	НТТНТННТТН	0.27136	0.27136

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