Topology of Optimal Control Landscapes for Classical Mechanical Systems

Carlee Joe-Wong

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Research Context

- **Control chemical systems** by passing them through an electric field.
- **Optimize** reaction yield, drive molecule to target energy level, etc.
- Shape the electric field to achieve this goal, assuming system follows **dynamical equations**.
    - Dynamical equations can be classical or quantum.
    - Previous work assumes **quantum mechanics** (Schrödinger's equation).
    - I assume **classical mechanics** (Hamilton's equations).

Image from Professor Herschel Rabitz, Princeton University, CHM 510, Fall 2010.

Optimal Control Formulation

- Assume some chemical system with **specified goal** at final time T.
  - Use a **cost functional** J to specify the goal.
  - Let $z(t)$ denote the state of the system at time t, a $2n \times 1$ vector.
  - Let $\epsilon(t)$ be the control field at time t.

$$\min J = F(z(T)) \tag{1}$$

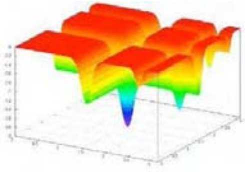
$$\text{s.t. } \dot{z} = f\big(z(t), \epsilon(t)\big) \tag{2}$$

$$z(0) = z_0 \tag{3}$$

- For instance, $F = z(T)^T z(T)$.
- Dynamic equation f either Schrödinger's equation or Hamilton's equations.
- An optimal control history ϵ produces $z(T)$ that **globally minimizes** J.

Search Algorithms and Quantum Results

- Compute optimal fields using **optimal control theory**.
- Start with an initial field and use **gradient search**.
- Problem with gradient search: gets stuck in local minima.



- Assume **fully controllable systems**: with appropriate control, can get from given initial state to any final state at time T.
- In controllable **quantum systems**, gradient search never gets stuck.
- **What about controllable classical mechanical systems?**

Classical Analysis: Zero Gradients

Gradient of the cost functional with respect to the control:

$$\frac{\delta J}{\delta \epsilon(t)} = \frac{\partial J}{\partial z(T)} \frac{\delta z(T)}{\delta \epsilon(t)} \tag{4}$$

- At **critical points**, this equation is 0 for all t.
- Also assume **regularity**: $\left\{ \frac{\delta z(T)}{\delta \epsilon(t)} \mid t \in [0, T] \right\}$ is surjective.
- In other words, this infinite set of vectors, indexed by time, contains $2n$ **linear independent vectors**.
- Then since $\frac{\partial J}{\partial z(T)}$ is independent of t in (4), at critical points $\frac{\partial J}{\partial z(T)} = 0$.

Classical Analysis: Defining the Cost Functional

From the previous slide, we have

$$\frac{\partial J}{\partial z(T)} = 0. \tag{5}$$

- Define an **observable** O, a function of the state (e.g. $O = z$).
- Let O be an $r \times 1$ vector-valued function.
- Suppose we want this observable to reach a **target value** O_t.

Then define

$$J = \left[O(z(T)) - O_t\right]^T \left[O(z(T)) - O_t\right]. \tag{6}$$

Taking the derivative, (5) gives

$$2\left[O(z(T)) - O_t\right]^T \frac{\partial O}{\partial z} = 0. \tag{7}$$

Critical Points as Global Minima

From the previous slide,

$$2\left[O(z(T)) - O_t\right]^T \frac{\partial O}{\partial z} = 0. \tag{8}$$

Note that $\left[O(z(T)) - O_t\right]^T$ is a $1 \times r$ vector and $\frac{\partial O}{\partial z}$ an $r \times 2n$ matrix.

- Suppose $M = \frac{\partial O}{\partial z}$ is an r-rank matrix.
- Then MM^T is an $r \times r$ matrix of rank r, and therefore invertible.

$$2\left[O(z(T)) - O_t\right]^T \frac{\partial O}{\partial z} M^T (MM^T)^{-1} = 0M^T(MM^T)^{-1}, \tag{9}$$

so

$$\left[O(z(T)) - O_t\right]^T = 0, \text{ i.e. } O(z(T)) = O_t \tag{10}$$

and J **is globally minimized**.

- For instance, target states or scalar O.

Numerical Example

- State $z = (q, p)$: position and momentum.
- Target and final states $(q, p) = (0{,}0)$ and (1.728e-5,-4.50e-6).

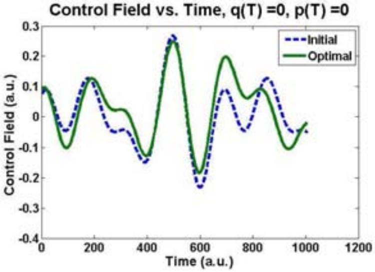


Figure: Control field evolution.

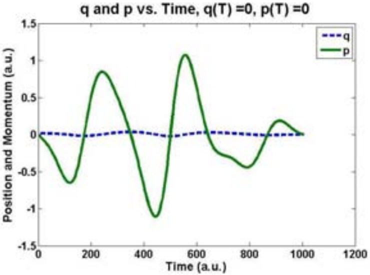


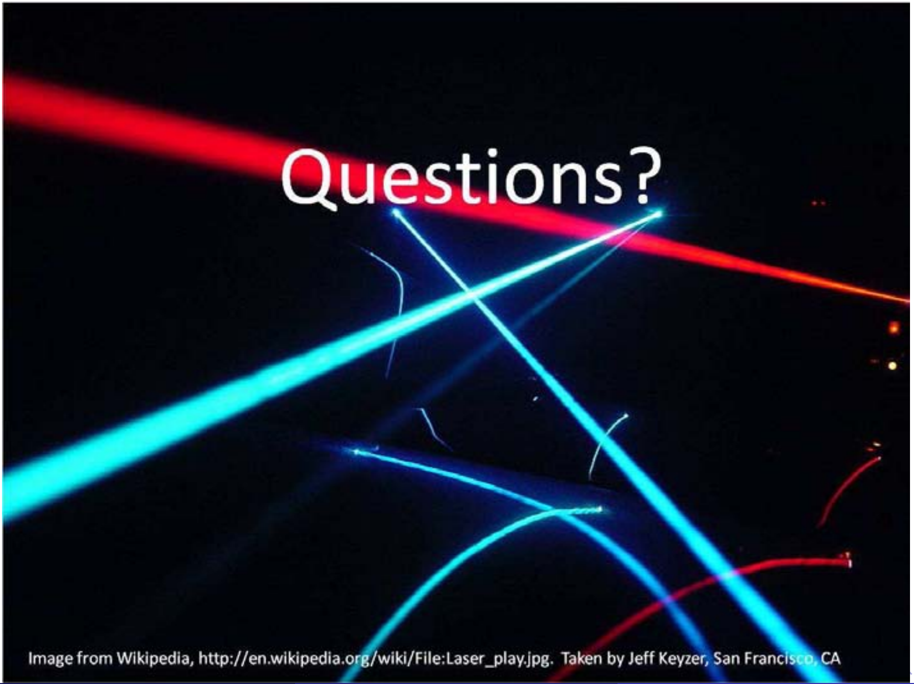
Figure: Final position and momentum trajectories.

Past, Present and Future Work

- Lots of **other numerical simulations**–none revealed a local trap!
  - Multi-particle systems.
  - Scalar objective.
  - Partial target state (e.g. target q but no target p).
- **Hessian derivation and analysis**: very similar to quantum expressions.
- Preliminary study of **singular (non-regular) controls**.
- Currently studying **non-deterministic systems**: initial state spread over a probability distribution.

Future research directions:

- Singular controls.
- Infinite-dimensional systems.
- Non-controllable systems: these have traps on the quantum side.


Questions?
Image from Wikipedia, http://en.wikipedia.org/wiki/File:Laser_play.jpg. Taken by Jeff Keyzer, San Francisco, CA