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Non-smooth optimal control of quantum systems

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The L^1-optimal control problem

$$\min_{x,u} \quad J(x,u) := \frac{1}{2}\|x(T) - x_T\|^2 + \frac{\nu}{2}\|u\|^2_{L^2} + \beta\|u\|_{L^1}$$

$$\text{s.t.} \quad \dot{x} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right] x \ , \ t \in (0,T] \ , \ x(0) = x_0$$

$$u \in U_{ad} \subset L^2((0,T);\mathbb{R}^{N_C})$$

The bilinear system can be a representation of Liouville equation, Pauli equation, semidiscrete Schrödinger equation, etc.

An optimal control solution of this L^1-optimization problem has a sparse structure, which resembles the control pulses usually considered in nuclear magnetic resonance and in other quantum control applications. This sparsity property of the controls can be advantageous for physical analysis and an adequate implementation in laboratory pulse shapers. Mathematically, this is explained by the following theorem.

Theorem [Vossen and Maurer 2006] If $u_n(t_j)u_n(t_k) < 0$ holds for two points $t_j < t_k$ in $[0,T]$, then there exist $\tilde{t}_j$ and $\tilde{t}_k$ in $[0,T]$ with $t_j < \tilde{t}_j < \tilde{t}_k < t_k$, such that $u_n = 0$ holds on $[\tilde{t}_j, \tilde{t}_k]$.

Optimality system and non-smoothness

In the space of solutions of constraint $(x = x(u))$ and adjoint equations $(p = p(u))$, the first-order optimality system can be written as the following root problem

$$\mathcal{F}_r(u) = 0$$

where for $n = 1, ..., N_C$ and $\theta > 0$, we have

$$\begin{aligned}(\mathcal{F}_r(u))_n := u_n &- \max\big(0, u_n + \theta(\mu_n(u) - \beta)\big) \\ &- \min\big(0, u_n + \theta(\mu_n(u) + \beta)\big) \\ &+ \max\big(0, u_n - b + \theta(\mu_n(u) - \beta)\big) \\ &+ \min\big(0, u_n + b + \theta(\mu_n(u) + \beta)\big)\end{aligned}$$

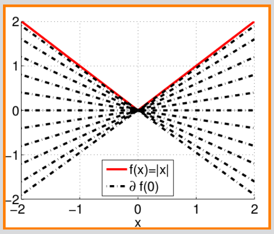
with $\mu_n(u) = \langle B_n x(u), p(u)\rangle - \nu u_n$.

The map $u \mapsto \mathcal{F}_r(u)$ is non-smooth and non-smooth calculus is required to construct a generalized Jacobian and to obtain semi-smoothness of $\mathcal{F}_r$.

Semi-smooth Newton method

To construct a semi-smooth Newton method, we consider the so-called sub-differential $\partial f(\tilde{x})$ of a function f at $\tilde{x}$. It represents the set of all sub-gradients or generalized derivative of f at $\tilde{x}$.

For example, the sub-differential of $f(x) = |x|$ at $x = 0$ is the set of all linear functionals $f' = c$ with $c \in [-1,1]$.



The semi-smooth Newton iteration is consequently defined as

- choose $\mathcal{J}_r(u_k) \in \partial\mathcal{J}_r(u_k)$;
- solve $\mathcal{J}_r(u_k)\delta u_k = -\mathcal{F}_r(u)$;
- update $u_{k+1} = u_k + \delta u_k$;

This semi-smooth Newton method is capable to obtain very accurate optimal control solutions and is proved to be locally superlinear convergent.

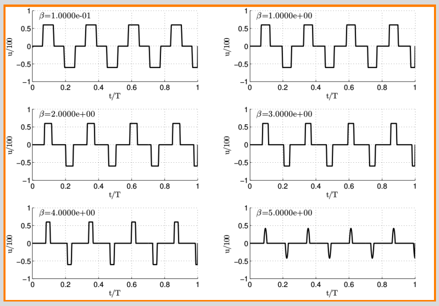
Theoretical characterization of the optimal controls

Under appropriate stability conditions of the trajectories $x(t)$, it holds that

- the optimal control posses a sparse structure;
- the map $\beta \mapsto \Phi(\beta) := u_\beta$ is continuous;
- there exists a $\hat{\beta} > 0$ such that the problem is solved by $u = 0$ for all $\beta \geq \hat{\beta}$;
- let $u \neq 0$ be an optimal control corresponding to $\nu > 0$ and $\beta > 0$, then it holds that

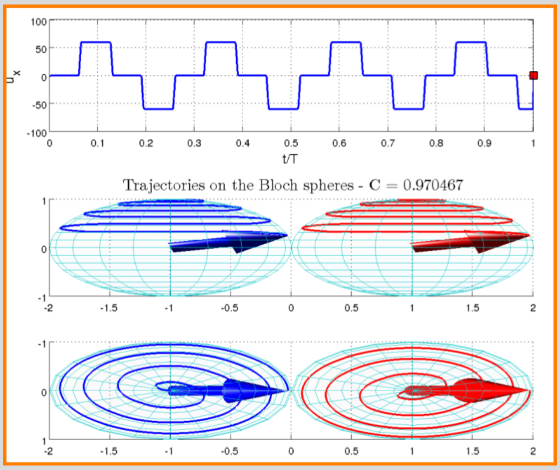
$$\|u\|_{L^1} \leq \min\big(O(\beta^{-1}), O(\nu^{-1/3})\big)$$

Numerical experiments validated this theoretical results and demonstrated that the sparsity of the solution increases when β steps up.



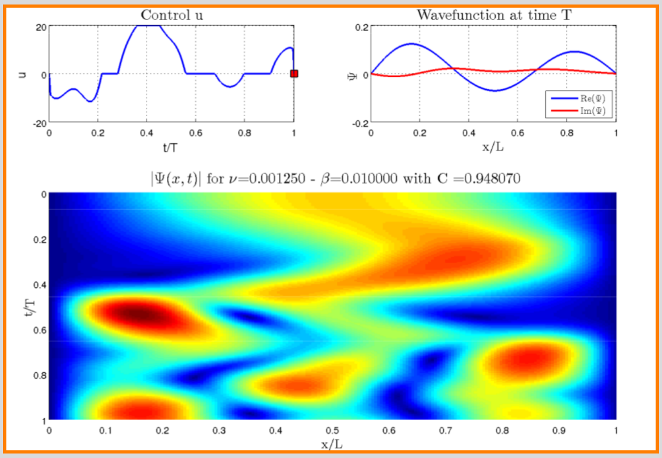
Control of a system of 2 uncoupled spins

The L^1-optimization framework is used for the control of a system of two uncoupled spins with opposite values of Larmor frequencies. The purpose is to steer each trajectory from the north-pole to the equator of the Bloch sphere.



Dipole control of a charged particle

The L^1-optimization framework is used for the control of a charged particle confined in an infinite potential well. The purpose is to steer the wavefunction from the ground state $\psi_1(x) = \sin(\pi x/L)$ to the third energy state $\psi_3(x) = \sin(3\pi x/L)$.



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