Geometric optimal control of dissipative quantum systems

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Optimal control of quantum dynamics

$$i\hbar\frac{\partial}{\partial t}\psi(t) = [H_0 + u(t)H_1]\psi(t)$$

Control: $\psi(0) = \psi_i \Longrightarrow \psi(T) = \psi_f$

Rem. 1: controllability (accessible set).
Rem. 2: optimal: minimization of a cost.

$$\text{Energy}: \int_0^T [u(t)^2]dt$$
$$\text{Time}: \ T \text{ with } |u| \leq 1$$

Ref: Numerical analysis by direct methods

Geometric optimal control theory

- Pontryagin maximum principle
- Analysis of the geometry of the Hamiltonian dynamics (extremals)
- Indirect numerical methods (homotopy)
- second-order optimality conditions (conjugate point)

Ref: A. Agrachev, J.-P. Gauthier, B. Bonnard, U. Boscain, V. Jurdjevic...

In quantum physics:

- Conservative case (U. Boscain et al)
- Sudden case (N. Khaneja, S. Glaser et al)

Pontryagin Maximum principle

Time-minimal control with $u_1^2 + u_2^2 \leq 1$:

$$\dot{x} = F_0(x) + u_1 F_1(x) + u_2 F_2(x)$$

We introduce a pseudo-Hamiltonian:

$$\mathcal{H} = p \cdot (F_0(x) + u_1 F_1(x) + u_2 F_2(x)) + p_0$$

with $p_0 \leq 0$.
The final time is not fixed $\Rightarrow \mathcal{H} = 0$.
$(p, p_0) \in \mathbb{R}^{n+1,*}$ is defined up to a scalar factor.

Theorem

PMP: The extremal dynamics are given almost everywhere by

$$\dot{x} = \frac{\partial \mathcal{H}}{\partial p}, \ \dot{p} = -\frac{\partial \mathcal{H}}{\partial x}$$

with the condition $H(x, p) = \max_{u_1, u_2 \in U} \mathcal{H}(x, p, u_1, u_2)$.

Time-minimal control

In the regular case:

$$u_1 = p \cdot F_1(x) / \sqrt{(p \cdot F_1(x))^2 + (p \cdot F_2(x))^2}$$

$$u_2 = p \cdot F_2(x) / \sqrt{(p \cdot F_1(x))^2 + (p \cdot F_2(x))^2}$$

with $(p \cdot F_1(x))^2 + (p \cdot F_2(x))^2 \neq 0$ and $|u| = 1$.
Smooth extremals are given by the corresponding Hamiltonian:

$$H(x, p) = p \cdot F_0(x) + \sqrt{(p \cdot F_1(x))^2 + (p \cdot F_2(x))^2}.$$

In the singular case: $p \cdot F_1(x) = p \cdot F_2(x) = 0$.

Dissipative quantum dynamics

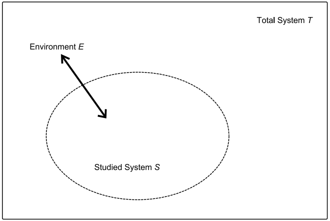

Figure: Open quantum systems

Lindblad form of dissipative dynamics:

$$i\hbar\frac{\partial}{\partial t}\rho(t) = [H_0 + u(t)H_1, \rho(t)] + \mathcal{L}[\rho(t)]$$

with $\mathrm{Tr}[\rho] = 1$ and $\mathrm{Tr}[\rho^2] \leq 1$

Dissipative two-level quantum systems

- A spin 1/2 particle in a magnetic field (B_x and B_y)
- The first two levels of a molecular system interacting with an electric field (E_x and E_y).

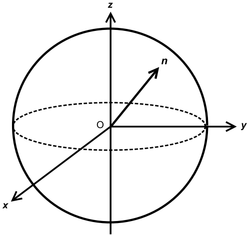

Figure: The Bloch ball

$$\mathrm{Tr}[\rho^2] \leq 1 \Leftrightarrow x^2 + y^2 + z^2 \leq 1$$

Control of two-level quantum systems

$$\begin{cases} \dot{x} = -\Gamma x + u_2 z \\ \dot{y} = -\Gamma y - u_1 z \\ \dot{z} = (\gamma_{12} - \gamma_{21}) - (\gamma_{12} + \gamma_{21})z + u_1 y - u_2 x \end{cases}.$$

We introduce $\gamma_+ = \gamma_{12} + \gamma_{21}$ and $\gamma_- = \gamma_{12} - \gamma_{21}$ such that $2\Gamma \geq \gamma_+ \geq |\gamma_-|$.

Hyp.:

- u_1 and u_2 envelopes of the two control fields.
- laser in resonance with the two-level system.
- Rotating wave approximation ($u \ll \omega$)

The single-input case

We consider the case $u_2 = 0$. (general case if the initial point is a pole).

$$\left\{ \begin{array}{l} \dot{y} = -\Gamma y - u_1 z \\ \dot{z} = (\gamma_{12} - \gamma_{21}) - (\gamma_{12} + \gamma_{21})z + u_1 y \end{array} \right. .$$

System on $\mathbb{R}^2$ of the form: $\dot{x} = F_0(x) + uF_1(x)$

$$PMP: \ \mathcal{H} = p \cdot F_0(x) + up \cdot F_1(x) + p_0$$

with $|u| \leq 1$.
We introduce the switching function ϕ:

$$\phi(x, p) = p \cdot F_1(x)$$

- **Regular case**: $\phi(x, p) \neq 0$, $u = \mathrm{sign}[\phi]$
- **Singular case**: $\phi(x, p) = 0$, u_s such that $\frac{d\phi}{dt} = 0$.

Example of solution

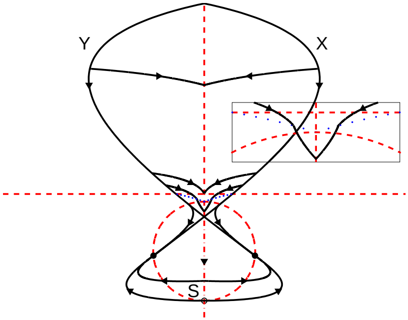

Figure: Optimal synthesis for $\Gamma = 3$, $\gamma_+ = 0.4$ and $\gamma_- = -0.2$.

Rem: Complete classification in B. Bonnard, M. Chyba and D. Sugny, to appear in IEEE AC.

The double-input case

We introduce the spherical coordinates (ρ, θ, ϕ)

$$
\begin{aligned}
H &= [\gamma_- \cos\phi - \rho(\gamma_+ \cos^2\phi + \Gamma \sin^2\phi)] p_\rho + \\
& p_\phi[-\frac{\gamma_- \sin\phi}{\rho} + \frac{\sin(2\phi)}{2}(\gamma_+ - \Gamma)] + \\
& \sqrt{p_\phi^2 + p_\theta^2 \cot^2\phi}
\end{aligned}
$$

Rem:

- p_θ is a constant of the motion (symmetry of revolution).
- ρp_ρ is a constant of the motion if $\gamma_- = 0$

$\Rightarrow$ H is integrable.

- Grushin model for $\Gamma = \gamma_+$. (dissipation in the radial direction)

The Grushin model on the sphere

$$H = \sqrt{p_\phi^2 + p_\theta^2 \cot^2 \phi}$$

Rem:

- Three-level quantum systems in the conservative case.
- Two-level dissipative quantum systems for $\Gamma = \gamma_+$ (independent of the purity).

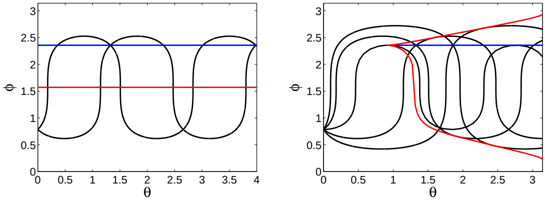

Figure: Conjugate and cut loci.

The concept of conjugate point

Local optimality: $\frac{\partial \mathcal{H}}{\partial u}=0,\ \frac{\partial^2 \mathcal{H}}{\partial u^2}\leq 0$

$$\left\{\begin{array}{l} \dot{\delta x}=\frac{\partial^2 H}{\partial x \partial p}\delta x+\frac{\partial^2 H}{\partial p^2}\delta p \\ \dot{\delta p}=-\frac{\partial^2 H}{\partial x^2}\delta x-\frac{\partial^2 H}{\partial x \partial p}\delta p \end{array}\right. ,$$

with $\delta x(0)=0$ and $\delta p(0)\cdot p(0)=0$.
Conjugate point: $\mathrm{Rank}(\delta x_1(t_c),\delta x_2(t_c),\cdots,\delta x_{n-1}(t_c))\leq n-2$

Ref.: The CotCot code (J.-B. Caillau)

The Integrable case

Deformation of the Grushin case with $\Gamma \neq \gamma_+$ and $\gamma_- = 0$.
Two different behaviors: $|\Gamma - \gamma_+| < 2$ and $|\Gamma - \gamma_+| > 2$

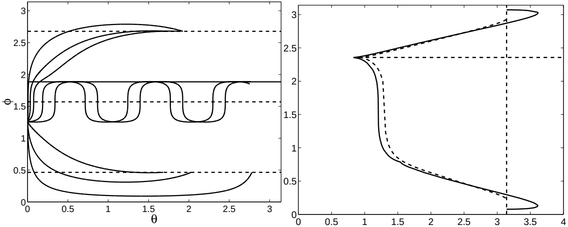

Figure: Projections of the extremals and of the conjugate locus.

Rem: Some properties are preserved when Γ and γ_+ vary.
Ref.: B. Bonnard and D. Sugny, SIAM J. Control Optim. 48, 1289 (2009).

The generic case

Deformation of the integrable case with $\gamma_- \neq 0$: not trivial!
$\Rightarrow$ Numerical simulations: Two cases.

1. Asymptotic dynamics for $|\Gamma - \gamma_+| > 2$:
   $\lim_{t\to+\infty} |p_\phi(t)| = +\infty$, $(\rho, \theta, \phi) \to (\rho_f, \theta_f, \phi_f)$
   No conjugate point.
2. Periodic dynamics for $|\Gamma - \gamma_+| < 2$:
   $\lim_{t\to+\infty} |\phi(t)| = 0, \pi$, $\rho \to \rho_f$
   Conjugate points.

Ref: B. Bonnard, M. Chyba and D. Sugny, IEEE Trans. AC.

Example of the continuation method: The two-dimensional case

We determine $(p_\phi(0), t_f)$ to reach the point (θ_f, ϕ_f) from the initial point (θ_i, ϕ_i): $(\theta_i, \phi_i) \to (\theta_f, \phi_f)$

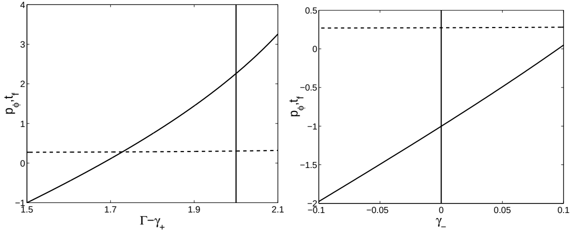

Figure: Continuation method from $\Gamma = 3.5$, $\gamma_+ = 2$ and $\gamma_- = 0$.

Rem:

- constant step
- Newton algorithm

Conclusion and perspectives

- Analytical proofs of numerical conjectures
- Generalization to more complex dynamics, quantum computing
- Coupling between indirect and direct methods
- Experimental applications in spin systems (NMR)

Bibliography

This work has been done in collaboration with B. Bonnard (Institut de Mathématiques de Bourgogne).

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