Optimal control landscape for the generation of unitary transformations

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The generation of specific unitary transformations is central to a variety of quantum control problems. Given a target unitary transformation, the optimal control landscape is defined as the Hilbert-Schmidt distance between the target and controlled unitary transformation as a function of the control variables. The critical topology of the landscape is analyzed for controllable quantum systems evolving under unitary dynamics over a finite dimensional Hilbert space. It is found that the critical regions of the landscape corresponding to global optima are isolated points, and the local optima are Grassmannian submanifolds. The volumes of the critical submanifolds corresponding to suboptimal critical values asymptotically vanish in the limit of large Hilbert space dimension. Furthermore, these critical submanifolds have saddle-point topology, which cannot act as traps when searching for optimal controls. These favorable properties of the local optima suggest that the landscape topology is generally amenable to optimization. The analysis is independent of the particular structure of the system Hamiltonian, except for the assumption of full controllability, and the results are universal to the control of unitary transformations of any quantum system.

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I. INTRODUCTION

The realization of many goals in quantum control [1] and quantum information processing [2] requires the generation of specific unitary transformations to a high degree of fidelity. For control problems in which the underlying dynamics are well understood, the control variables in the system Hamiltonian can be determined from first principles [3,4]. However, for the common case of complex systems whose dynamics are not sufficiently understood, optimal control experimental (OCE) methods can be used to obtain the desired unitary transformation by adaptive learning algorithms [5]. The OCE method has been applied successfully to a broad and growing variety of physical control experiments [6]. In all such experiments, the discovery of effective control fields is directed by an adaptive learning algorithm which uses a feedback signal to direct the controls. The computer simulation analog to OCE is optimal control theory (OCT) [7], which generally employs classical variational methods to optimize the dynamical outcomes [8]. In principle, OCE and OCT may be used for the optimal generation of unitary transformations as well. In this case, the learning algorithm could use quantum process tomography or other data for a metric of fidelity to evaluate the merit of the trial control parameters giving rise to a particular unitary transformation. Recently, OCT methods have been adapted for the generation of target unitary transformations with an encouraging degree of success [9]. Successful optimal searching for unitary transformations with genetic algorithms has also been demonstrated in model systems [10,11]. These results indicate that the generation of unitary transformations is amenable to optimal searching, and points toward the prospect of implementing such searches in the laboratory through OCE. These searches are conducted over an optimal control landscape, and understanding the topology of such landscapes can provide useful insights for practical implementations and aid in elucidating any intrinsic limitations to such efforts.

Section II presents the formal definition of the optimal control landscape. In Sec. III, we enumerate the critical regions of the landscape as a function of system Hilbert space dimension N, identify the topology of the critical regions as that of Grassmannian submanifolds, and discuss methods of computing their effective volumes. Section IV presents the explicit relation between the cost function value J at these critical submanifolds and the signs of the eigenvalues for the Hessian of J on those submanifolds. Section V presents concluding remarks.

II. CONTROL LANDSCAPE CONCEPT

Consider a quantum system defined over an N-dimensional Hilbert space whose dynamics are given by the Schrödinger equation

$$i\hbar \frac{d}{dt}U(t,0) = H(\kappa,t)U(t,0), \tag{1}$$

where $H(\kappa,t)$ is a time-dependent Hamiltonian whose control variables are collectively denoted as κ. The propagator $U(t,0)$ over the time interval $0 \leq t \leq T$ is the $N \times N$ unitary transformation

$$U(T,0) = \mathbf{T} \exp\left(-i\int_0^T dt H(\kappa,t)\right), \tag{2}$$

where $\mathbf{T}$ is the time-ordering operator and $U = U(T,0)$ is implicitly understood to be a function of κ.

The system is assumed to be controllable in a manner such that (i) any desired U can be generated by some κ within a finite T, and (ii) any local variation of U can be generated via some variation in κ. Given this degree of accessibility of all unitary transformations, the optimal control of the system dynamics can be viewed as the optimization of a real-valued cost function defining a landscape over the compact unitary Lie group $U(N)$. In lieu of working with the *dynamical* degrees of freedom κ at the Hamiltonian level, the following landscape analysis is based on the *kinematic* degrees of freedom of $U(N)$, in particular, a N^2-dimensional representation of the propagators $U \in U(N)$. By choosing kinematic degrees of freedom as the control variables of the landscape, the outcome of the analysis will depend only on the topology of $U(N)$ and not on the explicit structure of the Hamiltonian. Thus, the following analysis draws on no aspects of the dynamics other than unitarity and controllability as specified, and thus is fully general to all quantum systems satisfying these criteria.

A natural measure of fidelity between a controlled unitary transformation U and a target unitary transformation W is the Hilbert-Schmidt distance $\|U-W\|=2N-2\,\mathrm{Re}\,\mathrm{Tr}(W^\dagger U)$, whose nonconstant part we take to be the cost function J specifying the control landscape

$$J = \mathrm{Re}\,\mathrm{Tr}(W^\dagger U). \tag{3}$$

The attainment of the global extrema $J=N$ or $J=-N$, corresponding, respectively, to the cases of $U=W$ and $U=-W$. However, the search may be impeded by suboptimal stationary regions on the landscape. We enumerate and characterize the structure of such regions in the following analysis and find that (i) their enumeration scales favorably with N and (ii) such stationary regions have the topology of saddle points, and not local extrema traps that may potentially stop a control field search at a suboptimal value of J. It is important to note that the favorable topology of the landscape does not depend on the use of the kinematic representation. In a forthcoming work [12], it is shown that such topological features arise similarly in a dynamical representation of the variables.

III. GLOBAL LANDSCAPE TOPOLOGY

A. Critical submanifolds

Optimization algorithms are designed to seek values of the control variables corresponding to the critical values of J (ideally, the global extrema values). As a result, the critical topology of the landscape is of fundamental interest. Let the diagonal representation of the target unitary transformation be $W=Qe^{i\lambda}Q^\dagger$. In a prior analysis [13], it was shown that the critical points $\hat{U}$ satisfying $\delta J=0$ are of the form

$$\hat{U} = Qe^{i(\lambda+\sigma)}Q^\dagger, \tag{4}$$

with

$$\sigma = \sum_{k=1}^{N} \sigma_k |k\rangle\langle k|, \tag{5}$$

where $\{|k\rangle\}$ is an N-fold orthonormal basis and each σ_k is an integral multiple of π. If σ_k for all k are an even-integer multiples (odd-integer multiples) of π for all k, $\hat{U}$ is the global maximum (minimum) solution. For all other cases, $\hat{U}$ is a local critical solution. The objective of optimization is generally to reach either the global maximum or minimum.

Before proceeding, we remark that since the left multiplication $U \to W^\dagger U = V$ is an automorphism on $U(N)$, the landscape defined by the degrees of freedom of the unitary operator U is topologically equivalent to that for the degrees of freedom of operator V. In the following, J will refer to $J[V]=\mathrm{Re}\,\mathrm{Tr}(V)$ unless otherwise indicated. Recalling the expressions for the optimal solutions in Eq. (4), it is evident that the critical points of the landscape in the V representation are, up to conjugation by Q, the diagonal operators

$$\langle k|V|k\rangle = e^{i\sigma_k} = \delta_k, \tag{6}$$

$$\text{where } \delta_k = \begin{cases} +1 & \text{if } \sigma_k \equiv 0 \bmod 2\pi \\ -1 & \text{if } \sigma_k \equiv \pi \bmod 2\pi. \end{cases} \tag{7}$$

In the following we will ignore the conjugation by Q in the argument of J because of the cyclic invariance of the trace operation. Without loss of generality, we rearrange the matrix elements of V such that $V=-I_m \oplus I_{N-m} \equiv V_m$, where I_m and I_{N-m} are $m\times m$ and $(N-m)\times(N-m)$ identity operators respectively.

Consider the conjugation transformation of the unitary matrix V by T as a group action $\mathcal{G}: U(N)\times U(N) \to U(N)$, where $U(N)$ is both the acting group and the $\mathcal{G}$-*set* as follows:

$$\mathcal{G}(T,V) = TVT^\dagger. \tag{8}$$

The orbit of the $\mathcal{G}$-action with respect to a particular $V \in U(N)$ is defined as

$$\mathrm{Orb}(V) = \{SVS^\dagger : S \in U(N)\}. \tag{9}$$

Since the acting group $U(N)$ is compact, the $\mathcal{G}$-orbits are smooth, compact submanifolds of $U(N)$. Furthermore, since $J[V]$ is invariant under conjugation $V \to TVT^\dagger$ of its argument, the $\mathcal{G}$-orbits of the critical points $\{V_m\}$ are precisely the critical submanifolds of J [14].

The topological structure of the critical submanifolds of J can be further elucidated by noting that since the action group $U(N)$ is a compact Lie group, there is a diffeomorphism [14] between the $\mathcal{G}$-orbit $\mathrm{Orb}(V_m)$ and the quotient space $U(N)/\mathrm{Stab}(V_m)$, where $\mathrm{Stab}(V_m)$ is the stabilizer group of V_m, defined by

$$\mathrm{Stab}(V_m) = \{R \in U(N) : \mathcal{G}(R,V) = V\}. \tag{10}$$

Since $V_m=-I_m \oplus I_{N-m}$, the stabilizer group of V_m is just $\mathrm{Stab}(V_m)=\{U_m \oplus U_{N-m} : U_m \in U(m), U_{N-m} \in U(N-m)\}$. Therefore, the critical submanifold is the complex Grassmannian manifold

$$G(m,N) = \frac{U(N)}{U(m)\times U(N-m)}, \tag{11}$$

of dimension

$$\dim G(m,N) = \dim U(N) - [\dim U(m) + \dim U(N-m)] \tag{12}$$

$$= N^2 - [m^2 + (N-m)^2] \tag{13}$$

$$= 2m(N-m). \tag{14}$$

From Eq. (11), it is evident that the global optimal points with $m=0$ and $m=N$ correspond to isolated points over the landscape. The saddle-point regions with $m=1,\ldots,N-1$ correspond to submanifolds embedded in $U(N)$. The conclusion of this analysis is twofold. First, the number of suboptimal critical regions grows only linearly with respect to the system Hilbert space dimension N. Second, the nonzero volume of the saddle-point submanifolds may reduce the efficiency of identifying the global optima, which in contrast are merely isolated points. However, in the next section, we will evaluate the asymptotic scaling of these saddle-point submanifold volumes in the limit of large system dimension N and observe that these volumes rapidly approach zero.

B. Volumes of critical regions

The problem of evaluating the volumes of the critical Grassmannian submanifolds is implemented using a convenient heuristic method [15] that obviates the need for the algebraically difficult direct integrations in the foregoing statement of the problem. By identifying the unitary group $U(N)$ as the product

$$U(N)=\frac{U(N)}{U(N-1)}\times\frac{U(N-1)}{U(N-2)}\times\cdots\times\frac{U(2)}{U(1)}\times U(1), \tag{15}$$

and recalling that $\frac{U(m)}{U(m-1)}=S^{2m-1}$, where S^{2m-1} is the real $2m-1$-dimensional unit sphere, the volume of $U(N)$ is given by

$$\mathrm{Vol}[U(N)]=\prod_{j=1}^{N}\frac{2\pi^j}{(j-1)!}=2^N\frac{\pi^{(1/2)N(N+1)}}{0\,!\,1\,!\,\cdots(N-1)!}. \tag{16}$$

Recalling that $G(m,N)=U(N)/U(m)\times U(N-m)$, we have $\mathrm{Vol}[G(m,N)]=\frac{\mathrm{Vol}[U(N)]}{\mathrm{Vol}[U(m)]\times\mathrm{Vol}[U(N-m)]}$. This gives

$$\mathrm{Vol}[G(m,N)]=\frac{0\,!\,1\,!\,\cdots(m-1)!}{(N-m)\,!\,\cdots(N-2)\,!\,(N-1)!}\pi^{m(N-m)}. \tag{17}$$

It is important to note that the numerical values of the manifold volumes must be interpreted in the "volume units" dictated by their respective volume forms. In this sense the volumes given by Eqs. (16) and (17) are of incommensurate units, and are not meant to be compared directly. The property of interest in Eq. (17) is the scaling of the submanifold volume in the limit as N is large, which corresponds to the expected circumstance in many real physical systems where the Hilbert space dimension can be very large.

The critical submanifolds corresponding to the global extrema at $m=0$ or $m=N$ are isolated points for any value of N. Consider next a saddle-point submanifold corresponding to some $m\neq 0, N$. Since factorial growth dominates exponential growth, $\lim_{N\to\infty}\mathrm{Vol}\,G(m,N)=0$. In the asymptotic limit of large N, the relative volumes of the saddle-point submanifolds rapidly approach zero in their respective subspaces. Though they may still act as unstable attractors for optimal search processes, their volumes become vanishingly small as the system dimension increases.

IV. HESSIAN ANALYSIS OF THE CRITICAL REGIONS

Consider now the local structure of the function J at its critical points. The stability properties of a critical point $\hat{V}$ on the landscape are determined by the eigenvalue structure of the Hessian operator of J, defined by

$$\mathcal{H}_{i'i}(\hat{V})=\frac{\partial^2 J}{\partial x_{i'}\,\partial x_i}, \tag{18}$$

where $\{x_i\}$ are a suitable set of local coordinates around the point $\hat{V}\in U(N)$. In particular, the enumeration of the positive, negative, and zero eigenvalues of the Hessian at a critical point V_m, respectively, corresponds to that of the upward, downward, and flat directions at that point.

To obtain this enumeration, we calculate the Hessian quadratic form (HQF) of J by first parametrizing the argument $\hat{V}$ and J locally around a critical point $\hat{V}$ via the Cayley transform [16] as follows:

$$\hat{V}\to(1+iA)(1-iA)^{-1}\hat{V}, \tag{19}$$

where A is an arbitrary infinitesimal Hermitian matrix. Taylor expanding $(1-A)^{-1}$ and keeping terms up to second order in A, we obtain $\hat{V}=(1+2iA-2A^2)\hat{V}$. Writing the cost functional as $J=\mathrm{Re}\,\mathrm{Tr}[(1+2iA-2A^2)\hat{V}]$, and retaining only the second order terms yields the HQF

$$\mathcal{H}_A(\hat{V})=\mathrm{Re}\,\mathrm{Tr}(-2A^2\hat{V}). \tag{20}$$

We define $A_{ij}\equiv\alpha_{ij}+i\beta_{ij}$ for $A_{ij}=A^*_{ji}$. Evaluating $\mathcal{H}_A(\hat{V})$ explicitly at a critical point $\hat{V}=\Sigma_{j=1}^N\delta_j|j\rangle\langle j|$, where $\{|j\rangle\}$ is an N-fold orthonormal basis, we obtain

$$\mathcal{H}_A(\hat{V})=-2\left[\sum_{j=1}^{N}\alpha_{jj}^2\delta_j+\sum_{1\le k<\ell\le N}^{N}(\alpha_{k\ell}^2+\beta_{k\ell}^2)(\delta_k+\delta_\ell)\right]. \tag{21}$$

Direct computation with the HQF is illustrated with the following example.

Example. Consider the target transformation W as the SWAP operation

$$W=\begin{pmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{pmatrix}, \tag{22}$$

such that for $W=Qe^{i\lambda}Q^\dagger$,

$$e^{i\lambda}=\begin{pmatrix}e^{(2k+1)i\pi}&0&0&0\\0&e^{2ki\pi}&0&0\\0&0&e^{2ki\pi}&0\\0&0&0&e^{2ki\pi}\end{pmatrix}, \tag{23}$$

where k is any integer. Consider now the degrees of freedom of U where all critical points of $J[U]$ are of the form $Qe^{i(\lambda+\sigma)}Q^\dagger$ with σ defined in Eq. (5). The Hessian will be evaluated at a particular saddle-point solution for illustration,

$$\sigma = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \pi & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{24}$$

Returning to the V representation, this corresponds to the critical point

$$\hat{V} = W^{\dagger}\hat{U} = Q\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}Q^{\dagger}, \tag{25}$$

where the diagonal elements have been rearranged to proceed from negative to positive. Thus, in Eq. (21) $\delta_1=\delta_2=1$ and $\delta_3=\delta_4=-1$, implying that

$$\mathcal{H}_A(V) = -2[-\alpha_{11}^2 - \alpha_{22}^2 + \alpha_{33}^2 + \alpha_{44}^2 - 2\alpha_{12}^2 - 2\beta_{12}^2 + 2\alpha_{34}^2 + 2\beta_{34}^2]. \tag{26}$$

There are four positive and four negative terms. Since there are $N^2=16$ terms in the HQF, the remaining eight terms are zero valued. Therefore, we have four positive, four negative, and eight flat directions at the critical point $\hat{V}$.

In general, it can be seen from Eq. (21) that for any critical point $V_m \in G(m,N)$, the enumeration of positive (h_+), negative (h_-), and zero (h_0) eigenvalues of the Hessian of J are [11]

$$h_+ = m^2, \tag{27a}$$

$$h_- = (N-m)^2, \tag{27b}$$

$$h_0 = 2Nm - 2m^2. \tag{27c}$$

When seeking global optimal control, the enumeration in Eqs. (27) demonstrates that the saddle submanifolds with landscape values close to the global optima values of $J=N$, $-N$ may be a greater hindrance to the search effort, as the ratio $\frac{h_+}{h_-}$ $(\frac{h_-}{h_+})$ of favorable and unfavorable directions leading upward (downward) toward $J=N$ $(J=-N)$ decreases as the values approach that of the global maximum (minimum). Furthermore, the enumeration h_0 of the local flat directions [corresponding to the dimension of $G(m,N)$] shows that the saddle-point submanifolds corresponding to J values furthest from the global optima have the highest dimension. Both of these observations suggest that the topology of J at the saddle-point suboptima may produce unfavorable search conditions, perhaps especially for local search algorithms (e.g., gradient-following). The key implication of this analysis is that the success of optimization algorithms must be able to efficiently distinguish between the favorable and unfavorable directions. For low values of N, this situation may cause no substantial difficulties, but for large N, passage through a saddle-point submanifold may introduce difficulties as the number of desirable directions leading to the global extrema become increasingly lost among the directions leading away. Nevertheless, the saddle-point topology of all such regions assures that they will not act as local extrema traps in any search effort, and in this sense the landscape topology does not pose a fundamental obstacle to optimization.

V. CONCLUSIONS AND OPEN QUESTIONS

This work presents an assessment of the quantum optimal control landscape for creating a unitary transformation U targeted to reach a desired form W. It was found that the critical regions of J possess the topology of Grassmannian submanifolds, and that the number of such critical submanifolds scales only linearly with system dimension N. The global optima corresponding to perfect solutions (up to a global phase) are isolated points. However, the saddle-point submanifold volumes approach zero in the limit of large N, and as such the saddle-point regions are not expected to be deleterious attractors to trap searches for the global optima. The evaluation of the Hessian quadratic form reveals that the signs of the directions of J at its critical points generate an intrinsic bias away from the global extrema values of the landscape. For saddle-point submanifolds corresponding to J values close to the global optima, the number of favorable directions is at a minimum. Nevertheless, the existence of at least one direction leading toward an improvement in optimization outcome in all critical submanifolds assures that a sufficiently intelligent search algorithm should be able to overcome this hindrance.

There are several open issues relevant to the landscape analysis meriting further investigation. The kinematic controllability assumptions require that any $\hat{U} \in U(N)$ can be arbitrarily perturbed via some corresponding perturbation in $H(\kappa,t)$. Assessing the matter entails identifying the necessary conditions on a Hamiltonian $H(\kappa,t)$ that ensure that the kinematic controllability conditions are fulfilled. The present analysis is also restricted to N-level systems, although N may be arbitrarily large. In practice, continuous systems may still be adequately treated in this fashion, but a full formal analysis of the continuous limit would be desirable.

The generation of arbitrary unitary transformations is a fundamental goal for many endeavors in quantum control and quantum information processing. For large physical systems where controls cannot be designed from first principles, OCE methods may be the only feasible route to control. Any control process, including OCE, must necessarily pass over the landscape, and a clear understanding of the topological structure of the landscape is essential to developing the most effective control operations. In this analysis, we demonstrated that the landscape has generic topology that is generally favorable to optimal control, providing an optimistic outlook for future efforts.

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