# Second Order Analysis for Optimal Control Problems with Singular Arcs

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# Semigroup setting

Framework: reflexive Banach space $H$ (later: Hilbert space).

$C_0$ **(or strongly continous) semigroup**: Family $T(t)$, for $t \geq 0$, of bounded linear operators such that $T(0) = I$ and

$$T(s+t) = T(s)T(t), \quad s, t \geq 0$$

$$x = \lim_{t \downarrow 0} T(t)x, \quad \text{for all } x \in H.$$

Then (easy) there exists $M \geq 1$, $\omega \geq 0$ such that

$$\|T(t)\| \leq Me^{\omega t} \quad \text{for all } t \geq 0.$$

# Infinitesimal generator of a of $C_0$ semigroup

(Unbounded) linear operator $A$ in $H$ such that

$$Ax = \lim_{t \downarrow 0} \frac{T(t)x - x}{t}$$

with domain the set of $x$ such that the above limit exists.

# Characterization of $C_0$ semigroups

If $\lambda I + A$ is onto with a bounded inverse, we say that $\lambda$ belongs to the **resolvent set** $\rho(A)$ and denote by $R_\lambda(A) := (\lambda I + A)^{-1}$ the **resolvent**.

**Theorem 1.** *A linear operator $A$ is the infinitesimal generator of a $C_0$ semigroup $T(t)$ such that $\|T(t)\| \leq Me^{\omega t}$, iff $A$ is closed with dense domain, and for all $\lambda > \omega$, $\lambda \in \rho(A)$ and*

$$\|R_\lambda(A)^{-n}\| \leq M/(\lambda - \omega)^n, \quad n = 1, 2, \ldots$$

If $M = 1$, $\omega = 0$ we have a contraction semigroup: $\|T(t)\| \leq 1$.

Ref: A. Pazy, Semigroups of linear operators and applications to partial differential equations, Springer, 1983 (with convention $-A$ instead of $A$).

# Differential equations

In the sequel, $T(t)$ denoted by $e^{-tA}$. If $A \in L(H)$ then

$$e^{-tA} = I - tA + \frac{1}{2}t^2A^2 + \cdots$$

For $f \in L^1(0, T; H)$ consider the differential equation over $(0, T)$:

$$\dot{y} + Ay = f; \quad y(0) = y_0.$$

The mild, or semigroup solution is by the definition

$$y(t) = e^{-tA}y_0 + \int_0^t e^{-(t-s)A} f(s)\mathrm{d}s.$$

# Nonlinear differential equations

If $F : H \to H$ we define the solution of

$$\dot{y}(t) + Ay(t) = F(y(t)) + f(t);\ t \in (0, T); \quad y(0) = y_0.$$

by

$$y(t) = e^{-tA}y_0 + \int_0^t e^{-(t-s)A}(F(y(t)) + f(s))\mathrm{d}s$$

whenever is fixed-point equation is well-defined (as is e.g. if $F$ is Lipschitz).

# Dual semigroup

If $A$ linear operator in $H$ with domain $D(A)$: its **adjoint** $A^*$ is the linear operator over $H^*$ with domain

$$\{x^* \in H;\ \ \exists y^* \in H^*;\ \langle x^*, Ax\rangle = \langle y^*, x\rangle, \quad \text{for all } x \in D(A)\ \}.$$

If $\lambda \in \rho(A)$ then $R_\lambda(A)^* = R_\lambda(A^*)$.

**Theorem 2.** *Let $A$ be the infinitesimal generator of a $C_0$ semigroup $e^{-tA}$. Then the semigroup $(e^{-tA})^*$ over $H^*$ is $C_0$ and its generator is $A^*$.*

This theorem does not hold if $H$ is not reflexive.

# Adjoint equation

Consider the direct and adjoint differential equation, where $a \in L(H)$, $f \in L(0,T;H)$, $g \in L(0,T;H^*)$:

$$\dot{z}(t) + Az(t) = az(t) + f(t); \ t \in (0,T); \quad z(0) = z_0.$$

$$-\dot{p}(t) + A^*p(t) = a^*p(t) + g(t); \ t \in (0,T); \quad p(T) = p_T.$$

The semigroup solutions in $C(0,T;H)$ and $C(0,T;H^*)$ are

$$z(t) = e^{-tA} z_T + \int_0^t e^{-(t-s)A} (a^* z(s) + f(s)) \mathrm{d}s$$

$$p(t) = e^{-(t-T)A^*} p_T + \int_t^T e^{-(t-s)A^*} (a^* p(s) + g(s)) \mathrm{d}s$$

# Integration by parts (IBP)

We have that

$$\langle p(T), z(T)\rangle + \int_0^T \langle g(t), z(t)\rangle \mathrm{d}t = \langle p(0), z(0)\rangle + \int_0^T \langle p(t), b(t)\rangle \mathrm{d}t.$$

Application to optimal control:

$z$ solution of linearized state equation

$p$ costate

LHS $=$ directional derivative of cost

RHS $=$ expression of reduced gradient

# Another integration by parts formula

Let $w$ be the primitive of $v \in L^1(0,T)$. Then

$$\int_0^T \dot{w}(t)\langle p(t), z(t)\rangle \mathrm{d}t = \big[w(t)\langle p(t), z(t)\rangle\big]_0^T - \int_0^T w(t)\Big(\langle p(t), b(t)\rangle - \langle g(t), z(t)\rangle\Big)\mathrm{d}t$$

# The optimal control problem

Here $H$ Hilbert space, $\mathcal{B}_1 \in H$, $\mathcal{B}_2 \in L(H)$. Bilinear state equation

$$\dot{\Psi} + A\Psi = f + u(\mathcal{B}_1 + \mathcal{B}_2\Psi); \quad \Psi(0) = \Psi_0. \tag{1}$$

Cost function

$$J(u,\Psi) := \alpha \int_0^T u(t)\mathrm{d}t + \frac{a_1}{2}\int_0^T \|\Psi(t) - \Psi_d(t)\|^2_{\mathcal{H}}\mathrm{d}t + \frac{a_2}{2}\|\Psi(T) - \Psi_{dT}\|^2_{\mathcal{H}}; \tag{2}$$

Costate equation

$$-\dot{p} + \mathcal{A}^* p = a_1(\Psi - \Psi_d) + u\mathcal{B}_2^* p; \quad p(T) = a_2(\Psi(T) - \Psi_{dT}(T)). \tag{3}$$

# Control set

Control space (scalar)

$$\mathcal{U} := L^2(0,T)$$

Control constraints

$$u_m \leq u(t) \leq u_M.$$

# First order optimality conditions

Solution of state equation $\Psi[u]$

Reduced cost $F(u) := J(u, \Psi[u])$; Reduced gradient (based on IBP)

$$DF(u)v = \int_0^T \langle p(t), \mathcal{B}_1 + \mathcal{B}_2 \Psi(t) \rangle v(t) \mathrm{d}t$$

Assume (for ease of exposition) solution $\hat{u}$ unconstrained, associated state $\hat{\Psi}$ and costate $\hat{p}$: then

$$\langle p(t), \mathcal{B}_1 + \mathcal{B}_2 \hat{\Psi}(t) \rangle = 0 \quad \text{a.e. on } (0, T).$$

# Refs on semigroup approach to optimal control

- X. Li, Y. Yao, in LNCIS 75, 1985.
- X. Li, J. Yong, SICOPT 1991, Birkhäuser, 1995.
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# Second order optimality conditions

Lagrangian (formally)

$$J(u,\Psi) + \int_0^T \langle p(t), f(t) + u(t)(\mathcal{B}_1 + \mathcal{B}_2\Psi(t)) - \dot{\Psi}(t) - \mathcal{A}\Psi(t)\rangle \mathrm{d}t$$

# Second order optimality conditions II

Hessian of reduced cost (formally) assuming $a_1 = 1$ and no final cost

$$Q(v) := \int_0^T \left( \|z(t)\|^2 + v(t)\langle \hat{p}(t), \mathcal{B}_2 z(t)\rangle \right) \mathrm{d}t$$

where $z = z[v]$ solution of linearized equation (formally)

$$\dot{z} + \mathcal{A}z = \hat{u}\mathcal{B}_2 z + v(\mathcal{B}_1 + \mathcal{B}_2 \hat{\Psi}); \quad z(0) = 0.$$

**Theorem 3.** *If $\hat{u}$ local solution then $Q(v) \geq 0$ for any $v \in L^1(0,T)$.*

# Goh transform for the linearized system

Set

$$\xi := z - w(\mathcal{B}_1 + \mathcal{B}_2 \hat{\Psi}); \quad w(t) := \int_0^t v(s)\mathrm{d}s$$

Then $\xi(0) = 0$ and formally, with $[\mathcal{A}, \mathcal{B}_2] := \mathcal{A}\mathcal{B}_2 - \mathcal{B}_2\mathcal{A}$:

$$\dot{\xi} + \mathcal{A}\xi = \hat{u}\mathcal{B}_2\xi - w([\mathcal{A}, \mathcal{B}_2]\hat{\Psi} + \mathcal{A}\mathcal{B}_1).$$

Note that $v$ does not appear here !

We assume that $\hat{\Psi} \in \mathrm{dom}([\mathcal{A}, \mathcal{B}_2])$ and that $[\mathcal{A}, \mathcal{B}_2]\hat{\Psi} \in L^\infty(0, T; H)$. Then we can take $\xi$ as semigroup solution of the above equation.

# Goh transform in the second variation

We have that $Q(v) = \Omega(w,h)$, where $h = w(T)$ and setting $\mathcal{B} := \mathcal{B}_1 + \mathcal{B}_2\hat{\Psi}$:

$$\Omega := \Omega_t + \Omega_b, \tag{4}$$

$$\Omega_t(w,h) := \int_0^T \|\xi + w\mathcal{B}\|_{\mathcal{H}}^2 \,\mathrm{d}t, \tag{5}$$

$$\Omega_b(w,h) := \Omega_b^1(w,h) + \frac{1}{2}\Omega_b^2(w,h) \tag{6}$$

for

$$\begin{aligned}\Omega_b^1(w,h) :=\ & h(\hat{p}_T, \mathcal{B}_2\xi_T)_{\mathcal{H}} + \int_0^T w(t)(\hat{\Psi}(t) - \Psi_d(t), \mathcal{B}_2\xi(t))_{\mathcal{H}}\mathrm{d}t \\ & - \int_0^T w(t)(\hat{p}(t), [\mathcal{A}, \mathcal{B}_2]\xi(t))_{\mathcal{H}}\mathrm{d}t, \\ \Omega_b^2(w,h) :=\ & h^2(\hat{p}_T, \mathcal{B}_2^2\hat{\Psi}_T + \mathcal{B}_{2,T}\mathcal{B}_{1,T})_{\mathcal{H}} + \int_0^T w(t)^2(\hat{\Psi}(t) - \Psi_d(t), \mathcal{B}_2^2\hat{\Psi}(t))_{\mathcal{H}}\mathrm{d}t \\ & + \int_0^T w(t)^2(\hat{p}(t), [\mathcal{A}, \mathcal{B}_2^2]\hat{\Psi}(t) - [\mathcal{A}, \mathcal{B}_2]\mathcal{B}_1)_{\mathcal{H}}\mathrm{d}t \\ & - \int_0^T w(t)^2(\hat{p}(t), \mathcal{B}_2^2 f(t) + \mathcal{B}_2\mathcal{A}\mathcal{B}_1 + \hat{u}\mathcal{B}_2\mathcal{B}_1 - \mathcal{B}_2 b_z(t))_{\mathcal{H}}\mathrm{d}t.\end{aligned} \tag{7}$$

# Need for regularity

For the above expressions to be well-defined we need that

$$[\mathcal{A}, \mathcal{B}_2]\xi \in L^\infty(0, T; H) \quad \text{with} \quad \xi = z - w(\mathcal{B}_1 + \mathcal{B}_2\hat{\Psi})$$

Critical step

$$[\mathcal{A}, \mathcal{B}_2]\xi \in L^\infty(0, T; H)$$

Remember that $\xi(0) = 0$ and

$$\dot{\xi} + \mathcal{A}\xi = \hat{u}\mathcal{B}_2\xi - w([\mathcal{A}, \mathcal{B}_2]\hat{\Psi} + \mathcal{A}\mathcal{B}_1).$$

Again if $[\mathcal{A}, \mathcal{B}_2]\hat{\Psi} \in L^\infty(0, T; H)$ this will follow from specific regularity results.

# Second order optimality conditions III

**Corollary 1.** *If $\hat{u}$ local solution then*

$$\Omega(w,h) \geq 0, \quad \textit{for any } (w,h) \in L^2(0,T) \times \mathbb{R}.$$

Proof based on
- continuity of $\Omega$ in the $L^2(0,T) \times \mathbb{R}$ topology
- In the limit, $w$ and $h$ independent

## Taylor expansion of cost function using $w$

We have the Taylor expansion where $w(t) := \int_0^t v(s)\mathrm{d}s$:

$$F(\hat{u} + v) = F(\hat{u}) + DF(\hat{u})v + \tfrac{1}{2}\Omega(w) + o(\|w\|_1^2)$$

Second order sufficient condition: for some $\alpha > 0$:

$$\Omega(w) \geq 2\alpha\|w\|_2^2, \quad \text{for all } w \in L^2(0,T). \qquad (SOSC)$$

**Theorem 4.** *If $(SOSC)$ holds, then $\hat{u}$ satisfies the weak quadratic growth condition*

$$F(\hat{u} + v) \geq F(\hat{u}) + DF(\hat{u})v + \tfrac{1}{2}\alpha\|w\|_2^2$$

# Heat equation

**I: Setting**: $\Omega \subset \mathbb{R}^3$ open, bounded, smooth boundary

**Heat equation**: $b \in H_0^1(\Omega) \cap W^{2,\infty}(\Omega)$, $y_0 \in C(\bar{\Omega}) \cap H_0^1(\Omega)$, $y = y(x,t)$

$$\begin{cases} \dot{y} - \Delta y = u(t) b(x) y \quad \text{in } Q := \Omega \times [0,T] \\ y = 0 \text{ on } \partial\Omega \times [0,T]; \quad y(\cdot, 0) = y_0. \end{cases} \tag{8}$$

**Cost function**

$$J(u) = \tfrac{1}{2} \int_Q (y(x,t) - y_d(x,t))^2 \mathrm{d}x \mathrm{d}t \tag{9}$$

# Semigroup property

We need to study for $\lambda \geq 0$

$$\lambda y - \Delta y = f \in L^2(\Omega).$$

Then integrating by parts (Dirichlet boundary conditions)

$$\lambda \|y\|_2^2 + \int_\Omega |\nabla y(x)|^2 \mathrm{d}x = \int_\Omega y(x) f(x) \mathrm{d}x \leq \|y\|_2 \|f\|_2$$

implying that the heat equation corresponds to a contraction semigroup.

## Well-posedness of $\xi$ equation

Here $\mathcal{A} = -\Delta$ with domain $D(\mathcal{A}) := H_0^1(\Omega) \cap H^2(\Omega)$.

We have to compute (cancellation of $b\Delta y$)

$$[-\Delta, b]y = (-\Delta b)y + 2\nabla b \cdot \nabla y.$$

Known regularity result: if $y_0 \in H_0^1(\Omega)$ and $\hat{u} \in L^2(0,T)$ then

$$y \in C(0,T; H_0^1(\Omega)) \quad \Rightarrow \quad [-\Delta, b]y \in C(0,T; L^2(\Omega)).$$

Same analysis gives $[-\Delta, b]\xi \in C(0,T; L^2(\Omega))$.

## Schroedinger equation

Here $\Omega$ as before and $\Psi(x,t) \in \mathbb{C}$:

$$\dot{\Psi} - i\Delta\Psi = f$$

Semigroup property: consider

$$\lambda\Psi - i\Delta\Psi = f$$

Multiply by $\hat{\Psi}$ (conjugate), integrate over $\Omega$:

$$\lambda\|\Psi\|_2^2 + i\int_\Omega |\nabla\Psi|^2 \mathrm{d}x = \int_\Omega f(x)\Psi(x)\mathrm{d}x$$

Use Cauchy-Schwarz and take real parts: obtain contraction semigroup

Here $\mathcal{A} = -i\Delta$ with domain (complex spaces) $D(\mathcal{A}) := H_0^1(\Omega) \cap H^2(\Omega)$.

We have to compute (cancellation of $b\Delta y$)

$$[-i\Delta, b]y = (-i\Delta b)y + 2i\nabla b \cdot \nabla y.$$

Regularity result: if $y_0 \in H_0^1(\Omega) \cap H^2(\Omega)$ and $\hat{u} \in L^\infty(0,T)$ then

$$y \in C(0,T; H_0^1(\Omega)) \quad \Rightarrow \quad [-i\Delta, b]y \in C(0,T; L^2(\Omega)).$$

Same analysis gives $[-i\Delta, b]\xi \in C(0,T; L^2(\Omega))$.

**Numerical experiment I**

**Do such singular arcs really occur in practice ?**

Or is the solution bang-bang ?

**Numerical experiment support the existence of singular arcs !**

Computations based on the (free software) optimal toolbox

**http://bocop.org**

**Numerical experiment I**: Optimal control by the Neumann BC at $x = 0$
$nx = 50$, $nt = 200$, implicit Euler scheme, $y_0 = 1$, $y_d = 0$, $\alpha = 0$.

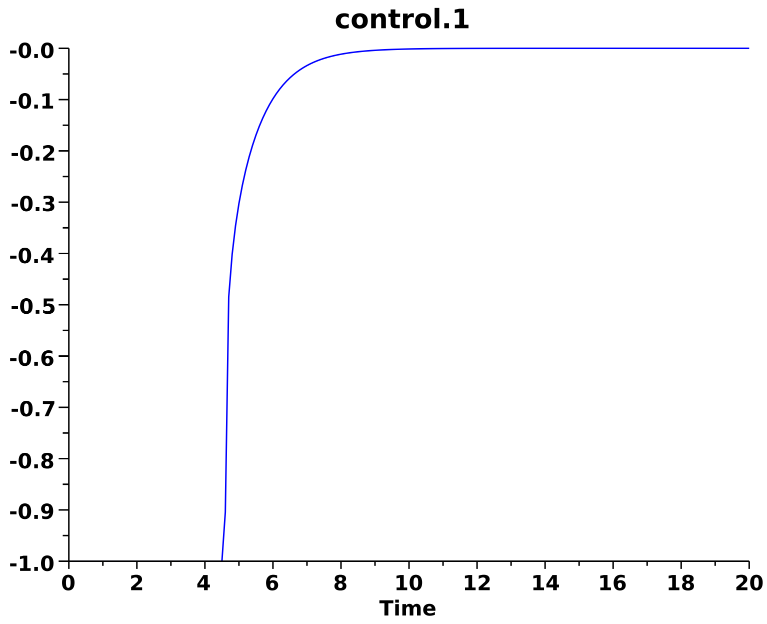


Figure 1: Optimal control: $u \in [-1, 1]$.

## A Fuller type phenomenon

- Ad constraint $\dot{u} \in [-1, 1]$

- Infinite dimensional extension of the classical Fuller problem
- The Goh transform should be performed twice, see (5).
- Known chattering phenomenon in Fuller's problem: infinite sequence of bang arcs before entering the singular arc.
- Similar behavior for the control of the heat equation ?

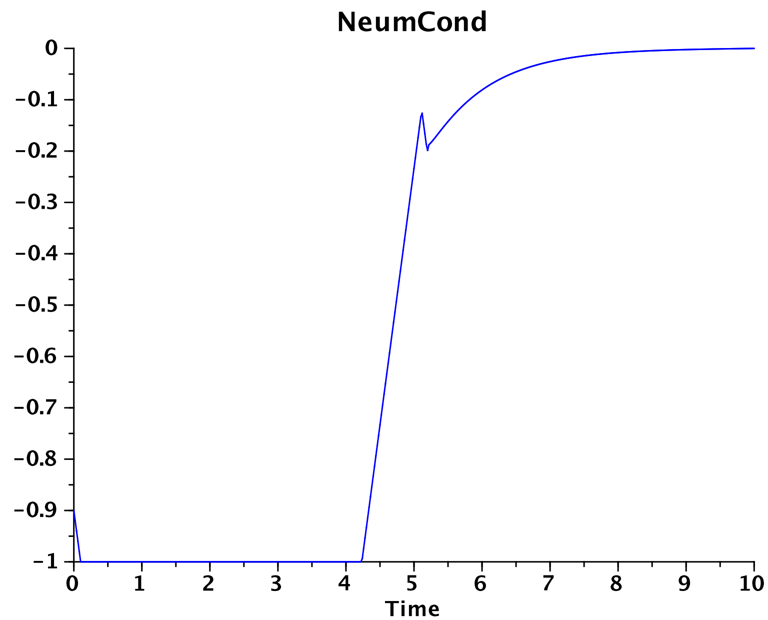


Figure 2: Neumann condition $u \in [-1, 1]$ with bounded derivative.

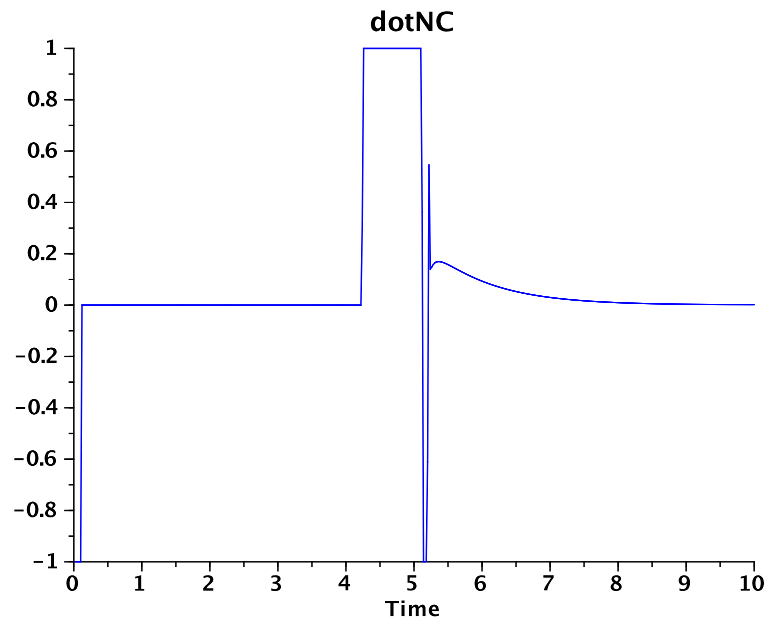


Figure 3: Derivative of the Neumann condition, restricted to $[-1, 1]$.

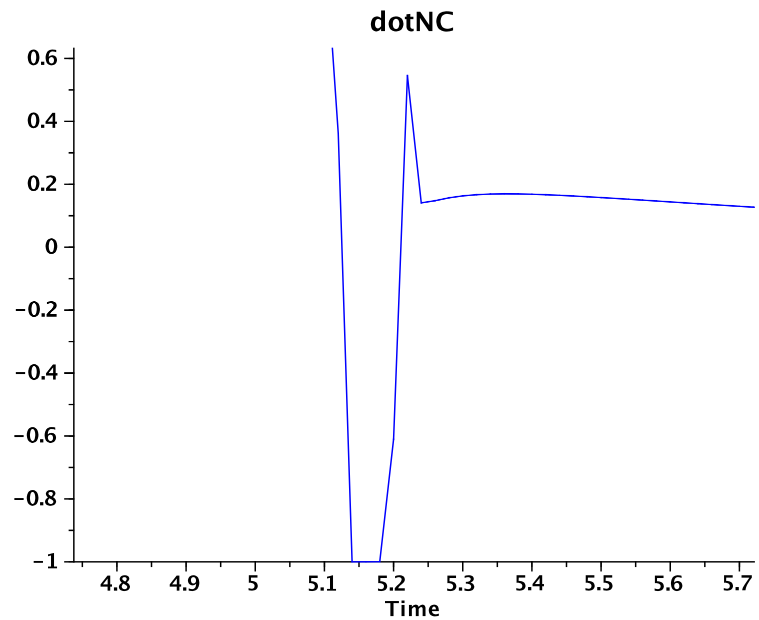


Figure 4: Zoom on the derivative of the Neumann condition.

# Singular arc in the Schrödinger equation

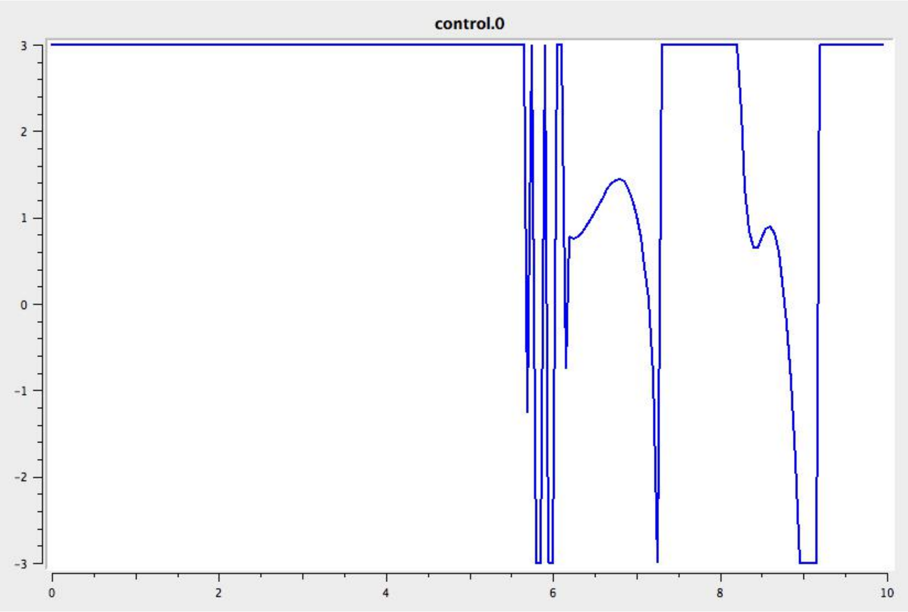


Figure 5: Presence of singular arcs, Schrödinger equation

## Questions and comments

- Partial extension of optimality conditions in (1).
  Elliptic case: link with recent work by Casas (4).

- Coefficients of $u$ functions of $y$ ?

- Final constraints, sensitivity analysis ?

- Related article (3).

- Link with the shooting algorithm (2)

## References

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