Robust Trajectory Optimization on a Quantum System

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The ability to engineer high-fidelity gates on quantum processors in the presence of systematic errors remains the primary challenge requisite to achieving quantum advantage. Quantum optimal control methods have proven effective in experimentally realizing high-fidelity gates, but they require exquisite calibration to be performant. We apply robust trajectory optimization techniques to suppress gate errors arising from system parameter uncertainty. We propose a derivative-based approach that maintains computational efficiency by using forward-mode differentiation. Additionally, the effect of depolarization on a gate is typically modeled by integrating the Lindblad master equation, which is computationally expensive. We employ a computationally efficient model and utilize time-optimal control to achieve high fidelity gates in the presence of depolarization. We apply these techniques to a two level approximation of a fluxonium qubit and suppress simulated gate errors due to parameter uncertainty below 10^{-7} for static parameter deviations on the order of 1%.

I. INTRODUCTION

Quantum optimal control (QOC) is a class of optimization algorithms for accurately and efficiently manipulating quantum systems. Early techniques were proposed for nuclear magnetic resonance experiments [1–7], and applications now include superconducting circuits [8–14], neutral atoms and ions [15–25], nitrogen-vacancy centers in diamond [26–32], and Bose-Einstein condensates [33, 34]. In the context of quantum computation, optimal control is employed to achieve high-fidelity gates while adhering to experimental constraints. Experimental errors such as parameter drift, noise, and finite control resolution cause the system to deviate from the model used in optimization, leading to poor experimental performance TODO: could be a good place for a citation here? It obviosuly makes sense in principle, but I'm not aware of a paper that tried to implement optimal control and failed for these reasons. *on reading further* Maybe the Zhou book from below. Robust control improves upon standard optimal control by encoding model parameter uncertainties in optimization objectives, yielding performance guarantees over a range of parameter values [35–37]. We adapt robust control techniques from the robotics community to mitigate parameter uncertainty errors for a superconducting fluxonium qubit.

Analytically-dervied control pulses that mitigate parameter uncertainty errors include composite pulses [38–41], pulses designed by considering dynamic and geometric phases [42, 43], and pulses obtained with the DRAG scheme [44]. These techniques are not amenable to arbitrary experimental constraints, so recent work has sought to achieve robustness in quantum optimal control frameworks using closed-loop methods [45–48] and open-loop methods [31, 49–53].

In this work, we study three robust control techniques that make the system's quantum state trajectory less sensitive to static and time-dependent parameter uncertainty:

1. A sampling method, similar to the work of [3, 31, 49–51, 54].
2. An unscented sampling method adapted from the unscented transform used in state estimation [55–58].
3. A derivative method, which penalizes the sensitivity of the quantum state trajectory to uncertain parameters.

We apply these techniques to the fluxonium qubit presented in [59]. We also show that QOC can solve important problems associated with fluxonium-based qubits: exploiting the T_1-dependence of the controls to mitigate depolarization and synchronizing the phase of qubits with distinct frequencies. To mitigate depolarization, we perform time-optimal control and employ an efficient depolarization model for which the computational cost is independent of the Hilbert space dimension. Leveraging recent advances in trajectory optimization within the field of robotics, we solve these optimization problems using ALTRO (Augmented Lagrangian TRajectory Optimizer) [60], which can enforce constraints on the quantum state trajectory and control parameters.

This paper is organized as follows. First, we describe ALTRO in the context of QOC in Section II. We outline realistic constraints for operating the fluxonium and define the associated QOC problem in Section III. Then, we formulate a method for supressing depolarization in Section IV. Next, we describe three techniques for achieving robustness to static parameter uncertainties in Section

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V. We adapt the same techniques to mitigate $1/f$ flux noise in Section VI.

II. BACKGROUND

In this section, we review the QOC problem statement and describe the ALTRO solver [60]. QOC concerns a vector of time-dependent control parameters $u(t)$ that steer the evolution of a (quantum) state $|\psi(t)\rangle$. The evolution of the state is governed by the time-dependent Schrödinger equation (TDSE),

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H(u(t),t)\,|\psi(t)\rangle\,. \tag{1}$$

The Hamiltonian $H(u(t),t)$ is determined by the quantum system. The QOC problem is to find the controls that minimize a functional $J(u(t))$. To make the problem numerically tractable, the controls and state are discretized into N knot points (time steps). In the case of a single state-transfer problem, the functional is the infidelity of the desired final state and the initial state evolved to the final knot point, $J(u) = 1-|\langle\psi_f|\psi_N(u)\rangle|^2$. In general, $J(u)$ is a linear combination of cost functions on the state as well as cost functions on the controls. Standard QOC solvers compute derivatives of the functional $\nabla_u J(u)$, which can easily be used to implement first-order optimization methods [3, 13, 61, 62].

Alternatively, the QOC problem can be formulated as a trajectory optimization problem and solved using a variety of specialized solvers developed by the robotics community [60, 63–65]. The functional $J(u)$ is divided into its constituent cost functions at each knot point $\ell_k(x_k,u_k)$, where $k \in \{1,...,N\}$ denotes the knot point, x_k is the augmented state vector, and u_k is the augmented control vector. The augmented state contains all relevant variables that are dependent upon the controls, for example the state $|\psi_k\rangle \subseteq x_k$. The augmented state trajectory obeys the physics of the system if the dynamics constraint is satisfied $x_{k+1} = f(x_k,u_k)$. For QOC, the discrete dynamics function $f(x_k,u_k)$ propagates the state by integrating the TDSE 1 with Runge-Kutta methods [66] or exponential integrators [67–70].

Additional constraints on the augmented controls and augmented states are encoded in constraint functions. The constraint functions are put into a form such that, when the constraint is satisfied, inequality constraint functions obey $g_k(x_k,u_k) \leq 0$ and equality constraint functions obey $h_k(x_k,u_k) = 0$. The constraint functions may be vector-valued to encode multiple constraints of each type. If a constraint function takes a positive value, the value is called the constraint's violation. The trajectory optimization problem can be stated concisely,

$$\underset{x_{1:N},\,u_{1:N-1}}{\text{minimize}} \quad \ell_N(x_N) + \sum_{k=1}^{N-1}\ell_k(x_k,u_k) \tag{2a}$$

$$\text{subject to} \quad x_{k+1} = f(x_k,u_k), \tag{2b}$$

$$g_k(x_k,u_k) \leq 0, \tag{2c}$$

$$h_k(x_k,u_k) = 0. \tag{2d}$$

Standard techniques for solving (2a)-(2d) typically fall into two categories: direct methods [71, 72] and indirect methods [73]. For indirect methods, the augmented controls are the decision variables–the variables the optimizer adjusts to solve the problem. The augmented states are obtained from the augmented controls using the discrete dynamics function, and are then used to evaluate derivatives of the cost functions (2a). Then, the derivative information is employed to update the augmented controls. This is the approach taken by standard QOC solvers such as GOAT [61], GRAPE [3, 13], and Krotov's method [62]. Conversely, direct methods treat both the augmented controls and the augmented states as decision variables. In addition to minimizing the cost functions, the optimizer uses derivative information for the discrete dynamics function to satisfy the dynamics constraint (2b) to a specified tolerance. In this sense, the TDSE (1) is a constraint which may be violated for intermediate steps of the optimization, where the states need not be physical. The direct approach lends itself to a nonlinear program formulation, for which a variety of general purpose solvers exist [74, 75]. Recent state-of-the-art solvers, such as ALTRO, have combined principles from both of these approaches. ALTRO uses an iterative linear-quadratic regulator (iLQR) algorithm [76] as the internal solver of an augmented Lagrangian method (ALM) [77, 78] and employs a projected Newton method [79, 80] in its final solving stage.

iLQR is an indirect method for solving the dynamically constrained trajectory optimization problem (2a)-(2b), and its update procedure is based on the differential-dynamic-programming approach [81]. First, iLQR uses an initial guess for the augmented controls to obtain the augmented states with the discrete dynamics function. iLQR then constructs quadratic models for each cost function using their zeroth-, first- and second-order derivatives in a Taylor expansion about the current augmented controls and augmented states. These models are used to derive a recurrence relation between knot points which gives the locally optimal update for the augmented controls. Finally, a line search [82] is performed in the direction of this update to ensure a decrease in the sum of the cost functions. This procedure is repeated until convergence.

Indirect solvers such as iLQR are popular because they are very computationally efficient and maintain high accuracy for the discrete dynamics throughout optimization. However, standard implementations have no ability to handle nonlinear equality and inequality constraints

(2c)-(2d). Projected gradient methods are a typical approach to handle constraints [83–86]. Unfortunately, within the indirect framework, they can only be used for constraints on the augmented controls, not the augmented states. Another technique, which is popular for QOC [13], is to add the constraint functions to the objective (2a). This strategy does not guarantee that the constraints are satisfied as the solver trades minimization of the cost functions and constraint functions against each other. ALM remedies this issue by adaptively adjusting a Lagrange multiplier estimate for each constraint function to ensure the constraints are satisfied. ALM adds terms that are linear and quadratic in the constraint functions to the objective. The new objective is then minimized with iLQR. If the solution obtained with iLQR does not satisfy the constraints, the prefactors for the constraint terms in the objective are increased intelligently and the procedure is repeated.

ALM converges superlinearly, but poor numerical conditioning may lead to small decreases in the constraint violations near the locally optimal solution [87]. To address this shortcoming, ALTRO projects the solution from the ALM stage onto the constraint manifold using a (direct) projected Newton method, achieving ultra-low constraint violations $\sim 10^{-8}$. For more information on the details of the ALTRO solver, see [60, 88].

As opposed to standard QOC solvers, ALTRO can satisfy constraints on both the augmented controls and the augmented states to tight tolerances. This advantage is crucial for this work, where multiple medium-priority cost functions are minimized subject to many high-priority constraints.

III. QOC FOR THE FLUXONIUM

In the following, we optimize quantum gates (unitary transformations) for the fluxonium qubit. The fluxonium is a promising building block for quantum computers, and the accurate two-level approximation of its Hamiltonian makes QOC on a classical computer inexpensive. To high accuracy, we approximate the Hamiltonian near the flux frustration as a spin-1/2 system:

$$H/h = f_q \frac{\sigma_z}{2} + a(t)\frac{\sigma_x}{2}, \tag{3}$$

where f_q is the qubit frequency at the flux frustration point, $a(t)$ is the flux bias, h is Planck's constant, and σ_z, σ_x are Pauli matrices. Although we use an approximation for the Hamiltonian, our noise model is realistic and considers the full Hilbert space. We optimize $X/2$, $Y/2$, and $Z/2$ gates for the fluxonium presented in [59], and compare them to the analytically constructed gates for that device.

First, we outline the constraints for the fluxonium gate problem. All gates in this work satisfy these constraints to a tolerance of $\sim 10^{-8}$. The initial conditions on the states are $\left|\psi_1^0\right\rangle = |0\rangle$, $\left|\psi_1^1\right\rangle = |1\rangle$ (6c) where the superscript is an index $i \in \{0, 1\}$, and the subscript indicates the knot point $k = 1$. The states at the final knot point are constrained to be the image of the initial states under the desired gate U, $\left|\psi_N^i\right\rangle = U\left|\psi_1^i\right\rangle \ \forall\ i$ (6d). Furthermore, we impose the normalization constraint $\left|\langle\psi_k^i|\psi_k^i\rangle\right|^2 = 1 \ \forall\ i, k$ (6e) to ensure the solver does not take advantage of discretization errors in numerical integration. To refer to the discrete moments of the flux, we introduce the notation $\int_{t_1}^{t_k} a(t)\ \mathrm{d}t \equiv \int_t a_k$, $a(t_k) \equiv a_k$, $\partial^n a(t)/\partial t^n\ |_{t=t_k} \equiv\ \partial_t^n a_k$. We impose the zero net flux constraint $\int_t a_N = 0$ TODO: seems kind of funny to be referencing the equations so far below - might be nicer to introduce the equations, referencing Eqs. (2)a-(2)d, then talk about what they mean. (6f) which mitigates the inductive drift ubiquitous in flux-bias lines [59, 89, 90]. The flux is constrained by $|a_k| \leq 0.5$ GHz $\forall\ k$ (6g) to ensure the two-level approximation (3) remains valid. We also enforce the boundary condition $a_1 = a_N = 0$ (6h) so the gates may be concatenated arbitrarily. Additionally, we have the initial condition $\int_t a_1 = \partial_t a_1 = 0$ (6i).

Next, we introduce the augmented control and augmented state:

$$u_k = \left[\partial_t^2 a_k\right], \quad x_k = \begin{bmatrix} \left|\psi_k^0\right\rangle \\ \left|\psi_k^1\right\rangle \\ \int_t a_k \\ a_k \\ \partial_t a_k \end{bmatrix}. \tag{4}$$

The variables in the augmented state are derived from the decision variable in the augmented control via coupled, first-order differential equations in the the discrete dynamics function (6b). We integrate the states according to the TDSE (1) and the fluxonium Hamiltonian (3) and integrate the second-derivative of the flux amplitude to obtain the first-derivative, proportional, and integral moments. The ALTRO implementation we use does not currently support complex numbers, so we repesent the states in the isomorphism $\mathcal{H}(\mathbb{C}^n) \cong \mathcal{H}(\mathbb{R}^{2n})$ given in [13],

$$H\left|\psi\right\rangle \cong \begin{bmatrix} H_{\mathrm{re}} & -H_{\mathrm{im}} \\ H_{\mathrm{im}} & H_{\mathrm{re}} \end{bmatrix} \begin{bmatrix} \left|\psi\right\rangle_{\mathrm{re}} \\ \left|\psi\right\rangle_{\mathrm{im}} \end{bmatrix}. \tag{5}$$

The cost function at each knot point is $\ell_k(x_k, u_k) = (x_k - x_f)^T Q_k (x_k - x_f) + u_k^T R_k u_k$ where Q_k and R_k are diagonal matrices we supply TODO: didn't we say above that iLQR constructs quadratic models for each cost function? Is that what's going on here? How do we reconcile then that "we supply" Q and R?. The Q_k term penalizes deviations from the final augmented state x_f, which is given by the constraints we have imposed on $\left|\psi_N^i\right\rangle$, $\int_t a_N$, and a_N in addition to $\partial_t a_f = 0$. The R_k term penalizes the norm of $\partial_t^2 a_k$, mitigating AWG ringing due to high-frequency transitions. Stated succinctly,

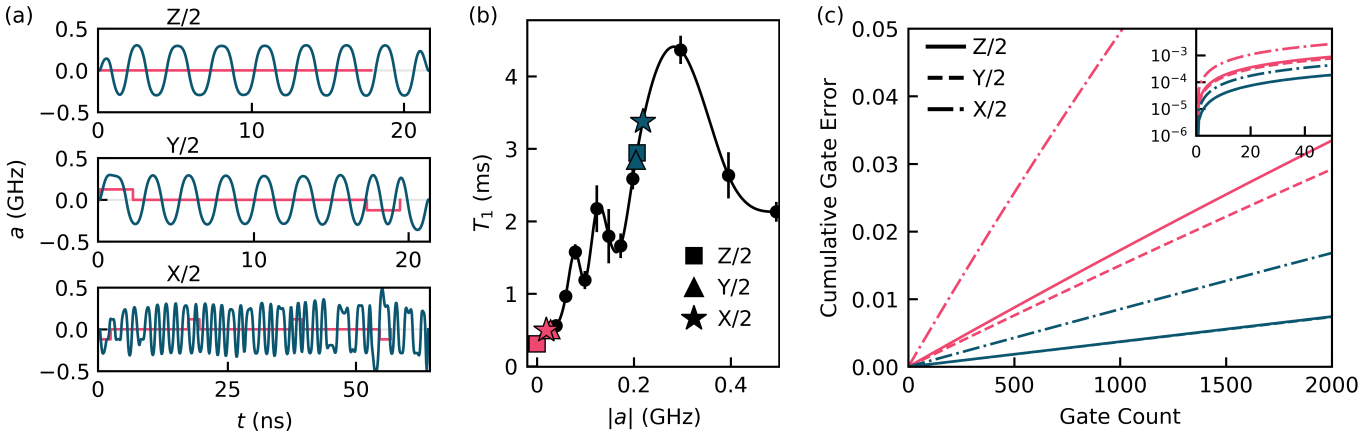

Figure 1: (a) Flux pulses for the numerical gates (dark blue) and the analytic gates (light pink). (b) T_1 interpolation function used in optimization. Circle markers indicate measured T_1 times. Non-circle markers are plotted at the time-averaged, absolute amplitude of each flux pulse TODO: seems a bit odd to plot these on this figure - it looks like you're assigning a T1 value to the entire pulse, which I'm not sure how to interpret. (c) Cumulative gate errors due to depolarization as a function of the number of gates applied. Cumulative gate errors for the numerical $Z/2$ and $Y/2$ gates are indistinguishable. Inset shows log-scaled cumulative gate errors for small gate counts.

the optimization problem takes the form:

$$\underset{x_{1:N},\, u_{1:N\text{-}1}}{\text{minimize}} \quad \sum_{k=1}^{N} (x_k\text{-}x_f)^T Q_k (x_k\text{-}x_f) + \sum_{k=1}^{N-1} {u_k}^T R_k u_k \tag{6a}$$

$$\text{subject to} \quad x_{k+1} = f(x_k, u_k), \tag{6b}$$

$$|\psi_1^0\rangle = |0\rangle\,, |\psi_1^1\rangle = |1\rangle\,, \tag{6c}$$

$$|\psi_N^i\rangle = U\,|\psi_1^i\rangle \;\forall\; i, \tag{6d}$$

$$|\langle\psi_k^i|\psi_k^i\rangle|^2 = 1 \;\forall\; i,k, \tag{6e}$$

$$\textstyle\int_t a_N = 0, \tag{6f}$$

$$|a_k| \le 0.5 \text{ GHz} \;\forall\; k, \tag{6g}$$

$$a_1 = a_N = 0, \tag{6h}$$

$$\textstyle\int_t a_1 = \partial_t a_1 = 0. \tag{6i}$$

IV. DEPOLARIZATION MITIGATION

In this section, we outline a method for optimizing the flux to mitigate depolarization. For many superconducting circuits, the $1/e$ depolarization time (T_1) is independent of the control parameters, so the fastest possible gate incurs the least depolarization error [91]. For the fluxonium, however, T_1 is strongly dependent on the flux. We enable the optimizer to trade longer gate times for lower depolarizaiton times or vice-versa by making the gate time a decision variable. Additionally, previous work has modeled the gate error due to depolarization by evolving density matrices under a master equation [31, 91] or evolving a large number of states in a quantum trajectory approach [92]. We avoid the increase in computational complexity required for these techniques by penalizing the integrated depolarization rate in optimization. Using this metric as a proxy for the gate error incurred is reasonable because depolarization errors are incoherent and therefore increase monotonically in time without interference.

The integrated depolarization rate is given by,

$$D_1(t) = \int_0^t T_1^{-1}(a(t'))dt'. \tag{7}$$

This value is appended to the augmented state (4) and its norm is penalized in the objective (6a) by setting the corresponding element of the final augmented state to zero. $T_1(a_k)$ is obtained at each knot point by evaluating a spline fit to experimental data of the form $\{(a, T_1)\}$, see Figure 1b. It is also possible to fit a spline to theoretically obtained data. However, experimental data often deviates from theoretical predictions because it is difficult to account for all loss channels [59], and T_1 values often fluctuate on hour time scales [93]. TODO: You could cut this - starting from "It is also" to end of paragraph - no need to justify using experimental data if you've got it! Maybe just cite where the data is coming from, if published.

We allow the optimizer to tune the gate time by making the time step between each knot point a decision variable. The square root of the time step $\sqrt{\Delta t_k}$ is appended to the augmented control (4) and its square $|\Delta t_k|$ is used for numerical integration in the discrete dynamics function (6b). To ensure numerical integration accuracy is maintained, we constrain the bounds of the time step at each knot point. We promote the time steps to decision variables, rather than the number of knot points N,

to ensure each cost function depends only on the augmented state and augmented controls at its own knot point $\ell_k(x_k, u_k)$, which is necessary for iLQR.

We analyze the effect of depolarization on the $X/2$, $Y/2$, and $Z/2$ gates obtained with our numerical method and the analytic gates. We use the Lindblad master equation to simulate T_1 dissipation for successive gate applications, and compute the cumulative gate error after each application, see Appendix A. The gate error reported in this text is the infidelity of the evolved state and the target state averaged over 1000 pseudo-randomly generated initial states. The flux pulses for the numerical gates are approximately periodic with amplitudes ~ 0.2GHz, see Figure 1a. They are reminiscent of the analytically determined Floquet operations for a fluxonium described in [94] and realized in [95]. The numerical gate times are greater than the analytic gate times, but the numerical flux pulses spend more time at higher amplitudes, achieving higher T_1 times. The single gate errors for both the analytic and numerical gates are less than 10^{-4}, which makes them sufficient for quantum error correction–a prerequisite for fault-tolerant quantum computing [96–98]. However, the numerical gates achieve single gate errors ~ 5 times less than those for the analytic gates, which tracks closely with their relative improvement on the integrated depolarization rate metric, see Appendix A. This single gate error advantage corresponds to a significant reduction in error correction resources TODO: this seems like a strong statement - citation?. Furthermore, for successive gate applications, the gate error due to depolarization is approximately linear in the gate count, which we expect for $t \ll T_1$, see Figure 1c. The gate error reduction for large gate counts is important for noisy, intermediate-scale quantum (NISQ) applications. These improvements are significant for the constraints we have imposed on the gates, and do not represent a fundamental limit to the optimization methods we have employed.

V. ROBUSTNESS TO STATIC PARAMETER UNCERTAINTY

We have formulated the QOC problem as an open-loop optimization problem; equivalently, we do not incorporate feedback from the experiment in optimization. However, the device's parameters deviate from the parameters we use in optimization, leading to poor experimental performance. We combat errors of this form using robust control techniques, making the state evolution insensitive to parameter uncertainty. As an example, we mitigate errors arising from the drift and finite measurement precision of the qubit frequency which modifies the fluxonium Hamiltonian (3) by $f_q \to f_q + \delta f_q$. We consider three robust control techniques to accomplish this task: a sampling method, an unscented sampling method, and a derivative method.

The sampling method incentivizes the optimizer to ensure multiple copies of a state, each of which evolves with a distinct value of the uncertain parameter, achieve the same target state. Variants of this technique have been proposed in the context of QOC [3, 31, 49, 51, 54] and applied experimentally [50]. For each initial state, we add two sample states $|\psi^{\pm}\rangle$ to the augmented state (4). The discrete dynamics function (6b) is modified so the sample states evolve under the fluxonium Hamiltonian (3) with $f_q \to f_q \pm \sigma_{f_q}$ for a fixed hyperparameter σ_{f_q} which is the standard deviation of the qubit frequency. We penalize the infidelities of the sample states and their target state by adding a cost function to the objective (6a) of the form $\sum_{k,\pm} b_k (1 - |\langle \psi_k^{\pm} | U | \psi_1 \rangle|^2)$ where b_k is a constant we supply. TODO: I thought of this question here but it applies also to when we first write down the objective 6a. Doesn't the sum over k imply that we are penalizing the time it takes to complete the gate? Why do we need to append Δt_k to the augmented state vector? For this method, the standard orthonormal basis states are an insufficient choice for the initial states. As an example, a $Z/2$ gate achieved by idling at the flux frustration point $a_k = 0 \; \forall \; k$ will be robust to qubit frequency detunings for the initial states $|0\rangle$ or $|1\rangle$ because the infidelity metric is insensitive to global phases, but this gate will not be robust for any other initial states. Therefore, we choose four initial states so that their outer products span the operators on the Hilbert space $\{|0\rangle, |1\rangle, (|0\rangle + i|1\rangle)/\sqrt{2}, (|0\rangle - |1\rangle)/\sqrt{2}\}$ [99], which we refer to as the operator basis.

Whereas the sampling method penalizes the deviations of the sample states from the target state, the unscented sampling method penalizes the deviations of the sample states from the nominal state [55, 57, 58]. Accordingly, the cost function we add to the objective (6a) takes the form $\sum_{k,j} c_k (\psi_k^j - \psi_k)^T (\psi_k^j - \psi_k)$, where c_k is a constant we supply, ψ_k is the evolved initial state (nominal state), and ψ_k^j is a sample state that evolves under a modified Hamiltonian similar to that in the sampling method. We omit bra-ket notation here to emphasize that the states are real vectors, and are given by the right-hand-side of the isomorphism (5). Additionally, the unscented sampling method employs the unscented transform [56, 100] to prevent the sample states from drifting too far or close to the nominal state during evolution, which would result in exceedingly large or small deviations in the cost function. In particular, the sample states are chosen to encode a unimodal distribution over the $2n$ TODO: at this point the reader has forgotten what lower-case n refers to elements of the nominal state, modeling the uncertainty in the state as a result of the uncertainty in the parameter. The unscented transform accurately propagates the mean and covariance of this distribution between knot points, or equivalently, through the transformation of the TDSE. For this method, we sample on one initial state $(|0\rangle + i|1\rangle)/\sqrt{2}$, and do not observe a performance increase using more initial states, for example those from the operator basis. A detailed procedure for the unscented transformation is given in Appendix B.

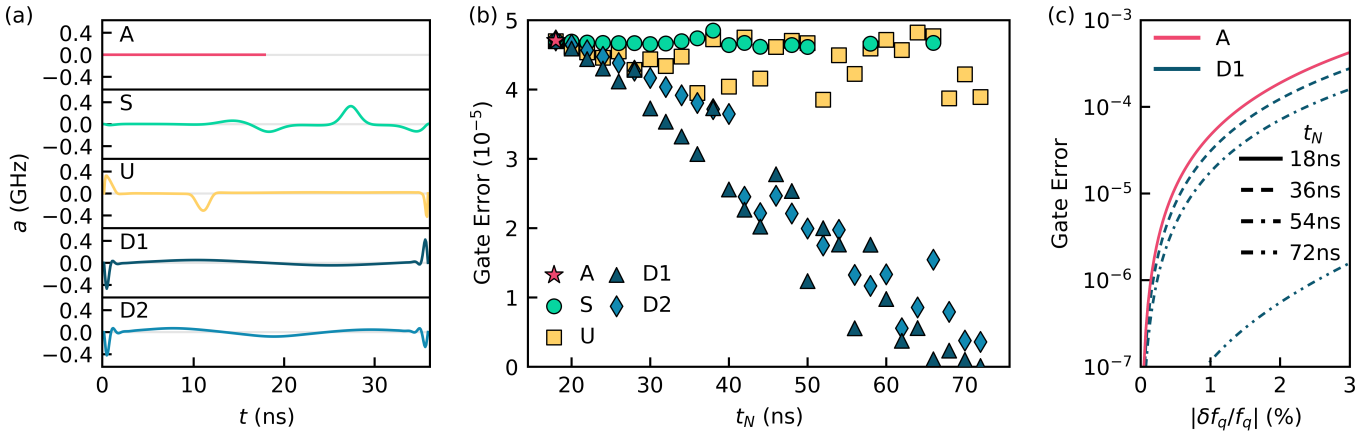

Figure 2: (a) Flux pulses for $Z/2$ gates robust to qubit frequency detunings constructed with the analytic (A), sampling (S), unscented sampling (U), and the 1st- and 2nd-order derivative methods (D1, D2). The flux pulses shown for the sampling, unscented sampling, and derivative methods are optimized for twice the gate time of the analytic gate. (b) Single gate error at a one-percent qubit frequency detuning as a function of the gate time. Missing data points represent gates with a gate error greater than $5 \cdot 10^{-5}$ TODO: ...what's going on here? Should I be concerned? This seems like a relatively big thing that goes unexplained. (c) Single gate error as a function of the qubit frequency detuning. The gate errors for the analytic and 1st-order derivative methods are shown for gate times which are multiples of $1/4f_q \sim 18$ns. The gate errors for the two methods are indistinguishable at the gate time 18ns.

TODO: this seems far more complicated than the sampling method - if it truly is necessary, perhaps earlier we could fully flesh out what the issues are? Does this drifting too close to the nominal state actually occur in practice? And if so, it isn't clear to me why that is a bad thing, as for example if it drifts close to the nominal state, then great, isn't the optimizer doing its job?

The derivative method penalizes the sensitivity of the state to the uncertain parameter, which is encoded in the l^{th}-order state derivative $\partial_{f_q}^l |\psi\rangle$ TODO: seems funny to change from l to m immediately after introduction. In the m^{th}-order derivative method, we append all state derivatives of order $1, \ldots, m$ to the augmented state vector (4) for each initial state. We use the initial state $|0\rangle$ for this method, and observe no advantage to using more initial states TODO: comment on why you've chosen different states for this vs. unscented?. We penalize the norms of the state derivatives in the objective (6a) by setting the corresponding elements of the final augmented state to zero TODO: this isn't totally obvious to me - why should this be the right way to penalize? Also the wording seems a bit off - surely you don't mean that you're penalizing the norm of the state derivative with itself? Isn't it normalized?. We could obtain the state derivatives at each knot point with backward-mode differentiation. In a naive automatic differentiation scheme, the discrete dynamics function at knot points $1, \ldots, k-1$ would be differentiated to obtain the state derivative at knot point k, requiring $O(N^2)$ matrix multiplications. Instead, we employ forward-mode differentiation on the TDSE (1) to obtain coupled, first-order ODEs which require $O(N)$ matrix multiplications to integrate. For example, the dynamics for the 1st-order derivative method are:

$$i\hbar \frac{d}{dt} |\psi\rangle = H |\psi\rangle , \tag{8}$$

$$i\hbar \frac{d}{dt} \left|\partial_{f_q}\psi\right\rangle = H \left|\partial_{f_q}\psi\right\rangle + (\partial_{f_q} H) |\psi\rangle . \tag{9}$$

We integrate the coupled ODEs with exponential integrators in the discrete dynamics function (6b), see Appendix C. For runtimes of the three robust control techniques, consult Appendix D.

TODO: you have obviously made the choice to first present all three methods as theoretical tools, then discuss their results together, which is fine. It might make sense to also consider presenting a method and presenting results associated with that method, before moving on to the next one. Might make it easier to justify, e.g., the complexity of the unscented sampling method if there are deficiencies to be addressed that are clear from the results of the sampling method. We examine the gate errors due to a static qubit frequency detuning for the $Z/2$ gates obtained with the robust control techniques and the analytic $Z/2$ gate. To compute the gate error, an initial state is evolved under the fluxonium Hamiltonian (3) two separate times with the transformations $f_q \to f_q \pm \delta f_q$ at the stated qubit frequency detuning δf_q. The reported gate error is the infidelity of the evolved state and the target state averaged over the two transformations for each of 1000 pseudorandomly generated initial states. We set $\sigma_{f_q}/f_q = 1\%$ for the sampling and unscented sampling methods. TODO: right so reading further - this paragraph has nothing to do with the previous two - might

make sense to put this with the corresponding explanation of the method.

The analytic gate corresponds to idling at the flux frustration point $a_k = 0 \ \forall \ k$, see Figure 2a. Its gate time $1/4f_q \sim 18$ns is the shortest possible for a $Z/2$ gate on the device. The gate's erroneous rotation angle $2\pi\delta f_q/4f_q$ is linear in the qubit frequency detuning, resulting in a gate error that is quadratic in the detuning. At a one-percent detuning ($|\delta f_q|/f_q = 1\%$), the gate error is $\sim 4.5 \cdot 10^{-5}$, which is sufficient for quantum error correction. Although the gate performs well, it cannot be extended to gate times other than $1/4f_q$. The ability to perform phase gates in any given time is critical for multi-qubit experiments, where the qubits operate at different frequencies. We can find solutions using the numerical methods at all gate times above 18ns, see Figure 2b. These numerical methods offer an effective scheme for synchronizing multi-qubit experiments. TODO: this seems like a funny way to end this paragraph - I was told that static parameter deviations were the issue the whole time, and suddenly it's that analytic pulses aren't flexible enough w.r.t. the time it takes to complete them. I would stress instead that you can do better than $\sim 4.5 \cdot 10^{-5}$! The time issue, though important, feels like it should be more of an aside given the things you've emphasized are the issues you're trying to solve.

The flux pulse produced by the sampling method transitions smoothly away from idles at the flux frustration point, whereas that for the unscented sampling method employs three distinct transitions. The gate error at a one-percent qubit frequency detuning for the sampling method does not improve substantially over the range of gate times. Conversely, the gate error at a one-percent detuning for the unscented sampling method reaches a minimum of $\sim 3.9 \cdot 10^{-5}$ near fractions of the Larmor period $2/4f_q \sim 36$ns, $3/4f_q \sim 54$ns, $4/4f_q \sim 72$ns.

The two derivative methods converge on qualitatively similar flux pulses that use fast triangle pulses at the boundaries and idle near the flux frustration point, similar to the flux pulse produced by the unscented sampling method. The gate errors at a one-percent qubit frequency detuning for both derivative methods decrease super-linearly in their gate times. The 2^{nd}-order method does not offer a substantial improvement over the 1^{st}-order method for most gate times. TODO: I would say the second order method as compared to the first order method feels the same as the sampling method as compared to the unscented method. You say here that there is no improvement, but improvement for unscented looks mostly like noise to me, even if you have some idea of where it's coming from (larmor period fractions). I would just be careful with how these things are framed - seems opportunistic to claim that unscented gives some sort of serious advantage here. The gate error at a one-percent detuning for the 1^{st}-order method reaches 10^{-7} at the Larmor period $1/f_q \sim 72$ns, see Figure 2c. This result mimics the ability of composite pulses to mitigate parameter uncertainty errors to arbitrary order with sufficiently many pulses [41]. It is difficult to choose an appropriate composite pulse for the problem studied here due to our Hamiltonian and experimental constraints. We propose comparisons between composite pulses and numerical techniques for future work.

VI. ROBUSTNESS TO TIME-DEPENDENT PARAMETER UNCERTAINTY

An additional source of experimental error arises from time-dependent parameter uncertainty. For many flux-biased and inductively-coupled superconducting circuit elements, magnetic flux noise is a significant source of coherent errors TODO: good place for a citation. Flux noise modifies the fluxonium Hamiltonian (3) by $a(t) \rightarrow a(t) + \delta a(t)$. The spectral density of the flux noise $\delta a(t)$ is observed to follow a $1/f$ distribution [101–104], so the noise is dominated by low-frequency components. The analytic gate considered here takes advantage of the low-frequency characteristic and treats the noise as quasi-static, performing a generalization of the spin-echo technique to compensate for erroneous drift [105, 106].

Additionally, we modify the robust control techniques presented in the previous section to combat $1/f$ flux noise. The unscented sampling method is modified so that the sample states are subject to $1/f$ flux noise. The noise is generated by filtering white noise sampled from a standard normal distribution with a finite impulse response filter [107]. The noise is then scaled by the flux noise amplitude of our device $A_\Phi = 5.21\mu\Phi_0 \implies \sigma_a = 2.5 \cdot 10^{-5}$GHz. In principle, we could modify the sampling method similarly; however, we choose to subject the sample states to static noise $a(t) \rightarrow a(t) \pm \sigma_a$ for comparison. The derivative methods require no algorithmic modification from the static case, but the TDSE is now differentiated with respect to $a(t)$ instead of f_q as in (9).

We analyze the gate errors due to $1/f$ flux noise for the $X/2$ gates constructed with the robust control techniques and the analytic $X/2$ gate. To compute the gate error, an initial state is evolved under the fluxonium Hamiltonian (3) where the optimized flux is modified $a(t) \rightarrow a(t) + \delta a(t)$. The flux noise is generated as we described for the unscented sampling method. The reported gate error is the infidelity averaged over 1000 pseudorandomly generated initial states, each of which is subject to a distinct pseudorandomly generated flux noise instance. To observe the effect of interfering coherent errors, we simulate successive applications of the gate constructed by each method and compute the cumulative gate error after each application, see Figure 3. Both the analytic and numerical gates yield single gate errors sufficient for quantum error correction. Despite converging on qualitatively different solutions, the numerical gates perform similarly in the concatenated gate application comparison. Their gate errors after 200 gate applications $\sim 11\mu$s are two orders of magnitude less than the gate

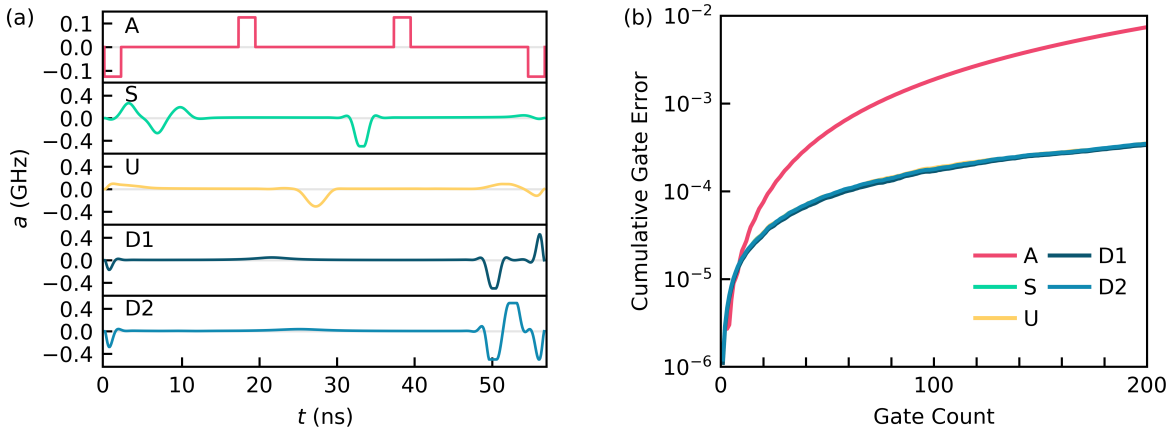

Figure 3: (a) Flux pulses for $X/2$ gates robust to flux offsets constructed with the analytic (A), sampling (S), unscented sampling (U), and the 1st- and 2nd-order derivative methods (D1, D2). (b) Cumulative gate error due to $1/f$ flux noise for successive gate applications. The cumulative gate errors for the sampling, unscented sampling, and the derivative methods are indistinguishable.

error produced by the analytic gate. $1/f$ flux noise is a significant source of coherent errors in NISQ applications and these numerical techniques offer effective avenues to mitigate it.

VII. CONCLUSION

We have applied state-of-the-art trajectory optimization techniques to mitigate decoherence and achieve robustness to parameter uncertainty errors on a quantum system. We have proposed a scheme for suppressing depolarization with time-optimal control and the integrated depolarization rate model. The computational cost of this model is independent of the dimension of the Hilbert space, enabling inexpensive optimization on high-dimensional quantum systems (hmm, this seems like something that definitely wasn't emphasized in the text - could be worth talking about this a little earlier. Also doesn't seem totally true right? Re Eq.(5)). We have also proposed the derivative method for robust control which achieves super-linear gate error reductions in the gate time for the static parameter uncertainty problem we studied. We have shown that the derivative, sampling, and unscented sampling methods can mitigate $1/f$ flux noise errors–which dominate coherent errors for flux controlled qubits. These robust control techniques can be applied to any Hamiltonian, allowing experimentalists in all domains to engineer robust operations on their quantum systems. These methods can be used to achieve the low gate errors required for fault-tolerant quantum computing applications. Our implementations of the techniques described in this work are available at `https://github.com/SchusterLab/rbqoc`. TODO: static code?

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Appendix A: Depolarization

We comment on the depolarization metrics and then give our procedure for integrating the Lindblad master equation. The integrated depolarization rate and the gate error due to depolarization metrics are compared in Table I for the numerical experiment described in Section IV. The relative performance of the analytic and numerical techniques is similar across the two metrics.

Gate	$D_{1\mathrm{A}}$ (10^{-5})	$D_{1\mathrm{N}}$ (10^{-5})	$D_{1\mathrm{A}}/D_{1\mathrm{N}}$	$\mathrm{GE_A}$ (10^{-5})	$\mathrm{GE_N}$ (10^{-5})	$\mathrm{GE_A}/\mathrm{GE_N}$
Z/2	5.745	1.149	5.000	1.776	0.371	4.787
Y/2	5.253	1.157	4.540	1.539	0.370	4.159
X/2	16.251	2.660	6.109	5.347	0.863	6.196

Table I: Single gate integrated depolarization rate (D_1) and single gate error due to depolarization (GE). Values are reported for the analytic (A) and numerical (N) gates.

We employ the Lindblad master equation to compute the gate error due to depolarization. This equation takes

the form:

$$\frac{d}{dt}\rho = \frac{-i}{\hbar}[H,\rho] + \sum_i \gamma_i (L_i \rho L_i^\dagger - \frac{1}{2}\{L_i^\dagger L_i, \rho\}), \quad \text{(A1)}$$

where $\rho = |\psi\rangle\langle\psi|$ is the density matrix, $[\cdot,\cdot]$ is the algebraic commutator, and $\{\cdot,\cdot\}$ is the algebraic anti-commutator. For depolarization $\gamma_\uparrow = T_{1,\uparrow}^{-1}$, $\gamma_\downarrow = T_{1,\downarrow}^{-1}$, $L_\uparrow = \sigma^+/2$, and $L_\downarrow = \sigma^-/2$ where $\sigma^\pm = \sigma_x \pm i\sigma_y$. Both $T_{1,\uparrow}$ and $T_{1,\downarrow}$ are obtained at each knot point from the spline shown in Figure 1b. We obtain the T_1 values in this spline by driving the qubit at the desired flux amplitude and monitoring the resultant decay. For more details on these measurements, consult [59].

So that we may use exponential integrators, we employ the Vectorization/Choi-Jamiolkowski isomorphism [108],

$$\frac{d}{dt}\text{vec}(\rho) = \hat{\mathcal{L}}\text{vec}(\rho), \quad \text{(A2)}$$

$$\begin{aligned}\hat{\mathcal{L}} &= -i(I\otimes H - H^T \otimes I) \\ &+ \sum_i \gamma_i (L_i^* \otimes L_i - \frac{1}{2}(I \otimes L_i^\dagger L_i - L_i^T L_i^* \otimes I)),\end{aligned} \quad \text{(A3)}$$

where $\rho = \sum_{i,j}\alpha_{i,j}|i\rangle\langle j|$ and $\text{vec}(\rho) = \sum_{i,j}\alpha_{i,j}|i\rangle\otimes|j\rangle$. We use zero-order hold on the controls–equivalently, $a(t)$ is piecewise-constant on the intervals $[t_k, t_{k+1}]$. Therefore, $H(a(t))$, $L(a(t))$, and $\gamma_i(a(t))$ are also piecewise-constant. So, the exact solution is $\text{vec}(\rho_{k+1}) = \exp(\Delta t_k \hat{\mathcal{L}}_k)\text{vec}(\rho_k)$. This isomorphism transforms $(n\times n)\times(n\times n)$ matrix-matrix multiplications to $(n^2\times n^2)\times n^2$ matrix-vector multiplications. For small n and zero-order hold on the controls, we find that it is faster to use an exponential integrator on the vectorized equation than to perform Runge-Kutta on the unvectorized equation. The latter requires decreasing the integration time step to maintain accuracy, resulting in more knot points.

Appendix B: Unscented Transformation

In this section, we outline the full unscented sampling procedure. In the unscented sampling method, we consider a state $\psi \in \mathbb{R}^{2n}$, an uncertain parameter $\lambda \in \mathbb{R}^d$, and discrete dynamics $\psi_{k+1} = f(\psi_k, \lambda_k)$ (maybe choose one between this and $x_{k+1} = f(x_k, u_k)$).. We omit braket notation to emphasize that the state is a real vector, and it is given by the right-hand-side of the isomorphism (5). The nominal initial state is given by $\bar{\psi}_1$ with an associated covariance matrix $P_1 \in \mathbb{S}_{++}^{2n}$ which describes the uncertainty in the initial state. We use the notation $\mathbb{S}_{++}^m$ to denote the set of real, symmetric, and positive-definite $m\times m$ matrices. P_1 is typically non-zero even if the state preparation error is negligible. The uncertain parameter has zero-mean and its distribution is given by the covariance matrix $L_k \in \mathbb{S}_{++}^d$ at knot point k. The zero-mean assumption is convenient for deriving the update procedure. A non-zero mean can be encoded in the discrete dynamics function $f(\psi_k, \lambda_k)$.

The initial $4n+2d$ sample states and initial $4n+2d$ uncertain parameters are sampled from the initial distributions,

$$\begin{bmatrix}\psi_1^j \\ \lambda_1^j\end{bmatrix} = \begin{bmatrix}\bar{\psi}_1 \\ 0\end{bmatrix} \pm \beta \sqrt{\begin{bmatrix}P_1 & 0 \\ 0 & L_1\end{bmatrix}}^j. \quad \text{(B1)}$$

β is a hyperparameter that controls the spacing of the covariance contour. The $(\pm)$ is understood to take $(+)$ for $j \in \{1,\ldots,2n+d\}$ and $(-)$ for $j \in \{2n+d+1,\ldots,4n+2d\}$. We use the Cholesky factorization to compute the square root of the joint covariance matrix, though other methods such as the principal square root may be employed. The superscript on the matrix square root indicates the j^{th} column (mod $2n+d$) of the lower triangular Cholesky factor. Then, the sample states are normalized,

$$\psi_1^j \to \frac{\psi_1^j}{\sqrt{{\psi_1^j}^T \psi_1^j}}. \quad \text{(B2)}$$

The sample states are propagated to the next knot point,

$$\psi_2^j = f(\psi_1^j, \lambda_1^j). \quad \text{(B3)}$$

The mean and covariance of the sample states are computed,

$$\bar{\psi}_2 = \frac{1}{4n+2d}\sum_{j=1}^{4n+2d}\psi_2^j, \quad \text{(B4)}$$

$$P_2 = \frac{1}{2\beta^2}\sum_{j=1}^{4n+2d}(\psi_2^j - \bar{\psi}_2)(\psi_2^j - \bar{\psi}_2)^T. \quad \text{(B5)}$$

The sample states are then resampled and propagated to the next knot point using (B1), (B2), and (B3). Our choice of sample states (sigma points) follows equation 11 of [56]. Prescriptions that require fewer sigma points exist [109].

Appendix C: Derivative Method

Here, we outline how to efficiently integrate the dynamics for the derivative method using exponential integrators. General exponential integrators break the dynamics into a linear term and a non-linear term. For example, the dynamics of the first state derivative in units of $i\hbar = 1$ (is setting i=1 something that is done? Seems fraught and scary...just leave it in there bro and set hbar to 1 like the rest of us!)are $\frac{d}{dt}|\partial_\lambda\psi\rangle = H|\partial_\lambda\psi\rangle + (\partial_\lambda H)|\psi\rangle$. The linear term is $L = H$ and the non-linear term is $N = (\partial_\lambda H)|\psi\rangle$. With zero-order hold on the

controls the exact solution is:

$$|\partial_\lambda \psi_{k+1}\rangle = \exp(\Delta t_k L_k)\,|\partial_\lambda \psi_k\rangle + \int_0^{\Delta t_k} \exp\Big((\Delta t_k - t^{'})L_k\Big) N(t_k + t^{'}) dt^{'}. \tag{C1}$$

General exponential integrators proceed by breaking the integral in (C1) into a discrete sum, similar to the procedure for Runge-Kutta schemes. We use a simple approximation known as the Lawson-Euler method [68],

$$|\partial_\lambda \psi_{k+1}\rangle \approx \exp(\Delta t_k L_k)\,|\partial_\lambda \psi_k\rangle + \exp(\Delta t_k L_k) N_k \Delta t_k. \tag{C2}$$

This method provides a good tradeoff between accuracy and efficiency, requiring one unique matrix exponential computation per stage. Integration accuracy is not of the utmost importance because the state derivatives guide the optimization, and do not correspond to experimental parameters which must be realized with high accuracy.

Appendix D: Computational Performance

We provide runtimes for our optimizations and comment on the problem size of the robustness methods. The runtimes for the base optimization in Section III, the depolarization optimization in Section IV, and the robust optimizations in Section V are presented in Table II for a $Z/2$ gate at gate times which are multiples of $1/4f_q \sim 18$ns. We performed optimizations on a single core of an AMD Ryzen Threadripper 3970X 32-Core Processor. Future work will parallelize the robustness methods using GPUs [13], which will enable fast optimizations on high-dimensional Hilbert spaces.

	Average Runtime (s)		
t_N (ns)	18	36	72
Base	0.155 ± 0.008	7.0 ± 0.4	15.9 ± 0.8
Depol.	1.69 ± 0.08	-	-
S	1.77 ± 0.09	48 ± 2	280 ± 10
U	75 ± 4	340 ± 20	400 ± 20
D1	6.1 ± 0.3	27 ± 1	65 ± 3
D2	15.7 ± 0.8	17.3 ± 0.9	54 ± 3

Table II: Average runtimes for $Z/2$ optimizations using the base, depolarization, sampling (S), unscented Sampling (U), and the 1st- and 2nd-order derivative methods (D1, D2). (comment on empty table slots?)

Now we note the size of the augmented state vector for the robustness methods. For the sampling method, the size of the augmented state vector is $O(dn^3)$, where d is the number of uncertain parameters and n is the dimension of the Hilbert space. There are n^2 initial states in the operator basis, $2d$ sample states per initial state, and each state has $2n$ real numbers. For the unscented sampling method, the size of the augmented state vector is $O(dn^3 + n^4)$. There are n^2 initial states in the operator basis, $2(2n + d)$ sample states per initial state, and each state has $2n$ real numbers. For the m^{th}-order derivative method, the size of the augmented state vector is $O(dmn^3)$. There are n^2 initial states in the operator basis, dm state derivatives per initial state, and each state has $2n$ real numbers. TODO: maybe add comment about auto-diff

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