Total variation regularization of multi-material topology optimization

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joint work with Florian Kruse and Karl Kunisch

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Motivation: hybrid discrete optimization

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

- $\mathcal{F}$ 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

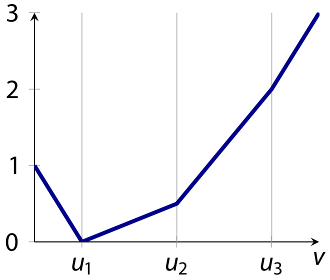
- convex relaxation: replace U by convex hull $u(x) \in [u_1, u_d]$
- works only for $d = 2$, cf. bang-bang control ($\alpha = 0$)
- $\rightsquigarrow$ promote $u(x) \in \{u_1, \dots, u_d\}$ by convex pointwise penalty

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

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

Motivation: penalty

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



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

- pointwise penalty $\rightsquigarrow$ add total variation regularization

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

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

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

Convex analysis approach

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

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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)

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

Convex analysis approach

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

Approach: pointwise

1. compute subdifferential ∂g (or Fenchel conjugate g^*)
2. compute conjugate subdifferential ∂g^*
3. compute proximal mapping $\mathrm{prox}_{\gamma g^*}$
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 $\quad [\partial \mathcal{G}^*_\gamma(p)](x) = \partial g^*_\gamma(p(x))$

Multi-bang penalty

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

piecewise differentiable $\rightsquigarrow$ subdifferential convex hull of derivatives

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

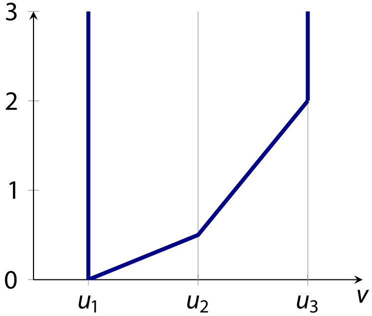
Multi-bang penalty

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

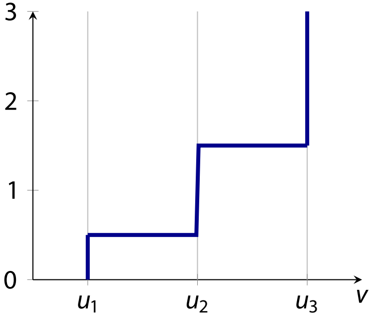
convex inverse function theorem:

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

Multi-bang penalty: sketch

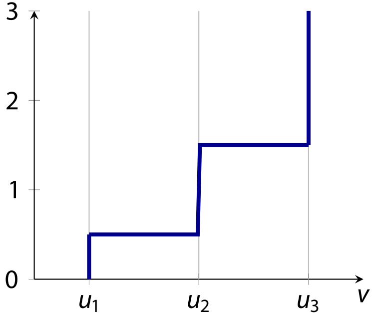


(a) g ($u_1 = 0, u_2 = 1, u_3 = 2$)

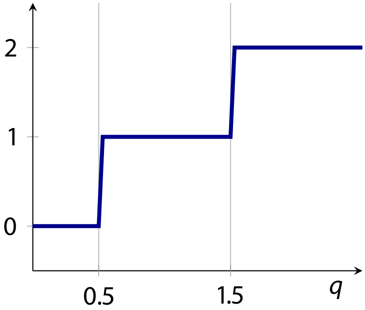


(b) ∂g ($u_1 = 0, u_2 = 1, u_3 = 2$)

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 conditions

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

- singular arc

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

- 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)

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

Moreau–Yosida regularization

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

case-wise inspection of subdifferential:

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

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

Moreau–Yosida regularization

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

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

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

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

Regularized optimality system

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

- optimality conditions for $\mathcal{F}(u) + \alpha\, \mathcal{G}(u) + \frac{\gamma}{2}\|u\|^2$ (non-smooth)
- $\rightsquigarrow$ unique solution (u_γ, p_γ)
- $(u_\gamma, p_\gamma) \rightharpoonup (\bar{u}, \bar{p})$ as $\gamma \to 0$
- 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

Nonlinear forward mapping

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: $\bar{u} \in L^\infty(\Omega) \quad \rightsquigarrow \quad S$ 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 $\partial \mathcal{G}_\gamma^*$ (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

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

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

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

TV regularization: existence

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

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

TV regularization: optimality conditions

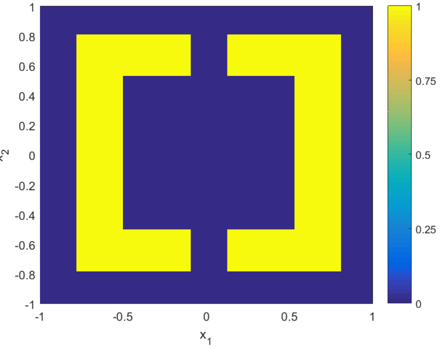
$$\begin{cases} 0 = F'(\Phi_\varepsilon(\bar{u}))\Phi'_\varepsilon(\bar{u}) + \alpha\bar{q} + \beta\bar{\xi} \\ \bar{u} \in \partial G^*(\bar{q}) \\ \bar{\xi} \in \partial TV(\bar{u}) \end{cases}$$

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

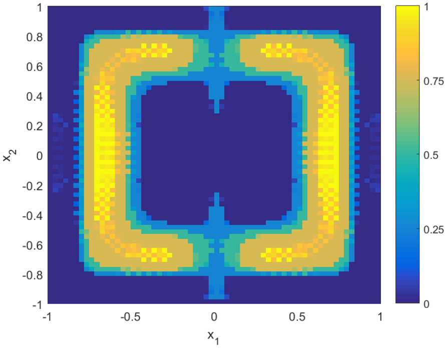
TV regularization: numerical solution

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 $\partial TV(u_h) = -\mathrm{div}_h \partial(\|\cdot\|_1)(\nabla_h u_h)$
- 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

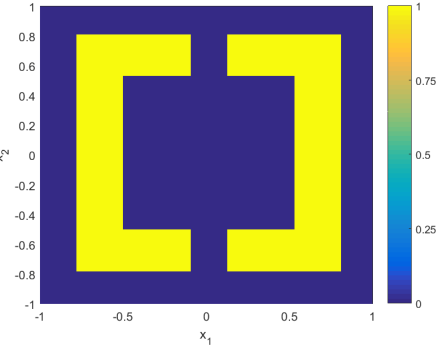


(a) $u^{\dagger}$

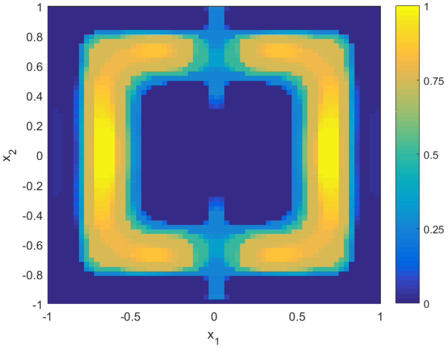


(b) $\alpha = 10^{-3}, \beta = 0$

Numerical example: topology optimization

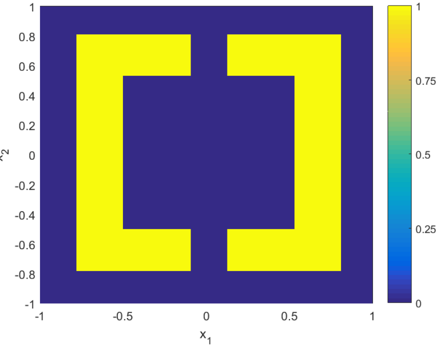


(c) $u^\dagger$

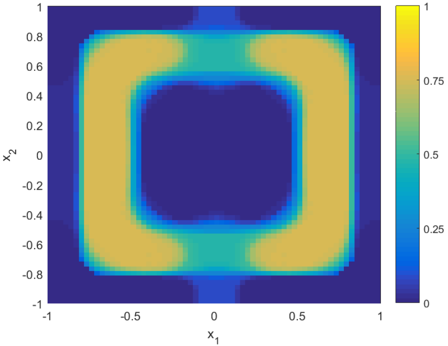


(d) $\alpha = 10^{-3}, \beta = 10^{-6}$

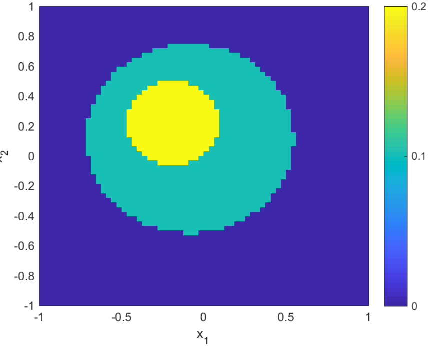
Numerical example: topology optimization



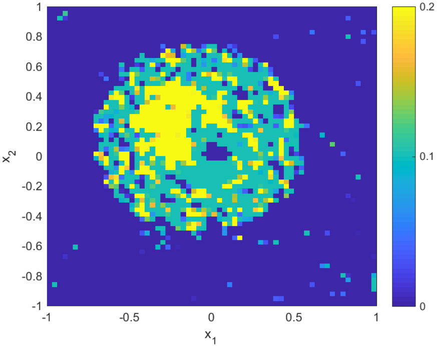
(e) $u^\dagger$



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

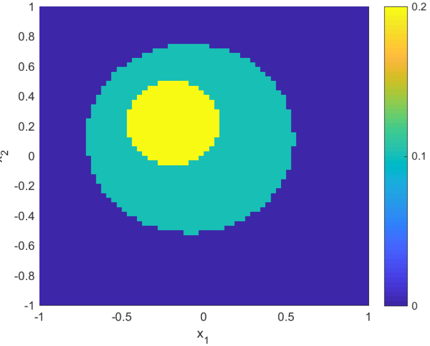


(a) $u^\dagger$

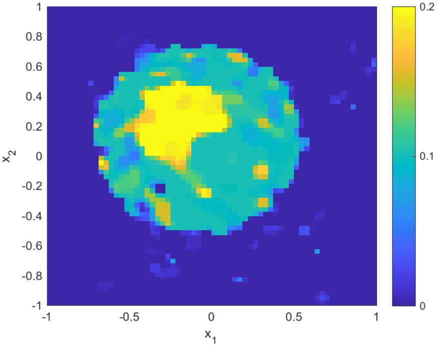


(b) $\alpha = 5 \cdot 10^{-4}, \beta = 0$

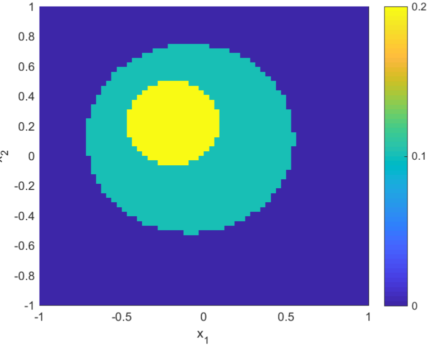
Numerical example: inverse problem



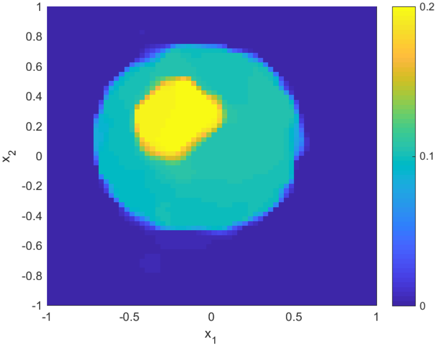
(c) $u^\dagger$



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



(e) $u^{\dagger}$



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

Conclusion

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