

Total variation regularization of multi-material topology optimization

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joint work with Florian Kruse and Karl Kunisch

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

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

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

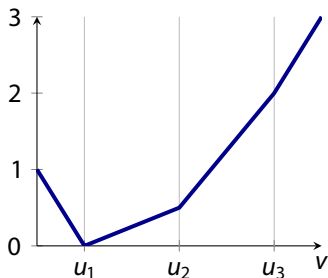
- u_1, \dots, u_d given voltages, velocities, materials, ...
(assumed here: ranking by magnitude possible!)
- motivation: topology optimization, medical imaging

- **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 $\frac{1}{2}\|u\|^2 + \delta_U$
 - **multi-bang** (generalized bang-bang) control
 - \rightsquigarrow non-smooth optimization in function spaces
- pointwise penalty \rightsquigarrow add **total variation regularization**

- 1 Overview
- 2 Multi-bang penalty
- 3 Total variation regularization

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

- 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:

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

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

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

- 4 Moreau–Yosida regularization (semismooth)

$$\begin{cases} -p_\gamma \in \partial\mathcal{F}(u_\gamma) \\ u_\gamma = \partial\mathcal{G}_\gamma^*(p_\gamma) \end{cases}$$

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

Approach: pointwise

- 1 compute subdifferential ∂g (or Fenchel conjugate g^*)
 - 2 compute conjugate subdifferential ∂g^*
 - 3 compute proximal mapping $\text{prox}_{\gamma g^*}$
 - 4 compute Moreau–Yosida regularization ∂g_{γ}^*
 - 5 compute Newton derivative $D_N \partial g_{\gamma}^*$
- ↪ semismooth Newton method, continuation in γ for
superposition operator $[\partial \mathcal{G}_{\gamma}^*(p)](x) = \partial g_{\gamma}^*(p(x))$

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

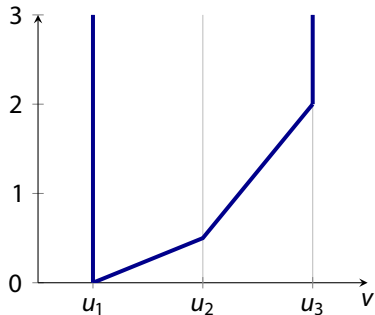
piecewise differentiable \rightsquigarrow subdifferential convex hull of derivatives

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

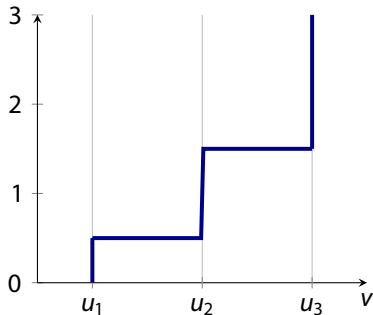
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convex inverse function theorem:

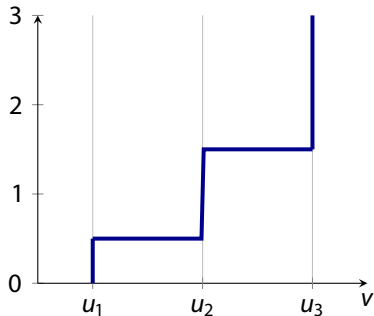
$$\partial g^*(q) \in \begin{cases} \{u_1\} & q \in (-\infty, \frac{1}{2}(u_1 + u_2)) \\ [u_i, u_{i+1}] & q = \frac{1}{2}(u_i + u_{i+1}), \quad 1 \leq i < d \\ \{u_i\} & q \in (\frac{1}{2}(u_{i-1} + u_i), \frac{1}{2}(u_i + u_{i+1})) \quad 1 < i < d, \\ \{u_d\} & q \in (\frac{1}{2}(u_{d-1} + u_d), \infty)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



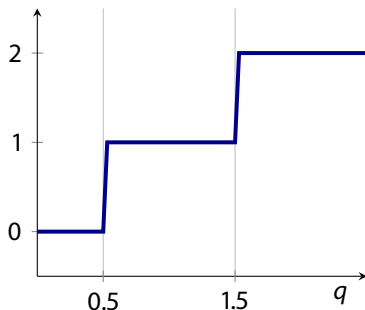
(a) $g(u_1 = 0, u_2 = 1, u_3 = 2)$



(b) $\partial g(u_1 = 0, u_2 = 1, u_3 = 2)$



(c) $\partial g(u_1 = 0, u_2 = 1, u_3 = 2)$



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

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

■ singular arc

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

- 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 $\text{prox}_{\gamma g^*}(q) = w$ iff $q \in \{w\} + \gamma \partial g^*(w)$

case-wise inspection of subdifferential:

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

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

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

Lipschitz continuous, piecewise $C^1 \rightsquigarrow$ **Newton derivative**

$$D_N \partial g_Y^*(q) = \begin{cases} 0 & q \in Q_i^Y \\ \frac{1}{\gamma} & q \in Q_{i,i+1}^Y \end{cases}$$

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

$$\begin{cases} p_\gamma \in \mathcal{F}(u_\gamma) \\ u_\gamma = \partial \mathcal{G}_\gamma^*(p_\gamma) \end{cases}$$

- optimality conditions for $\mathcal{F}(u) + \alpha \mathcal{G}(u) + \frac{\gamma}{2} \|u\|^2$ (non-smooth)
- \rightsquigarrow unique solution (u_γ, p_γ)
- $(u_\gamma, p_\gamma) \rightarrow (\bar{u}, \bar{p})$ as $\gamma \rightarrow 0$
- norm gap $p_\gamma \in V \hookrightarrow L^p(\Omega), p > 2$
- \rightsquigarrow semismooth Newton method in function space
- only number of sets Q_i^γ depends on $d \rightsquigarrow$ linear complexity

- 1 Overview
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Goal: application to topology optimization, EIT

- $\mathcal{F}(u) = \frac{1}{2} \|S(u) - z\|^2,$

$$S : u \mapsto y \quad \text{solving} \quad -\nabla \cdot (u \nabla y) = f$$

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

- 1 lack of existence of minimizer ($\bar{y} \neq S(\bar{u})$, cf. homogenization)

- 2 lack of convergence $\gamma \rightarrow 0$

- 3 lack of Newton differentiability of $\partial \mathcal{G}_\gamma^*$ (no norm gap)

- **remedies:** higher regularity of y or u by

- 1 local smoothing: consider $-\nabla \cdot \left(\int_{B_\varepsilon(x)} u(s) ds \nabla y \right)$

- 2 **TV regularization:** add $\|Du\|_{\mathcal{M}} \rightsquigarrow u \in BV(\Omega) \cap L^\infty(\Omega) \hookrightarrow_c L^p(\Omega)$

Difficulty:

- existence requires box constraints \rightsquigarrow use penalty

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

(here: G multi-bang 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 $u \in L^1(\Omega)$

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

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

- **existence** of optimal $\bar{u} \in BV(\Omega) \cap L^\infty(\Omega)$ for $\varepsilon \geq 0$
- tracking term Fréchet differentiable in $\Phi_\varepsilon(u) \in L^\infty$ 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 $L^r(\Omega)$, $r > 1$

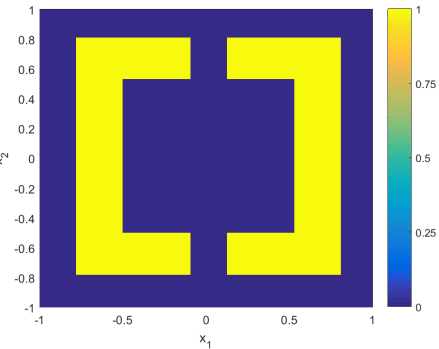
$$\begin{cases} 0 = F'(\Phi_\varepsilon(\bar{u}))\Phi'_\varepsilon(\bar{u}) + \alpha\bar{q} + \beta\bar{\xi} \\ \bar{u} \in \partial G^*(\bar{q}) \\ \bar{\xi} \in \partial TV(\bar{u}) \end{cases}$$

- $F'(\Phi_\varepsilon(\bar{u})) = (\nabla\bar{y} \cdot \nabla\bar{p}) \in L^r(\Omega)$ (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)

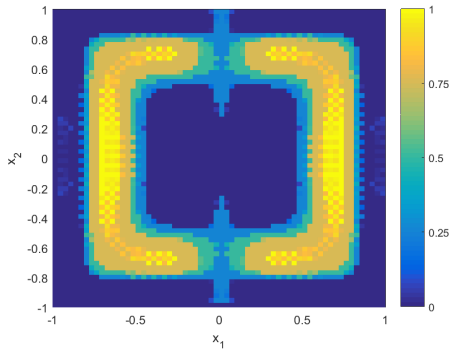
Approach: discretize before optimize

- consider finite element discretization of problem (p.w. linear)
- include projection in multi-bang penalty, eliminate Φ_ε
- apply sum rule, chain rule for $\partial TV(u_h) = -\operatorname{div}_h \partial(\|\cdot\|_1)(\nabla_h u_h)$
- apply Moreau–Yosida regularization to $\partial \mathcal{G}^*, \partial(\|\cdot\|_1)^*$
- \rightsquigarrow semi-smooth Newton-type method
(modified Newton step to avoid kernel of div_h ; line search)
- local convergence: path-following with extrapolation

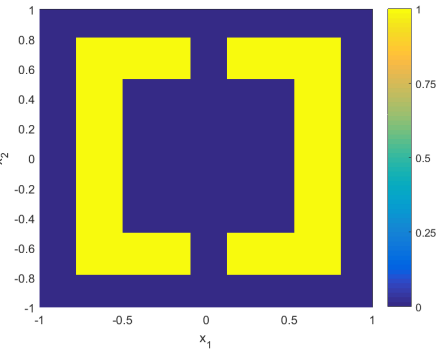
Numerical example: topology optimization



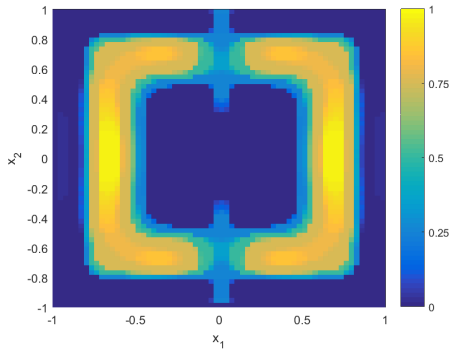
(a) u^\dagger



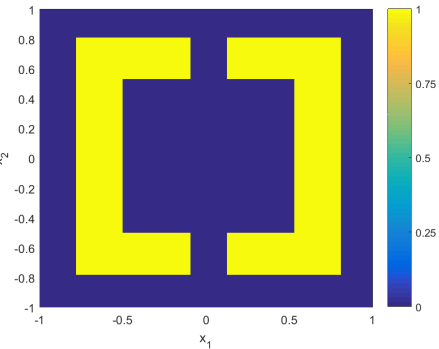
(b) $\alpha = 10^{-3}, \beta = 0$



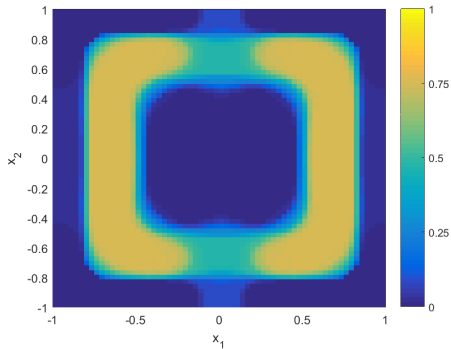
(c) u^\dagger



(d) $\alpha = 10^{-3}, \beta = 10^{-6}$

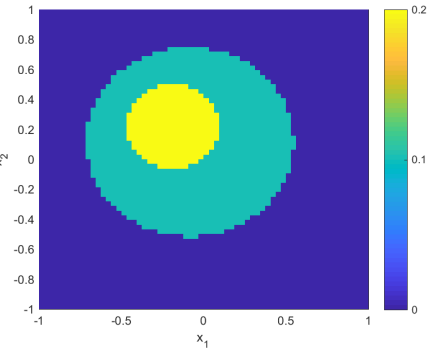


(e) u^\dagger

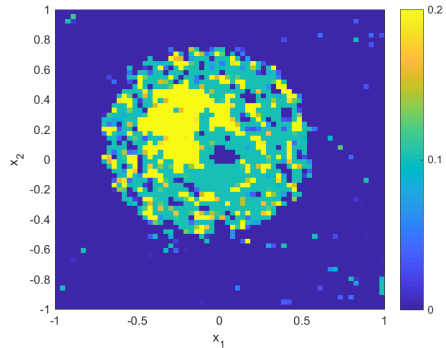


(f) $\alpha = 10^{-3}, \beta = 5 \cdot 10^{-5}$

Numerical example: inverse problem

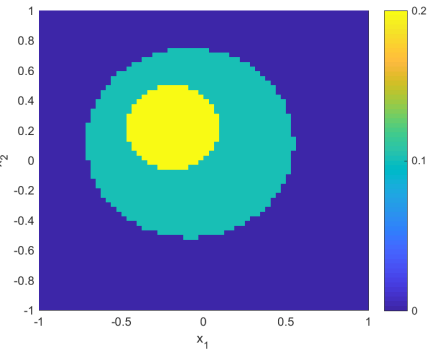


(a) u^\dagger

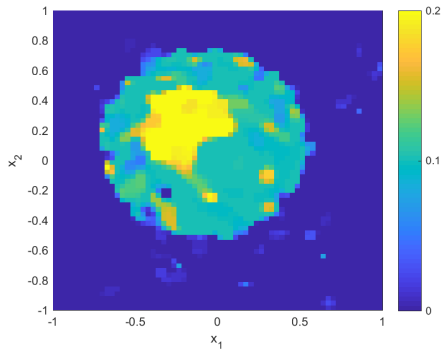


(b) $\alpha = 5 \cdot 10^{-4}, \beta = 0$

Numerical example: inverse problem

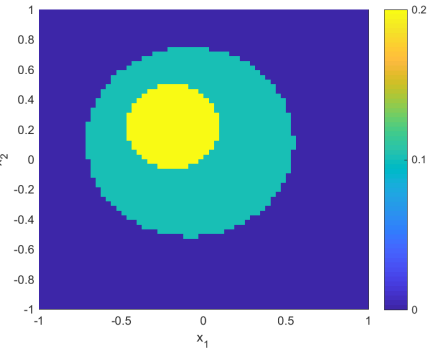


(c) u^\dagger

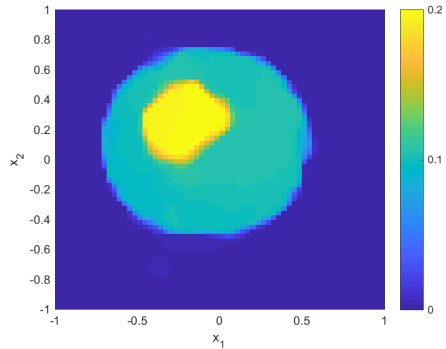


(d) $\alpha = 5 \cdot 10^{-4}, \beta = 10^{-5}$

Numerical example: inverse problem



(e) u^\dagger



(f) $\alpha = 5 \cdot 10^{-4}, \beta = 10^{-5}$

Convex relaxation of discrete–continuous control problems

- strong structural properties
- efficient numerical solution (superlinear convergence)
- can be combined with total variation regularization

Outlook:

- sufficient second-order conditions?
- finite element error estimates?
- vector-valued multi-bang
- other hybrid discrete–continuous problems (switching)

Preprint:

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