Convex relaxation of (some) hybrid discrete-continuous control problems

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Motivation: discrete optimization

$$\min_{u \in U} \mathcal{F}(u) + \frac{\alpha}{2}\|u\|^2$$

- $\mathcal{F}$ tracking, discrepancy term (involving PDEs)
- U discrete set,

$$U = \left\{u \in L^p(\Omega) : u(x) \in \{u_1, \dots, u_d\} \text{ a.e.}\right\}$$

- $u_1, \dots, u_d$ given voltages, velocities, materials, … (assumed here: ranking by magnitude possible!)
- motivation: topology optimization, medical imaging

Motivation: penalty

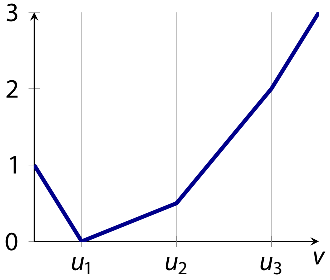
- convex relaxation: replace U by convex hull
- works only for $d = 2$, cf. bang-bang control ($\alpha = 0$)
- $\rightsquigarrow$ promote $u(x) \in \{u_1, \dots, u_d\}$ by convex pointwise penalty

$$\mathcal{G}(u) = \int_\Omega g(u(x))\,dx$$

- generalize L^1 norm: polyhedral epigraph with vertices $u_1, \dots, u_d$
- not exact relaxation/penalization (in general)!

Motivation: penalty

- generalize L^1 norm: polyhedral epigraph with vertices $u_1, \ldots, u_d$



- motivation: convex envelope of $\frac{1}{2}\|u\|^2 + \delta_U$
- multi-bang (generalized bang-bang) control
- $\rightsquigarrow$ non-smooth optimization in function spaces

Convex analysis: motivation

$f : \mathbb{R} \to \mathbb{R}$ differentiable:

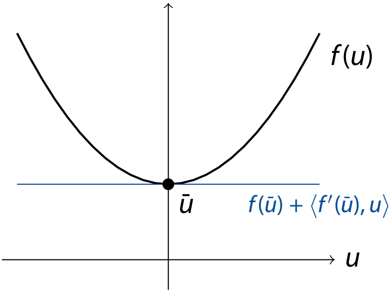
- derivative:

$$f'(u) = \lim_{h \to 0} \frac{f(u+h) - f(u)}{h}$$

- geometrically:
  $f'(u)$ tangent slope

- $f(\bar{u}) = \min_u f(u) \Rightarrow f'(\bar{u}) = 0$

- calculus for f'



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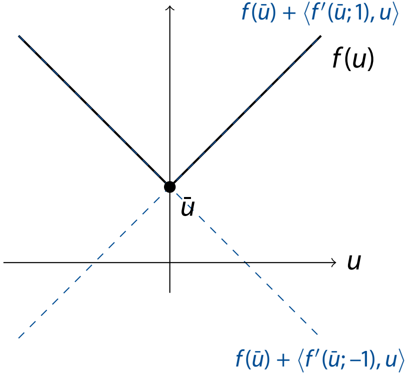
$f : \mathbb{R} \to \mathbb{R}$ not differentiable, convex:

- directional derivative:

$$f'(u;h) = \lim_{t \to 0^+} \frac{f(u+th) - f(u)}{t}$$

- but: for all h,

$$f'(\bar{u};h) \neq 0$$



Convex relaxation: motivation

$f : \mathbb{R} \to \mathbb{R}$ not differentiable, convex:

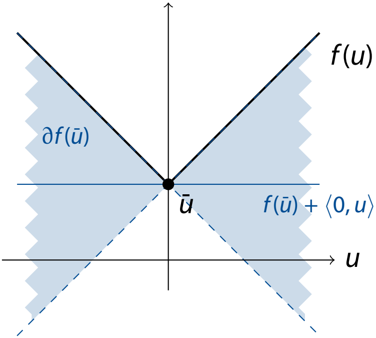
- subdifferential:

  $$\partial f(u) = \left\{ u^* : \langle u^*, h \rangle \leqslant f'(u;h) \right\}$$

- geometrically: $\partial f(u)$ set of tangent slopes

- $f(\bar{u}) = \min_u f(u) \Rightarrow 0 \in \partial f(\bar{u})$

- calculus for ∂f



$f : V \to \overline{\mathbb{R}} := \mathbb{R} \cup \{+\infty\}$ convex, V Banach space, V^* dual space

- subdifferential

$$\partial f(\bar v) = \left\{ v^* \in V^* : \langle v^*, v - \bar v\rangle_{V^*,V} \leqslant f(v) - f(\bar v) \quad \text{for all } v \in V \right\}$$

- Fenchel conjugate (always convex)

$$f^* : V^* \to \overline{\mathbb{R}}, \qquad f^*(v^*) = \sup_{v \in V} \langle v^*, v\rangle_{V^*,V} - f(v)$$

- "convex inverse function theorem":

$$v^* \in \partial f(v) \quad \Leftrightarrow \quad v \in \partial f^*(v^*)$$

Fenchel duality: application

$$\mathcal{F}(\bar{u}) + \mathcal{G}(\bar{u}) = \min_u \mathcal{F}(u) + \mathcal{G}(u)$$

1. Fermat principle: $0 \in \partial\left(\mathcal{F}(\bar{u}) + \mathcal{G}(\bar{u})\right)$

2. sum rule: $0 \in \partial\mathcal{F}(\bar{u}) + \partial\mathcal{G}(\bar{u})$, i.e., there is $\bar{p} \in V^*$ with

$$\begin{cases} -\bar{p} \in \partial\mathcal{F}(\bar{u}) \\ \bar{p} \in \partial\mathcal{G}(\bar{u}) \end{cases}$$

3. Fenchel duality:

$$\begin{cases} -\bar{p} \in \partial\mathcal{F}(\bar{u}) \\ \bar{u} \in \partial\mathcal{G}^*(\bar{p}) \end{cases}$$

Regularization

$\mathcal{G}$ non-smooth $\rightsquigarrow$ subdifferential $\partial\mathcal{G}^*$ set-valued $\rightsquigarrow$ regularize

$u, p \in L^2(\Omega)$ Hilbert space $\rightsquigarrow$ consider for $\gamma > 0$

Proximal mapping

$$\operatorname{prox}_{\gamma\mathcal{G}^*}(p) = \arg\min_{w} \mathcal{G}^*(w) + \frac{1}{2\gamma}\|w - p\|^2$$

- single-valued, Lipschitz continuous
- coincides with resolvent $(\mathrm{Id} + \gamma\partial\mathcal{G}^*)^{-1}(p)$
- (also required for primal-dual first-order methods)

Regularization

Proximal mapping

$$\operatorname{prox}_{\gamma \mathcal{G}^*}(p) = \arg\min_w \mathcal{G}^*(w) + \frac{1}{2\gamma}\|w - p\|^2$$

Complementarity formulation of $u \in \partial\mathcal{G}^*(p)$

$$u = \frac{1}{\gamma}\left((p + \gamma u) - \operatorname{prox}_{\gamma \mathcal{G}^*}(p + \gamma u)\right)$$

- equivalent for every $\gamma > 0$
- single-valued, Lipschitz continuous, implicit

Regularization

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Proximal mapping

$$\operatorname{prox}_{\gamma\mathcal{G}^*}(p) = \arg\min_w \mathcal{G}^*(w) + \frac{1}{2\gamma}\|w - p\|^2$$

Moreau–Yosida regularization of $u \in \partial\mathcal{G}^*(p)$

$$u = \frac{1}{\gamma}\left(p - \operatorname{prox}_{\gamma\mathcal{G}^*}(p)\right) =: \partial\mathcal{G}^*_\gamma(p)$$

- $\partial\mathcal{G}^*_\gamma = \partial\left(\mathcal{G} + \frac{\gamma}{2}\|\cdot\|^2\right)^* \to \partial\mathcal{G}^*$ as $\gamma \to 0$
- single-valued, Lipschitz continuous, explicit
  $\rightsquigarrow$ nonsmooth operator equation, Newton method

Generalized Newton method

Consider Banach spaces X, Y, mapping $F : X \to Y$

Newton-type method for $F(x) = 0$

- choose $x^0 \in X$ (close to solution x^*)
- for $k = 0, 1, \ldots$
  1. choose $M_k \in \mathcal{L}(X, Y)$ invertible
  2. solve for s^k:

$$M_k s^k = -F(x^k)$$

  3. set $x^{k+1} = x^k + s^k$

Convergence of Newton method

Set $d^k = x^k - x^* \rightsquigarrow$

$$\frac{\|x^{k+1} - x^*\|_X}{\|x^k - x^*\|_X} = \frac{\|M_k^{-1}(F(x^* + d^k) - F(x^*) - M_k d^k)\|_X}{\|d^k\|_X}$$

$\rightsquigarrow$ superlinear convergence if

1. regularity condition

$$\|M_k^{-1}\|_{\mathcal{L}(Y,X)} \leqslant C \qquad \text{for all } k$$

2. approximation condition

$$\lim_{\|d^k\|_X \to 0} \frac{\|F(x^* + d^k) - F(x^*) - M_k d^k\|_Y}{\|d^k\|_X} = 0$$

Semismooth Newton method

Goal: define Newton derivative $M_k =: D_N F(x^k)$ such that

$$x^{k+1} = x^k - D_N F(x^k)^{-1} F(x^k)$$

converges superlinearly for $F(x) = 0$ nonsmooth

- $\mathbb{R}^n$: F Lipschitz $\rightsquigarrow$ $D_N F$ from Clarke subdifferential (Rademacher)
  [Mifflin 1977, Kummer 1992, Qi/Sun 1993]
- function space: Clarke subdifferential not explicit
  $\rightsquigarrow$ define $D_N F$ via approximation condition
  [Chen/Nashed/Qi 2000, Hintermüller/Ito/Kunisch 2002]
- $f : \mathbb{R}^N \to \mathbb{R}$ semismooth $\rightsquigarrow$ superposition operator
  $F : L^p(\Omega) \to L^q(\Omega)$ semismooth for $p > q$
  [Ulbrich 2002/03/11, Schiela 2008]

Numerical solution: summary

For (non)convex $\mathcal{G} : L^2(\Omega) \to \mathbb{R}$, $\quad \mathcal{G}(u) = \int_\Omega g(u(x))\,dx$,

Approach: pointwise

1. compute subdifferential ∂g (or Fenchel conjugate g^*)
2. compute subdifferential ∂g^*
3. compute proximal mapping $\text{prox}_{\gamma g^*}$
4. compute Moreau–Yosida regularization ∂g^*_γ
5. compute Newton derivative $D_N \partial g^*_\gamma$

$\rightsquigarrow$ semismooth Newton method, continuation in γ for

superposition operator $\quad [\partial \mathcal{G}^*_\gamma(p)](x) = \partial g^*_\gamma(p(x))$

Formulation

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$$\begin{cases} \displaystyle\min_{u\in L^2(\Omega)} \frac{1}{2}\|y-z\|_{L^2}^2 + \alpha\, \mathcal{G}(u) \\ \text{s. t. } Ay = u, \quad u_1 \leqslant u(x) \leqslant u_d \text{ a.e.} \end{cases}$$

- $u_1 < \cdots < u_d$ given parameter values $(d > 2)$
- $z \in L^2(\Omega)$ target (or noisy data)
- $A : V \to V^*$ isomorphism for Hilbert space $V \hookrightarrow L^2(\Omega) \hookrightarrow V^*$
  (e.g., elliptic differential operator with boundary conditions)
- $\rightsquigarrow \mathcal{F}(u) = \frac{1}{2}\|A^{-1}u - z\|_{L^2}^2$ smooth
- $\mathcal{G}$ multi-bang penalty (will include control constraints from now)

Multi-bang penalty

$$g : \mathbb{R} \to \overline{\mathbb{R}}, \qquad v \mapsto \begin{cases} \frac{1}{2}\left((u_i + u_{i+1})v - u_i u_{i+1}\right) & v \in [u_i, u_{i+1}] \\ \infty & \text{else} \end{cases}$$

piecewise differentiable $\rightsquigarrow$ subdifferential convex hull of derivatives

$$\partial g(v) = \begin{cases} \left(-\infty, \frac{1}{2}(u_1 + u_2)\right] & v = u_1 \\ \left\{\frac{1}{2}(u_i + u_{i+1})\right\} & v \in (u_i, u_{i+1}) \quad 1 \leqslant i < d \\ \left[\frac{1}{2}(u_{i-1} + u_i), \frac{1}{2}(u_i + u_{i+1})\right] & v = u_i \qquad 1 < i < d \\ \left[\frac{1}{2}(u_{d-1} + u_d), \infty\right) & v = u_d \end{cases}$$

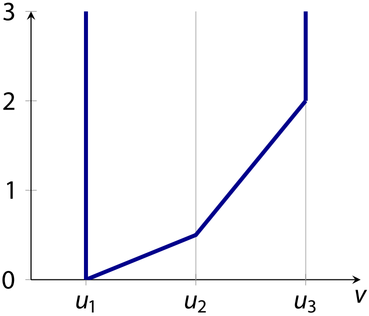
Multi-bang penalty

$$\partial g(v) = \begin{cases} \left(-\infty, \frac{1}{2}(u_1 + u_2)\right] & v = u_1 \\ \left\{\frac{1}{2}(u_i + u_{i+1})\right\} & v \in (u_i, u_{i+1}) \quad 1 \leqslant i < d \\ \left[\frac{1}{2}(u_{i-1} + u_i), \frac{1}{2}(u_i + u_{i+1})\right] & v = u_i \quad 1 < i < d \\ \left[\frac{1}{2}(u_{d-1} + u_d), \infty\right) & v = u_d \end{cases}$$

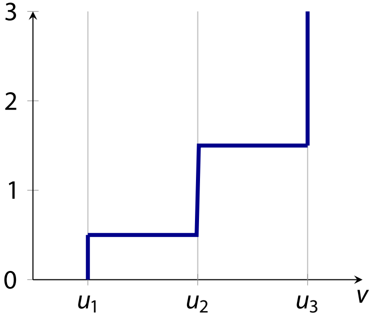
convex inverse function theorem:

$$\partial g^*(q) \in \begin{cases} \{u_1\} & q \in \left(-\infty, \frac{1}{2}(u_1 + u_2)\right) \\ [u_i, u_{i+1}] & q = \frac{1}{2}(u_i + u_{i+1}), \quad 1 \leqslant i < d \\ \{u_i\} & q \in \left(\frac{1}{2}(u_{i-1} + u_i), \frac{1}{2}(u_i + u_{i+1})\right) \quad 1 < i < d, \\ \{u_d\} & q \in \left(\frac{1}{2}(u_{d-1} + u_d), \infty\right) \end{cases}$$

Multi-bang penalty: sketch

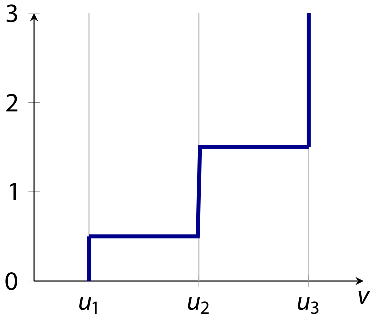


(a) g ($u_1 = 0, u_2 = 1, u_3 = 2$)

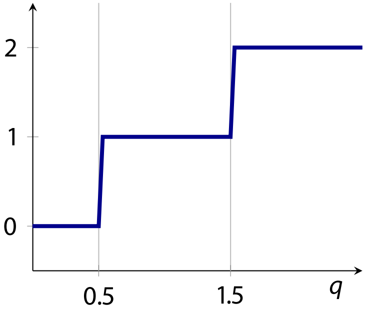


(b) ∂g ($u_1 = 0, u_2 = 1, u_3 = 2$)

Multi-bang penalty: sketch



(c) ∂g ($u_1 = 0, u_2 = 1, u_3 = 2$)



(d) ∂g^* ($u_1 = 0, u_2 = 1, u_3 = 2$)

Optimality system

$$\bar{p} = \frac{1}{\alpha} S^*(z - S\bar{u})$$

$$\bar{u} \in \partial\mathcal{G}^*(\bar{p}) = \begin{cases} \{u_i\} & \bar{p}(x) \in Q_i \\ [u_i, u_{i+1}] & \bar{p}(x) \in \overline{Q}_i \cap \overline{Q}_{i+1} \end{cases}$$

- $S : u \mapsto y$ control-to-state mapping, S^* adjoint
- $\rightsquigarrow$ unique solution $(\bar{u}, \bar{p}) \in L^2(\Omega) \times L^2(\Omega)$
- singular arc $\mathcal{S} = \left\{x : \bar{u}(x) \notin \{u_i\}\right\} \subset \{x : \bar{p}(x) = \frac{1}{2}(u_i + u_{i+1})\}$
- for suitable A, $\bar{p}(x)$ constant implies $[A^*\bar{p}](x) = [z - \bar{y}](x) = 0$

$\rightsquigarrow$ $|\{x : \bar{y}(x) = z(x)\}| = 0 \;\Rightarrow\; \bar{u} \in \{u_1, \dots u_d\}$ a. e., true multi-bang

Moreau–Yosida regularization

Proximal mapping $\quad \mathrm{prox}_{\gamma g^*}(q) = w \;\text{ iff }\; q \in \{w\} + \gamma \partial g^*(w)$

case-wise inspection of subdifferential:

$$\partial g_\gamma^*(q) = \frac{1}{\gamma}\left(q - \mathrm{prox}_{\gamma g^*}(q)\right) = \begin{cases} u_i & q \in Q_i^\gamma \\ \frac{1}{\gamma}\left(q - \frac{1}{2}(u_i + u_{i+1})\right) & q \in Q_{i,i+1}^\gamma \end{cases}$$

$$Q_i^\gamma = \left(\tfrac{1}{2}(u_{i-1} + u_i) + \gamma u_i, \tfrac{1}{2}(u_i + u_{i+1}) + \gamma u_i\right)$$
$$Q_{i,i+1}^\gamma = \left[\tfrac{1}{2}(u_i + u_{i+1}) + \gamma u_i, \tfrac{1}{2}(u_i + u_{i+1}) + \gamma u_{i+1}\right]$$

Regularized optimality system

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$$\begin{cases} p_\gamma = \frac{1}{\alpha} S^*(z - Su_\gamma) \\ u_\gamma = \partial \mathcal{G}_\gamma^*(p_\gamma) \end{cases}$$

- optimality conditions for $\mathcal{F}(u) + \alpha\, \mathcal{G}(u) + \frac{\gamma}{2}\|u\|^2$
- $\rightsquigarrow$ unique solution (u_γ, p_γ)
- $(u_\gamma, p_\gamma) \rightharpoonup (\bar{u}, \bar{p})$ as $\gamma \to 0$
- ∂g_γ^* Lipschitz continuous, piecewise C^1, norm gap $V \hookrightarrow L^2(\Omega)$
- $\rightsquigarrow$ semismooth Newton method

Regularized optimality system

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$$\begin{cases} A^* p_\gamma = \frac{1}{\alpha}(z - y_\gamma) \\ A y_\gamma = \mathcal{G}_\gamma^*(p_\gamma) \end{cases}$$

- optimality conditions for $\mathcal{F}(u) + \alpha\,\mathcal{G}(u) + \frac{\gamma}{2}\|u\|^2$
- $\rightsquigarrow$ unique solution (u_γ, p_γ)
- $(u_\gamma, p_\gamma) \rightharpoonup (\bar u, \bar p)$ as $\gamma \to 0$
- ∂g_γ^* Lipschitz continuous, piecewise C^1, norm gap $V \hookrightarrow L^2(\Omega)$
- $\rightsquigarrow$ semismooth Newton method
- introduce $y_\gamma = S u_\gamma$, eliminate $u_\gamma = \mathcal{G}_\gamma^*(p_\gamma)$

Semismooth Newton method

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$$\begin{pmatrix} \frac{1}{\alpha}\,\mathrm{Id} & A^* \\ A & -D_N\mathcal{G}_\gamma^*(p) \end{pmatrix} \begin{pmatrix} \delta y \\ \delta p \end{pmatrix} = -\begin{pmatrix} A^*p + \frac{1}{\alpha}(y-z) \\ Ay - \mathcal{G}_\gamma^*(p) \end{pmatrix}$$

$$[D_N\mathcal{G}_\gamma^*(p)\delta p](x) = \begin{cases} \frac{1}{\gamma}\delta p(x) & p(x) \in Q_{i,i+1}^\gamma \\ 0 & \text{else} \end{cases}$$

- symmetric, but: local convergence
- $\rightsquigarrow$ continuation in $\gamma \to 0$
- $\rightsquigarrow$ backtracking line search based on residual norm
- only number of sets Q_i^γ depends on d $\rightsquigarrow$ linear complexity

Numerical example

- $\Omega = [0,1]^2, \quad A = -\Delta$

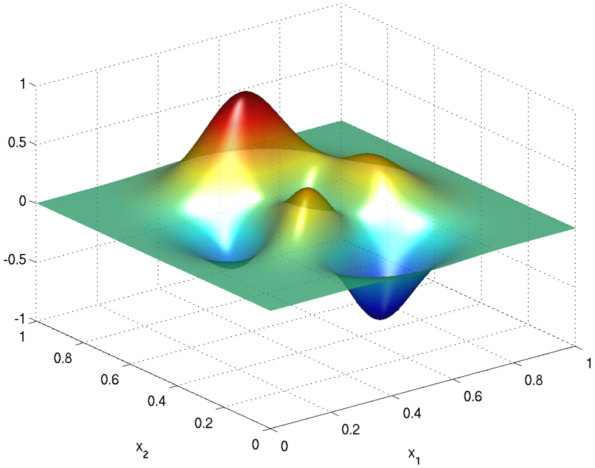
- finite element discretization: uniform grid, 256×256 nodes
- state, adjoint: piecewise linear
- parameter: eliminated (variational discretization)

- $d = 5, \quad (u_1, \ldots, u_5) = (-2, 1, 0, 1, 2)$

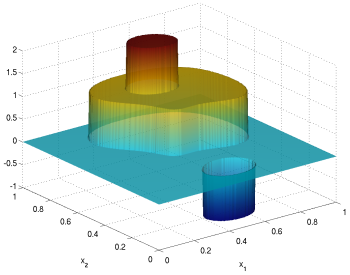
- $\gamma = 0$: regularized active sets empty, true multi-bang

  $\gamma > 0$: terminated with 2–21 nodes in regularized active sets

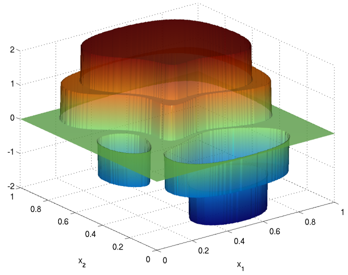
Numerical examples: desired state



Multi-bang controls



(a) $\alpha = 5 \cdot 10^{-3}$ $(\gamma = 0)$



(b) $\alpha = 10^{-3}$ $(\gamma \approx 10^{-7})$

Parameters: effect of d

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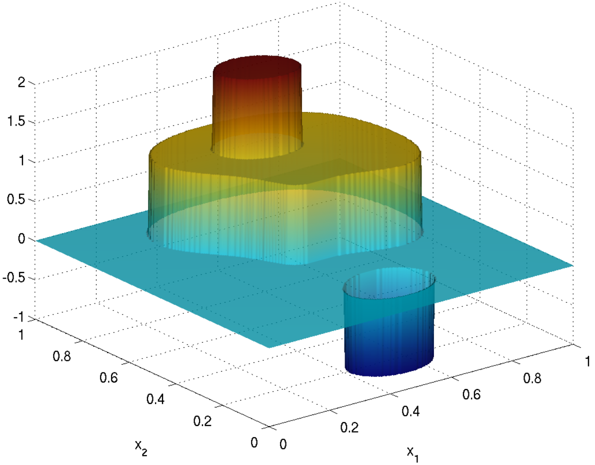
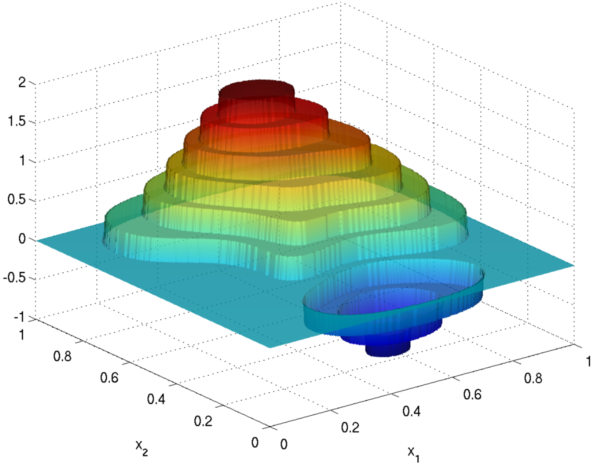


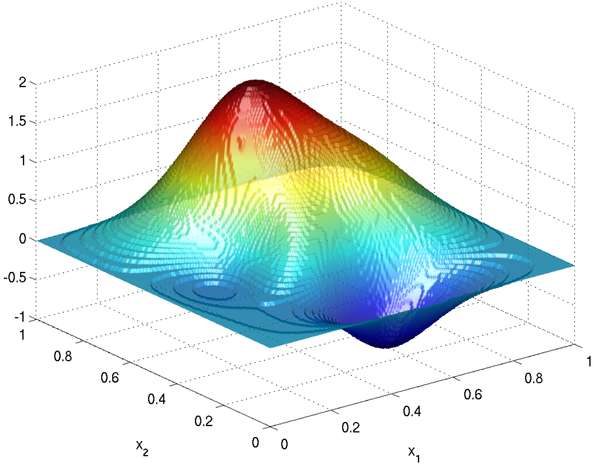
(a) $d = 5$ ($\gamma = 0$)

Parameters: effect of d



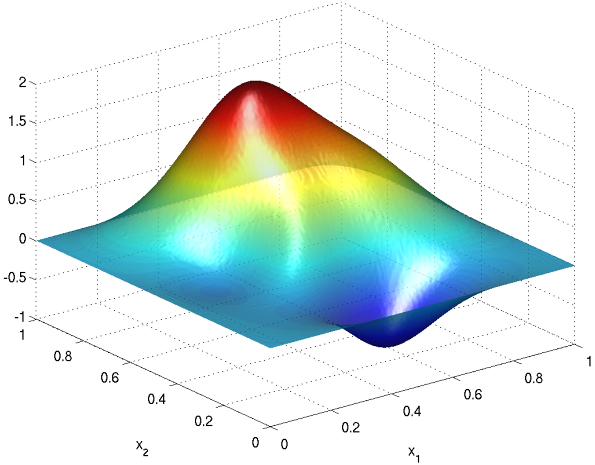
(b) $d = 15$ ($\gamma = 0$)

Parameters: effect of d



(c) $d = 101$ ($\gamma \approx 10^{-9}$)

Parameters: effect of d



(d) $d = 1001$ ($\gamma \approx 10^{-11}$)

Nonlinear control-to-state mapping

Control-to-state mapping $S : u \mapsto y$ nonlinear:

- approach applicable if S
  1. weak-to-weak continuous
  2. twice Fréchet-differentiable
- example: $u \mapsto y$ solving $-\Delta y + uy = f$
- existence, optimality conditions

$$\begin{cases} -\bar{p} = S'(\bar{u})^* (S(\bar{u}) - z) \\ \bar{u} \in \partial \mathcal{G}^*(\bar{p}) \end{cases}$$

- semismooth Newton method (regularity condition technical)

Nonlinear control-to-state mapping

Goal: application to topology optimization / EIT

- $S : u \mapsto y$ solving
$$-\nabla \cdot (u \nabla y) = f$$
- difficulty: $\bar{u} \in L^\infty(\Omega) \quad \rightsquigarrow \quad S$ not weakly-$*$ closed
  1. lack of existence of minimizer ($\bar{y} \neq S(\bar{u})$, cf. homogenization)
  2. lack of convergence $\gamma \to 0$
  3. lack of Newton differentiability of H_γ (no norm gap)
- remedies: higher regularity of y or u by
  1. local smoothing: consider $\quad -\nabla \cdot \left(\int_{B_\varepsilon(x)} u(s)\, ds \nabla y \right)$
  2. TV regularization: add $\|Du\|_{\mathcal{M}} \quad \rightsquigarrow u \in BV(\Omega) \cap L^\infty(\Omega) \hookrightarrow_c L^p(\Omega)$

Difficulty:

- existence requires box constraints $\rightsquigarrow$ use penalty

$$G(u) + TV(u) + \delta_{[u_1,u_d]}(u)$$

- but: $TV(u) + \delta_{[u_1,u_d]}(u)$ not continuous on $L^p(\Omega)$, $p < \infty$
- but: multipliers $\xi \in \partial TV(u)$, $q \in \partial G(u)$ not pointwise on BV, L^∞

- $\rightsquigarrow$ replace box constraints by ($C^{1,1}$) projection of $u \in L^1(\Omega)$

$$[\Phi(u)](x) = \mathrm{proj}^{\varepsilon}_{[u_1,u_d]}(u(x)) \qquad \text{a.e. } x \in \Omega$$

TV regularization: existence

$$\begin{cases} \min_{u \in BV(\Omega)} \frac{1}{2}\|y - z\|^2_{L^2(\Omega)} + \alpha\, G(u) + \beta\, TV(u) \\ \text{s.t.} \quad -\nabla \cdot (\Phi(u)\nabla y) = f \text{ in } \Omega \\ \qquad\qquad\qquad\qquad y = 0 \text{ on } \partial\Omega \end{cases}$$

- existence of optimal $\bar{u} \in BV(\Omega) \cap L^\infty(\Omega)$ for $\varepsilon \geqslant 0$
- tracking term Fréchet differentiable in $\Phi(u) \in L^\infty$ for $\varepsilon > 0$
- regularity of state, adjoint $\rightsquigarrow$ derivative in $L^r(\Omega)$, $r > 1$ (instead of $L^\infty(\Omega)^*$)
- $\rightsquigarrow$ sum rule applicable, subgradients in $L^r(\Omega)$, $r > 1$

TV regularization: optimality conditions

$$\begin{cases} 0 = F'(\Phi(\bar{u}))\Phi'(\bar{u}) + \alpha\bar{q} + \beta\bar{\xi} \\ \bar{u} \in \partial G^*(\bar{q}) \\ \bar{\xi} \in \partial TV(\bar{u}) \end{cases}$$

- $F'(\Phi(\bar{u})) = (\nabla\bar{y} \cdot \nabla\bar{p}) \in L^r(\Omega)$ (optimal state, adjoint)
- $\bar{q} \in L^r(\Omega)$, $r > 1 \rightsquigarrow$ pointwise multi-bang
- $\bar{\xi} \in L^r(\Omega)$, $r > 1 \rightsquigarrow$ characterization via *full trace* [Bredies/Holler '12]
- $\rightsquigarrow$ pointwise optimality conditions
- semi-smooth Newton (after discretization, regularization)

Vector-valued multi-bang control

Discrete vector-valued controls $u : \Omega \to U \subset \mathbb{R}^m$

Example: optimal control of Bloch equation: $\Omega = [0, T]$, $m = 2$

$$\frac{d}{dt}M(t) = M(t) \times B(t), \qquad M(0) = M_0$$

- $M(t) \in \mathbb{R}^3$ describes temporal evolution of spin ensemble
- $B(t) = (u_1(t), u_2(t), \omega)^T$ controlled time-dependent magnetic field
- ω resonance frequency (material parameter)
- applications in magnetic resonance imaging, spectroscopy
- control-to-state mapping $S : u \to M$ bilinear

Vector-valued multi-bang: penalty

Here: admissible control set U of d radially distributed states, origin

$$U = \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \omega_0 \cos\theta_1 \\ \omega_0 \sin\theta_1 \end{pmatrix}, \dots, \begin{pmatrix} \omega_0 \cos\theta_d \\ \omega_0 \sin\theta_d \end{pmatrix} \right\}$$

- fixed amplitude $\omega_0 > 0$
- phases $0 \leqslant \theta_1 < \dots < \theta_d < 2\pi$

multi-bang penalty $g = \left(\frac{1}{2}|\cdot|_2^2 + \delta_U\right)^{**}$ convex envelope

$$g^*(q) = \left(\left(\tfrac{1}{2}|\cdot|_2^2 + \delta_U\right)^{**}\right)^*(q) = \left(\tfrac{1}{2}|\cdot|_2^2 + \delta_U\right)^*(q)$$

$$= \begin{cases} 0 & \langle q, u_i\rangle \leqslant \frac{1}{2}\omega_0^2 \text{ for all } 1 \leqslant i \leqslant d \\ \langle q, u_i\rangle - \frac{1}{2}\omega_0^2 & \frac{\theta_{i-1}+\theta_i}{2} \leqslant \angle q \leqslant \frac{\theta_i+\theta_{i+1}}{2}, \langle q, u_i\rangle \geqslant \frac{1}{2}\omega_0^2 \end{cases}$$

Vector-valued multi-bang: subdifferential

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Fenchel conjugate

$$g^*(q) = \begin{cases} 0 =: u_0 & q \in \overline{Q}_0 \\ \langle q, u_i \rangle - \frac{1}{2}\omega_0^2 & q \in \overline{Q}_i \end{cases}$$

Subdifferential

$$\partial g^*(q) = \begin{cases} \{u_i\} & q \in Q_i \qquad 0 \leqslant i \leqslant d \\ \operatorname{co}\{u_{i_1}, \dots, u_{i_k}\} & q \in Q_{i_1 \dots i_k} \qquad 0 \leqslant i_1, \dots, i_k \leqslant d \end{cases}$$

Vector-valued multi-bang: subdifferential

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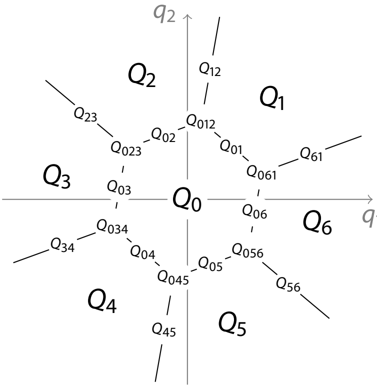
Subdifferential

$$\partial g^*(q) = \begin{cases} \{u_i\} & q \in Q_i \qquad 0 \leqslant i \leqslant d \\ \operatorname{co}\{u_{i_1}, \dots, u_{i_k}\} & q \in Q_{i_1 \dots i_k} \qquad 0 \leqslant i_1, \dots, i_k \leqslant d \end{cases}$$

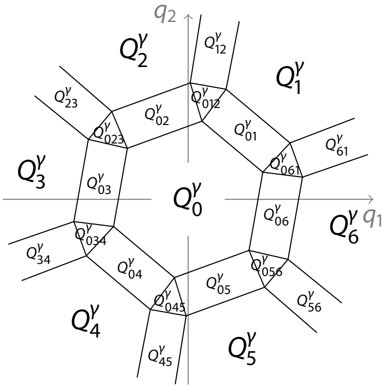
Moreau–Yosida regularization

$$(\partial g^*)_\gamma(q) = \begin{cases} u_i & q \in Q_i^\gamma \\ \left(\frac{\langle q, u_i\rangle}{\gamma\omega_0^2} - \frac{\alpha}{2\gamma}\right) u_i & q \in Q_{0,i}^\gamma \\ \frac{u_i + u_{i+1}}{2} + \frac{\langle q, u_i - u_{i+1}\rangle (u_i - u_{i+1})}{\gamma |u_i - u_{i+1}|_2^2} & q \in Q_{i,i+1}^\gamma \\ \frac{q}{\gamma} - \frac{\alpha}{\gamma}\left(\frac{\omega_0}{|u_i + u_{i+1}|_2}\right)^2 (u_i + u_{i+1}) & q \in Q_{0,i,i+1}^\gamma. \end{cases}$$

Vector-valued multi-bang: subdifferential



(a) subdomains for ∂g^*



(b) subdomains for $(\partial g^*)_\gamma$

Vector-valued multi-bang: examples

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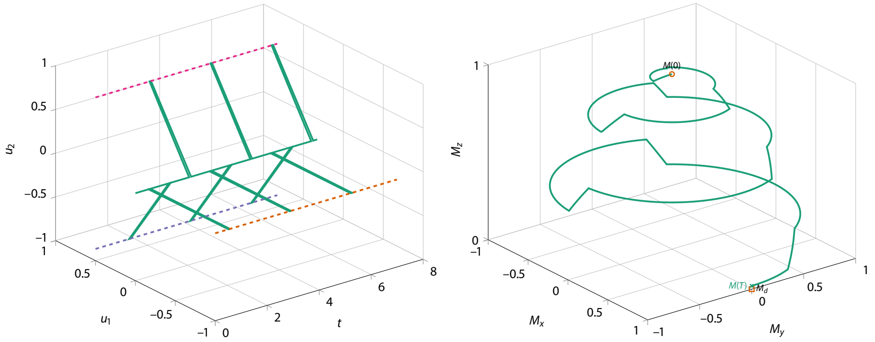
- goal: shift magnetization from $M_0 = (0,0,1)^T$ at $t = 0$
  to $M_d = (1,0,0)^T$ at $t = T$
- $d = 3, 6$ radially distributed admissible control states
- $n = 1, 4$ isochromats with different resonance frequencies
  1. shift all isochromats
  2. shift only one isochromat
- $\alpha = 10^{-1}, \omega_0 = 1$
- example motivated by [Dridi/Lapert/Salomon/Glaser/Sugny '15]
- matrix-free Krylov method for semismooth Newton step
- discretization, adjoint from [Aigner/Clason/Rund/Stollberger '16]

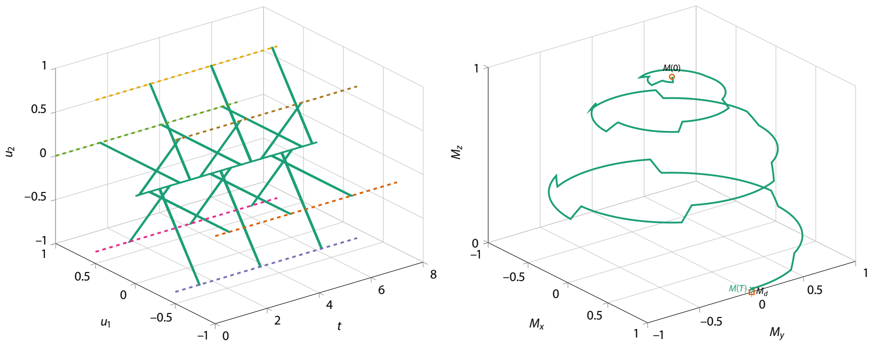
Vector-valued multi-bang: examples



(a) control $u(t)$ (b) state $M(t)$

Figure: $n = 1$ isochromat, $d = 3$ control states

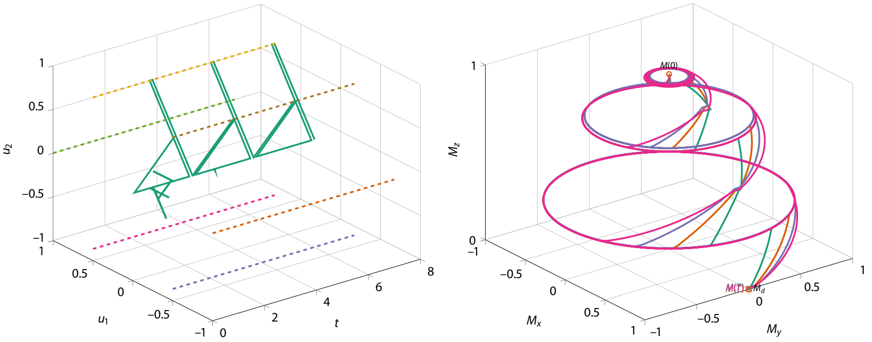
Vector-valued multi-bang: examples



(a) control $u(t)$ (b) state $M(t)$

Figure: $n = 1$ isochromat, $d = 6$ control states

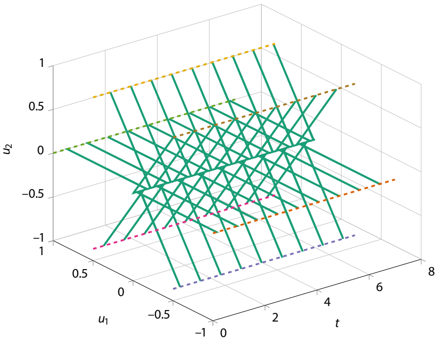
Vector-valued multi-bang: examples



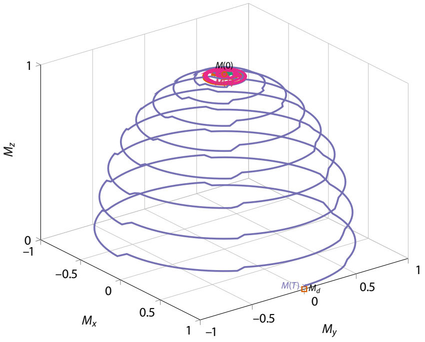
(a) control $u(t)$ (b) state $M(t)$

Figure: $n = 4$ isochromats, same target

Vector-valued multi-bang: examples



(a) control $u(t)$



(b) state $M(t)$

Figure: $J = 4$ isochromats, different targets

Conclusion

Discrete controls:

- can be promoted by convex penalties
- linear complexity in number of parameter values
- $\rightsquigarrow$ efficient numerical solution (superlinear convergence)
- applicable to nonlinear, vector-valued problems

Outlook:

- nonlinear inverse problems: electrical impedance tomography
- combination with BV regularization
- regularization properties, parameter choice
- other discrete–continuous problems: switching, networks

Preprint, MATLAB/Python codes:

http://www.uni-due.de/mathematik/agclason/clason_pub.php