Exploring quantum control landscape structure

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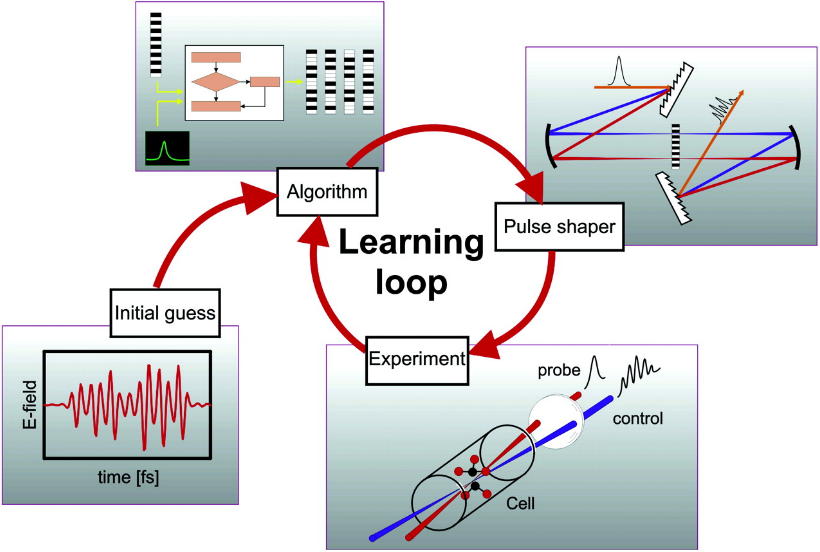
Quantum control



Basics

The dynamics is given by the Schrodinger equation

$$i\hbar \frac{\partial U(t)}{\partial t} = H(t)U(t), \qquad U(0) = \mathbb{1}.$$

Add the interaction to the Hamiltonian

$$H(t) = H_0 - \mu E(t)$$

in order to "control" the observable

$$P_{i\to f} = |\langle f|U(T;0)|i\rangle|^2.$$

D-MORPH

How to achieve control?

Parameterize the electric field using a continuous variable s.

To require

$$\frac{dP_{i\to f}}{ds} = \int_0^T \frac{\delta P_{i\to f}}{\delta E(s,t)} \frac{\partial E(s,t)}{\partial s} dt \geq 0$$

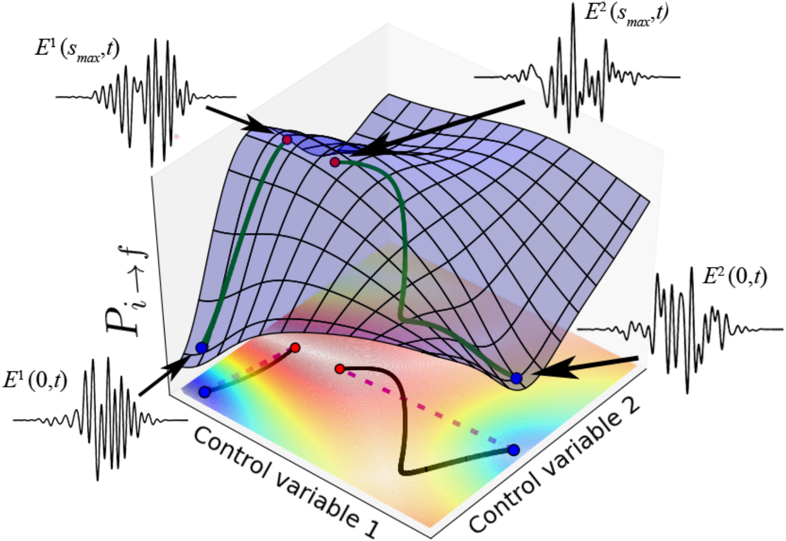
we set

$$\frac{\partial E(s,t)}{\partial s} = \frac{\delta P_{i\to f}}{\delta E(s,t)},$$

where

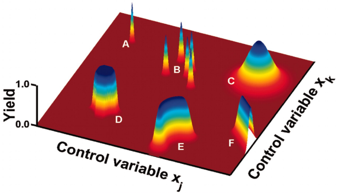
$$\frac{\delta P_{i\to f}}{\delta E(t)} = -\frac{2}{\hbar} \Im \left\{ \left\langle i \middle| U^\dagger(T;0) \middle| f \right\rangle \left\langle f \middle| U(T;0) U^\dagger(t;0) \mu U(t;0) \middle| i \right\rangle \right\}.$$

Quantum control landscape



Structure vs. topology

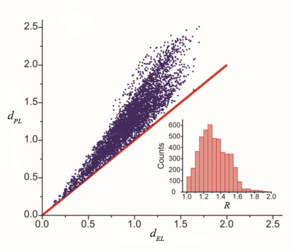
H. Rabitz, M. Hsieh, C. Rosenthal *Science* (2004) examined the *topology* of the quantum control landscape.



Results very encouraging: no sub-optimal extrema!

Our work is to examine the *structure*, using the linearity metric R.

Figure from J. Roslund and H. Rabitz *Phys. Rev. A* (2009)



Results again very encouraging: landscape is structurally simple.

What is R?

Optimizations are trajectories in *control space*.

The path length of a trajectory is

$$d_{PL} = \int_0^{s_{max}} \left[\int_0^T \left(\frac{\partial E(s,t)}{\partial s} \right)^2 dt \right]^{\frac{1}{2}} ds.$$

The Euclidean distance is

$$d_{EL} = \left[\int_0^T \left(E(s_{max}, t) - E(0,t) \right)^2 dt \right]^{\frac{1}{2}}$$

The ratio R is defined by

$$R = \frac{d_{PL}}{d_{EL}}.$$

Statistical behavior of R

Perform random optimizations and calculate R.

$$H_0 = \begin{pmatrix} -10 & 0 & 0 & 0 & 0 \\ 0 & -7 & 0 & 0 & 0 \\ 0 & 0 & -3 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 8 \end{pmatrix}$$

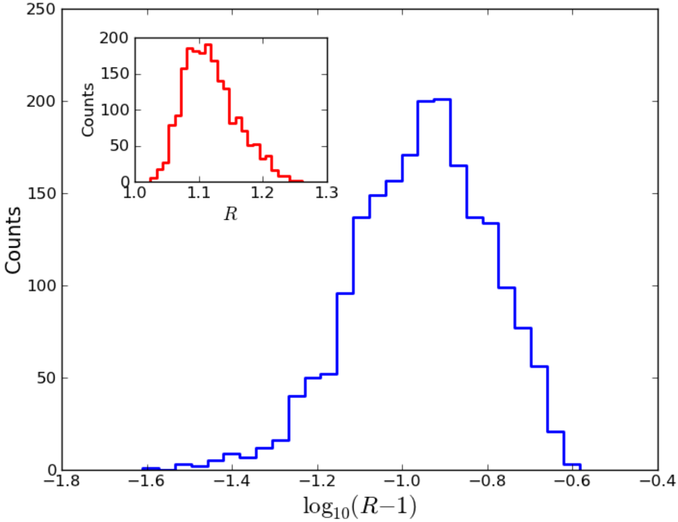
and

$$\mu = \begin{pmatrix} 0 & \pm 1 & \pm 0.5 & \pm 0.5^2 & \pm 0.5^3 \\ \pm 1 & 0 & \pm 1 & \pm 0.5 & \pm 0.5^2 \\ \pm 0.5 & \pm 1 & 0 & \pm 1 & \pm 0.5 \\ \pm 0.5^2 & \pm 0.5 & \pm 1 & 0 & \pm 1 \\ \pm 0.5^3 & \pm 0.5^2 & \pm 0.5 & \pm 1 & 0 \end{pmatrix}.$$

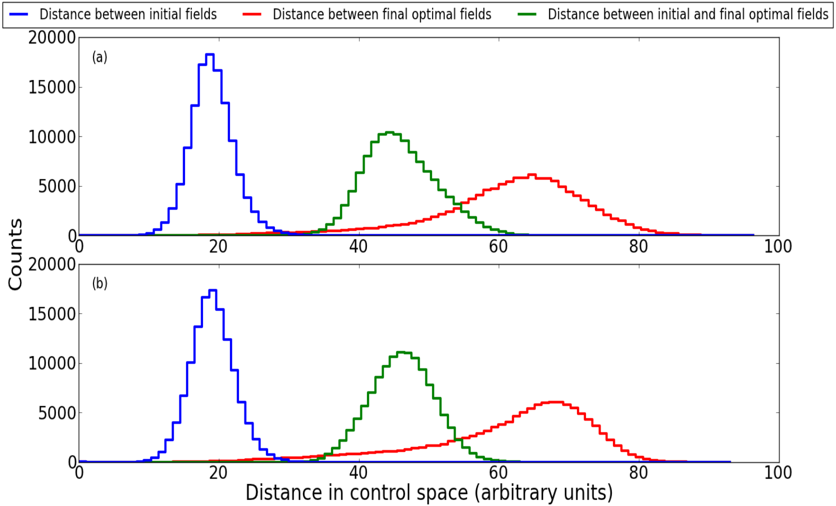
Initial field parametrized in the form

$$E(t) = \frac{1}{F} \sum_{n=1}^{20} \exp[-0.3(t - \frac{T}{2})^2] a_n \sin(\omega_n t + \phi_\omega).$$

Statistical behavior of R



Statistical behavior of R

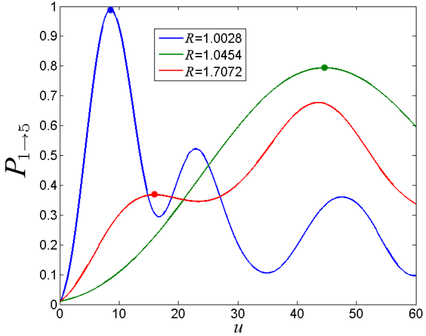


“Straight shot” assessment and algorithm

How straight is “straight”?

$$E(u,t) = \left(\frac{\delta P^I_{i\to f}}{\delta E(s=0,t)} \right) u + E(0,t), \quad u \geq 0.$$

Could be another method to optimize.



Minimizing R

Use the Particle Swarm Optimization (PSO) algorithm to search for low R.

Particles updated through

$$E_k^g = E_k^{g-1} + v_k^g.$$

Velocities of particles given by

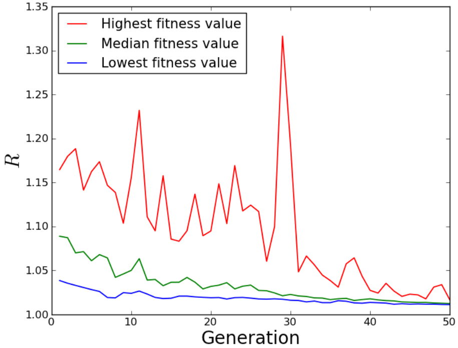
$$v_k^g = C_0 v_k^{g-1} + C_1 S_1 (E_{swarm}^{best,g-1} - E_k^{best,g-1}) + C_2 S_2 (E_{swarm}^{best,g-1} - E_k^{g-1})$$

PSO algorithm is a *stochastic* optimization algorithm.

Minimizing R

With our landscape, $R - 1$ can be driven down to $\sim 10^{-4}$, two orders of magnitude lower than random trajectories.

R can also be maximized, highest values are $R \sim 1.7$.

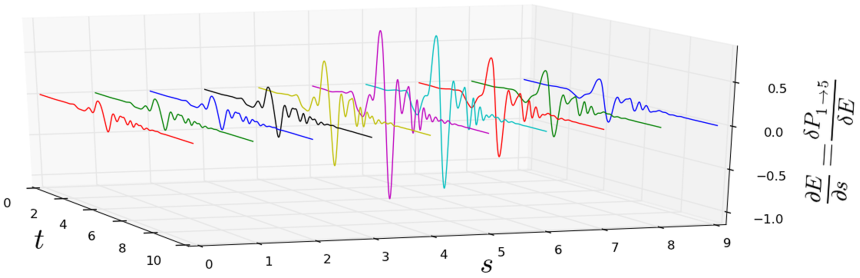


Mathematics of straight trajectories

In order to achieve $R = 1$, the gradient function must be separable

$$\frac{\partial E(s,t)}{\partial s} = \frac{\delta P_{i\to f}}{\delta E(s,t)} = \alpha(s) \times \beta(t).$$

The slope-intercept equation for a line in infinite dimensions.



Mathematics of straight trajectories

If $R = 1$, then the gradient points in the same direction everywhere on the path.

More precisely, $\frac{\delta P_{i\to f}}{\delta E}$ should be proportional to itself at two points on the path.

Sliding from point to point involves translating by $\frac{\delta P_{i\to f}}{\delta E}$ itself, so

$$\begin{aligned}\frac{\delta P_{i\to f}}{\delta E}[E] &\propto \frac{\delta P_{i\to f}}{\delta E}\left[E + \frac{\delta P_{i\to f}}{\delta E} \times const.\right] \\ &\approx \frac{\delta P_{i\to f}}{\delta E}\left[E\right] + \frac{\delta^2 P_{i\to f}}{\delta E \delta E}\left[E\right] \cdot \frac{\delta P_{i\to f}}{\delta E}\left[E\right] \times const.\end{aligned}$$

Mathematics of straight trajectories

This implies that

$$\frac{\delta^2 P_{i\to f}}{\delta E \delta E} \cdot \frac{\delta P_{i\to f}}{\delta E}[E_1] \propto \frac{\delta P_{i\to f}}{\delta E}[E_1]$$

which *appears* to say that the gradient is an eigenvector of the Hessian.

Can we then find the eigenvalue? Exact relation:

$$\int \frac{\delta^2 P_{i\to f}}{\delta E(t) \delta E(t')}[E(s',\tau)] \frac{\delta P_{i\to f}}{\delta E(t')}[E(s',\tau)]\, \mathrm{d}t' = \frac{\alpha'(s')}{\alpha(s')} \cdot \frac{\delta P_{i\to f}}{\delta E(t)}[E(s',\tau)].$$

Mathematics of straight trajectories

We can factor the Hessian

$$\frac{\delta^2 P_{i\to f}}{\delta E(s,t')\delta E(s,t)} = \beta^{[2]}(s) \times K^{[2]}(t,t')$$

where $K^{[2]}(t,t)$ is a symmetric kernel that leaves the gradient invariant, and $\beta^{[2]}(s) = \frac{\alpha'(s)}{\alpha(s)}$.

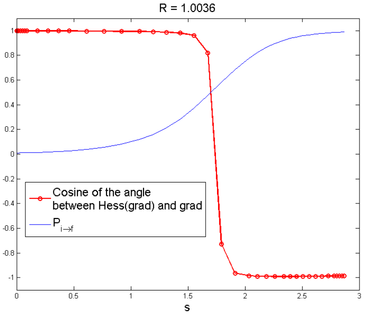
More generally, every higher-order derivative factors

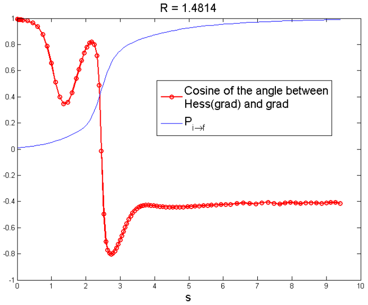
$$\frac{\delta^n P_{i\to f}}{\delta E(s,t_n)\cdots\delta E(s,t_1)} = \beta^{[n]}(s) \times K^{[n]}(t_n,\cdots,t_1)$$

with $K^{[n]}$ a symmetric kernel and

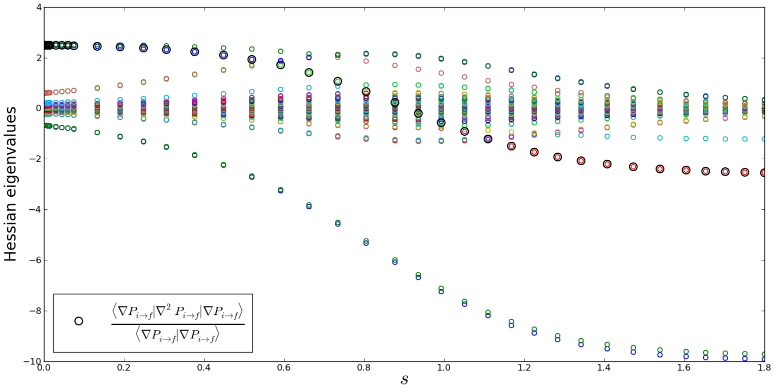
$$\beta^{[n]}(s) = \frac{1}{\alpha(s)}\frac{d\beta^{[n-1]}(s)}{ds}, \qquad \beta^{[1]}(s) = \alpha(s).$$

Hessian-gradient eigenrelation

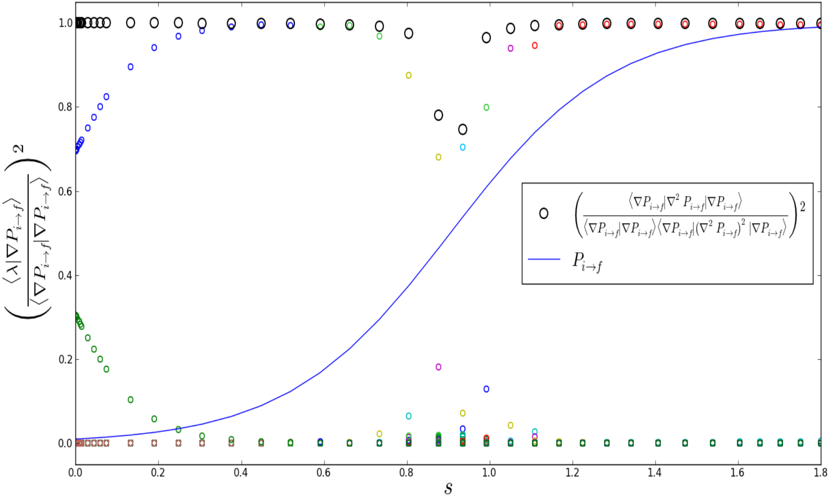




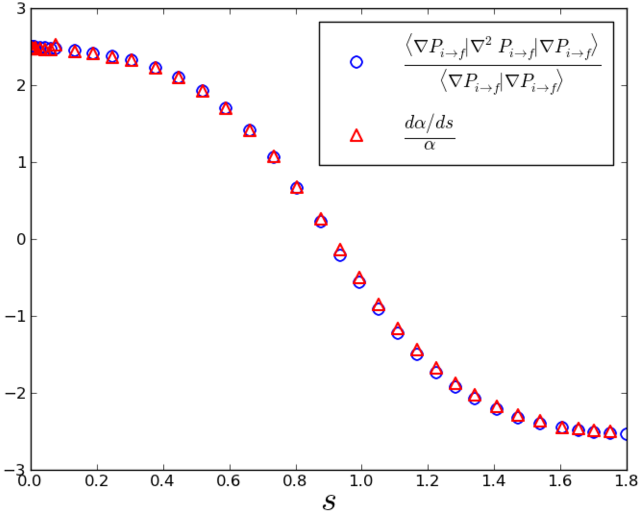
Hessian-gradient eigenrelation



Hessian-gradient eigenrelation



Hessian-gradient eigenrelation



Additional optimization objectives

Can optimize unitary transformations

$$J = ||W - U(T)||^2$$

Gradient is then

$$\frac{\delta J}{\delta E(t)} = 2 \ \mathrm{Tr} \ \Im \Big\{ W^\dagger U \mu(t) \Big\}.$$

Or optimize arbitrary observables

$$J = \mathrm{Tr} \ \Big(\rho(T) O \Big)$$

Gradient is then

$$\frac{\delta J}{\delta E(t)} = 2 \ \Im \Big\{ \mathrm{Tr} \ U \rho \mu(t) U^\dagger O \Big\}.$$

Saddle points

Topology of landscape is now more complex; consequently, so is the structure.

Kinematics: view landscape as Lie Group $\mathcal{U}(N)$.

Additional critical points appear in the middle of the landscape, but always *saddle points*.

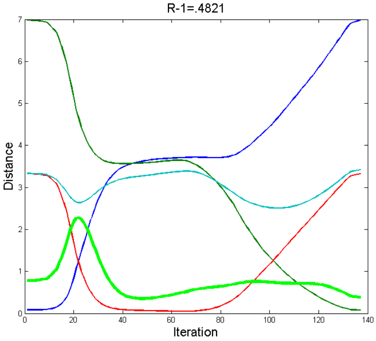
For W problem, critical submanifolds occur when

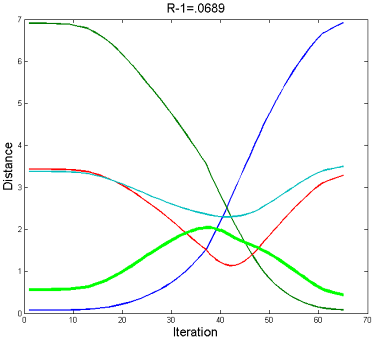
$$\mathrm{Tr}\,(W^{\dagger}U) = -N, -N+2, \cdots, N.$$

For $\mathrm{Tr}\,(\rho O)$ problem, critical submanifolds correspond to the double cosets

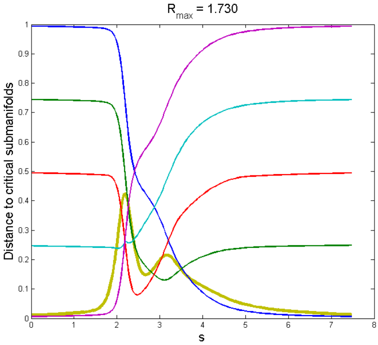
$$\bigcup_{\pi \in \mathcal{P}(N)} \mathcal{U}(m)\pi\mathcal{U}(n)$$

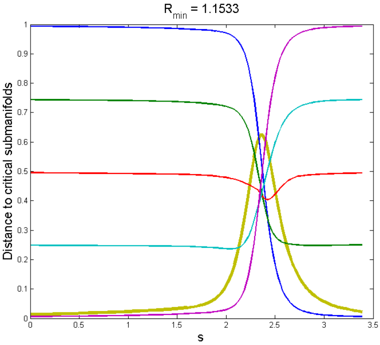
Saddle points $(\mathrm{Tr}\,(\rho O))$





Saddle points (W)





References

A. Nanduri, A. Donovan, T. S. Ho, and H. Rabitz, Exploring quantum control landscape structure, Phys. Rev. A **88**, 033425 (2013).

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