Optimal Control of PDEs with Non-smooth Cost Functionals

K. Kunisch

Institute for Mathematics and Scientific Computing
University of Graz, Austria
Radon Institute, Austrian Academy of Sciences, Linz, Austria

in collaboration with E. Casas, C. Clason, F. Henneke, K. Ito, K. Pieper, A. Rund, P. Trautmann, B. Vexler

Luminy, November 9-13, 2015

To start

$$
\begin{cases}
\min \frac{1}{2}\int_0^{T_\infty} |y-z|^2\,dt + \frac{\alpha}{2}\int_0^{T_\infty} |u|^2\,dt \\
\text{subject to} \\
\frac{d}{dt}y(t) = Ay(t) + Bu(t) \text{ for } t > 0 \\
y(0) = y_0 \\
u(t) \in U
\end{cases}
$$

where $T^\infty \in (0,\infty],\ \alpha > 0.$

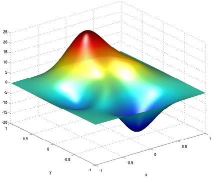
Motivation: LQR, LQG, differentiability,...

Fact: Extra regularity: $\alpha u^*(t) = P_U(p(t))$

Focus on the cost functional

motivation

$$\begin{cases} \min\limits_{u \in \mathcal{X}} \|y - z\|^2_{L^2(\Omega)} + \alpha \mathcal{N}(\|u\|) \\ \text{s.t.} \quad Ay = u \end{cases} \qquad (\mathcal{P})$$

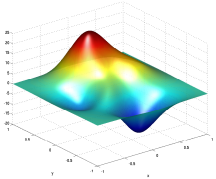


$\int_\Omega |u(x)|^2 \, dx$

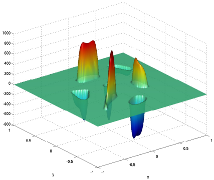
Focus on the cost functional

motivation

$$\begin{cases} \min\limits_{u \in \mathcal{X}} \|y - z\|^2_{L^2(\Omega)} + \alpha \mathcal{N}(\|u\|) \\ \text{s.t.} \quad Ay = u \end{cases} \qquad (\mathcal{P})$$



$\int_\Omega |u(x)|^2 \, dx$

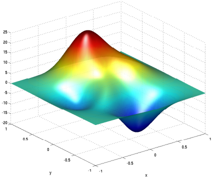


$\int_\Omega |u(x)| \, dx$

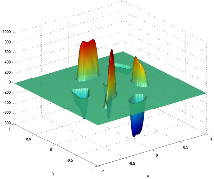
Focus on the cost functional

motivation

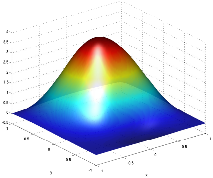
$$\left\{\begin{array}{ll}\min\limits_{u\in\mathcal{X}} \|y-z\|^2_{L^2(\Omega)} + \alpha\,\mathcal{N}(\|u\|) \\ \text{s.t.} \qquad Ay = u\end{array}\right. \qquad (\mathcal{P})$$



$\int_\Omega |u(x)|^2\,dx$



$\int_\Omega |u(x)|\,dx$

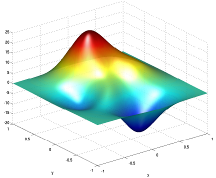


$\int_\Omega |\nabla u(x)|^2\,dx$

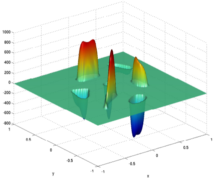
Focus on the cost functional

motivation

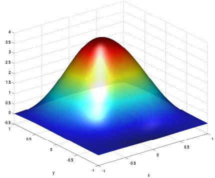
$$\left\{ \begin{array}{ll} \min\limits_{u \in \mathcal{X}} \|y - z\|^2_{L^2(\Omega)} + \alpha \mathcal{N}(\|u\|) & \\ \text{s.t.} \quad Ay = u & \end{array} \right. \qquad (\mathcal{P})$$



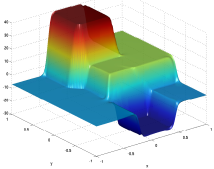
$\int_\Omega |u(x)|^2 \, dx$



$\int_\Omega |u(x)| \, dx$



$\int_\Omega |\nabla u(x)|^2 \, dx$



$\int_\Omega |\nabla u(x)| \, dx$

Short computations

$$\min \frac{1}{2}|u-z|^2 + \frac{\alpha}{2}|u|^2$$

$$u^*(z) = \frac{z}{1+\alpha}$$

$$\min \frac{1}{2}|u-z|^2 + \beta|u|$$

$$u^*(z) = \begin{cases} 0 & \text{if } |z| < \beta \\ z-\beta & \text{if } z \geq \beta \\ z+\beta & \text{if } z \leq -\beta \end{cases}$$

$$\min \frac{1}{2}|u-z|^2 + \beta|u|^0$$

$$u^*(z) = \begin{cases} 0 & \text{if } |z| < \sqrt{2\beta} \\ z & \text{if } |z| \geq \sqrt{2\beta} \end{cases}$$

$$\min \frac{1}{2}|u-z|^2 + \frac{\alpha}{2}|u|^2 + \beta|u|^0$$

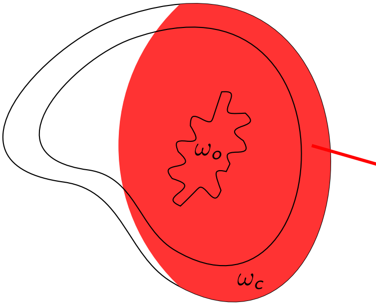
$$u^*(z) = \begin{cases} 0 & \text{if } |z| < \sqrt{2(1+\alpha)\beta} \\ \frac{z}{1+\alpha} & \text{if } |z| \geq \sqrt{2(1+\alpha)\beta} \end{cases}$$

Motivation for sparsity constraints

- Proportionality
- Eliminate 'small' controls
- Optimal actuator placement
- Inverse source problems

Motivation for sparsity constraints

- Optimization of light source locations in diffusive optical tomography
- Goal: Homogeneous illumination (application in photochemotherapy)
- Standard approach (discrete): combinatorial explosion with DOFs
- Here: Consider fictitious distributed "control field", apply sparse control techniques
  $\rightsquigarrow$ localization of sources



$$
\begin{aligned}
-\nabla \cdot (\kappa \nabla y) + \mu y &= u \chi_{\omega_c} \text{ in } \Omega \\
\kappa \nu \cdot \nabla y + \rho y &= 0 \text{ on } \partial\Omega
\end{aligned}
$$

diffusive approximation of radiative transfer to model steady state light propagation

in scattered media, Brunner-Clason-Freiberger-Scharfetter

'Table of contents'

Optimal control with sparsity constraints for elliptic equations

$$\begin{cases} \min_{u \in L^1(\Omega)} J(u) = \frac{1}{2}\|y - z\|^2_{L^2(\Omega)} + \alpha\|u\|_{L^1(\Omega)} \\ \text{subject to} \quad Ay = u \quad \text{in } \Omega \\ \qquad\qquad\quad\;\; y = 0 \quad \text{on } \partial\Omega \end{cases}$$

No guaranteed existence! Remedy: control constraints or measures

$$(P) \begin{cases} \min_{u \in \mathcal{M}(\Omega)} J(u) = \frac{1}{2}\|y - z\|^2_{L^2(\Omega)} + \alpha\|u\|_{\mathcal{M}(\Omega)} \\ \text{subject to} \quad Ay = u \quad \text{in } \Omega \\ \qquad\qquad\quad\;\; y = 0 \quad \text{on } \partial\Omega \end{cases}$$

Optimal control with sparsity constraints for elliptic equations

$$\left\{\begin{array}{l} \displaystyle\min_{u\in L^1(\Omega)} J(u) = \frac{1}{2}\|y-z\|^2_{L^2(\Omega)} + \alpha\|u\|_{L^1(\Omega)} \\ \\ \text{subject to} \quad \begin{array}{rcll} Ay & = & u & \text{in } \Omega \\ \\ y & = & 0 & \text{on } \partial\Omega \end{array} \end{array}\right.$$

No guaranteed existence! Remedy: control constraints or measures

$$(P)\left\{\begin{array}{l} \displaystyle\min_{u\in \mathcal{M}(\Omega)} J(u) = \frac{1}{2}\|y-z\|^2_{L^2(\Omega)} + \alpha\|u\|_{\mathcal{M}(\Omega)} \\ \\ \text{subject to} \quad \begin{array}{rcll} Ay & = & u & \text{in } \Omega \\ \\ y & = & 0 & \text{on } \partial\Omega \end{array} \end{array}\right.$$

Analysis of the state equation

Theorem

For any $u \in \mathcal{M}(\Omega)$ *and* $q \in (0, \frac{n}{n-1})$

$$\begin{cases} Ay = u, & \text{in } \Omega, \\ y = 0, & \text{on } \partial\Omega, \end{cases}$$

has a unique solution $y \in W_0^{1,q}(\Omega)$*:*

$$\|y\|_{W_0^{1,q}(\Omega)} \leq C\|u\|_{\mathcal{M}(\Omega)}.$$

Recall $W_0^{1,q'}(\Omega) \subset C_0(\bar{\Omega})$ where $q' = \frac{q}{q-1}$.

Existence

Proposition (existence)

$$\min_{u \in \mathcal{M}} \frac{1}{2}\|y - z\|^2_{L^2(\Omega)} + \alpha\|u\|_{\mathcal{M}}$$

$$\begin{cases} Ay = u, & \text{in } \Omega, \\ y = 0, & \text{on } \partial\Omega, \end{cases}$$

has a unique minimizer u^*.

$$\mathcal{L}(u, y, p) = \frac{1}{2}\|y - z\|^2_{L^2(\Omega)} + \alpha\|u\|_{\mathcal{M}(\Omega)} - \langle p, Ay - u\rangle_{C(\Omega),\mathcal{M}(\Omega)}$$

Theorem (necessary optimality)

$$\begin{cases} Ay^* = u^*, & \text{in } \Omega, \quad y^* = 0, \quad \text{on } \partial\Omega, \\ A^* p^* = y^* - z, & \text{in } \Omega, \quad p^* = 0, \quad \text{on } \partial\Omega, \\ ??? & \end{cases}$$

Necessary optimality

$$\mathcal{L}(u, y, p) = \frac{1}{2}\|y - z\|^2_{L^2(\Omega)} + \alpha \int_\Omega \|u\| dx - \langle p, Ay - u\rangle_{C(\Omega),\mathcal{M}(\Omega)}$$

$$-\frac{1}{\alpha}p^* \in \partial\varphi(u^*) \Leftrightarrow u^* \in \partial\varphi^*(-\frac{1}{\alpha}p^*)$$

Theorem (necessary optimality)

$$\begin{cases} Ay^* = u^*, & \text{in } \Omega, \quad y^* = 0, \quad \text{on } \partial\Omega, \\ A^*p^* = y^* - z, & \text{in } \Omega, \quad p^* = 0, \quad \text{on } \partial\Omega, \\ \langle u^*, p^* - p\rangle_{\mathcal{M},C} \leq 0, & p \in C_0(\Omega) \text{ with } \|p\|_{C_0(\Omega)} \leq \alpha. \\ \|p^*\|_{C_0(\Omega)} \leq \alpha, & \end{cases}$$

$$\begin{cases} \langle u^*, p^* - p\rangle_{\mathcal{M},C} \leq 0, & p \in C(\Omega) \text{ with } |p|_{C(\Omega)} \leq \alpha. \\ |p^*|_{C(\Omega)} \leq \alpha, \end{cases}$$

" $p^* = Proj_C(-u^*)$" where $C = \{p : |p(x)| \leq \alpha\}$

Jordan decomposition $u^* = u^*_+ - u^*_-$,

$$\begin{cases} supp(u^*_+) \subset \{x \in \Omega : p^*(x) = -\alpha\}, \\ supp(u^*_-) \subset \{x \in \Omega : p^*(x) = +\alpha\}. \end{cases}$$

Corollary

$$\exists \eta > 0 \text{ such that } supp\, \bar{u} \in \{x \in \Omega | dist(x, \delta\Omega) > \eta\}$$
$$dist(supp\,(u^*_+), supp\,(u^*_-)) > \eta.$$

Theorem

If $z \in L^\infty(\Omega)$ and $\Omega = \Omega_c = \Omega_0$, then $\|y^*\|_{L^\infty(\Omega)} \leq \|z\|_{L^\infty(\Omega)}$ and $\|u^*\|_{H^{-1}(\Omega)} \leq \|\nabla y^*\|_{L^2(\Omega)}$.

cf. Pieper-Vexler

$$\begin{cases} \langle u^*, p^* - p\rangle_{\mathcal{M},C} \le 0, \quad p \in C(\Omega) \text{ with } |p|_{C(\Omega)} \le \alpha. \\ \\ |p^*|_{C(\Omega)} \le \alpha, \end{cases}$$

"$p^* = Proj_C(-u^*)$" where $C = \{p : |p(x)| \le \alpha\}$

Jordan decomposition $u^* = u^*_+ - u^*_-$,

$$\begin{cases} supp(u^*_+) \subset \{x \in \Omega : p^*(x) = -\alpha\}, \\ supp(u^*_-) \subset \{x \in \Omega : p^*(x) = +\alpha\}. \end{cases}$$

formal:

$$u^* + \max(0, -u^* + c(p^* - \alpha)) + \min(0, -u^* + c(p^* + \alpha)) = 0$$

for any $c > 0$.

$$\begin{cases} \langle u^*, p^* - p\rangle_{\mathcal{M},C} \le 0, \quad p \in C(\Omega) \text{ with } |p|_{C(\Omega)} \le \alpha. \\ |p^*|_{C(\Omega)} \le \alpha, \end{cases}$$

"$p^* = Proj_C(-u^*)$" where $C = \{p : |p(x)| \le \alpha\}$

Jordan decomposition $u^* = u^*_+ - u^*_-$,

$$\begin{cases} supp(u^*_+) \subset \{x \in \Omega : p^*(x) = -\alpha\}, \\ supp(u^*_-) \subset \{x \in \Omega : p^*(x) = +\alpha\}. \end{cases}$$

formal:

$$u^* + \max(0, -u^* + c(p^* - \alpha)) + \min(0, -u^* + c(p^* + \alpha)) = 0$$

for any $c > 0$.

Semi-smooth Newton method

Definition

$F : D \subset X \to Z$ is called Newton differentiable in $U \subset D$, if there exist $G : U \to \mathcal{L}(X, Z)$:

$$(A)\ lim_{h\to 0} \frac{1}{\|h\|_Y} \|F(x+h) - F(x) - G(x+h)h\|_Z = 0, \text{ for all } x \in U.$$

Example

$F : L^p(\Omega) \to L^q(\Omega)$,

$F(\varphi) = \max(0, \varphi)$, $q < p$ is Newton differentiable and

$$G_{\max}(\varphi)(x) = \begin{cases} 1 & \text{if } \varphi(x) > 0 \\ 0 & \text{if } \varphi(x) < 0 \\ \delta & \text{if } \varphi(x) = 0,\ \delta \in \mathbb{R} \text{ arbitrary.} \end{cases}$$

Semi-smooth Newton method

Theorem

Let $F(x^*) = 0$, F Newton differentiable in $U(x^*)$, and $\{||G(x)^{-1}||_{\mathcal{L}(X,Z)} : x \in U(x^*)\}$ bounded.

Then the Newton iteration converges locally superlinearly.

Remark: Rate of convergence, calculus for semi-smoothness

Ref.: Hintermüller-Ito-K, Chen-Nashed, Kummer, M. Ulbrich.

Semi-smooth Newton method

Theorem

Let $F(x^*) = 0$, F Newton differentiable in $U(x^*)$, and $\{||G(x)^{-1}||_{\mathcal{L}(X,Z)} : x \in U(x^*)\}$ bounded.

Then the Newton iteration converges locally superlinearly.

Remark: Rate of convergence, calculus for semi-smoothness

Ref.: Hintermüller-Ito-K, Chen-Nashed, Kummer, M. Ulbrich.

Nonlinear equation

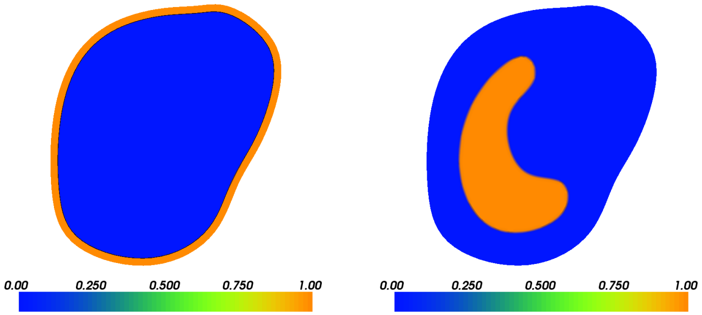
$$F(u_h, y_h, p_n) = 0 \qquad \Longleftrightarrow$$

$$\begin{cases} A_h y_h - u_h = 0 \\ A_h^* p_h - (y - z) = 0 \\ u_h + max(0, -u_h + p_h - \alpha) + min(0, -u_h + p_h + \alpha) = 0 \end{cases}$$

Solve by semi-smooth Newton method

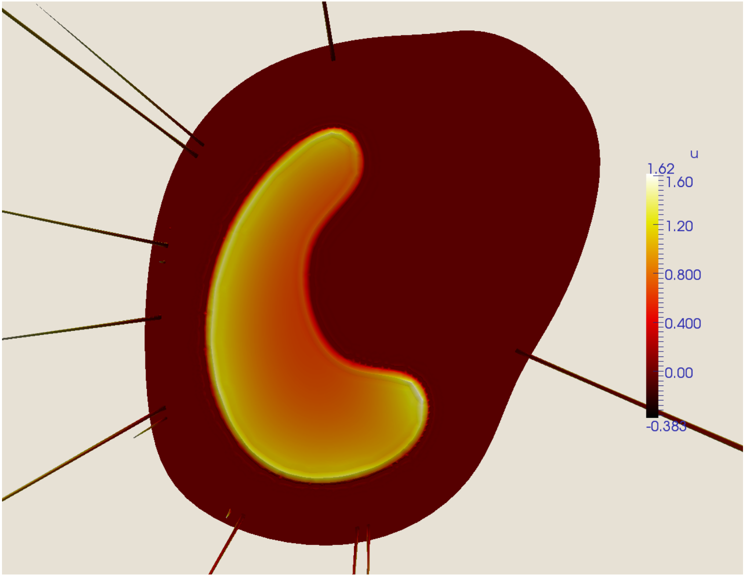
Remark: Convergence rate estimates for FE-discretizations, $\|u_h\|_{\mathcal{M}} \to \|u^*\|_{\mathcal{M}}$

Example: geometry

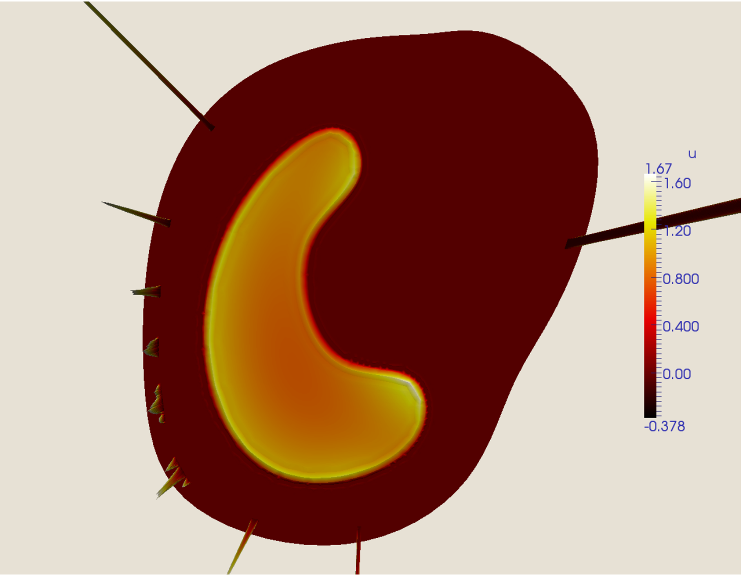


control domain observation domain

Example: $\alpha = 10^{-1}$



Example: $\alpha = 10^{-4}$

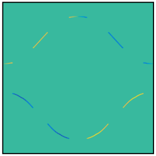


Comparison of $L^2(I, \mathcal{M}(\Omega_c))$ and $\mathcal{M}(\Omega_c, L^2(I))$

$\boxed{L^2(I, \mathcal{M}(\Omega_c))}$

- Time-dependent measure:
$$u(t) \in \mathcal{M}(\Omega_c),$$
$$\text{a.e. } t \in I$$

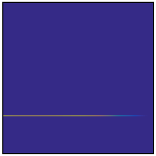
- Typical element:
$$u(t) = \sum_{i=1}^{N} u_i(t)\delta_{x_i(t)}$$



$\boxed{\mathcal{M}(\Omega_c, L^2(I))}$

- Time-independent measure:
$$u = u'(x,t) \cdot |u|, \ |u| \in \mathcal{M}(\Omega_c)^+,$$
$$u' \in L^1(\Omega_c, |\mu|, L^2(I))$$

- Typical element:
$$u(t) = \sum_{i=1}^{N} u_i(t)\delta_{x_i}$$



$$\boxed{\mathcal{M}(\Omega_c, L^2(I)) \hookrightarrow L^2(I, \mathcal{M}(\Omega_c))}$$

Optimal control of wave equation with sparsity constraints

- Simple model for seismic events:

$$u(t) = \sum_{i=1,\dots,N} u_i(t)\delta_{x_i} \qquad \text{(PS)}$$

- Approximation of seismic waves by acoustic waves

$$\partial_{tt} y - \Delta y = u \quad \text{in } I \times \Omega \; + \text{B.C.} + \text{I.C.} \qquad \text{(WE)}$$

- Aim: Reconstruction of (PS) from M (noisy) mean values

$$O_j y(t) = \frac{1}{|P_j|} \int_{P_j} y(t,\cdot)\,\mathrm{d}x$$

  on spatial patches $P_j \subset \Omega$

- Direct optimization of N, x_i and u_i:

$$\min_{X,U} \frac{1}{2M} \sum_{j=1,\dots,M} \|O_j y - z_j\|^2_{L^2(I)} + \alpha \sum_{i=1,\dots,N} \|u_i\|_{L^2(I)} \quad \text{s.t. (WE)}$$

  $\Rightarrow$ non-convex problem $\Rightarrow$ convex "relaxation"

Convex problem

$$\min_{u\in\mathcal{M}_T, y\in Y} J(u,y) = \frac{1}{2}\|y-z\|^2_{L^2(Q)} + \alpha\|u\|_{\mathcal{M}_T} \qquad (\mathcal{P})$$

s.t.

$$\begin{cases} \partial_{tt} y - \Delta y = u & \text{in } Q = I\times\Omega, \\ y = 0 & \text{on } I\times\partial\Omega, \\ y = 0, \partial_t y = 0 & \text{in } \{0\}\times\Omega. \end{cases} \qquad \text{(SE)}$$

with $\mathcal{M}_T = L^2(I,\mathcal{M}(\Omega_c))$, or $\mathcal{M}_T = \mathcal{M}(\Omega_c, L^2(I))$.

- Measures on the compact control set $\Omega_c \subset \Omega$: $\mathcal{M}(\Omega_c)$ with total variation norm $\|u\|_{\mathcal{M}(\Omega_c)}$
- Bochner space: $L^2(I,\mathcal{M}(\Omega_c))$ with norm

$$\|u\|_{L^2(I,\mathcal{M}(\Omega_c))} = \left(\int_0^T \|u(t)\|^2_{\mathcal{M}(\Omega_c)}\,\mathrm{d}t\right)^{1/2}$$

- $L^2(I)$-valued measures: $\mathcal{M}(\Omega_c, L^2(I))$, total variation norm $\|u\|_{\mathcal{M}(\Omega_c,L^2(I))}$

Well posedness of the state equation

Theorem

Let $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$ and $u \in L^2(I, \mathcal{M}(\Omega_c))$. Then there exits a unique very weak solution

$$y \in Y = \mathcal{C}(\bar{I}, H^{-d/2+1-\varepsilon}(\Omega)) \cap \mathcal{C}^1(\bar{I}, H^{-d/2-\varepsilon}(\Omega))$$

of the state equation for any $\varepsilon > 0$ which satisfies

$$\|y\|_Y \leq c\,\|u\|_{L^2(I,\mathcal{M}(\Omega_c))}$$

- $L^2(I, \mathcal{M}(\Omega_c)) \hookrightarrow L^2(I, H^{-\frac{d}{2}-\varepsilon}(\Omega))$ for $d = 1, 2, 3$ $\Rightarrow$ Existence, uniqueness and regularity follows by classical arguments.
- However: $y \in L^2(I \times \Omega)$ and $p \in L^2(I, \mathcal{C}(\Omega_c))$ only for $d = 1$ guaranteed $\Rightarrow$ Well-posedness and optimality conditions
- Sharpness?: Yes for $d = 1$
  - $u = \delta_t \Rightarrow y$ with moving jump discontinuity in space $\Rightarrow$ $y \notin \mathcal{C}(\bar{I}, H^{1/2}(\Omega))$

Improved regularity for $u \in \mathcal{M}(\Omega_c, L^2(I))$

Theorem

Let Ω_c be compact and $u \in \mathcal{M}(\Omega_c, L^2(I))$. Then the solution of the state equation satisfies

$$y \in Y = \mathcal{C}(\bar{I}, [H_0^1(\Omega), L^2(\Omega)]_{\theta_d}) \cap \mathcal{C}^1(\bar{I}, [L^2(\Omega), H^{-1}(\Omega)]_{\theta_d})$$

with $\theta_d = (d-1)/2$ and

$$\|y\|_Y \leq c\|u\|_{\mathcal{M}(\Omega_c, L^2(I))}.$$

- Here: $y \in L^2(I \times \Omega)$ and $p \in \mathcal{C}(\Omega_c, L^2(I))$ for $d = 1, 2, 3$ guaranteed
  $\Rightarrow$ Well-posedness and optimality conditions

Improved regularity for $u \in \mathcal{M}(\Omega_c, L^2(I))$, continued

Theorem

Let Ω_c be compact and $u \in \mathcal{M}(\Omega_c, L^2(I))$, $y_0 \in H_0^1(\Omega)$, $y_1 \in L^2(\Omega)$. Then the solution of the state equation satisfies

$$y \in \mathcal{C}(\bar{I}, [H_0^1(\Omega), L^2(\Omega)]_{\theta_d}) \cap \mathcal{C}^1(\bar{I}, [L^2(\Omega), H^{-1}(\Omega)]_{\theta_d})$$

with $\theta_d = (d-1)/2$.

Idea behind the proof:

- $S_{x_0}\colon L^2(I) \to L^2(I, [H_0^1(\Omega), L^2(\Omega)]_{\theta_d})$, $h \mapsto y$ bounded[1], y solution of (SE) for $u = h\delta_{x_0}$, $x_0 \in \Omega_c$
- Duality: $S_{x_0}^*\colon L^2(I, [L^2(\Omega), H^{-1}(\Omega)]_{\theta_d}) \to L^2(I)$, $\phi \mapsto p(t, x_0)$ bounded, p solution of (AE) for a source term ϕ
- Compactness of Ω_c: $S^*\colon L^2(I, [L^2(\Omega), H^{-1}(\Omega)]_{\theta_d}) \to \mathcal{C}(\Omega_c, L^2(I))$, $\phi \mapsto p$ bounded
- Duality: $S\colon \mathcal{M}(\Omega_c, L^2(I)) \to L^2(I, [H_0^1(\Omega), L^2(\Omega)]_{\theta_d})$, $u \mapsto y$ bounded

[1] R. Triggiani, Regularity with interior point control. Part 1: Wave and Euler-Bernoulli equations

First order optimality conditions

- Optimality condition: u^* is an optimal control iff

$$-p^* = \delta(\alpha \|u^*\|_{\mathcal{M}_T})$$

- Adjoint state: $p^* \in {}^*(\mathcal{M}_T)$ solves

$$\begin{cases} \partial_{tt} p^* - \Delta p^* = y^* - z & \text{in } \Omega \times I \\ p^* = 0 & \text{on } \partial\Omega \times I \\ p^* = 0,\ \partial_t p^* = 0 & \text{on } \{T\} \times \Omega \end{cases} \tag{AE}$$

Structural properties of the optimal control

$\mathcal{M} = L^2(I, \mathcal{M}(\Omega_c))$:

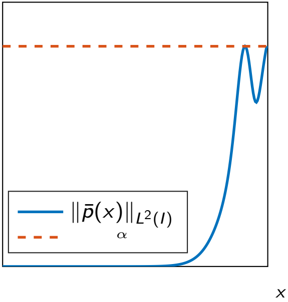
- Time-dependent support of $\bar{u}$:

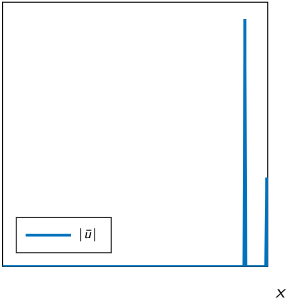
$$\operatorname{supp}(u^*)^{\pm}(t) \subseteq \{x \in \Omega_c \mid p^*(x,t) = \mp \|p^*(t)\|_{\mathcal{C}(\Omega_c)}\} \quad \text{a.e. } t \in I$$

$\mathcal{M} = \mathcal{M}(\Omega_c, L^2(I))$:

- Optimal Radon-Nikodym derivative: $u^{*\prime}(t,x) = -\frac{1}{\alpha} p^*(t,x)$
- Time-independent support of the total variation measure $|u^*|$:

$$\operatorname{supp}|u^*| \subseteq \{x \in \Omega_c \mid \|p^*(x)\|_{L^2(I)} = \alpha\}.$$

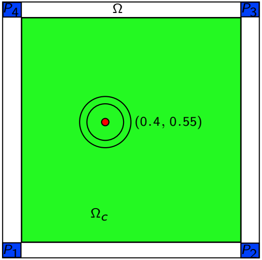




Solution of the inverse source problem

- Point sources static $\Rightarrow \mathcal{M}_T = \mathcal{M}(\Omega_c, L^2(I))$
- Optimization problem:

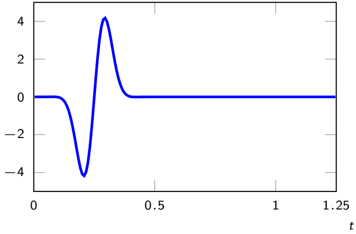
$$\min_{u \in \mathcal{M}(\Omega_c, L^2(I))} \frac{1}{2M} \sum_{j=1,\ldots,M} \|O_j \circ Su - z_j\|^2_{L^2(I)} + \alpha \|u\|_{\mathcal{M}(\Omega_c, L^2(I))} \quad \text{s.t. (SE)}$$



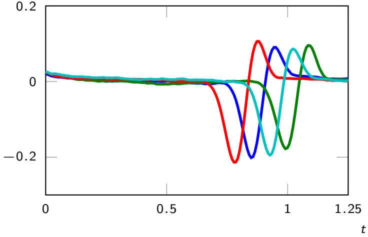
- Avoid reflections on the boundary of $\Omega \Rightarrow$ (approximative) absorbing boundary conditions
- Artificial data: $z_j = O_j S u^\dagger + n_j$ (n_j noise), $u^\dagger$ exact source

Exact state, exact intensity and noisy measurements

(a) Exact state

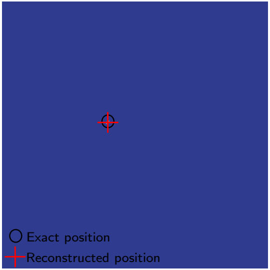


(b) Exact Intensity



(c) Measurements

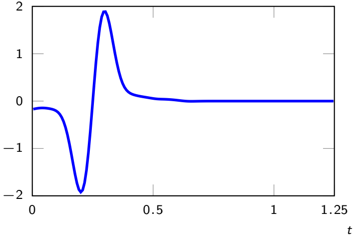
Reconstructions



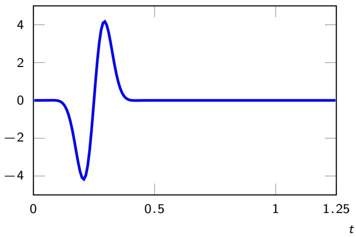
(a) $|\bar{u}|$ on Ω

Exact	$(0.4, 0.55)$
Reconstructed	$(0.39, 0.547)$

(b) Positions



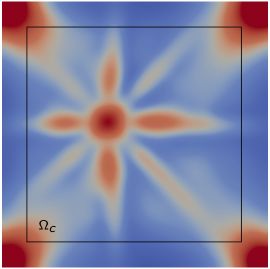
(c) Reconstructed intensity



(d) Exact intensity

Adjoint state and its $L^2(I)$-norm

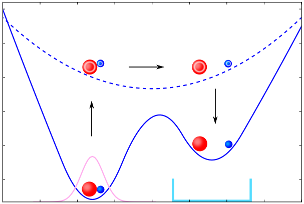
(a) Optimal adjoint state $\bar{p}$



(b) $\|\bar{p}(x)\|_{L^2(I)}$ on Ω

Remark: time reversal
Remark: difference to parabolic case.

Prototype problem: chemical reaction dynamics



- multilevel Born–Oppenheimer approximation

$$\Psi(R,x,t) \approx \sum_{j=1}^{2} \overbrace{\psi_j(R,t)}^{\text{nuclei}} \overbrace{\phi_j^R(x)}^{\text{electrons}}$$

- electric field $v(t)$: $[0,T] \to \mathbb{R}$

System of Schrödinger equations on 2 potential energy surfaces

$$i\partial_t \begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix} = \left[\begin{pmatrix} -\frac{1}{2}\Delta + V_1 & 0 \\ 0 & -\frac{1}{2}\Delta + V_2 \end{pmatrix} + v(t) \begin{pmatrix} \mu_{11} & \mu_{12} \\ \mu_{21} & \mu_{22} \end{pmatrix} \right] \begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix}$$

control mechanisms

- movement on surface
- transitions between surfaces through Bohr frequencies

Optimal quantum control

motivation of optimal control

- constructive, applicable to complex systems

Traditional optimal control formulation (Pierce/Daleh/Rabitz '88)

$$\underset{\psi,v}{\text{Minimize}} \ \frac{1}{2} \overbrace{\langle \psi(T), \mathcal{O}\psi(T)\rangle}^{\text{physically relevant}} + \frac{\alpha}{2} \overbrace{\|v\|^2_{L^2(0,T) \text{ or } H^1_0(0,T)}}^{\text{mathematical tool}}$$

$$i\partial_t \psi = (H_0 + v(t)H_1)\psi, \quad \psi(0) = \psi_0$$

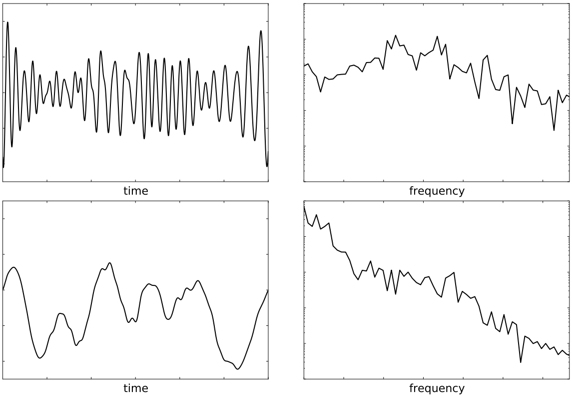
H_0, H_1, $\mathcal{O}$ selfadj. op.; $v\colon [0, T] \to \mathbb{R}$ control field

Why use a different approach?

Problems with traditional optimal quantum control

$L^2(0, T)$

$H^1_0(0, T)$



time frequency

- fail to capture Bohr frequencies
- have nonsparse frequency structure

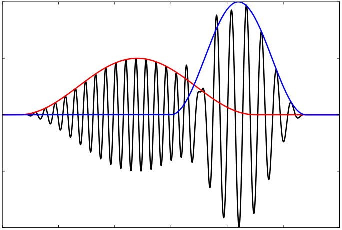
frequency of transition between two quantum states (is eigenvalue difference.)

Ansatz by experimentalists

ansatz for control field,
low dimensional parametrization

$$v(t) = \sum_{k=1}^{K} b_k(t) \cos(\omega_k t)$$

Auger, Ben, Yedder, Cances, LeBris et al '02; Turinici et al. '04; Sharma et al '10; Ruetzel et al '11

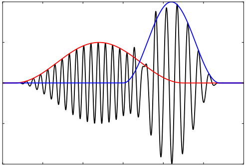


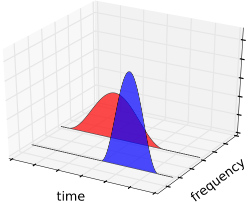
- results in pysically intuitive controls
- but: not flexible, a priori knowledge necessary

our goal

- obtain experimentalists controls using optimal control theory

Our approach





- time-frequency control (quantum physics)

$$v(t) = (Bu)(t) = \operatorname{Re} \int_\Omega u(\omega, t) e^{i\omega t} \, \mathrm{d}\omega$$

- sparsity enhancing costs

$$\|u\|_{\mathcal{M}(\Omega; H_0^1(0,T))} = \int_\Omega \|u(\omega, \cdot)\|_{H_0^1(0,T)} \, \mathrm{d}\omega$$

physically intuitive fields $v \longleftrightarrow$ sparse controls u

$$v(t) = \sum_k b_k(t) \cos(\omega_k t) \longleftrightarrow u(\omega, t) = \sum_k \delta_{\omega_k}(\omega) b_k(t)$$

General framework

Optimal control problem in $\mathcal{M}(\Omega; \mathcal{U})$

$$\begin{aligned} &\underset{\psi,u}{\text{Minimize}} \; \frac{1}{2}\langle \psi(T), \mathcal{O}\psi(T)\rangle_{\mathcal{H}} + \alpha \|u\|_{\mathcal{M}(\Omega;\mathcal{U})} \\ &i\partial_t \psi(t) = [H_0 + (Bu)(t) H_1]\,\psi(t), \quad \psi(0) = \psi_0 \end{aligned} \tag{P}$$

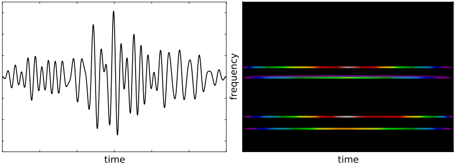
- Ω sparsity domain $\rightsquigarrow$ sparse in frequency
- $\mathcal{U}$ Hilbert space $\rightsquigarrow$ smooth in time
- B control operator $\rightsquigarrow$ assembles field

Examples

$\Omega = [\omega_{\min}, \omega_{\max}] \subset \mathbb{R}^+$, $\quad (Bu)(t) = \mathrm{Re} \int u(\omega, t) e^{i\omega t}\, \mathrm{d}\omega$ (2-scale synth)

1. simplest case:

$$\mathcal{U} = H_0^1(0, T; \mathbb{C})$$

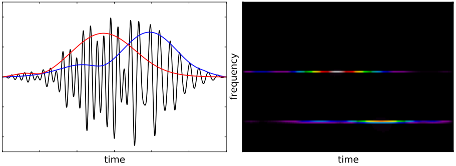


2. deconvolution space:

$$\mathcal{U} = \mathcal{U}_G =$$

$$\{\, b \in L^2(0, T) \mid (G*\cdot)^{-1/2} b \in L^2 \,\}$$

with G Gaussian kernel

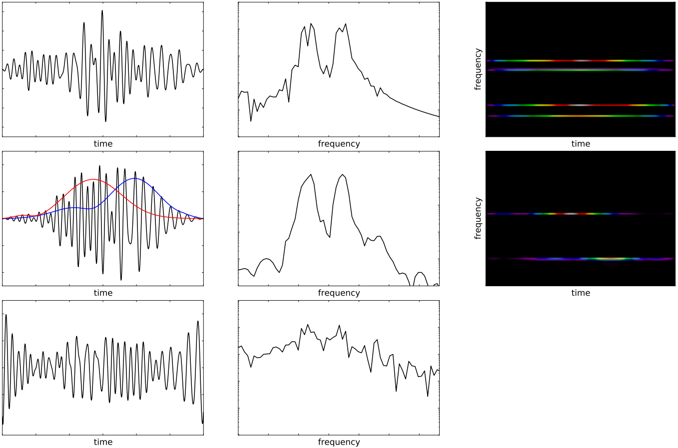


Numerical results

$\mathcal{M}(\Omega; H_0^1)$

$\mathcal{M}(\Omega; \mathcal{U}_G)$

$L^2(0, T)$



time | frequency | time-frequency

Switching control

$$\begin{cases} \displaystyle\min_{u\in L^2(0,T;\mathbb{R}^N)} \frac{1}{2}\|y-z\|^2_{L^2(0,T;L^2(\omega_{\mathrm{obs}}))} + \frac{\alpha}{2}\int_0^T |u(t)|_1^2\,dt, \\ \text{s. t.} \quad \partial_t y + Ay = Bu, \quad y(0)=y_0, \end{cases} \tag{P}$$

where

$$(Bu)(t,x) = \sum_{i=1}^{N} \chi_{\omega_i}(x)u_i(t),$$

WHAT IS IT ? WHY ?

$$g:\mathbb{R}^N \to \mathbb{R}, \qquad g(v) = \frac{\alpha}{2}|v|_1^2 = \frac{\alpha}{2}\Big(\sum_{i=1}^{N}|v_i|\Big)^2.$$

$$g(v) = \frac{\alpha}{2}|v|_2^2 + \alpha \sum_{\substack{i,j=1\\ i<j}}^{N} |v_i v_j|,$$

Switching control

$$\left\{\begin{array}{l} \displaystyle\min_{u\in L^2(0,T;\mathbb{R}^N)} \frac{1}{2}\|y-z\|^2_{L^2(0,T;L^2(\omega_{\mathrm{obs}}))} + \frac{\alpha}{2}\int_0^T |u(t)|_1^2\,dt, \\ \text{s. t.} \quad \partial_t y + Ay = Bu, \quad y(0)=y_0, \end{array}\right. \tag{P}$$

where

$$(Bu)(t,x) = \sum_{i=1}^N \chi_{\omega_i}(x)u_i(t),$$

WHAT IS IT ? WHY ?

$$g:\mathbb{R}^N \to \mathbb{R}, \qquad g(v) = \frac{\alpha}{2}|v|_1^2 = \frac{\alpha}{2}\Big(\sum_{i=1}^N |v_i|\Big)^2.$$

$$g(v) = \frac{\alpha}{2}|v|_2^2 + \alpha \sum_{\substack{i,j=1\\ i<j}}^N |v_i v_j|,$$

Switching control: competitive Lotka-Volterra equation

$$\min \int_0^{100} -(\sigma_1 c_1 N_1 u_1 + \sigma_2 c_2 N_2 u_2)\, dt + \frac{\alpha}{2}\|u\|^2_{L^2(0,T)} + \alpha\|u_1 u_2\|_{L^1(0,T)}$$

s.t. the competitive Lotka–Volterra equation with two species on $t \in I = (0, 100)$

$$\dot{N}_1 = c_1 N_1 \left(1 - \frac{N_1 + d_1 N_2}{k_1} - u_1\right),$$
$$\dot{N}_2 = c_2 N_2 \left(1 - \frac{N_2 + d_2 N_1}{k_2} - u_2\right),$$

N_1/N_2:	number of prey/predators	$N_1(0) = 2000$, $N_2(0) = 10$
$c_i > 0$	birth rates	$c_1 = c_2 = 0.1$
d_i	interaction rates	$d_1 = 2$, $d_2 = -0.1$
k_i	carrying capacities of the habitat	$k_1 = 1000$, $k_2 = 100$
u_i	harvesting rates	
σ_i	prices	$\sigma_1 = 10$, $\sigma_2 = 100$

Switching control: competitive Lotka-Volterra equation

$$\min \int_0^{100} -(\sigma_1 c_1 N_1 u_1 + \sigma_2 c_2 N_2 u_2)\, dt + \frac{\alpha}{2}\|u\|^2_{L^2(0,T)} + \alpha \|u_1 u_2\|_{L^1(0,T)}$$

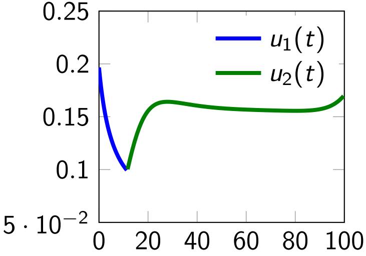
s.t. the competitive Lotka–Volterra equation with two species on $t \in I = (0, 100)$

$$\dot{N}_1 = c_1 N_1 \left(1 - \frac{N_1 + d_1 N_2}{k_1} - u_1\right),$$
$$\dot{N}_2 = c_2 N_2 \left(1 - \frac{N_2 + d_2 N_1}{k_2} - u_2\right),$$

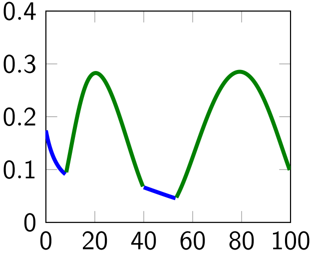
N_1/N_2:	number of prey/predators	$N_1(0) = 2000$, $N_2(0) = 10$
$c_i > 0$	birth rates	$c_1 = c_2 = 0.1$
d_i	interaction rates	$d_1 = 2$, $d_2 = -0.1$
k_i	carrying capacities of the habitat	$k_1 = 1000$, $k_2 = 100$
u_i	harvesting rates	
σ_i	prices	$\sigma_1 = 10$, $\sigma_2 = 100$

Switching control: competitive Lotka-Volterra equation

- 300 dof per control function,
- globalization by trust-region (TR-SN)



(c) $\sigma_2 = 100$



(d) $\sigma_2 = 100(1 + sin(t/10))$

Figure: Optimal controls for different prices σ_2.

Structure of optimality condition

$$g : \mathbb{R}^N \to \mathbb{R}, \qquad g(v) = \frac{\alpha}{2}|v|_1^2 = \frac{\alpha}{2}\Big(\sum_{i=1}^{N} |v_i|\Big)^2.$$

Proposition

The minimizer $u^* \in L^2(0,T;\mathbb{R}^N)$ and the adjoint $p \in L^2(0,T;\mathbb{R}^N)$

$$\begin{cases} -\partial_t p + Ap &= y^* - z \quad \text{in } (0,T)\times\Omega, \\ p &= 0 \quad \text{on } (0,T)\times\partial\Omega, \\ p(x,T) &= 0 \quad \text{in } \Omega. \end{cases}$$

satisfy for almost every $t \in (0,T)$ and $1 \le j \le N$

$$u_j^*(t) \in \begin{cases} \left\{ \frac{1}{\alpha} p_j(t) \right\} & \text{if } |p_j(t)| = \max_i |p_i(t)| \text{ and } |p_j(t)| > |p_i(t)|,\ i \neq j, \\ \{0\} & \text{if } |p_j(t)| < \max_i |p_i(t)|, \\ \left\{ \frac{s_j}{\alpha} p_j(t) : s_j \ge 0, \sum_{i=1}^N s_i = 1 \right\} & \text{if } |p_j(t)| = \max_i |p_i(t)| \text{ and } |p_j(t)| = |p_i(t)|,\ i \neq j. \end{cases}$$

Perfect switching

$$\mathcal{S} := \{t \in (0,T) : |p_{j_1}(t)| = |p_{j_2}(t)| = \max_i |p_i(t)| \text{ for } j_1 \neq j_2\},$$

meas $(\mathcal{S}) = 0$ implies perfect switching

Remark (some difficulties:)

- *characterize* $\partial g(v) = \partial(\frac{\alpha}{2}|v|_2^2 + \alpha \sum_{\substack{i,j=1 \\ i<j}}^N |v_i v_j|)$ *and/or its conjugate*
- *regularize*

Remark

$$g(v) = g_\infty^{**}$$

where

$$g_\infty(v) := \frac{\alpha}{2}|v|_2^2 + \delta_{\{v: v_1 v_2 = 0\}}(v) := \begin{cases} \frac{\alpha}{2}|v|_2^2 & \text{if } v_1 v_2 = 0, \\ \infty & \text{else,} \end{cases}$$

Perfect switching

$$\mathcal{S} := \{t \in (0,T) : |p_{j_1}(t)| = |p_{j_2}(t)| = \max_i |p_i(t)| \text{ for } j_1 \neq j_2\},$$

meas $(\mathcal{S}) = 0$ implies perfect switching

Remark (some difficulties:)

- *characterize* $\partial g(v) = \partial(\frac{\alpha}{2}|v|_2^2 + \alpha \sum_{\substack{i,j=1 \\ i<j}}^N |v_i v_j|)$ *and/or its conjugate*
- *regularize*

Remark

$$g(v) = g_\infty^{**}$$

where

$$g_\infty(v) := \frac{\alpha}{2}|v|_2^2 + \delta_{\{v : v_1 v_2 = 0\}}(v) := \begin{cases} \frac{\alpha}{2}|v|_2^2 & \text{if } v_1 v_2 = 0, \\ \infty & \text{else,} \end{cases}$$

Switching control: heat equation in 2D

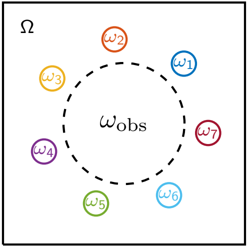


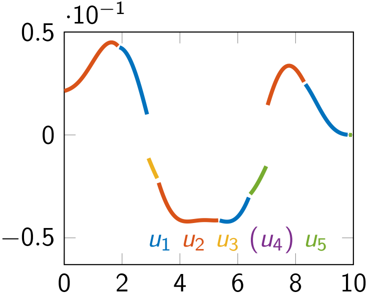
Figure: Problem setting for $N = 7$ control components

$$z_{des} = \sum_{i=1}^{N} \cos(i + t) \sin^2\left(2\pi \frac{t}{T}\right) |x - x_i|^2.$$

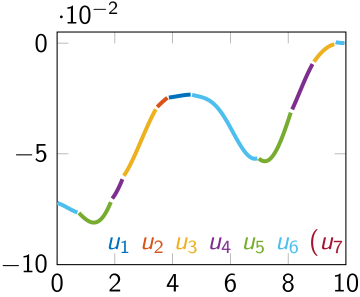
Discretization:

- linear FE in space, cG(1) Petrov-Galerkin method in time
- 200 degrees of freedom per control component

Optimal controls for $\alpha = 10^{-1}$



(a) $N = 5$



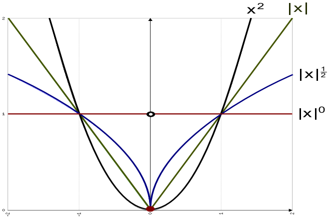
(b) $N = 7$

Alternatives for mixed continuous-discrete decision processes

L^p and ℓ^p functionals, with $p \in [0, 1)$

NOT CONVEX

$$|x|^0 = \begin{cases} 0 \text{ if } x = 0 \\ 1 \text{ if } x \neq 0 \end{cases}$$



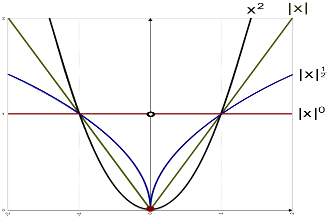
No topological tools to argue existence, compare ℓ^p

Alternatives for mixed continuous-discrete decision processes

L^p and ℓ^p functionals, with $p \in [0, 1)$

NOT CONVEX

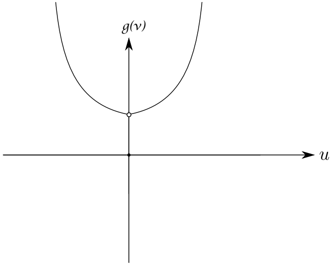
$$|x|^0 = \begin{cases} 0 \text{ if } x = 0 \\ 1 \text{ if } x \neq 0 \end{cases}$$

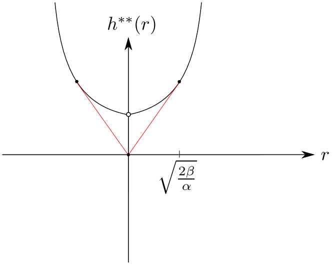


No topological tools to argue existence, compare ℓ^p

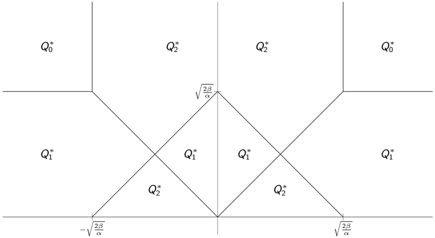
Convex relaxation

$$g(v) = \frac{\alpha}{2}|v|^2 + \beta|v|^0$$





$$g^{**}(v) = \begin{cases} \frac{\alpha}{2} v_1^2 + \sqrt{2\alpha\beta}|v_2| & \text{if } v \in Q_1^*, \\ \frac{\alpha}{2} v_2^2 + \sqrt{2\alpha\beta}|v_1| & \text{if } v \in Q_2^*, \\ \frac{\alpha}{2}(v_1^2 + v_2^2) + \beta & \text{if } v \in Q_0^*, \end{cases}$$



Multi-bang control

$$\begin{cases} \min\limits_{u,y} \ \dfrac{1}{2}\|y-z\|_{L^2}^2 + \dfrac{\alpha}{2}\|u\|_{L^2}^2 + \beta \displaystyle\int_\Omega \prod_{i=1}^{d} |u(x)-u_i|^0 \, dx \\ \text{s. t. } \ Ay = u, \qquad u_1 \le u(x) \le u_d, \ \text{ for a.e. } x \in \Omega. \end{cases}$$

Convexify

$$\begin{cases} \min\limits_{u,y} \ \dfrac{1}{2}\|y-z\|_{L^2}^2 + \mathcal{G}^{**}(u) \\ \text{s. t. } \ Ay = u, \qquad u_1 \le u(x) \le u_d, \ \text{ for a.e. } x \in \Omega. \end{cases}$$

Multi-bang control

Proposition (Generalized bang-bang)

The multi-bang problem admits a solution u^*. If $\frac{2\beta}{\alpha} \geq \frac{1}{2}(u_{i+1} - u_i)$ for all $i = 1, \ldots d$, then

$$\Omega = \bigcup_{i=1}^{d} \{x \in \Omega : u^*(x) = u_i\} \cup \{x \in \Omega : y^*(x) = z(x)\}.$$

$u^*(x) = u_i$ if $\frac{\alpha}{2}(u_{i-1} + u_i) < p^*(x) < \frac{\alpha}{2}(u_i + u_{i+1})$

Proposition (Estimate the duality gap)

$$J(u^*) \leq J(u) + \beta \; meas\; (\mathcal{C}(p^*))$$

Multi-bang control

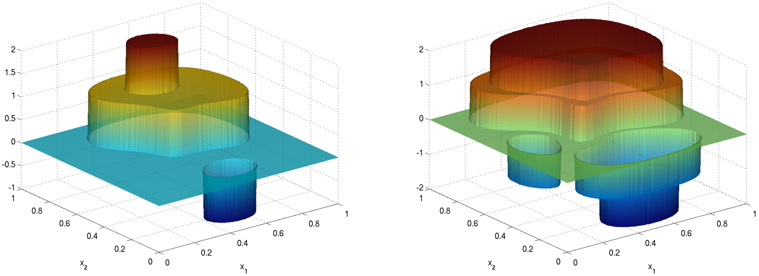


Figure: Effect of α, β on the structure of the control u, left: $\alpha = 5.10^{-3}, \beta = 10^{-3}$, right: $\alpha = 10^{-3}$, $\beta = 10^{-3}$.

Conclusions and perspectives

- Convex analysis techniques are a powerful tool for nonstandard cost functionals
- Necessary optimality conditions can be solved efficiently
- Improved analysis on duality gaps
- Applications
- (Choice of α)

Some contributers

- Hante - Sager (relaxation technique with rounding strategy)
- Herzog
- Leugering
- Seidman
- Stadler
- D. Wachsmuth
- G. Wachsmuth
- Zuazua (controlability)

Thank You