ARE THERE TRAPS IN QUANTUM CONTROL LANDSCAPES?

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PRELIMINARIES

Quantum control is a powerful tool for controlling the dynamics of physical processes on the atomic and molecular scale. A fundamental issue in quantum control which is currently attracting great interest is the analysis of quantum control landscapes. Given an objective functional $J(\varepsilon)$ that depends on a control field ε, the dynamical landscape is defined by the properties of the Hessian $\delta^2 J/\delta\varepsilon^2$ at the critical points $\delta J/\delta\varepsilon = 0$. We discuss an important discovery in quantum control landscape of special trapping critical points—second-order traps—which can slow down the search for globally optimal controls.

FORMULATION

Formulation of a quantum control problem includes defining the following objects:

- Evolution equation: (for n-level quantum system)

$$\frac{dU_t^\varepsilon}{dt} = -i[H_0 + V\varepsilon(t)]U_t^\varepsilon$$

  Here H_0 and V are Hermitian $n \times n$ matrices.

- Control space $\mathcal{U}$: A function space of all admissible controls, for example $L^2([0,T])$, $L^\infty([0,T])$ ($T > 0$ is the final time), etc.

- Objective functional J: For a wide variety of problems,

$$J(\varepsilon) = \mathrm{Tr}[U_T^\varepsilon \rho_0 U_T^{\varepsilon\dagger} O] \to \max$$

  where O is a target operator and ρ_0 is the initial density matrix.

CONTROL LANDSCAPES AND TRAPS

The objective $J(\varepsilon)$ as a functional of the control $\varepsilon(t)$ defines the dynamical control landscape, the graph of $J(\varepsilon)$, whose structure determines the complexity of the underlying control problem. Important points on the landscape are:

- Optimal controls: Global maxima of $J(\varepsilon)$.
- Traps: Local maxima of $J(\varepsilon)$.
- Second-order traps: Controls ε where gradient of J is zero, $\nabla J_\varepsilon = 0$, Hessian $H_\varepsilon := \delta^2 J/\delta\varepsilon^2$ is negative semidefinite, $H_\varepsilon \le 0$, and $J(\varepsilon) < J_{\max} := \max\limits_{\varepsilon\in\mathcal{U}} J(\varepsilon)$.

Traps may significantly hinder the search for globally optimal controls with local algorithms. This circumstance motivates the importance of the analysis of traps for quantum control problems.

Definition: Landscape lifting is the mapping $J(\varepsilon) \to \widehat{J}(U) := \mathrm{Tr}[U\rho_0 U^\dagger O]$ of the functional $J(\varepsilon)$ to a function on $U(n)$. The graph of $\widehat{J}(U)$ is called the kinematic landscape.

Definition: A control ε_* is regular if the differential of the map $f : \mathcal{U} \to U(n)$, $f(\varepsilon) = U_T^\varepsilon$ is surjective at $\varepsilon = \varepsilon_*$.

Theorem: A regular control ε is a trap for $J(\varepsilon)$ if and only if $U := U_T^\varepsilon$ is a trap for $\widehat{J}(U)$.

LANDSCAPES FOR CLOSED SYSTEMS

The analysis of traps for kinematic landscapes for closed quantum systems can be traced back to the analysis of trace functions $f(U) := \mathrm{Tr}[UAU^\dagger B]$, where A, B are symmetric matrices with all distinct eigenvalues. Such functions were shown to have exactly one maximum and one minimum value, with all other stationary points being saddles over the sets of unitary and orthogonal matrices U by, respectively, J. von Neumann in *Tomsk Univ. Rev.* **1**, 286 (1937), and R. Brockett in *Lin. Alg. Appl.* **122/123/124**, 761 (1989). This result was generalized to non-symmetric A, B by S.J. Glaser *et al.* in *Science* **280**, 421 (1998).

REGULAR CONTROLS: NO TRAPS

In full generality, the properties of kinematic landscapes for closed quantum systems can be formulated as the following theorem.

Theorem [H. Rabitz, M. Hsieh, C. Rosenthal, *Science* **303**, 1998 (2004) and subsequent works]: The kinematic landscape of $\widehat{J}(U) = \mathrm{Tr}[U\rho_0 U^\dagger O]$ on the unitary group $U(n)$ has as critical points only global maxima/minima and saddles (all are found).

Conclusion: Regular controls are not traps for $J(\varepsilon)$.

However, non-regular controls are known to exist, and therefore the problem of presence or absence of traps remained open.

NON-REGULAR CONTROLS: SECOND-ORDER TRAPS

The question of ultimate interest is whether non-regular controls can be traps for dynamic landscapes. Recently, P. de Fouquieres and S.G. Schirmer in preprint `arXiv`:1004.3492 constructed an example of a second-order trap and numerically found a trap for a special case. We find that non-regular controls are second-order traps under rather general assumptions on H_0, V, ρ_0, and O, as opposed to previous expectations. This result in the simplest form is explicitly formulated as the following theorem.

Theorem: If $V_{ij} = 0$ for some $i \neq j$ in the eigenbasis $|i\rangle$ of H_0, then there exists an initial density matrix ρ_0 and infinitely many target operators O for which zero control $\varepsilon(t) \equiv 0$ is a second-order trap [theorem admits a generalization to any constant controls].[1]

The assumption in the theorem is consistent with controllability of the system; hence this result implies the existence of second-order traps for controllable systems. The theorem implies that local optimization methods will have low efficiency when starting from controls with small intensity of arbitrary temporal profile.[2] The difficulties may arise even for generally strong fields of intensities as high as $I \approx 10^{12} - 10^{13}$ W/cm^2.[3]

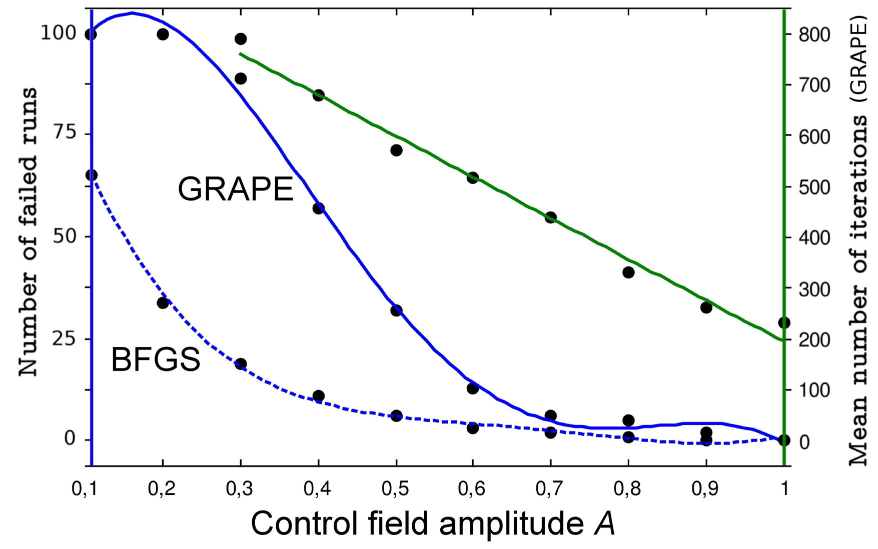

Figure 1: Percentage of failed runs of GRAPE and BFGS for various intensities of the initial control. For some realistic system parameters, $A = 0.1 - 0.2$ corresponds to intensity $I \approx 10^{12} - 10^{13}$ W/cm^2.

[1] A.N. Pechen, D.J. Tannor, *Phys. Rev. Lett.* **106**, 120402 (2011).
[2] A.N. Pechen, D.J. Tannor, *Israel J. Chemistry* **52**, 467 (2012).
[3] A.N. Pechen, D.J. Tannor, *Phys. Rev. Lett.* **108**, 198902 (2012).

LANDSCAPES FOR OPEN SYSTEMS

Often atomic and molecular controlled systems are open—they interact with their environment. Their evolution is completely positive instead of unitary and may be represented in the form

$$\rho_0 \to \rho_T = \sum_{i=1}^{\lambda(=n^2)} K_i \rho_0 K_i^\dagger, \qquad \sum_{i=1}^{\lambda} K_i^\dagger K_i = \mathbb{I}_n\,,$$

where matrices $K_i = K_i(T,\varepsilon)$ depend on time and on the control. The condition $\sum K_i^\dagger K_i = \mathbb{I}_n$ implies that the set of matrices $\{K_i\}$ can be identified with a point $S = (K_1;\ldots;K_\lambda)$ ($S^\dagger S = \mathbb{I}_n$) of the Stiefel manifold $S_n(\mathbb{C}^{\lambda n})$. Hence the landscape lifting for an open quantum system is a function over the Stiefel manifold:

$$J(\varepsilon) = \mathrm{Tr}[\rho_T^\varepsilon O] \longrightarrow \widehat{J}(S) = \mathrm{Tr}\left[S\rho S^\dagger(\mathbb{I}_{n^2} \otimes O)\right]$$

Theorem: The kinematic landscape of $\widehat{J}(S)$ on the Stiefel manifold $S_n(\mathbb{C}^{\lambda n})$ has as critical points only global maxima/minima and saddles (all are found).[4,5]

[4] A. Pechen, D. Prokhorenko, R. Wu, H. Rabitz, *J. Phys. A: Math. Theor.* **41**, 045205 (2008). [5] R. Wu, A. Pechen, H. Rabitz, M. Hsieh, B. Tsou, *J. Math. Phys.* **49**, 022108 (2008).

Acknowledgements: This research was supported by a Marie Curie International Incoming Fellowship within the 7th European Community Framework Programme.