Control Optimization Methods in Quantum Systems

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Zvenigorod, June 21, 2012

4th Traditional School
CONTROL, INFORMATION, OPTIMIZATION

1 General Statements of Optimal Control Problems

A general nonlinear optimal control problem (OCP)

$$I(\sigma) = F(x(T), w) + \int\limits_0^T f^0\left(t, x(t), u(t), w\right) dt \to \inf_{\sigma\in D}, \quad \left(\text{or} \quad \min_{\sigma\in D}\right) \qquad (1)$$

$$\dot{x}(t) = f\left(t, x(t), u(t), w\right), \quad x(0) = a, \qquad (2)$$

$$\begin{gathered} u(t) \in U \subseteq E^m, \quad t \in [0, T], \\ w \in W \subseteq E^z, \quad a \in A \subseteq E^n, \end{gathered} \qquad (3)$$

where

$u(\cdot)$ – program control vector function (piecewise-continuous),
$x(\cdot)$ – state vector function (piecewise differentiable),
w, a – control parameters,
U, W, A – convex sets,
D – set of admissible processes, $\sigma = (x(\cdot), u(\cdot), w, a) \in D$.

OCP (1) – (3) without control parameters

$$I(\sigma) = F(x(T)) + \int_0^T f^0(t, x(t), u(t))\, dt \to \inf_{\sigma \in D}, \tag{4}$$

$$\dot{x}(t) = f(t, x(t), u(t)), \quad x(0) = x_0, \tag{5}$$

$$u(t) \in U \subseteq E^m, \quad t \in [0, T], \quad \sigma = (x(\cdot), u(\cdot)) \in D. \tag{6}$$

where we have only control function $u(\cdot)$.

Auxiliary problem: improving the given control process σ^{I} on D

It's required to improve $\sigma^{\mathrm{I}} = \left(x^{\mathrm{I}}(\cdot), u^{\mathrm{I}}(\cdot)\right) \in D$ in OCP (1) – (3) (or OCP (4) – (6)): i.e. we have to compute process $\sigma^{\mathrm{II}} = \left(x^{\mathrm{II}}(\cdot), u^{\mathrm{II}}(\cdot)\right) \in D$ such that

$$\Delta I(\sigma^{\mathrm{II}}) = I(\sigma^{\mathrm{II}}) - I(\sigma^{\mathrm{I}}) \leq 0.$$

3 Large Number of Applications

Both traditional and new areas for application of optimal control theory and related numerical methods

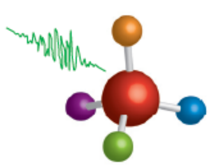
- Flight dynamics.
- Robotics.
- Chemistry, biosynthesis, immunological models.
- Laser control for quantum systems (including quantum information processing).

Etc.

4 Optimization methods for quantum physics

- C. Brif, R. Chakrabarti, H. Rabitz. *Control of Quantum Phenomena*. In "Advances in Chemical Physics. Vol. 148". 2011. John Wiley & Sons, Inc. (Rabitz Group, Princeton Univ.)
- V.F. Krotov. Global methods in optimal control theory. New York: Marcel Dekker, 1996. 408 p. (Institute of Control Sciences RAS.)

Laser pulse excites the electrons to higher-lying molecular orbitals



Ref.: K. Moore, H. Rabitz. Laser control. Manipulating molecules, *Nature. Chemistry*. Vol. 4, 2012.

5 Optimization methods for quantum physics

• D. Reich, M. Ndong, C.P. Koch. Monotonically convergent optimization in quantum control using Krotov's method. *J. Chem. Phys.* 136, 104103 (2012).

• R. Schmidt, A. Negretti, J. Ankerhold, et al. Optimal control of open quantum systems: cooperative effects of driving and dissipation. *Phys. Rev. Lett.* 107, 130404 (2011). http://arxiv.org/abs/1010.0940. [Using Krotov's method]

Optimal Control of Open Quantum Systems: Cooperative Effects of Driving and Dissipation

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(Dated: August 22, 2011)

We investigate the optimal control of open quantum systems, in particular, the mutual influence of driving and dissipation. A stochastic approach to open-system control is developed, using a generalized version of Krotov's iterative algorithm, with no need for Markovian or rotating-wave approximations. The application to a harmonic degree of freedom reveals cooperative effects of driving and dissipation that a standard Markovian treatment cannot capture. Remarkably, control can modify the open-system dynamics to the point where the entropy change turns negative, thus achieving cooling of translational motion without any reliance on internal degrees of freedom.

OCP for bilinear systems according to quantum control

Nonlinear cost functional:

$$I(x,u) = F(x(T)) \quad (\text{e.g.}, F(x) = \langle x, Mx \rangle). \tag{7}$$

Bilinear differential system:

$$\dot{x} = (A + Bu)x, \quad x(0) = x_0, \quad x \in E^n. \tag{8}$$

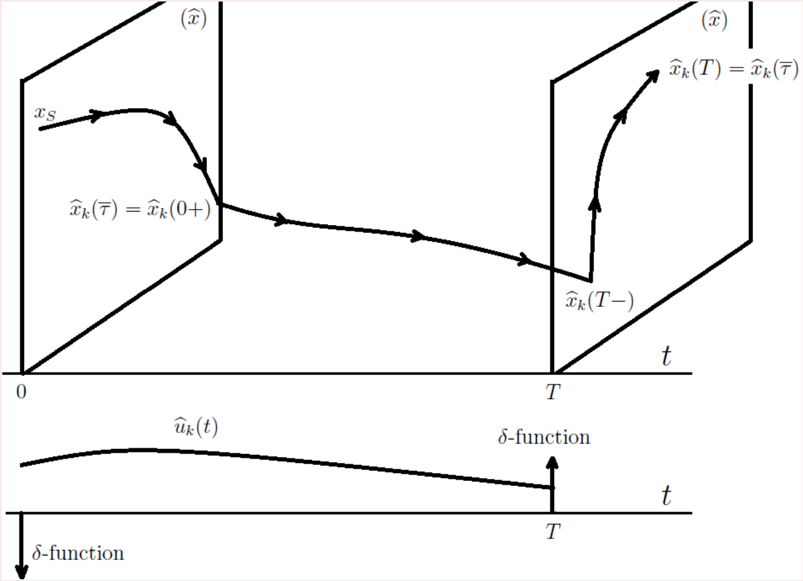
Ideas for OCP (7)–(8)

We develop ideas that deal with:

- Impulse and singular controls, discontinuous trajectories (and approximation using elements of D);
- Exact formulas for increment ΔI.

It'll be interesting for physics, because lasers can provide such controls.

7 Approaches for nonlocal improvement



Nonlocal improvements in nonlinear OCPs (1) – (3) and (4) – (6))

O.V. Morzhin. Nonlocal improvement of nonlinear controlled processes on the basis of sufficient optimality conditions. *Automation and Remote Control*. Vol. 71, No 8, 2010, pp. 1526-1539. www.springerlink.com/content/v6kv550252qm526l/.

O.V. Morzhin. Nonlocal improvement of control functions and parameters in nonlinear dynamic systems. *Automation and Remote Control*. Number 11, 2012. (In print.) **Issue according to the 3rd School "Control, Information, Optimization"(June 2011).**

Developing ideas: an exact increment formula and the correspondent conjugate system (in OCP (4) – (6))

$$\Delta I(\sigma) = I(\sigma) - I(\sigma^{\mathrm{I}}) =$$
$$= -\int_0^T \left\langle H_u(t, y(t), x(t), u^{\mathrm{I}}(t)) + d(t), \Delta u(t) \right\rangle dt, \quad \sigma, \sigma^{\mathrm{I}} \in D;$$
$$\dot{y}(t) = -H_x(t, y(t), x^{\mathrm{I}}(t), u^{\mathrm{I}}(t)) - r(t), \quad y(T) = -F_x(x^{\mathrm{I}}(T)) - q,$$
$$H(t, y(t), x(t), u^{\mathrm{I}}(t)) - H(t, y(t), x^{\mathrm{I}}(t), u^{\mathrm{I}}(t)) =$$
$$= \langle H_x(t, y(t), x^{\mathrm{I}}(t), u^{\mathrm{I}}(t)), \Delta x(t) \rangle + \langle r(t), \Delta x(t) \rangle,$$
$$F(x(T)) - F(x^{\mathrm{I}}(T)) = \langle F_x(x^{\mathrm{I}}(T)), \Delta x(T) \rangle + \langle q, \Delta x(T) \rangle,$$
$$H(t, y(t), x(t), u(t)) - H(t, y(t), x(t), u^{\mathrm{I}}(t)) =$$
$$= \langle H_u(t, y(t), x(t), u^{\mathrm{I}}(t)) + d(t), \Delta u(t) \rangle,$$

where increments $\Delta u(t) = u(t) - u^{\mathrm{I}}(t)$, $\Delta x(t) = x(t) - x^{\mathrm{I}}(t)$, $t \in [0, T]$.

Thank you for your attention!

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