Optimal Control of Families of Quantum Gates

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Quantum optimal control (QOC) enables the realization of accurate operations, such as quantum gates, and supports the development of quantum technologies. To date, many QOC frameworks have been developed, but those remain only naturally suited to optimize a single targeted operation at a time. We extend this concept to optimal control with a continuous family of targets, and demonstrate that an optimization based on neural networks can find families of time-dependent Hamiltonians realizing desired classes of quantum gates in minimal time.

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After concerted efforts in the development of synthetic quantum systems we have access to a variety of systems with sufficiently long coherence time to perform a series of coherent operations. In the community's effort to turn such systems into technological applications, quantum optimal control (QOC) [1,2] helps to increase the precision and rate of desired operations. Common problems successfully addressed by means of QOC include the realization of quantum gates or entangled states in few-body or many-body systems [3–11] and the refinement of metrology protocols [12,13].

Current tasks of optimal control are mostly focused on the realization of a single target operation, such as the preparation of one specific state or the implementation of one specific gate. Yet, as quantum technologies mature, it becomes important to enlarge the range of operations which can be accurately implemented on a device. For instance, in the context of noisy-intermediate scale quantum devices [14], augmenting the set of available elementary gates allows for a more compact compilation of quantum circuits, i.e., their decomposition into these elementary gates. Already the inclusion of continuous families of 2-qubit gates to a typical gate set, composed of 1-qubit rotations and a 2-qubit entangling gate, can lead to a significant reduction in gate count [15–17]. This, in turn, opens the possibility to run more expressive computations before the onset of decoherence, a key limitation in current technology. That is, the ability to implement a broader range of optimized operations has the potential to substantially increase the utility of current quantum hardware.

Despite the many flavors of QOC frameworks that have been proposed (e.g., Refs. [18–28]), the case remains that current methodologies are only naturally suited to consider a single control task at a time. We thus aim at lifting the original scope of QOC from the control of a single target operation to the control of continuous families of targets. This is achieved with a neural network (NN) modeling the dependency between Hamiltonians to be engineered and control tasks to be solved. Efficient training of the framework by means of gradient descent is facilitated by recent advances in the field of automatic differentiation [29]. Such a framework, dubbed family control, is sketched in Fig. 1 and is now explained in detail.

Typically, the central task in QOC is the identification of the time-dependent Hamiltonian $H(t)$ that induces a propagator $U(t)$ with desired properties. This is formulated in terms of a cost functional $\mathcal{I}[H(t)]$ to be minimized. A common example would be the task of realizing a target controlled-not gate $U^{\mathrm{tgt}} = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes \sigma_x$ at a given time T, with the cost $\mathcal{I}[H(t)] = \|U(T) - U^{\mathrm{tgt}}\|$ measuring the deviation between the controlled and target propagators. A corresponding task of family control could be the realization of the family of target gates $U_\alpha^{\mathrm{tgt}} = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes \exp(-i\alpha\sigma_x)$ with variable angle α. In this case, the overall task to be solved would be the identification of a continuum of Hamiltonians $H_\alpha(t)$, parametrized by the angle α, such that any of the propagators $U_\alpha = U_\alpha(t=T)$ induced by $H_\alpha(t)$ approximates the gate U_α^{tgt} as well as possible at $t = T$. The corresponding functional would thus become $\mathcal{I}[H_\alpha(t)] = \langle \|U_\alpha - U_\alpha^{\mathrm{tgt}}\| \rangle_\alpha$ with an average over α.

The general formulation of such a family-control problem can be given in terms of the individual costs $\mathcal{I}_\alpha[H_\alpha(t)]$, where the target parameter α can be a single scalar or a vector. The overall task to be solved is the identification of the continuum of time-dependent Hamiltonians $H_\alpha(t)$ that minimizes the averaged cost $\mathcal{I} = \langle \mathcal{I}_\alpha[H_\alpha(t)] \rangle_\alpha$.

In principle, this can be addressed as several control problems to be solved separately for a discretized set of target values $\{\alpha^{(i)}\}$, and, an additional step of interpolation for any new target with $\alpha \notin \{\alpha^{(i)}\}$. Hardly any control problem, however, has a unique solution, or at least a unique solution that can be found in practice. That is, there

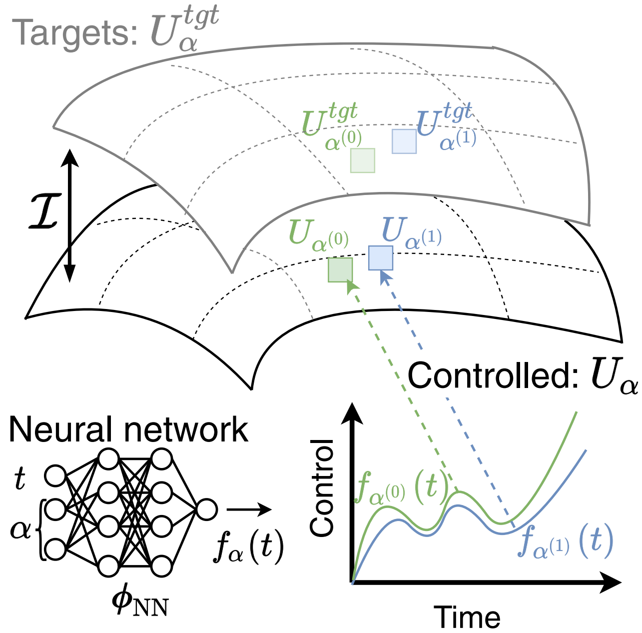

FIG. 1. Optimal control of a continuous family of target gates U_α^{tgt} indexed by the target parameter α which can be either a scalar or a vector. The time-dependent controls $f_\alpha(t)$ which now also depend on α are modeled by a neural network (NN). This NN effectively parametrizes a continuous family of controlled gates U_α where each point corresponds to the propagator obtained by evolving the system in time (dashed arrows) under the controls produced by the NN (illustrated for two sets of target parameters $\alpha^{(0)}$ and $\alpha^{(1)}$). Training of the framework consists in optimizing the weights ϕ_{NN} of the NN such that the deviation $\mathcal{I}$ between the controlled and target families of operations is minimized.

is no guarantee for two Hamiltonians $H_{\alpha^{(1)}}$ and $H_{\alpha^{(2)}}$ identified as optimal for similar values of $\alpha^{(1)}$ and $\alpha^{(2)}$, to be themselves similar. Any attempt to find an optimal Hamiltonian for a value of α between $\alpha^{(1)}$ and $\alpha^{(1)}$ in terms of an interpolation between $H_{\alpha^{(1)}}$ and $H_{\alpha^{(2)}}$ can thus result in a Hamiltonian that utterly fails to realize the desired task. To avoid this issue, it is desirable to require H_α to depend smoothly on α. Such a requirement can be realized by means of an appropriate parametrization of the dependence of $H_\alpha(t)$ on both α and t. Given that NNs provide the flexible structure to approximate multivariate continuous functions up to arbitrary precision [30], these are deemed ideally suited for the task at hand.

Time dependence in a Hamiltonian is typically realized in terms of temporally modulated electromagnetic fields that appear as one or several control functions $f_\alpha(t)$ in the Hamiltonian. The scope of the NN is thus to model these functions. To this intent, the parameters α and the time t are taken to be the inputs of the NN, and the control values $f_\alpha(t)$ its outputs. An example of such a NN is illustrated in Fig. 1 for the case of two-dimensional parameters α and a single control function $f_\alpha(t)$; it is readily adapted to arbitrary dimensions of the parameters and number of controls by varying the sizes of the inputs and outputs accordingly.

The optimization—i.e., training of the NN—can be achieved with a variety of techniques, but gradient-descent training has the advantage of simplicity and scalability to high-dimensional problems. Since the propagators U_α induced by the Hamiltonians H_α typically need to be constructed numerically, efficient means to take derivatives with respect to the control functions $f_\alpha(t)$ are essential. Recent advances in the field of automatic differentiation [29] give access to efficient differentiation over numerical solvers of differential equations. This allows one to combine seamlessly gradients over the evolution of the system and over the weights of the NN. Finally, even though the evaluation of the averaged cost $\mathcal{I}$ would always be based on a sum over discrete values of α rather than a proper integral, the output of the neural network is still continuous in α, and choosing different random sampling points at each step in the training process avoids finding solutions with artifacts resulting from the sampling. Implementation details can be found in Sec. I of the Supplemental Material [31].

The following discussion exemplifies the framework sketched so far, with the realization of quantum gates induced by the n-qubit Hamiltonian

$$\mathcal{H}_\alpha(t) = \sum_{i<j=1}^{n} f_\alpha^{ij}(t)\sigma_x^{(i)}\sigma_x^{(j)} + \sum_{i=1}^{n} f_\alpha^{iy}\sigma_y^{(i)}(t) + f_\alpha^{iz}(t)\sigma_z^{(i)}, \quad (1)$$

with 1-qubit Pauli $\sigma_y^{(i)}$ and $\sigma_z^{(i)}$ terms complemented with interactions $\sigma_x^{(i)}\sigma_x^{(j)}$ between pairs of qubits (i, j). Overall, $C = 2n + n(n-1)/2$ time-dependent functions have to be learned, including the 1-qubit $f_\alpha^{iy}(t)$ and $f_\alpha^{iz}(t)$, and 2-qubit controls $f_\alpha^{ij}(t)$. The Hamiltonian is sufficiently general so that any desired n-qubit unitary can be realized [45], but bounded control amplitudes $\{f_\alpha^{ij}, f_\alpha^{iy}, f_\alpha^{iz}\} \in [-1, 1]$ result in a finite minimal time required to realize a given unitary. Deviations between controlled and target gates are characterized by the gate infidelities

$$\mathcal{I}_\alpha[H_\alpha(t)] = 1 - \frac{1}{2^n}|\mathrm{Tr}[U_\alpha^\dagger U_\alpha^{\mathrm{tgt}}]|^2 \quad (2)$$

in the subsequent examples.

The basic workings of the framework can be illustrated with the task of realizing the manifold of 1-qubit gates

$$U_\alpha^1 = \exp\left(-i\frac{\alpha_1}{2}\sigma_z\right)\exp\left(-i\frac{\alpha_2}{2}\sigma_y\right)\exp\left(-i\frac{\alpha_3}{2}\sigma_z\right) \quad (3)$$

for the three-dimensional target parameters α with components $\alpha_{j=1,2,3} \in [0, \pi]$, given the 1-qubit version of $\mathcal{H}_\alpha(t)$ in Eq. (1) and a fixed gate time $T = \pi$. Here, and in all subsequent examples, the training stage is limited to 400

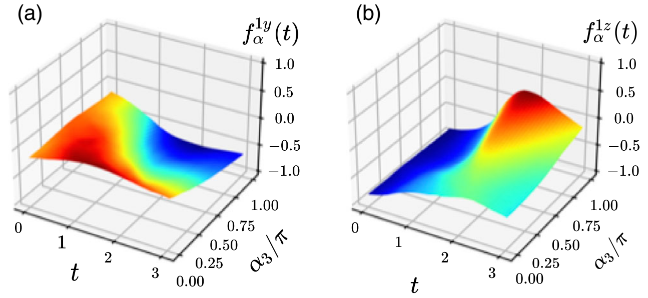

FIG. 2. Control of the family of arbitrary 1-qubit rotations U_α^1 defined in Eq. (3) with the Hamiltonian in Eq. (1). The framework is successfully trained to implement any of the target rotations, resulting in an average infidelity of $\bar{\mathcal{I}} = 2 \times 10^{-4}$ (assessed on new targets not seen during training). To visualize the controls produced by the NN, α_1 and α_2 are kept fixed to a value of $3\pi/4$ and α_3 is varied in the range $[0, \pi]$. The amplitudes of the two control fields f_α^{1y} (a) and f_α^{1z} (b) produced by the NN are plotted as a function of both the time t and α_3/π.

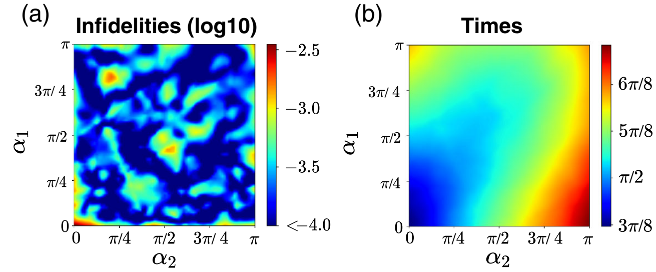

FIG. 3. Infidelities and times for the family U_α^1 of rotations when both the (target-dependent) control functions and times are learned concurrently. For the sake of visualization, results are plotted for a two-dimensional subset of the three-dimensional family of targets, with fixed parameter $\alpha_3 = 3\pi/4$, and discretized $\alpha_1, \alpha_2 \in [0, \pi]$ over a grid of 75×75 regularly spaced points. For each of the corresponding target gates a heat map indicates the values of the infidelities $\mathcal{I}_\alpha$ achieved [panel (a), in logarithmic scale] and the control times T_α entailed by the framework [panel (b)].

iterations, with each iteration corresponding to an average of the gate infidelity in Eq. (2) taken over 128 values of the parameters α uniformly sampled.

After training, the average gate infidelity $\bar{\mathcal{I}} = \langle \mathcal{I}_\alpha \rangle_\alpha$ resulting from the controls identified as optimal by the framework, is evaluated on an ensemble of 250 random values of α. Crucially, this average is taken with respect to new parameter values (i.e., corresponding to targets not seen during training), and thus probes the ability of the framework to realize any gates belonging to the targeted family. In this example, the average infidelity is as low as $\bar{\mathcal{I}} = 2[3] \times 10^{-4}$, where the number in brackets indicates the standard deviation of the distribution. Figure 2 depicts the two control functions $f_\alpha^{1y}(t)$ and $f_\alpha^{1z}(t)$ [panels (a) and (b) respectively] as functions of α_3/π and t for $\alpha_1 = \alpha_2 = 3\pi/4$, substantiating that the solutions produced by the NN are indeed well behaved, continuous functions of both the parameters α and time t.

A comparison between family control and current QOC approaches is provided in Sec. II of the Supplemental Material [31]. As discussed, the latter involves individual optimizations of a discrete set of gates, and a subsequent step of interpolation. Similar training complexity for the individual approach is found for a discretization of each α_i in Eq. (3) over less than $N_d = 10$ distinct values. Refining such coarse discretization results in substantially increased training effort—scaling cubically with N_d given the 3D nature of the gate's family. More crucially, interpolating between individual control solutions is found to often yield close-to-vanishing fidelities.

In addition to an optimization of control functions, the present framework is also well suited to identify a minimal gate time T, or even minimal target-dependent gate times T_α (Sec. IB of the Supplemental Material [31]). The latter is achieved by introducing a second neural network with the gate time T_α as an output. Given the new cost $\mathcal{I}_\alpha + \mu \times T_\alpha$ comprised of the gate infidelity and the gate time as a penalty weighted with a scalar factor $\mu > 0$, this second neural network can be trained similarly to the case discussed above.

In Fig. 3 the results from such an optimization are reported, with a small value $\mu = 10^{-2}$ of the weight suitable to find high-fidelity gates close to the minimally required time. Panel (a) depicts the infidelity $\mathcal{I}_\alpha$ of the resulting gates for $\alpha_3 = 3\pi/4$ as a function of α_1 and α_2. Typical values are smaller than 10^{-3}, and the average infidelity with the average taken over all three components of α is $\bar{\mathcal{I}} = 4[5] \times 10^{-4}$.

Figure 3(b) depicts the target-dependent minimized gate times, with again a fixed value of $\alpha_3 = 3\pi/4$ but varied α_1 and α_2. The shortest gate time is obtained for $\alpha_1 = \alpha_2 = 0$ (i.e., for the target parameters $\alpha^{(0)} = [0, 0, 3\pi/4]$) in which case the constant control amplitudes $f_{\alpha^{(0)}}^{1z}(t) = 1$ and $f_{\alpha^{(0)}}^{1y}(t) = 0$ induce the desired gate $U_{\alpha^{(0)}}^1 = \exp[-i(3\pi/8)\sigma_z]$ after a time $T_{\alpha^{(0)}} = 3\pi/8$. The obtained gate times grow with increasing values of α_1 and α_2, but always remain below the value of π used in the above example.

While the ability to realize 1-qubit gates is of substantial practical value, it is certainly not the challenging control problem that helps to demonstrate the actual strength of the framework. This is better achieved in terms of 2-qubit and 3-qubit gates that are building blocks of quantum algorithms or digital quantum simulations.

Table I summarizes the results for a few selected families of 2- and 3-qubit gates with the domain χ of the parameters α depicted in column 3 and the obtained average infidelities (in multiples of 10^{-4}) in column 4 (further details of the NNs used are reported in Sec. IC of the Supplemental Material [31]). The 2-qubit gates (i) to (iv) involve

TABLE I. Control under the Hamiltonian of Eq. (1) of families of $n = 2$ and 3 qubit gates, corresponding to $C = 5$ and 9 control functions to be learned respectively. For each problem the family of target $U_\alpha^{\rm tgt}$ considered and the domain χ of the target parameters α are reported. Results are provided in terms of the average (and standard deviations in brackets) infidelities $\bar{\mathcal{I}}$, and of the ratio R between the average gate times resulting from a decomposition in terms of elementary gates and the times necessitated by the framework. Additional elements of training the families (vi) and (vii) are provided in the main text.

	$U_\alpha^{\rm tgt}$	χ	$\bar{\mathcal{I}}[10^{-4}]$	R
(i)	$\vert 0\rangle\langle 0\vert \otimes I + \vert 1\rangle\langle 1\vert \otimes \exp(-i\alpha_1\sigma_z^{(2)})$	$[0,\pi]$	1[1]	2.0
(ii)	$\exp(-i\alpha_1\sigma_z^{(1)}\sigma_z^{(2)})$	$[0,(\pi/2)]$	0[0]	2.0
(iii)	$\vert 0\rangle\langle 0\vert \otimes I + \vert 1\rangle\langle 1\vert \otimes U_\alpha^1$	$[0,\pi]^3$	3[4]	2.1
(iv)	$\exp(-i\sum_{j\in\{x,y,z\}}\alpha_j\sigma_j^{(1)}\sigma_j^{(2)})$	$[0,(\pi/2)]^3$	4[4]	2.6
(v)	$\exp(-i\alpha_1\sigma_z^{(1)}\sigma_z^{(2)}\sigma_z^{(3)})$	$[0,(\pi/2)]$	1[0]	4.1
(vi)	$\exp(-i\sum_{j\in\{x,y,z\}}\alpha_j\sigma_j^{(1)}\sigma_j^{(2)}\sigma_j^{(3)})$	$[0,(\pi/2)]^3$	9[8]	> 10
(vii)	$(I - \vert 11\rangle\langle 11\vert)\otimes I + \vert 11\rangle\langle 11\vert \otimes U_\alpha^1$	$[0,\pi]^3$	6[5]	> 10

optimizations over $C = 5$ control functions, and the 3-qubit gates (v) to (vii) involve $C = 9$ control functions.

Consistently with the previous findings, low infidelities $\bar{\mathcal{I}} < 5\times 10^{-4}$ are achieved for any of the families of 2-qubit gates (i–iv) and for the one-dimensional family of 3-qubit gates (v).

A straightforward application of the above framework to the problems (vi) and (vii)—corresponding to nine time-dependent controls to be learned and three-dimensional families to be realized—however results in higher infidelities [$3[2.5]\times 10^{-3}$ for (vi) and $1.7[1.5]\times 10^{-3}$ for (vii)] than in the other cases. Yet, the results of the optimizations contain clear indications toward steps to reach higher fidelities that are now further discussed.

First, the lowest fidelities are systematically obtained for values of α close to the boundary of its admissible domain χ [as can also be seen in Fig. 3(a)]. Enlarging the range of values used for training by 20% resolves this effect. Second, the control functions identified as optimal have general properties that can be exploited to reduce the number of independent functions that need to be learned. In case (vi), the control solutions discovered by the framework satisfy the relation $f_\alpha^{13} = f_\alpha^{1z} = f_\alpha^{3z} = 0$, and in case (vii) they satisfy $f_\alpha^{1z} = f_\alpha^{2z} = 0$, $f_\alpha^{1y} = f_\alpha^{2y}$ and $f_\alpha^{13} = f_\alpha^{23}$. This indicates that only six and five independent control functions, out of the nine possible, are needed for cases (vi) and (vii) respectively. The infidelities listed in Table I, for families (vi) and (vii), result from an optimization with enlarged domain χ and reduced number of control functions, and their magnitude is comparable to those of the other cases.

While generally the nonuniqueness of solutions of optimal control problems makes it difficult to understand why a solution returned by a specific algorithm does achieve the goal that it is meant to achieve, it seems that the requirement of smooth dependence on the parameters α helps the NN to identify common features of all control pulses within the family and to avoid unnecessary terms in the Hamiltonian that would obscure its working principle.

Beyond this conceptual benefit and the low infidelities achieved, the gain in gate time is also of high practical relevance. Since state-of-the-art implementation of unitaries on quantum devices relies on their decompositions in terms of elementary gates, the times $T^{\rm dec}$ entailed by such decompositions provide well-defined baselines. Given the freedom offered by the control Hamiltonian in Eq. (1) these decompositions are performed in terms of the gate set of rotations generated by the 1-qubit σ_y and σ_z and 2-qubit $\sigma_x\sigma_x$ operators, for which Qiskit's [46] compiling routine is employed with the highest level of optimization available (Sec. II of Supplemental Material [31]).

Column 5 of Table I depicts the ratio R between the averaged durations $\langle T_\alpha^{\rm dec}\rangle_\alpha$ obtained with compiled gate circuits and the durations obtained with the present techniques. In all cases there is an improvement of at least a factor of 2, but, in cases (vi) and (vii), the improvement is substantially larger. This suggests that compilation techniques (i.e., discrete optimizations) struggle with these complex 3-qubit gates, whereas the continuous optimization realized in terms of NN does not suffer from these limitations.

The ability to accurately control entire families of gates in reduced time, especially for complex gates, highlights the benefits of family control. Given that the automatic differentiation techniques [29], that ensure the efficient training of the framework, can be applied to any system of ordinary differential equations (ODE), family control can find a direct application to a broad range of quantum systems, such as superconducting qubits. Since those are nonlinear oscillators with a ladder of excited states, further studies would include suppression of leakage to such states. Similarly, trapped ions or optomechanical systems with several interacting degrees of freedom pose control problems that can be addressed with the present techniques.

Applying QOC to open systems [47–50] allows one to take into account (and minimize) the detrimental effects of an external environment, and is within the direct reach of family control. The dynamics of open quantum systems is mostly described by means of a master equation, effectively an ODE, and is thus amendable to the methodology described. While simulating such dynamics is inherently more demanding than for closed systems, this overhead can be mitigated by evolving only a constant number of carefully selected initial states [48]. Going further, automatic differentiation has now been extended to the treatment of stochastic differential equations [51,52] such that family control can also be applied to open systems simulated with quantum trajectories [50] and could even generalize to problems of control with active feedback [53,54].

While optimal control is traditionally realized in terms of control pulses designed in numerical experiments, fundamental limitations in modeling and simulating the dynamics of composite quantum systems resulted in a shift toward designing control pulses in laboratory experiments [55–58]. Just like many techniques for individual control targets could be generalized to this setting, also family control could be trained based exclusively on experimental data, either in situations where gradients can be experimentally estimated [59], or by resorting to gradient-free optimization strategies [60].

Essentially, the methodology that was presented here enables the control of a quantum system in different *contexts*. In the examples investigated, this context was in one to one correspondence with the target gate to be realized, that is, the overall details of the system under control were kept fixed and only the targets were varied. More generally, the scheme based on NNs allows one to tailor controls to be applied to any relevant context variable. For instance, the inputs of the NN could also include intrinsic details of the controlled system (such as varied energy detunings [61] or sizes [62]) or extrinsic (such as environmental heating rates [63] or nearby operations inducing crosstalk [64]). Provided that the effects of these context variables can be simulated and that the corresponding optimal controls are expected to vary continuously with these variables, one would learn to accurately operate a quantum device in very broad situations.

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