

Optimal control of the principal coefficient in a scalar wave equation

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

- $\mathcal{F}$ discrepancy term (involving PDE)
- U discrete set

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

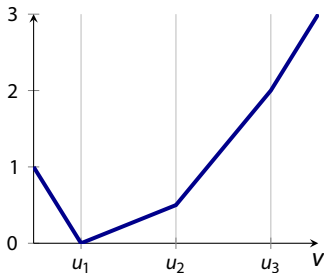
- $u_1, \dots, u_d$ given voltages, velocities, materials, ...
(assumed here: ranking by magnitude possible!)
- motivation: topology optimization, medical imaging

- **convex relaxation**: replace U by convex hull $u(x) \in [u_1, u_d]$
- 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)!

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



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

- 1 Overview
- 2 Multibang penalty
- 3 Wave equation and total variation
- 4 Numerical solution

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

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

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

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- 4 equivalent reformulation (for any $\sigma, \tau > 0$):

$$\begin{cases} \bar{p} = \text{prox}_{\sigma \mathcal{F}^*}(\bar{p} + \sigma \bar{u}) \\ \bar{u} = \text{prox}_{\tau \mathcal{G}}(\bar{u} - \tau \bar{p}) \end{cases}$$

For $\min_u \mathcal{F}(u) + \mathcal{G}(u)$, $\mathcal{G}(u) = \int_{\Omega} g(u(x)) dx$ convex, l.s.c.

Approach: pointwise

- 1 compute subdifferential ∂g (or Fenchel conjugate g^*)
- 2 compute conjugate subdifferential ∂g^*
- 3 compute proximal mapping $\text{prox}_{\gamma g}$

↪ optimality conditions, proximal splitting methods

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

piecewise differentiable $\rightsquigarrow$ subdifferential convex hull of derivatives

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

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convex inverse function theorem:

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

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

■ singular arc

$$\mathcal{S} = \{x : \bar{u}(x) \neq u_i\} \subset \{x : \bar{p}(x) = \tfrac{1}{2}(u_i + u_{i+1})\}$$

- for suitable $\mathcal{F}$: $\bar{p}(x)$ constant implies $[\bar{y} - z](x) = 0$
- (e.g., $\mathcal{F}$ quadratic with pure second-order elliptic PDE)

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

Proximal mapping $\text{prox}_{\gamma g}(v) = w$ iff $v \in \{w\} + \gamma \partial g(w)$

case-wise inspection of subdifferential:

$$\text{prox}_{\gamma g}(v) = \begin{cases} u_i & \text{if } v \in P_i^\gamma \\ v - \frac{\gamma}{2}(u_i + u_{i+1}) & \text{if } v \in P_{i,i+1}^\gamma \end{cases}$$

$$P_i^\gamma = \left[\left(1 + \frac{\gamma}{2}\right) u_i + \frac{\gamma}{2} u_{i-1}, \left(1 + \frac{\gamma}{2}\right) u_{i-1} + \frac{\gamma}{2} u_i \right]$$
$$P_{i,i+1}^\gamma = \left(\left(1 + \frac{\gamma}{2}\right) u_i + \frac{\gamma}{2} u_{i+1}, \left(1 + \frac{\gamma}{2}\right) u_{i+1} + \frac{\gamma}{2} u_i \right)$$

↪ generalized soft thresholding

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Goal: application to **coefficient inverse problem for wave equation**

- $K : u \mapsto y$ solving

$$\begin{cases} y_{tt} - \nabla \cdot (u \nabla y) = f \\ y(0) = y_0, \quad y_t(0) = 0 \end{cases}$$

- difficulty: $\bar{u} \in L^\infty(\Omega) \rightsquigarrow K$ **not** weakly-* closed

$\rightsquigarrow$ lack of existence of minimizer ($\bar{y} \neq K(\bar{u})$, cf. homogenization)

- $\rightsquigarrow$ **TV regularization**: add $TV(u) := \|Du\|_{\mathcal{M}}$

- $\rightsquigarrow u \in BV(\Omega) \cap L^\infty(\Omega) \hookrightarrow_c L^p(\Omega)$

Difficulty:

- existence requires box constraints $\rightsquigarrow$ use penalty

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

(here: G multibang penalty with $\text{dom } G = L^1(\Omega)$)

- **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 $u \in L^1(\Omega)$

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

- $\rightsquigarrow$ use higher regularity of solution to wave equation

$$\begin{cases} \int_0^T -(\partial_t y, \partial_t v) + (u \nabla y(t), \nabla v(t)) dt = \int_0^T (f(t), v(t)) dt \\ y(0) = y_0 \end{cases}$$

f.a. $v \in W := L^2(0, T; H^1) \cap H^1(0, T; L^2)$ with $v(T) = 0$ [Lions/Magenes '72]

solution mapping $S : u \mapsto y$ on $U := \{u \in L^\infty(\Omega) : u_1 \leq u \leq u_d \text{ a.e.}\}$

- $S(u)$ uniformly bounded in $W \cap H^2(0, T; H^{-1}) := Z$
- S Lipschitz continuous from L^∞ to $L^2(0, T; L^2)$
- $S(u_n) \rightharpoonup S(u)$ in Z if $u_n \rightarrow u$ in $L^r(\Omega)$, $r \in [1, \infty]$

$$\begin{cases} \int_0^T -(\partial_t y, \partial_t v) + (u \nabla y(t), \nabla v(t)) dt = \int_0^T (f(t), v(t)) dt \\ y(0) = y_0 \end{cases}$$

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Assumption:

- $f \in L^2(0, T; H^1)$, $y_0 \in H^2(\Omega)$, $\partial_\nu y_0 = 0$, $y_1 \in H^1(\Omega)$
- there is $\omega_c \subset \Omega$ with u constant on $\Omega \setminus \omega_c$, y_0 constant on ω_c

Then:

- $S(u)$ uniformly bounded in $L^\infty(0, T; W^{1,s})$ for some $s > 2$
(proof: combination of higher hyperbolic and maximal elliptic regularity [Wloka '87, Gröger '89])

$$\begin{cases} \min_{u \in BV(\Omega)} \frac{1}{2} \|y - y^\delta\|_{L^2(\Omega)}^2 + \alpha G(u) + \beta TV(u) \\ \text{s.t.} \quad y_{tt} - \nabla \cdot (\Phi_\varepsilon(u) \nabla y) = f \\ \quad y(0) = y_0, \quad y_t(0) = y_1 \end{cases}$$

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

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

- $F'(\Phi_{\varepsilon}(\bar{u})) = \int_0^T \nabla \bar{y} \cdot \nabla \bar{p} dt \in L^r(\Omega), r > 1$
($\bar{y}$ optimal state, $\bar{p}$ adjoint state)
- $\bar{q} \in L^r(\Omega), r > 1 \rightsquigarrow$ pointwise **multibang**
- $\bar{\xi} \in L^r(\Omega), r > 1 \rightsquigarrow$ characterization via *full trace*
[Bredies/Holler '12]
- $\rightsquigarrow$ **pointwise optimality conditions**

Approach: discretize before optimize

- consider finite element discretization of problem
 - piecewise linear in space
 - stabilized piecewise linear in time [Zlotnik '94]
 - discrete adjoint
- include projection in multi-bang penalty, eliminate Φ_ε
- apply sum rule, chain rule for $\partial TV(u_h) = -\operatorname{div}_h \partial(\|\cdot\|_1)(\nabla_h u_h)$
- $\rightsquigarrow$ apply nonlinear primal-dual proximal splitting

$$u^{k+1} = \text{prox}_{\tau\mathcal{G}} \left(u^k - \tau K'(u^k)^* p^k \right)$$

$$\bar{u}^{k+1} = 2u^{k+1} - u^k$$

$$p^{k+1} = \text{prox}_{\sigma\mathcal{F}^*} \left(p^k + \sigma K(\bar{u}^{k+1}) \right)$$

- nonlinear variant of Chambolle–Pock

[Valkonen '14, C./Mazurenko/Valkonen '18]

- $\tau, \sigma > 0$ step sizes

- local convergence in Hilbert space under

- 1 second-order type condition on K

- 2 τ, σ sufficiently small

- apply to $\mathcal{F}(y, q) = \|y - y^\delta\|_2^2 + \|q\|_2$, $K(u) = (S(u), \nabla_h u)$

$$u^{k+1} = \text{prox}_{\tau\alpha\mathcal{G}} \left(u^k - \tau S'_h(u^k)^*(r^k) - \tau \nabla_h^* \psi^k \right)$$

$$\bar{u}^{k+1} = 2u^{k+1} - u^k$$

$$r^{k+1} = \frac{1}{1 + \frac{\sigma}{v_1}} \left(r_1^k + \sigma(S_h(\bar{u}^{k+1}) - y^d) \right)$$

$$q^{k+1} = \psi^k + \sigma \nabla_h \bar{u}^{k+1}$$

$$\psi^{k+1} = \frac{\beta q^{k+1}}{\max\{\beta, |q^{k+1}|_2\}}$$

- $S_h(u)$ solution of wave equation
- $S'_h(u)^* r$ solution of wave, adjoint equation (with RHS r), integration
- proximal mappings pointwise ($\mathcal{G}$ includes projection)

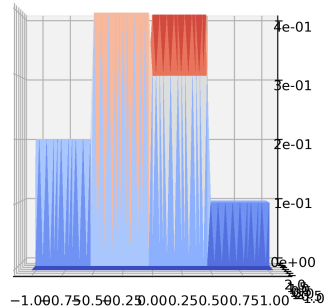
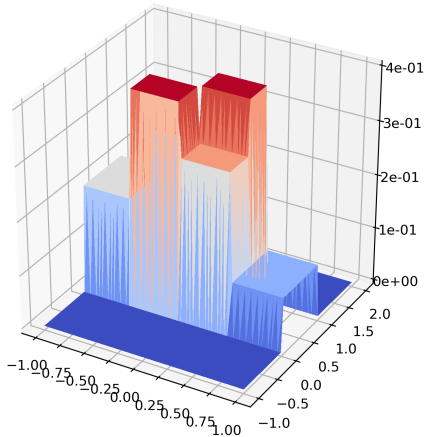


Figure: exact coefficient (front: sources; back: observation)

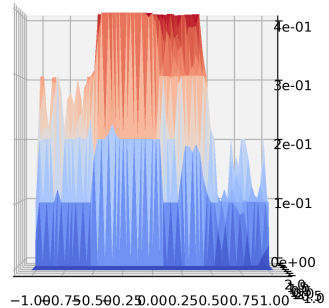
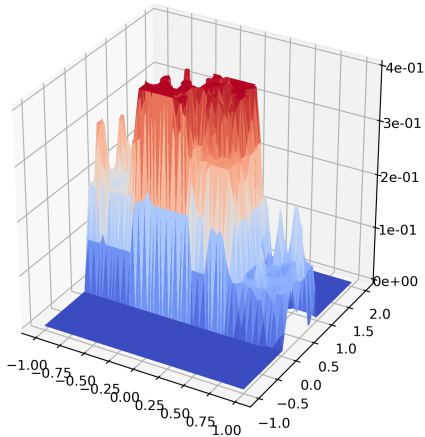


Figure: $\delta = 0.1, \alpha = 10^{-5}, \beta = 0, k = 300$

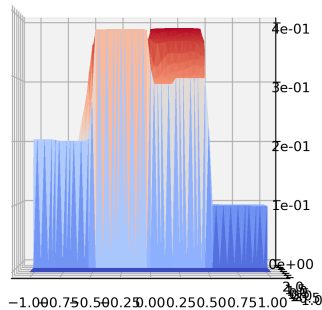
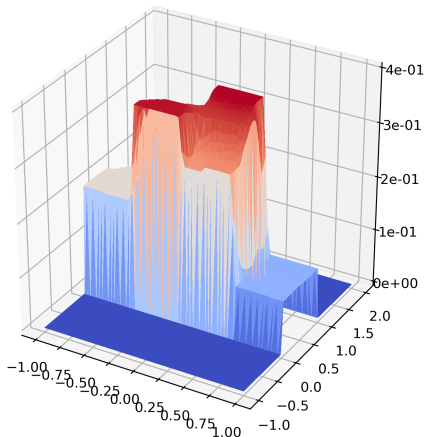


Figure: $\delta = 0.1, \alpha = 0, \beta = 10^{-4}, k = 300$

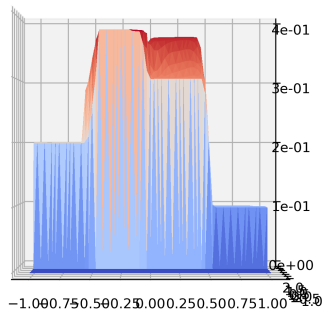
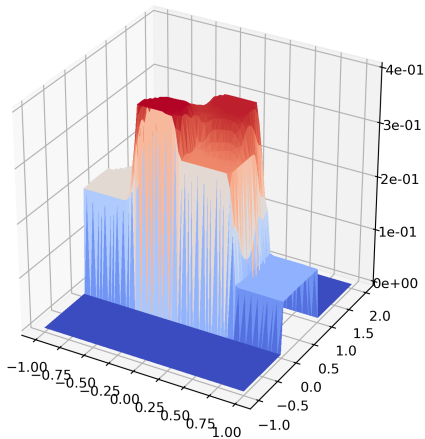


Figure: $\delta = 0.1$, $\alpha = 10^{-5}$, $\beta = 10^{-4}$, $k = 300$

Multibang regularization for discrete-valued optimization

- well-posed convex relaxation
- combination with total variation
- applicable to wave equation

Outlook:

- (block) acceleration of proximal splitting
- boundary observation
- vector-valued coefficient

Preprint, MATLAB/Python codes: (soon ...)

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