

# Convex regularization of discrete-valued inverse problems

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

■ *f* discrepancy term (involving PDEs)

#### U discrete set

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

u<sub>1</sub>,..., u<sub>d</sub> 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 (a = 0)
- ~→ promote  $u(x) \in \{u_1, \ldots, u_d\}$  by convex pointwise penalty

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

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



## • 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
- ••• non-smooth optimization in function spaces



#### 1 Overview

#### 2 Approach

- Convex analysis
- Moreau–Yosida regularization
- Semismooth Newton method
- Multi-bang penalty
- 3 Multi-bang regularization
  - Regularization properties
  - Structure and numerical solution
- 4 Nonlinear problems



 $\mathcal{F}: V \to \overline{\mathbb{R}} := \mathbb{R} \cup \{+\infty\}$  convex, V Banach space, V<sup>\*</sup> dual space

#### subdifferential

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

#### ■ Fenchel conjugate (always convex)

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

"convex inverse function theorem":

$$v^* \in \partial \mathcal{F}(v) \quad \Leftrightarrow \quad v \in \partial \mathcal{F}^*(v^*)$$

# **Fenchel duality: application**



- **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:

$$egin{cases} -ar{p}\in \partial {\mathbb F}(ar{u})\ ar{u}\in \partial {\mathbb G}^*(ar{p}) \end{cases}$$



 $\mathcal{G}$  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** 

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

- single-valued, Lipschitz continuous
- coincides with resolvent (Id + $\gamma \partial G^*$ )<sup>-1</sup>(*p*)
- (also required for primal-dual first-order methods)



### **Proximal mapping**

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

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

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

• equivalent for every  $\gamma > 0$ 

#### single-valued, Lipschitz continuous, implicit



### Proximal mapping

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

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

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

single-valued, Lipschitz continuous, explicit

 nonsmooth operator equation, Newton method



f locally Lipschitz, piecewise  $C^1$ :

$$f(\mathbf{v}) = 0, \qquad f: \mathbb{R}^n \to \mathbb{R}$$

Newton derivative

$$D_N f(v) \delta v \in \partial_C f(v) \delta v$$

Clarke generalized gradient: convex hull of piecewise derivatives

semismooth Newton method

$$D_N f(v^k) \delta v = -f(v^k), \qquad v^{k+1} = v^k + \delta v$$

converges locally superlinearly

f locally Lipschitz, piecewise  $C^1$ :

F(u) = 0,  $F: L^{r}(\Omega) \rightarrow L^{s}(\Omega),$  [F(u)](x) = f(u(x))

Newton derivative

 $[D_N F(u) \delta u](x) \in \partial_C f(\delta u(x)) \delta u(x)$ 

any measurable selection of Clarke generalized gradient

semismooth Newton method

$$D_N F(u^k) \delta u = -F(u^k), \qquad u^{k+1} = u^k + \delta u$$

converges locally superlinearly if r > s

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

#### Approach: pointwise

- **1** compute subdifferential  $\partial g$  (or Fenchel conjugate  $g^*$ )
- 2 compute subdifferential  $\partial g^*$
- 3 compute proximal mapping prox<sub>yq\*</sub>
- 4 compute Moreau–Yosida regularization  $\partial g_{v}^{*}$
- 5 compute Newton derivative  $D_N \partial g_{\nu}^*$
- →→ semismooth Newton method, continuation in γ for superposition operator  $[\partial G_v^*(p)](x) = \partial g_v^*(p(x))$



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

#### piecewise differentiable ~> subdifferential convex hull of derivatives

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

# **Multi-bang penalty**



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

#### convex inverse function theorem:

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

# Multi-bang penalty: sketch



# Multi-bang penalty: sketch



D<sub>E</sub>UIS<sub>EN</sub>URG Open-Minded

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

case-wise inspection of subdifferential:

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

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



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

•  $K: L^2(\Omega) \to Y$  (linear) forward mapping, weakly closed

- $y^{\delta} \in L^2(\Omega)$  noisy data with  $\|y y^{\delta}\|_Y \leqslant \delta$
- $u_1 < \cdots < u_d$  given parameter values (d > 2)
- 9 multi-bang penalty



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

#### ■ 9 multi-bang penalty convex:

1 existence of solution  $u_a^{\delta}$  for every a > 0

2 
$$\delta \rightarrow 0$$
 implies  $u_{\alpha}^{\delta} \rightarrow u_{\alpha}$  for every  $\alpha > 0$ 

3  $\delta \rightarrow$  0,  $a \rightarrow$  0,  $\delta a^{-2} \rightarrow$  0 implies  $u_a^{\delta} \rightharpoonup u^{\dagger}$ 

(standard arguments, e.g. [Burger/Osher 04, Ito/Jin 14])

# **Multi-bang regularization**



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

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

1 a priori choice  $a(\delta) = c\delta$ 2 a posteriori choice  $||Ku_{a(\delta)}^{\delta} - y^{\delta}||_{Y} \le \tau\delta, \tau > 1$ 

→ convergence rate

$$d^{p^{\dagger}}_{\mathfrak{S}}(u^{\delta}_{a},u^{\dagger})\leqslant C\delta$$

in Bregman distance

$$d_{\mathfrak{S}}^{p_1}(u_2, u_1) = \mathfrak{S}(u_2) - \mathfrak{S}(u_1) - \langle p_1, u_2 - u_1 \rangle_X, \qquad p_1 \in \mathfrak{d}\mathfrak{S}(u_1)$$



Pointwise definition of Bregman distance,  $\partial g$ :

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

$$d_g^{p^\dagger(x)}(u_{a(\delta)}^\delta(x),u^\dagger(x)) o 0 \qquad ext{ for }\delta o 0$$

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

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

•  $u_{a(\delta)}^{\delta} \rightarrow u^{\dagger}$  pointwise a.e. iff  $u^{\dagger}(x) \in \{u_1, \dots, u_d\}$  a.e.

■ (convergence not uniform ~>> no pointwise rates)



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

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

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

 $\rightsquigarrow |\{x : K\bar{u}(x) = y^{\delta}(x)\}| = 0 \implies \bar{u} \in \{u_1, \dots, u_d\}$  a.e. (true multi-bang)



$$\begin{cases} p_{\gamma} = \frac{1}{a} K^* (y^{\delta} - K u_{\gamma}) \\ u_{\gamma} = \partial \mathcal{G}^*_{\gamma} (p_{\gamma}) \end{cases}$$

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

# **Regularized optimality system**



$$\begin{cases} p_{\gamma} = \frac{1}{a} K^* (y^{\delta} - K u_{\gamma}) \\ u_{\gamma} = \partial \mathcal{G}^*_{\gamma} (p_{\gamma}) \end{cases}$$

- semismooth Newton method
- inverse source problem:  $K = A^{-1}$ , A elliptic differential operator
- introduce  $y_{\gamma} = Ku_{\gamma}$ , eliminate  $u_{\gamma} = \mathcal{G}^*_{\gamma}(p_{\gamma})$

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



$$\begin{pmatrix} \frac{1}{a} \operatorname{Id} & A^* \\ A & -D_N \mathcal{G}^*_{\gamma}(p) \end{pmatrix} \begin{pmatrix} \delta y \\ \delta p \end{pmatrix} = - \begin{pmatrix} A^* p + \frac{1}{a} (y - y^{\delta}) \\ A y - \mathcal{G}^*_{\gamma}(p) \end{pmatrix}$$

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

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

# **Example: linear inverse problem**

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

$$u^{\dagger}(x) = u_1 + u_2 \chi_{\{x:(x_1 - 0.45)^2 + (x_2 - 0.55)^2 < 0.1\}}(x) + (u_3 - u_2) \chi_{\{x:(x_1 - 0.4)^2 + (x_2 - 0.6)^2 < 0.02\}}(x)$$
$$d = 3, \quad u_1 = 0, \quad u_2 = 0.1, \quad u_3 \in \{0.15, 0.11\}$$

- finite element discretization: uniform grid, 256 × 256 nodes
- $a = a(\delta)$  by Morozov discrepancy principle
- terminate at  $\gamma < 10^{-12}$



















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





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Forward 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

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

semismooth Newton method (regularity condition technical)





**S** : 
$$u \mapsto y$$
 solving

$$-\Delta y + \mathbf{u}y = f$$

- **approach applicable, but**  $\mathcal{F}$  **nonconvex**
- numerical example:  $\Omega = [0, 1]^2$ ,  $f \equiv 1$

• 
$$u^{\dagger}(x) = u_1 + (u_2 - u_1) \chi_{\{x:(x_1 - 0.45)^2 + (x_2 - 0.55)^2 < 0.1\}}(x)$$
  
+  $(u_3 - u_2 - u_1) \chi_{\{x:(x_1 - 0.4)^2 + (x_2 - 0.6)^2 < 0.02\}}(x)$ 

•  $y^{\delta} = S(u^{\dagger}) + \xi$ •  $a = 3 \cdot 10^{-5}, \quad \gamma \to 10^{-12}$ 

# Numerical example: nonlinear problem





(a) noisy data  $y^{\delta}$ 

# Numerical example: nonlinear problem







#### Goal: application to EIT

**S** :  $u \mapsto y$  solving

$$-\nabla \cdot (\boldsymbol{u} \nabla \boldsymbol{y}) = \boldsymbol{f}$$

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

- 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  $H_{\gamma}$  (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  $||Du||_{\mathcal{M}} \longrightarrow u \in BV(\Omega) \cap L^{\infty}(\Omega) \hookrightarrow_{c} L^{p}(\Omega)$

### Difficulty:

■ existence requires box constraints ~→ 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,  $L^{\infty}$ 

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

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





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

- existence of optimal  $\bar{u} \in BV(\Omega) \cap L^{\infty}(\Omega)$  for  $\varepsilon \ge 0$
- 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  $L^{\infty}(\Omega)^{*}$ )
- $\rightarrow$  sum rule applicable, subgradients in  $L^r(\Omega)$ , r > 1

# TV regularization: optimality conditions



- $F'(\Phi_{\varepsilon}(\bar{u})) = (\nabla \bar{y} \cdot \nabla \bar{p}) \in L'(\Omega)$  (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]
- vointwise optimality conditions
- semi-smooth Newton (after discretization, regularization)

# Numerical example: total variation





# Numerical example: total variation





# Conclusion



- Convex relaxation of discrete regularization:
  - well-posed regularization method
  - pointwise convergence under general assumptions
  - strong structural regularization
  - efficient numerical solution (superlinear convergence)

Outlook:

- (heuristic) parameter choice
- nonlinear inverse problems: EIT
- vector-valued multibang
- other hybrid discrete-continuous problems

#### Preprint, MATLAB/Python codes:

http://www.uni-due.de/mathematik/agclason/clason\_pub.php