



Nonsmooth regularization of a coefficient inverse problem for the wave equation

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Motivation: coefficient inverse problem

Wave equation

$$\begin{cases} y_{tt} - \nabla \cdot (u \nabla y) = f & \text{on } \Omega \times [0, T] \\ \partial_\nu y = 0 & \text{on } \partial\Omega \times [0, T] \\ y(0) = y_0, \quad y_t(0) = 0 & \text{on } \Omega \end{cases}$$

Goal: recover u from (partial) measurement of y

Assumption: u piecewise constant (with known values?)

Approach:

1 add **total variation regularization** $\|\nabla u\|_1$
($\leadsto$ sparse gradient $\leadsto$ piecewise constant)

2 add **pointwise penalty** promoting known values

$\leadsto$ **nonsmooth regularization:** non-differentiable but convex

1 Overview

2 Pointwise regularization

- Multibang penalty
- Regularization properties

3 Wave equation and total variation

4 Numerical solution

Convex analysis approach

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

- 1 Fermat principle: $0 \in \partial (\mathcal{F}(K(\bar{u})) + \mathcal{G}(\bar{u}))$
- 2 sum, chain rule: $0 \in K'(\bar{u})^* \partial \mathcal{F}(K(\bar{u})) + \partial \mathcal{G}(\bar{u})$
 $\leadsto$ there is $\bar{p}$ with

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

- 3 Fenchel duality:

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

Convex analysis approach

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

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- 2 sum, chain rule: $0 \in K'(\bar{u})^* \partial \mathcal{F}(K(\bar{u})) + \partial \mathcal{G}(\bar{u})$
 $\leadsto$ there is $\bar{p}$ with

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

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

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

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 (for K linear)
[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
- can be accelerated if $\mathcal{F}$ and/or $\mathcal{G}$ strongly convex

Convex analysis approach

For $\min_u \mathcal{F}(K(u)) + \mathcal{G}(u)$, $\mathcal{G}(u) = \int_{\Omega} g(u(x)) dx$ 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

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Motivation: hybrid discrete optimization

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

- $\mathcal{F}$ discrepancy term, K forward operator (involving PDE solution)
- 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

Motivation: penalty

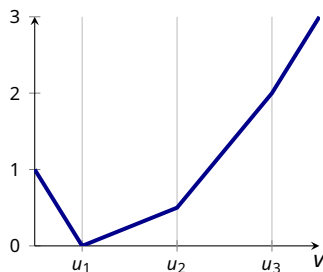
- **convex relaxation**: replace U by convex hull $u(x) \in [u_1, u_d]$
- works only for $d = 2$, cf. bang-bang control ($\alpha = 0$)
- $\leadsto$ promote $u(x) \in \{u_1, \dots, u_d\}$ by **convex pointwise penalty**

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

- 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 $u_1, \dots, u_d$



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

Multibang penalty

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

piecewise differentiable $\leadsto$ subdifferential convex hull of derivatives

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

Multibang penalty

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

Fenchel duality:

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

Proximal point mapping

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

case-wise inspection of subdifferential:

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

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

↪ generalized soft thresholding

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Multibang regularization

$$\min_{u \in L^2(\Omega)} \frac{1}{2} \|K(u) - y^\delta\|_Y^2 + \alpha \mathcal{G}(u)$$

- $K : L^2(\Omega) \rightarrow Y$ (nonlinear) forward mapping, weakly closed
- $y^\delta \in L^2(\Omega)$ noisy data with $\|y - y^\delta\|_Y \leq \delta$
- $u_1 < \dots < u_d$ given parameter values ($d > 2$)
- $\mathcal{G}$ multibang penalty
- $\alpha > 0$ regularization parameter (a priori, Morozov, heuristic, ...)

Multibang regularization

$$\min_{u \in L^2(\Omega)} \frac{1}{2} \|K(u) - y^\delta\|_Y^2 + \alpha \mathcal{G}(u)$$

■ $\mathcal{G}$ multibang penalty convex:

- 1 existence of solution u_α^δ for every $\alpha > 0$
- 2 $\delta \rightarrow 0$ implies $u_\alpha^\delta \rightarrow u_\alpha$ for every $\alpha > 0$
- 3 $\delta \rightarrow 0, \alpha \rightarrow 0, \delta^2 \alpha^{-1} \rightarrow 0$ implies $u_\alpha^\delta \rightarrow u^\dagger$

(standard arguments: [Burger/Osher '04, Scherzer et al. '09, Kaltenbacher et al. '12, Ito/Jin '14, ...])

Multibang regularization

$$\min_{u \in L^2(\Omega)} \frac{1}{2} \|K(u) - y^\delta\|_Y^2 + \alpha \mathcal{G}(u)$$

- standard source condition: $p^\dagger := K'(u^\dagger)^* w \in \partial \mathcal{G}(u^\dagger)$ for $w \in Y$,

- 1 a priori choice $\alpha(\delta) = c\delta$

- 2 a posteriori choice $\|K(u_{\alpha(\delta)}^\delta) - y^\delta\|_Y \leq \tau\delta, \tau > 1$

→ convergence rate

$$d_{\mathcal{G}}^{p^\dagger}(u_\alpha^\delta, u^\dagger) \leq C\delta$$

in Bregman divergence

$$d_{\mathcal{G}}^{p_1}(u_2, u_1) = \mathcal{G}(u_2) - \mathcal{G}(u_1) - \langle p_1, u_2 - u_1 \rangle_X, \quad p_1 \in \partial \mathcal{G}(u_1)$$

Multibang regularization

Pointwise definition of Bregman divergence, ∂g :

- $u^\dagger(x) = u_i$ and $p^\dagger \notin \left\{ \frac{1}{2}(u_{i-1} + u_i), \frac{1}{2}(u_i + u_{i+1}) \right\}$ implies

$$d_g^{p^\dagger(x)}(u_{\alpha(\delta)}^\delta(x), u^\dagger(x)) \rightarrow 0 \quad \text{for } \delta \rightarrow 0$$

- $u^\dagger(x) \in (u_i, u_{i+1})$ implies

$$d_g^{p^\dagger(x)}(u(x), u^\dagger(x)) = 0 \quad \text{for any } u(x) \in [u_i, u_{i+1}]$$

- $\rightsquigarrow u_{\alpha(\delta)}^\delta \rightarrow u^\dagger$ pointwise a.e. iff $u^\dagger(x) \in \{u_1, \dots, u_d\}$ a.e.
- (convergence not uniform $\rightsquigarrow$ no pointwise rates)

Optimality system

$$\bar{p} = \frac{1}{\alpha} K'(\bar{u})^* (y^\delta - K(\bar{u}))$$

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

■ $\leadsto$ unique solution $(\bar{u}, \bar{p}) \in L^2(\Omega) \times L^2(\Omega)$

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

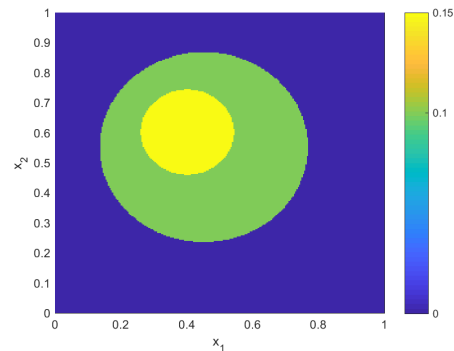
■ for suitable K , $\bar{p}(x)$ constant implies $[y^\delta - K(\bar{u})](x) = 0$
(e.g., $K = A^{-1}$ for A pure second-order elliptic)

$\leadsto |\{x : K(\bar{u}(x)) = y^\delta(x)\}| = 0 \Rightarrow \bar{u} \in \{u_1, \dots, u_d\}$ a.e. (true multibang)

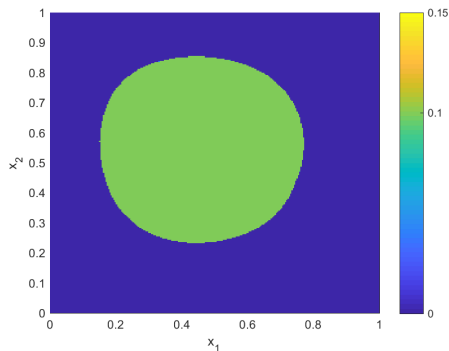
Example: linear inverse problem

- $\Omega = [0, 1]^2$, $K = A^{-1}$, $A = -\Delta$
- $u^\dagger(x) = u_1 + u_2 \chi_{\{(x_1-0.45)^2+(x_2-0.55)^2 < 0.1\}}(x)$
 $+ (u_3 - u_2) \chi_{\{(x_1-0.4)^2+(x_2-0.6)^2 < 0.02\}}(x)$
- $d = 3$, $u_1 = 0$, $u_2 = 0.1$, $u_3 \in \{0.15, 0.11\}$
- $y^\delta = y^\dagger + \xi$, $\xi \in \mathcal{N}(y^\dagger, \delta \|y^\dagger\|_\infty)$
- finite element discretization: uniform grid, 256×256 nodes
- solution by (regularized) semismooth Newton method ($\gamma < 10^{-12}$)
- $\alpha = \alpha(\delta)$ by Morozov discrepancy principle

Numerical example: $u_3 = 0.15$

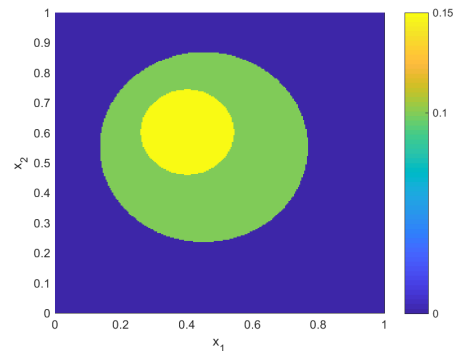


(a) $u^\dagger$

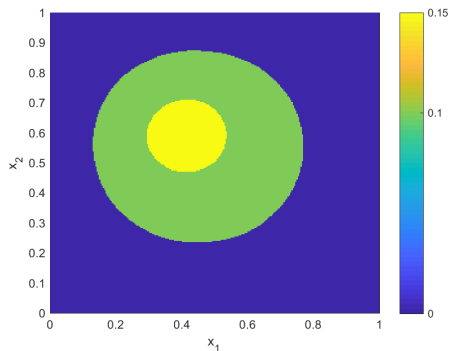


(b) $u_\alpha^\delta, \delta \approx 1.89 \cdot 10^{-1}$

Numerical example: $u_3 = 0.15$

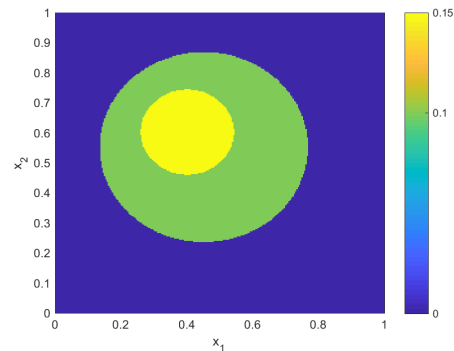


(c) $u^\dagger$

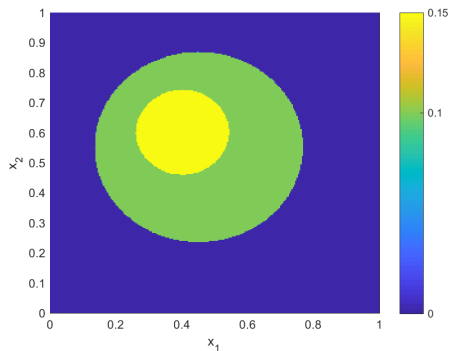


(d) $u_{\alpha}^{\delta}, \delta \approx 2.37 \cdot 10^{-2}$

Numerical example: $u_3 = 0.15$

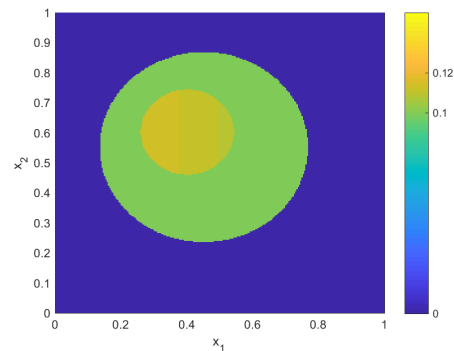


(e) $u^\dagger$

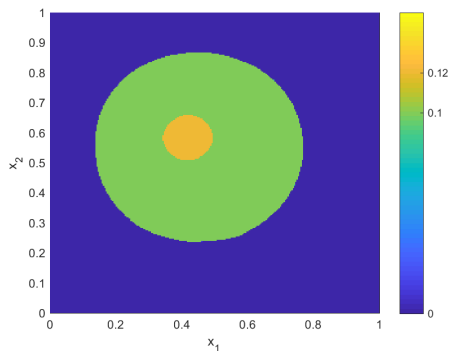


(f) $u_\alpha^\delta, \delta \approx 3.69 \cdot 10^{-4}$

Numerical example: $u_3(x) = 0.12(1 - x_1)$

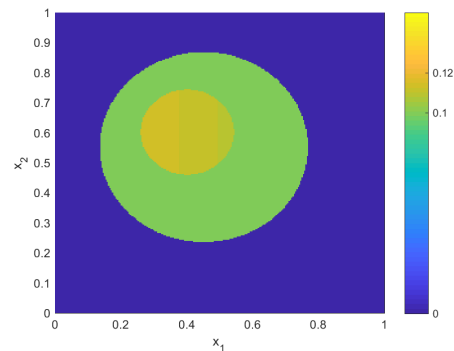


(a) $u^\dagger$

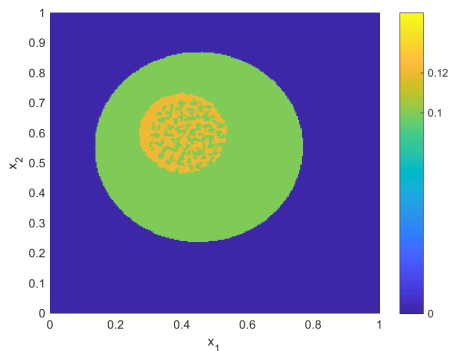


(b) $u_{\alpha}^{\delta}, \delta \approx 2.11 \cdot 10^{-2}$

Numerical example: $u_3(x) = 0.12(1 - x_1)$

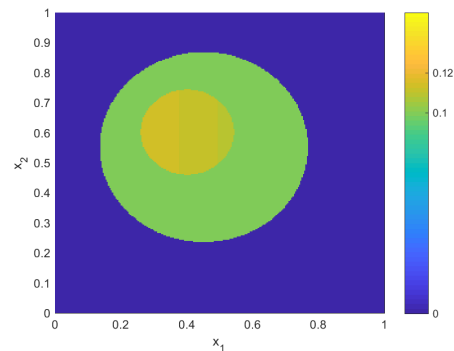


(c) $u^\dagger$

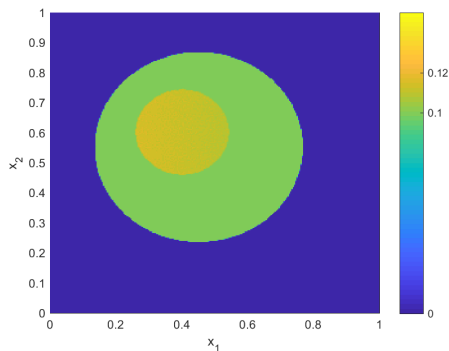


(d) $u_\alpha^\delta, \delta \approx 3.29 \cdot 10^{-4}$

Numerical example: $u_3(x) = 0.12(1 - x_1)$



(e) $u^\dagger$



(f) $u_\alpha^\delta, \delta \approx 1.29 \cdot 10^{-6}$

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Nonlinear forward mapping

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

- $K : u \mapsto y$ solving

$$\begin{cases} y_{tt} - \nabla \cdot (u \nabla y) = f & \text{on } \Omega \times [0, T] \\ \partial_\nu y = 0 & \text{on } \partial\Omega \times [0, T] \\ y(0) = y_0, \quad y_t(0) = 0 & \text{on } \Omega \end{cases}$$

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

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

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

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

TV regularization

Difficulty:

- existence requires box constraints $\leadsto$ 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^∞
- $\leadsto$ replace box constraints by $(C^{1,1})$ **projection** of $u \in L^1(\Omega)$

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

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

Wave equation

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

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

$\leadsto$ 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 $L^2(0, T; L^2)$
- $S(u_n) \rightarrow S(u)$ in Z if $u_n \rightarrow u$ in $L^r(\Omega)$, $r \in [1, \infty]$

Wave equation

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

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

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])

TV regularization: existence

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

- 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 $\leadsto$ derivative in $L^r(\Omega), r > 1$
(instead of $L^\infty(\Omega)^*$)
- $\leadsto$ sum rule applicable, subgradients in $L^r(\Omega), r > 1$

TV regularization: optimality conditions

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

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

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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 $\partial TV(u_h) = -\operatorname{div}_h \partial(\|\cdot\|_1)(\nabla_h u_h)$
- $\leadsto$ apply nonlinear primal-dual proximal splitting

Primal-dual proximal splitting

$$\begin{aligned}u^{k+1} &= \text{prox}_{\tau\mathcal{G}} \left(u^k - \tau K'(u^k)^* p^k \right) \\ \bar{u}^{k+1} &= 2u^{k+1} - u^k \\ p^{k+1} &= \text{prox}_{\sigma\mathcal{F}^*} \left(p^k + \sigma K(\bar{u}^{k+1}) \right)\end{aligned}$$

- 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 $\mathcal{F}(y, q) = \|y - y^\delta\|_2^2 + \|q\|_2\|_1$, $K(u) = (S(u), \nabla_h u)$

Primal-dual proximal splitting algorithm

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

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

$$r^{k+1} = \frac{1}{1 + \frac{\sigma}{\nu_1}} \left(r_1^k + \sigma(S_h(\bar{u}^{k+1}) - y^d) \right)$$

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

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

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

Numerical example

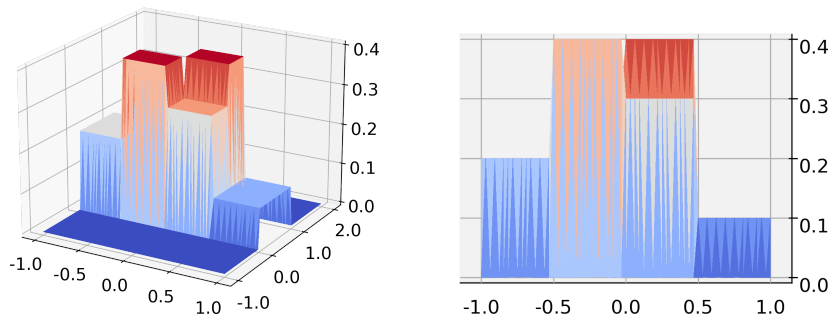


Figure: exact coefficient (front: sources; back: observation)

Numerical example

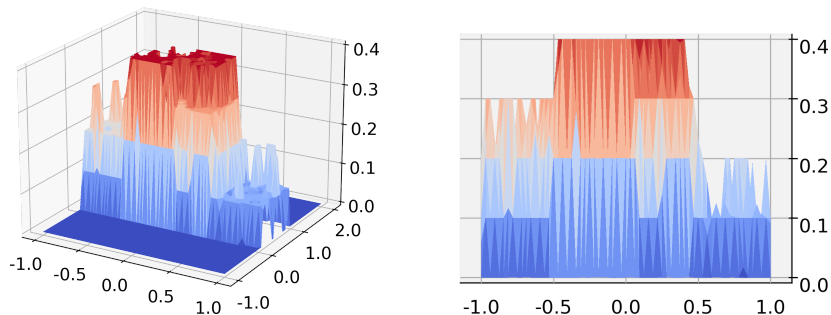


Figure: $\alpha = 10^{-5}$, $\beta = 0$, 3680 iterations

Numerical example

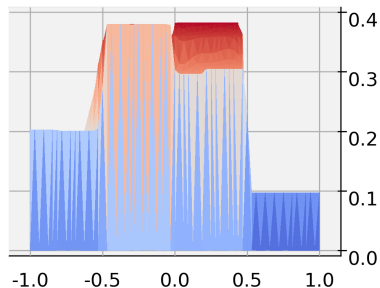
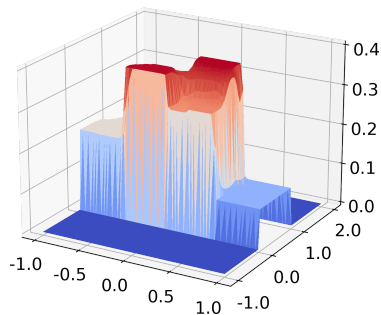


Figure: $\alpha = 0$, $\beta = 10^{-4}$, 1100 iterations

Numerical example

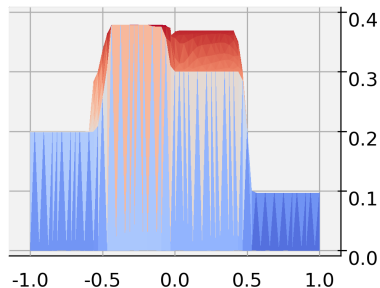
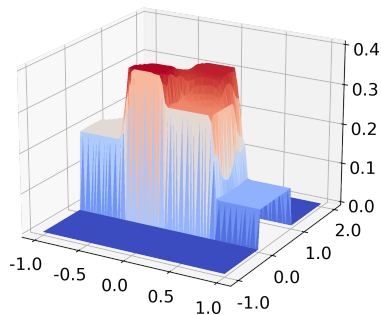


Figure: $\alpha = 10^{-5}$, $\beta = 10^{-4}$, 600 iterations

Numerical example

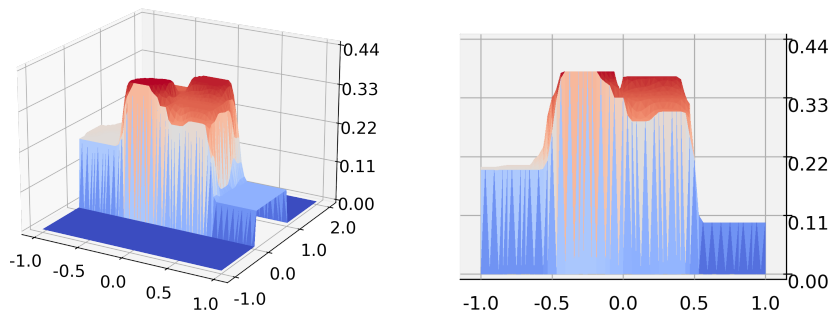


Figure: u_i overestimated, $\alpha = 10^{-5}$, $\beta = 10^{-4}$, 820 iterations

Conclusion

Multibang regularization for discrete-valued inverse problem

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

Outlook:

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

Preprints, codes:

<http://homepage.uni-graz.at/c.clason/publikationen>