

Robust Quantum Optimal Control

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This is a paper about robust quantum optimal control.

Introduction

(Existing work) The leading model of universal quantum computation is gate-based. The Quantum Optimal Control (QOC) literature has sought to answer the question "What is the best way to construct a quantum gate?". Analytic methods have been demonstrated to construct quantum gates [1? –4]. Most methods rely on solving the time-dependent Schroedinger equation analytically or deriving equations of motion from a suitable Lagrangian.

Some analytical methods have been presented to address realistic experimental constraints. Considering the dynamical and geometric phases of state evolution has led to methods for achieving robustness to pure dephasing in quantum systems [3? ?]. Additionally, suitable choices of bases have been demonstrated that allow the experimentalist to infer trade-offs in longitudinal and pure dephasing coherence times [2]. To date, however, no analytical method has been presented to construct a gate while satisfying all relevant experimental constraints. Furthermore, most analytic methods have only been demonstrated in the two-level approximation and become cumbersome to solve for larger Hilbert space sizes.

Numerical quantum control techniques have developed in parallel with the analytic frameworks. Numerical quantum control techniques integrate the time-dependent Schroedinger equation and use sensitivity analysis to optimize target metrics of the quantum gate, such as fidelity [5? –9]. These techniques typically employ zeroth- or first-order optimizers and make no guarantees of optimality. Further, they formulate the quantum control problem as unconstrained or use projective gradient methods [9]. The latter approach relies on constructing bases for constraint spaces—which is not always feasible—and may hinder convergence.

(This work) We employ the trajectory optimization literature to formulate the quantum optimal control problem as a constrained optimization problem. The trajectory optimization framework allows us to handle arbitrary constraints on the evolution

of the quantum state. Additionally, we introduce methods for constructing gates robust to longitudinal relaxation and pure dephasing, the dominant barrier to experimentally realizing practical quantum computing.

We study the quantum optimal control problem on the fluxonium qubit. We outline experimentally realistic constraints and map them to the trajectory optimization framework. For the device we study we achieve a 1.5x increase in T_1 times. We present two methods for achieving robustness to pure dephasing, and compare them to existing dynamic decoupling methods. We find that our methods mitigate dephasing by order X over dynamic decoupling.

(Outline) First we formulate the quantum optimal control problem in the trajectory optimization framework. Then, we introduce the dynamics of the fluxonium device and outline experimental considerations relevant to gate construction. Next we outline a method for making the optimization T_1 aware. Finally, we present some methods for engineering robustness to pure dephasing and compare them to existing techniques.

QOC + AL-iLQR

(QOC Problem Statement) Here we introduce the notation we will use throughout the paper, review the quantum optimal control problem statement, and introduce the trajectory optimization framework. Quantum optimal control concerns the evolution of a state $|\psi(t)\rangle$ governed by the time-dependent Schroedinger equation

$$\partial_t |\psi(t)\rangle = -\frac{i}{\hbar} H(\mathbf{u}(t), t) |\psi(t)\rangle \quad (1)$$

The evolution is sometimes cast with $\rho(t) = |\psi(t)\rangle \langle \psi(t)|$ and the Lindblad master equation to model the decoherence of the state explicitly. The Hamiltonian depends arbitrarily on the controls $\mathbf{u}(t)$.

Numerical quantum optimal control techniques make the problem tractable by discretizing the problem into N time steps. Typical integration techniques rely on approximating the analytical solution

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to the time-dependent Schroedinger equation or using explicit integration methods, e.g. Runge-Kutta, of the form

$$|\psi_{k+1}\rangle \approx |\psi_k\rangle + \partial_t |\psi_k\rangle \cdot \Delta t_k \quad (2)$$

Quantum optimal control seeks the control parameters that minimize a functional $J(u, |\psi_N(u)\rangle)$. In the simplest case the functional $J = 1 - |\langle \psi_f | \psi_N(u) \rangle|^2$ which is the infidelity between the initial state evolved to the final time step ($|\psi_N(u)\rangle$) and the target state ($|\psi_f\rangle$). In general J is a linear combination of cost functions on $|\psi_N(u)\rangle$, e.g. forbidden-state occupation, as well as cost functions on u , e.g. the norm of the control amplitudes [5].

(AL-iLQR Problem Statement) The trajectory optimization literature solves a more general class of non-linear programs that resemble the quantum optimal control problem. The quantum optimal control problem is a specific case of the linear quadratic regulator (LQR). LQR is so called because the dynamics are linear in the state and the cost function is quadratic in the state. In the LQR formulation the same functional is evaluated at each time step

$$J_{\text{LQR}} = \tilde{x}_N^T Q_N \tilde{x}_N + \sum_{k=0}^{N-1} \tilde{x}_k^T Q_k \tilde{x}_k + u_k^T R_k u_k \quad (3)$$

where $\tilde{x}_k = x_k - x_f$ is the difference between the current and final state and Q_k, R_k are matrices that define the penalty metric.

The advantage of the LQR formulation is that there exists a dynamic programming algorithm to compute the optimal update to the controls u_k at each time step based on the Ricatti recursion (see Appendix).

Trajectory optimization gives us gaurantees about our updates via Ricatti recursion and allows us to put constraints on our cost functions.

$$\begin{aligned} \min_{U: N-1 \times m} \mathcal{L}_N(x_N, \lambda_N, \mu_N) \\ + \sum_{k=1}^{N-1} \mathcal{L}_k(x_k, u_k, \lambda_k, \mu_k) \end{aligned} \quad (4)$$

$$\begin{aligned} \mathcal{L}_k(x_k, u_k, \lambda_k, \mu_k) = \\ (\lambda_k + \frac{1}{2} I_{\mu_k} c_k(x_k, u_k))^T c_k(x_k, u_k) \\ + (x_k - x_f)^T Q (x_k - x_f) + u_k^T R u_k \end{aligned} \quad (5)$$

The important point is that there is an update step (e.q. 17 from ALTRO paper) where we send $\lambda \rightarrow \infty$

and get all of the nice convergence properties. The weights are adjusted dynamically between iterations until all of our constraints are satisfied. The Markovian decision structure of the problem allows us to apply differentiable dynamic programming to guarantee that the update for each control U_k is optimal, as apposed to the greedy updates of first-order optimizers like the naive gradient descent.

QOC on the Fluxonium

(Fluxonium Device) In the two-level approximation we have

$$H/h = \omega_q \frac{\sigma_z}{2} + A(\Phi_{\text{ext}}) \frac{\sigma_x}{2} \quad (6)$$

This approximation is good up to the avoided crossing at $\Phi_{\text{ext}} = 0.35\Phi_0$. We get A by converting via $\langle g | \hat{\phi} | e \rangle$. We use the gates $X/2, Y/2, Z/2$. $X/2, Y/2$ are universal up to an arbitrary Z rotation.

(Constraints) We want constraints on our pulses. We want pulses start and end at zero for concatenation. We want pulses to have zero net flux to mitigate hysteresis in flux bias lines. We want the amplitude to be constrained $\delta\Phi_{\text{ext}} \sim 0.06\Phi_0$ so the two-level approximation stays valid. We want our state to obey normalization conditions, mitigating numerical error in simulaiton.

(T_1 and T_ϕ noise) Dissipation to the thermal bath via longitudinal relaxation (T_1) is an irreversible process that results in information loss. Pure dephasing (T_ϕ) is a reversible process. Dielectric loss, etc. contribute to T_1 . $1/f$ flux noise, etc. contribute to T_ϕ . There is a tradeoff between T_1 and T_ϕ . In the case of white noise we have that the sum of the noise weights W_1 and W_ϕ is constant [2]. In our case T_ϕ is saturated at the flux frustration point $\Phi_{\text{ext}} = 0.5\Phi_0$. T_ϕ decreases as we move away from the flux frustration point. Conversely, T_1 is at a minimum around the flux frustration point $T_1(0.5\Phi_0) = 0.315\text{ms}$, and increases away from the flux frustration point $T_1(0.43\Phi_0) = 4.3\text{ms}$. Given the nature of the decay processes and the tradeoff, we choose to optimize the flux bias to have high time-averaged T_1 times and employ some techniques to mitigate T_ϕ dephasing.

Robustness to T_1 -type Noise

(Strategy) We seek to minimize the probability that the qubit relaxes longitudinally. To this end we augment the state vector x_k with the longitudinal

Gate	Analytic	QOC	Speedup
	P_1 (10^{-5})	P_1 (10^{-5})	
Z/2	4.615	2.576	1.792
Y/2	2.826	1.888	1.496
X/2	9.562	5.080	1.882

Table I: Probability of longitudinal relaxation for each gate evaluated at the gate’s duration.

relaxation probability

$$P_1(t_k) = \int_0^{t_k} \gamma_1(\Phi_{\text{ext}}(t)) dt \quad (7)$$

where $\gamma_1 = T_1^{-1}$. Setting the target longitudinal relaxation probability to 0 results in a quadratic cost at each knot point of the form $|P_1(t_k)|^2$.

The value $T_1(\Phi_{\text{ext}}(t_k))$ is obtained at each knot point by evaluating a spline interpolant fit to experimentally obtained data of the form $\{(\Phi_{\text{ext}}, T_1)\}$. Calculating T_1 directly from theoretical considerations requires many high-dimensional eigendecompositions, which is computationally expensive. Additionally, T_1 values are known to fluctuate greatly with laboratory temperatures [10]. Interpolating T_1 from experimental data increases the fridge truth of the simulation.

Furthermore, the probability of longitudinal relaxation is dependent on the gate duration t_N . We allow the optimizer to tune the gate duration by augmenting the control vector u_k with the time step between knot points Δt_k . Promoting Δt_k to a decision variable, rather than the number of knot points N , preserves the Markovian decision structure of the trajectory optimization problem. To ensure numerical integration accuracy is maintained we add a bound constraint at each knot point $5\text{e-}3 \text{ ns} \leq \Delta t_k \leq 2\text{e-}2 \text{ ns}$. Note that this bound constraint is allowed to be broken for intermediate iterations of the optimization, so we use the absolute value of the time step $|\Delta t_k|$ to ensure that it is non-negative.

(Results) We achieve a factor of 1.5 decrease in the probability of longitudinal relaxation from the analytic gates we benchmark against. We simulate the performance of the gates using the lindblad master equation (see Appendix X). We repeatedly apply the basis gates and measure the fidelity of the resulting state as a function of time as shown in Fig. 1.

Figure 1: Master equation simulation with T_1 dissipation for all basis gates.

Figure 2: fidelity v.s. ω for the X/2 gate via analytic, 3-sample, 2-derivative (maybe add 5-sample and 3-derivative)

Robustness to T_ϕ -type Noise

(Strategy) System parameter deviations arise due to measurement error and noise injection. For example, we might measure ω_q inaccurately, which leads to a deviation from the the drive frequency ω_d . Further, we may have some temperature dependent gain in the lines leading to the device, or $1/f$ noise and $A(\Phi_{\text{ext}})$ comes out with some δA on the flux axis. Both of these effects lead to dephasing, uncertain dynamics, and thus erroneous computation.

These problems are typically attacked with dynamic decoupling sequence where an erroneous rotation is compensated for with one that cancels the δ . However, we can do better than the first order variants of these pulses.

We propose two methods for engineering robustness to system parameter deviations. The first we call the derivative method. We use the intuition that making the final state insensitive to changes in the system parameter is encoded in the derivative $\partial_\omega^l |\psi_N\rangle$. In particular, we find that going to the second derivative is good. The first derivative is already small, especially for the δA time, because, near the end of optimization, the optimizer is unable to improve the final state by changing the flux bias. The dynamics for propagating the derivative of the state are found by differentiating the schroedinger equation dynamics with respect to the parameter of interest. The scheme boils down to propagating sequential derivatives of the parameter you want to be robust to ∂_ω^l and penalizing thier norm $|\partial_\omega^l|^2$.

The other scheme we call the sampling method. This method is well-known in the trajectory optimization. In this scheme we propagate an array of states whose dynamics differ in that the parameter of interest is altered slightly for each state. In the 3-point sampling method we propagate ψ_\pm, ψ where $\omega_\pm = \omega \pm \delta\omega$. Here δ is typically taken at standard deviations of the parameter of interest.

(Results) We compare the simplest schemes for the derivative and sampling methods to the CORPSE dynamic decoupling sequence. They perform X better by Y metric.

We also find that longer gate durations allow for greater robustness.

Figure 3: fidelity at $\omega \pm \sigma_\omega$ v.s. time for the $X/2$ gate via analytic, 3-sample, 2-derivative (maybe add 5-sample and 3-derivative)

Figure 4: Master equation simulation with T_2 dissipation comparing the gates robust to $\delta\omega_q$ and δA against the analytic gate.

Discussion

We have proposed some schemes and they work well.

Ricatti Recursion

This will give the reader unfamiliar with trajectory optimization intuition for how the trajectory optimization update scheme works and why it is better than a more naive method.

Measurements

We measure T_1 using the standard experiment and T_2 using the Ramsey experiment. We fit with splines and the data looks like fig. 3 in Helin's paper [1]. We measure ω_q and σ_{ω_q} using X method.

ME Simulation

We model dissipation using the Lindblad master equation and standard collapse operators for longitudinal relaxation and dephasing of a two-level system.

Derivative Method

$$\partial_\omega^2 \partial_t \psi = \frac{-i}{\hbar} \left[2 \cdot \frac{\sigma_z}{2} \partial_\omega \psi + \left(\omega \frac{\sigma_z}{2} + A \frac{\sigma_x}{2} \right) \partial_\omega^2 \psi \right] \quad (8)$$

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- [1] H. Zhang, S. Chakram, T. Roy, N. Earnest, Y. Lu, Z. Huang, D. Weiss, J. Koch, and D. I. Schuster, Universal fast flux control of a coherent, low-frequency qubit, arXiv preprint arXiv:2002.10653 (2020).
 - [2] Z. Huang, P. S. Mundada, A. Gyenis, D. I. Schuster, A. A. Houck, and J. Koch, Engineering dynamical sweet spots to protect qubits from $1/f$ noise, arXiv preprint arXiv:2004.12458 (2020).
 - [3] Z. Han, Y. Dong, B. Liu, X. Yang, S. Song, L. Qiu, D. Li, J. Chu, W. Zheng, J. Xu, *et al.*, Experimental realization of universal time-optimal non-abelian geometric gates, arXiv preprint arXiv:2004.10364 (2020).
 - [4] J. Xu, S. Li, T. Chen, and Z.-Y. Xue, Nonadiabatic geometric quantum computation with optimal control on superconducting circuits, arXiv preprint arXiv:2004.10199 (2020).
 - [5] N. Leung, M. Abdelhafez, J. Koch, and D. Schuster, Speedup for quantum optimal control from automatic differentiation based on graphics processing units, Physical Review A **95**, 042318 (2017).
 - [6] M. H. Goerz, D. Basilewitsch, F. Gago-Encinas, M. G. Krauss, K. P. Horn, D. M. Reich, and C. P. Koch, Krotov: A python implementation of krotov's method for quantum optimal control, SciPost physics **7** (2019).
 - [7] P. Doria, T. Calarco, and S. Montangero, Optimal control technique for many-body quantum dynamics, Physical review letters **106**, 190501 (2011).
 - [8] M. Abdelhafez, D. I. Schuster, and J. Koch, Gradient-based optimal control of open quantum systems using quantum trajectories and automatic differentiation, Physical Review A **99**, 052327 (2019).
 - [9] S. Machnes, E. Assémat, D. J. Tannor, and F. K. Wilhelm, Gradient optimization of analytic controls: the route to high accuracy quantum optimal control, arXiv preprint arXiv:1507.04261 (2015).
 - [10] P. Klimov, J. Kelly, Z. Chen, M. Neeley, A. Megrant, B. Burkett, R. Barends, K. Arya, B. Chiaro, Y. Chen, *et al.*, Fluctuations of energy-relaxation times in superconducting qubits, Physical review letters **121**, 090502 (2018).