



Convex relaxation of (some) hybrid discrete-valued optimization problems

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Motivation: hybrid discrete optimization

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

- $\mathcal{F}$ tracking, 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

Motivation: penalty

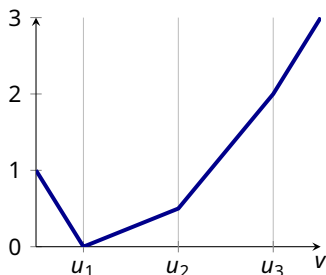
- **convex relaxation**: replace U by convex hull $u(x) \in [u_1, u_d]$
- works only for $d = 2$, cf. bang-bang control ($\alpha = 0$)
- $\leadsto$ promote $u(x) \in \{u_1, \dots, u_d\}$ by **convex pointwise penalty**

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

- 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 $\frac{1}{2}u^2 + \delta_U$
- **multi-bang** (generalized bang-bang) control
- $\leadsto$ non-smooth optimization in function spaces

1 Overview

2 Approach

- Convex analysis
- Moreau–Yosida regularization
- Semismooth Newton method

3 Multi-bang penalty

4 Vector-valued multi-bang penalty

Convex analysis: motivation

$f : \mathbb{R} \rightarrow \mathbb{R}$ differentiable:

■ derivative:

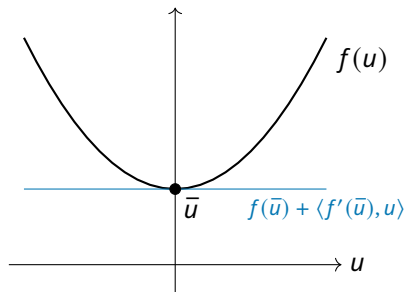
$$f'(u) = \lim_{h \rightarrow 0} \frac{f(u+h) - f(u)}{h}$$

■ geometrically:

$f'(u)$ tangent slope

■ $f(\bar{u}) = \min_u f(u) \Rightarrow f'(\bar{u}) = 0$

■ calculus for f'



Convex relaxation: motivation

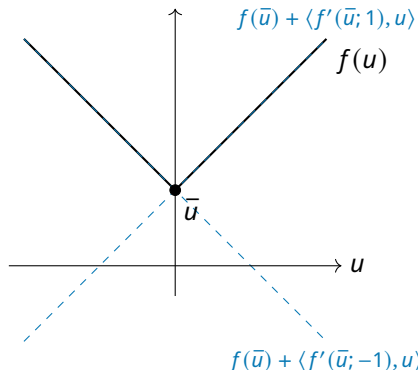
$f : \mathbb{R} \rightarrow \mathbb{R}$ not differentiable, **convex**:

■ **directional derivative**:

$$f'(u; h) = \lim_{t \rightarrow 0^+} \frac{f(u + th) - f(u)}{t}$$

■ **but**: for all h ,

$$f'(\bar{u}; h) \neq 0$$



Convex relaxation: motivation

$f : \mathbb{R} \rightarrow \mathbb{R}$ not differentiable, **convex**:

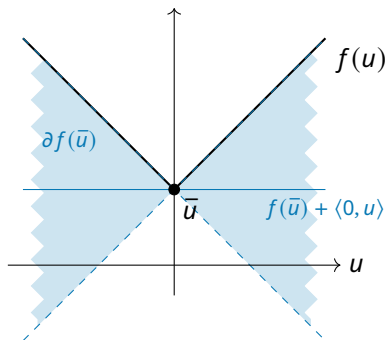
- **subdifferential**:

$$\partial f(u) = \{u^* : \langle u^*, h \rangle \leq f'(u; h)\}$$

- geometrically: $\partial f(u)$ **set of tangent slopes**

- $f(\bar{u}) = \min_u f(u) \Rightarrow 0 \in \partial f(\bar{u})$

- calculus for ∂f **under regularity conditions**



Fenchel duality

$\mathcal{F} : V \rightarrow \overline{\mathbb{R}} := \mathbb{R} \cup \{+\infty\}$ convex, V Banach space, V^* dual space

■ subdifferential

$$\partial \mathcal{F}(\bar{v}) = \{v^* \in V^* : \langle v^*, v - \bar{v} \rangle_{V^*, V} \leq \mathcal{F}(v) - \mathcal{F}(\bar{v}) \text{ for all } v \in V\}$$

■ Fenchel conjugate (always convex)

$$\mathcal{F}^* : V^* \rightarrow \overline{\mathbb{R}}, \quad \mathcal{F}^*(v^*) = \sup_{v \in V} \langle v^*, v \rangle_{V^*, V} - \mathcal{F}(v)$$

■ “convex inverse function theorem” (if $\mathcal{F}$ lower semicontinuous)

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

Fenchel duality: example

■ $\mathcal{G} : V \rightarrow \mathbb{R}, \quad v \mapsto \|v\|_V:$

$$\mathcal{G}^* : V^* \rightarrow \overline{\mathbb{R}}, \quad v^* \mapsto \delta_{\{\|\cdot\|_{V^*} \leq 1\}}(v^*) := \begin{cases} 0 & \text{if } \|v^*\|_{V^*} \leq 1 \\ \infty & \text{else} \end{cases}$$

■ $\mathcal{G} : V \rightarrow \overline{\mathbb{R}}, \quad v \mapsto \delta_{\{\|\cdot\|_V \leq 1\}}(v):$

$$\partial \mathcal{G}(\bar{v}) = \{v^* \in V^* : \langle v^*, v - \bar{v} \rangle_{V^*, V} \leq 0 \text{ for all } \|v\|_V \leq 1\}$$

↪ box-constrained optimization

Fenchel duality: application

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

- 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:

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

Regularization

$\mathcal{G}$ non-smooth $\leadsto$ subdifferential $\partial\mathcal{G}^*$ set-valued $\leadsto$ **regularize**

$u, p \in L^2(\Omega)$ Hilbert space $\leadsto$ consider for $\gamma > 0$

Proximal mapping

$$\text{prox}_{\gamma\mathcal{G}^*}(p) = \arg \min_w \mathcal{G}^*(w) + \frac{1}{2\gamma} \|w - p\|^2$$

- single-valued, Lipschitz continuous
- coincides with **resolvent** $(\text{Id} + \gamma\partial\mathcal{G}^*)^{-1}(p)$
- (also required for primal-dual first-order methods)

Regularization

Proximal mapping

$$\text{prox}_{\gamma \mathcal{G}^*}(p) = \arg \min_w \mathcal{G}^*(w) + \frac{1}{2\gamma} \|w - p\|^2$$

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

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

- **equivalent** for every $\gamma > 0$
- single-valued, Lipschitz continuous, **implicit**

Regularization

Proximal mapping

$$\text{prox}_{\gamma \mathcal{G}^*}(p) = \arg \min_w \mathcal{G}^*(w) + \frac{1}{2\gamma} \|w - p\|^2$$

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

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

- $\partial \mathcal{G}_\gamma^* = \partial \left(\mathcal{G} + \frac{\gamma}{2} \|\cdot\|^2 \right)^* \rightarrow \partial \mathcal{G}^*$ as $\gamma \rightarrow 0$ (no smoothing of $\mathcal{G}$!)
- single-valued, Lipschitz continuous, explicit
 $\leadsto$ nonsmooth operator equation, Newton method

Regularization: example

$$\mathcal{G}^* : V^* \rightarrow \overline{\mathbb{R}}, \quad p \mapsto \delta_{\{\|\cdot\|_{V^*} \leq 1\}}(p):$$

- Proximal mapping:

$$\text{prox}_{\mathcal{G}^*}(p) = \text{proj}_{\{\|\cdot\|_{V^*} \leq 1\}}(p)$$

- Moreau–Yosida regularization ($V^* = L^\infty(\Omega)$):

$$\partial \mathcal{G}_Y^*(p) = \frac{1}{Y} (\max(0, p - 1) + \min(0, p + 1))$$

(max, min pointwise almost everywhere)

Generalized Newton method

Consider Banach spaces X, Y , mapping $F : X \rightarrow Y$

Newton-type method for $F(x) = 0$

- choose $x^0 \in X$ (close to solution x^*)
- for $k = 0, 1, \dots$
 - 1 choose $M_k \in \mathcal{L}(X, Y)$ invertible
 - 2 solve for s^k :

$$M_k s^k = -F(x^k)$$

- 3 set $x^{k+1} = x^k + s^k$

Convergence of Newton method

Set $d^k = x^k - x^* \leadsto$

$$\frac{\|x^{k+1} - x^*\|_X}{\|x^k - x^*\|_X} = \frac{\|M_k^{-1}(F(x^* + d^k) - F(x^*) - M_k d^k)\|_X}{\|d^k\|_X}$$

$\leadsto$ superlinear convergence if

1 regularity condition

$$\|M_k^{-1}\|_{\mathcal{L}(Y,X)} \leq C \quad \text{for all } k$$

2 approximation condition

$$\lim_{\|d^k\|_X \rightarrow 0} \frac{\|F(x^* + d^k) - F(x^*) - M_k d^k\|_Y}{\|d^k\|_X} = 0$$

Semismooth Newton method

Goal: define **Newton derivative** $M_k =: D_N F(x^k)$ such that

$$x^{k+1} = x^k - D_N F(x^k)^{-1} F(x^k)$$

converges **superlinearly** for $F(x) = 0$ **nonsmooth**

- $\mathbb{R}^n$: F Lipschitz $\leadsto D_N F$ from Clarke subdifferential (Rademacher)
[Mifflin 1977, Kummer 1992, Qi/Sun 1993]
- **function space**: Clarke subdifferential not explicit
 $\leadsto$ define $D_N F$ via approximation condition
[Chen/Nashed/Qi 2000, Hintermüller/Ito/Kunisch 2002]
- $f : \mathbb{R} \rightarrow \mathbb{R}$ semismooth $\leadsto$ **superposition operator**
 $F : L^p(\Omega) \rightarrow L^q(\Omega)$ semismooth for $p > q$
[Ulbrich 2002/03/11, Schiela 2008]

Semismooth Newton method

f locally Lipschitz, piecewise C^1 :

$$f(v) = 0, \quad f : \mathbb{R}^n \rightarrow \mathbb{R}$$

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

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

converges **locally superlinearly**

Semismooth Newton method

f locally Lipschitz, piecewise C^1 :

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

Newton derivative

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

any measurable selection of Clarke generalized gradient

semismooth Newton method

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

converges locally superlinearly if $r > s$

Semismooth functions: example

■ $f : \mathbb{R} \rightarrow \mathbb{R}, \quad t \mapsto \max(0, t)$

$$D_N f(t) \in \partial_C f(t) = \begin{cases} \{0\} & t < 0 \\ \{1\} & t > 0 \\ [0, 1] & t = 0 \end{cases}$$

■ $F : L^p(\Omega) \rightarrow L^q(\Omega), \quad u(x) \mapsto \max(0, u(x)), \quad p > q$

$$[D_N F(u)h](x) = \begin{cases} 0 & u(x) < 0 \\ h(x) & u(x) \geq 0 \end{cases}$$

→ Moreau–Yosida regularization semismooth

Numerical solution: summary

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

Approach: pointwise

- 1 compute subdifferential ∂g (or Fenchel conjugate g^*)
 - 2 compute 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 $[\partial \mathcal{G}_{\gamma}^*(p)](x) = \partial g_{\gamma}^*(p(x))$

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Formulation

$$\begin{cases} \min_{u \in L^2(\Omega)} \frac{1}{2} \|y - z\|_{L^2}^2 + \alpha \mathcal{G}(u) \\ \text{s. t. } Ay = u, \quad u_1 \leq u(x) \leq u_d \text{ a.e.} \end{cases}$$

- $u_1 < \dots < u_d$ given parameter values ($d > 2$)
- $z \in L^2(\Omega)$ target (or noisy data)
- $A : V \rightarrow V^*$ isomorphism for Hilbert space $V \hookrightarrow L^2(\Omega) \hookrightarrow V^*$
(e.g., elliptic differential operator with boundary conditions)
- $\leadsto \mathcal{F}(u) = \frac{1}{2} \|A^{-1}u - z\|_{L^2}^2$ smooth
- $\mathcal{G}$ multi-bang penalty (will include control constraints from now)

Multi-bang 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

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

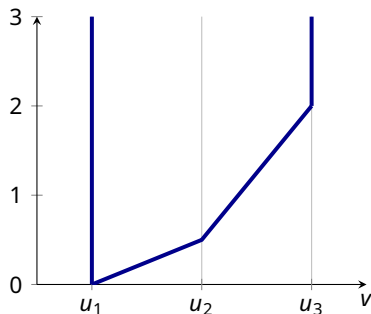
Multi-bang penalty

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

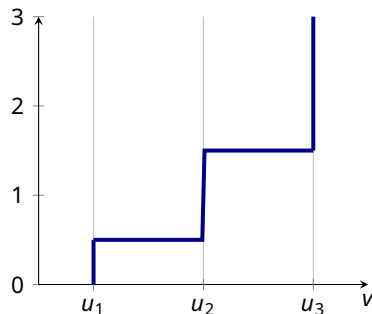
convex inverse function theorem:

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

Multi-bang penalty: sketch

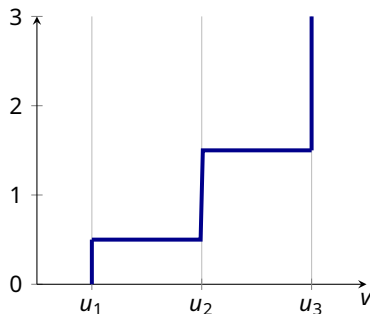


(a) $g(u_1 = 0, u_2 = 1, u_3 = 2)$

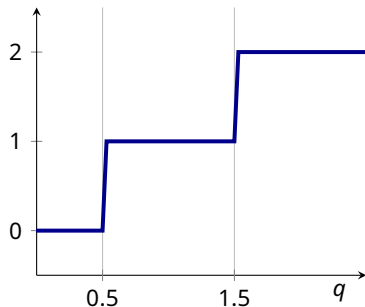


(b) $\partial g(u_1 = 0, u_2 = 1, u_3 = 2)$

Multi-bang penalty: sketch



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



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

Optimality system

$$\bar{p} = \frac{1}{\alpha} S^*(z - S\bar{u})$$

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

■ $S : u \mapsto y$ control-to-state mapping, S^* adjoint

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

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

■ for suitable A , $\bar{p}(x)$ constant implies $[A^* \bar{p}](x) = [z - \bar{y}](x) = 0$

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

Moreau–Yosida regularization

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

case-wise inspection of subdifferential:

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

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

Regularized optimality system

$$\begin{cases} p_Y = \frac{1}{\alpha} S^*(z - Su_Y) \\ u_Y = \partial \mathcal{G}_Y^*(p_Y) \end{cases}$$

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

Regularized optimality system

$$\begin{cases} A^* p_Y = \frac{1}{\alpha} (z - y_Y) \\ A y_Y = \mathcal{G}_Y^*(p_Y) \end{cases}$$

- optimality conditions for $\mathcal{F}(u) + \alpha \mathcal{G}(u) + \frac{\gamma}{2} \|u\|^2$
- $\leadsto$ unique solution (u_Y, p_Y)
- $(u_Y, p_Y) \rightarrow (\bar{u}, \bar{p})$ as $\gamma \rightarrow 0$
- ∂g_Y^* Lipschitz continuous, piecewise C^1 , norm gap $V \hookrightarrow L^2(\Omega)$
- $\leadsto$ **semismooth Newton method**
- introduce $y_Y = S u_Y$, eliminate $u_Y = \mathcal{G}_Y^*(p_Y)$

Semismooth Newton method

$$\begin{pmatrix} \frac{1}{\alpha} \text{Id} & A^* \\ A & -D_N \mathcal{G}_Y^*(p) \end{pmatrix} \begin{pmatrix} \delta y \\ \delta p \end{pmatrix} = - \begin{pmatrix} A^* p + \frac{1}{\alpha}(y - z) \\ Ay - \mathcal{G}_Y^*(p) \end{pmatrix}$$

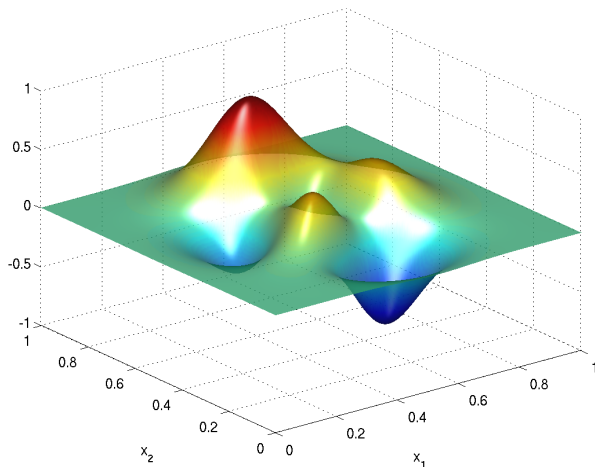
$$[D_N \mathcal{G}_Y^*(p) \delta p](x) = \begin{cases} \frac{1}{Y} \delta p(x) & p(x) \in Q_{i,i+1}^Y \\ 0 & \text{else} \end{cases}$$

- symmetric, but: local convergence
- $\leadsto$ continuation in $\gamma \rightarrow 0$
- $\leadsto$ backtracking line search based on residual norm
- only number of sets Q_i^Y depends on $d \leadsto$ **linear complexity**

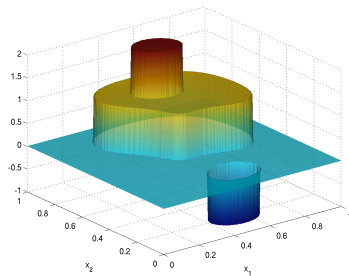
Numerical example

- $\Omega = [0, 1]^2$, $A = -\Delta$
- finite element discretization: uniform grid, 256×256 nodes
- state, adjoint: piecewise linear
- parameter: eliminated (variational discretization)
- $d = 5$, $(u_1, \dots, u_5) = (-2, 1, 0, 1, 2)$
- $\gamma = 0$: regularized active sets empty, true multi-bang
 $\gamma > 0$: terminated with 2–21 nodes in regularized active sets

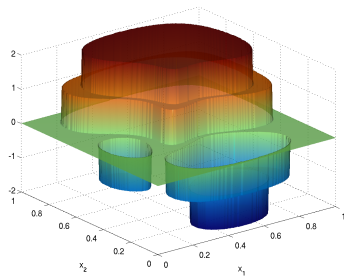
Numerical examples: desired state



Multi-bang controls

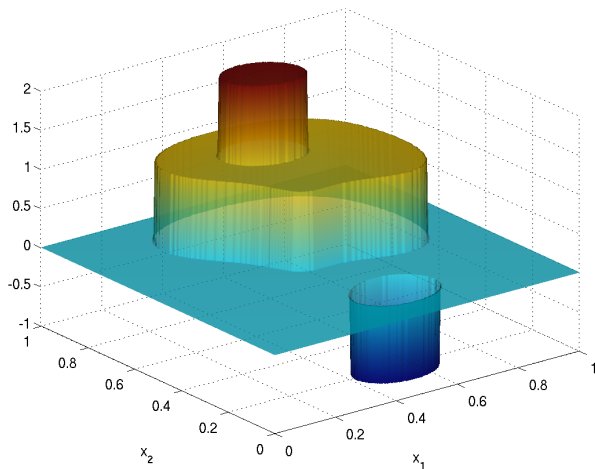


(a) $\alpha = 5 \cdot 10^{-3}$ ($\gamma = 0$)



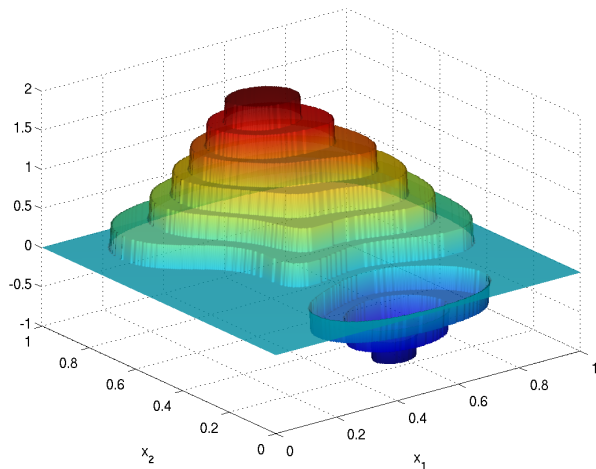
(b) $\alpha = 10^{-3}$ ($\gamma \approx 10^{-7}$)

Parameters: effect of d



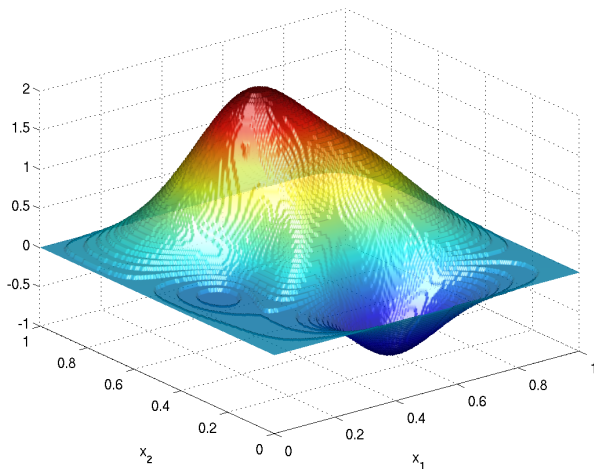
(a) $d = 5$ ($\gamma = 0$)

Parameters: effect of d



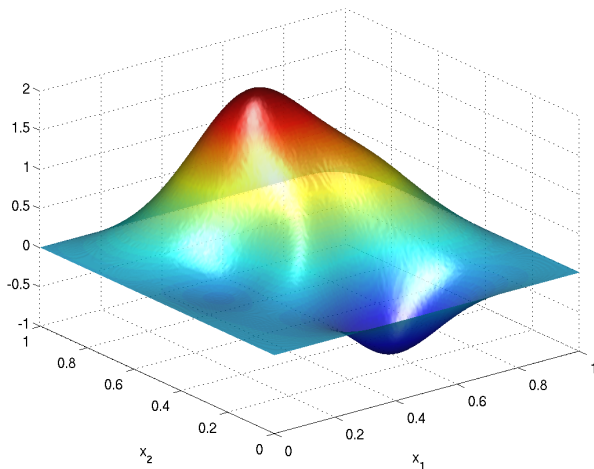
(b) $d = 15$ ($\gamma = 0$)

Parameters: effect of d



(c) $d = 101$ ($\gamma \approx 10^{-9}$)

Parameters: effect of d



(d) $d = 1001$ ($\gamma \approx 10^{-11}$)

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Vector-valued multi-bang control

Discrete **vector-valued** controls $u : \Omega \rightarrow U \subset \mathbb{R}^m$

Example: optimal control of **Bloch equation**: $\Omega = [0, T]$, $m = 2$

$$\frac{d}{dt}M(t) = M(t) \times B(t), \quad M(0) = M_0$$

- $M(t) \in \mathbb{R}^3$ describes temporal evolution of spin ensemble
- $B(t) = (u_1(t), u_2(t), \omega)^T$ **controlled** time-dependent magnetic field
- ω resonance frequency (material parameter)
- applications in magnetic resonance imaging, spectroscopy
- control-to-state mapping $S : u \rightarrow M$ **bilinear** ($\leadsto$ chain rule, Clarke)

Vector-valued multi-bang: penalty

Here: admissible control set U of d radially distributed states, origin

$$U = \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \omega_0 \cos \theta_1 \\ \omega_0 \sin \theta_1 \end{pmatrix}, \dots, \begin{pmatrix} \omega_0 \cos \theta_d \\ \omega_0 \sin \theta_d \end{pmatrix} \right\}$$

■ fixed **amplitude** $\omega_0 > 0$

■ **phases** $0 \leq \theta_1 < \dots < \theta_d < 2\pi$

multi-bang penalty $g = \left(\frac{1}{2}|\cdot|_2^2 + \delta_U\right)^{**}$ convex envelope

$$\begin{aligned} g^*(q) &= \left(\left(\frac{1}{2}|\cdot|_2^2 + \delta_U \right)^{**} \right)^* (q) = \left(\frac{1}{2}|\cdot|_2^2 + \delta_U \right)^* (q) \\ &= \begin{cases} 0 & \langle q, u_i \rangle \leq \frac{1}{2}\omega_0^2 \text{ for all } 1 \leq i \leq d \\ \langle q, u_i \rangle - \frac{1}{2}\omega_0^2 & \frac{\theta_{i-1} + \theta_i}{2} \leq \angle q \leq \frac{\theta_i + \theta_{i+1}}{2}, \langle q, u_i \rangle \geq \frac{1}{2}\omega_0^2 \end{cases} \end{aligned}$$

Vector-valued multi-bang: subdifferential

Fenchel conjugate

$$g^*(q) = \begin{cases} 0 =: u_0 & q \in \bar{Q}_0 \\ \langle q, u_i \rangle - \frac{1}{2}\omega_0^2 & q \in \bar{Q}_i \end{cases}$$

Subdifferential

$$\partial g^*(q) = \begin{cases} \{u_i\} & q \in Q_i & 0 \leq i \leq d \\ \text{co} \{u_{i_1}, \dots, u_{i_k}\} & q \in Q_{i_1 \dots i_k} & 0 \leq i_1, \dots, i_k \leq d \end{cases}$$

Vector-valued multi-bang: subdifferential

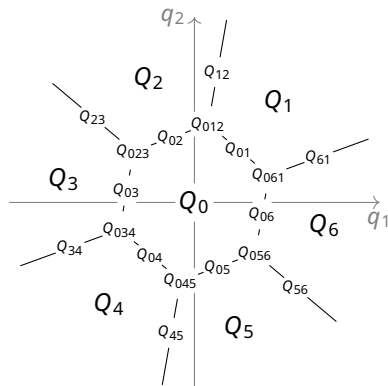
Subdifferential

$$\partial g^*(q) = \begin{cases} \{u_i\} & q \in Q_i \quad 0 \leq i \leq d \\ \text{co} \{u_{i_1}, \dots, u_{i_k}\} & q \in Q_{i_1 \dots i_k} \quad 0 \leq i_1, \dots, i_k \leq d \end{cases}$$

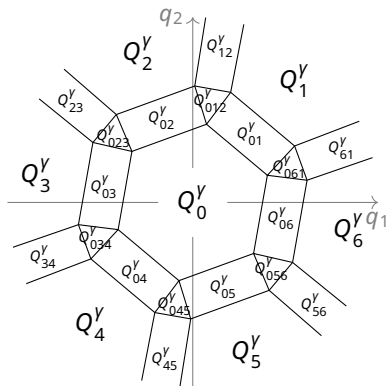
Moreau–Yosida regularization

$$(\partial g^*)_Y(q) = \begin{cases} u_i & q \in Q_i^Y \\ \left(\frac{\langle q, u_i \rangle}{\gamma \omega_0^2} - \frac{\alpha}{2\gamma} \right) u_i & q \in Q_{0,i}^Y \\ \frac{u_i + u_{i+1}}{2} + \frac{\langle q, u_i - u_{i+1} \rangle (u_i - u_{i+1})}{\gamma |u_i - u_{i+1}|_2^2} & q \in Q_{i,i+1}^Y \\ \frac{q}{\gamma} - \frac{\alpha}{\gamma} \left(\frac{\omega_0}{|u_i + u_{i+1}|_2} \right)^2 (u_i + u_{i+1}) & q \in Q_{0,i+1}^Y. \end{cases}$$

Vector-valued multi-bang: subdifferential



(a) subdomains for ∂g^*

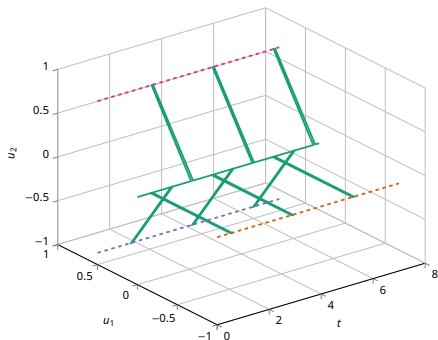


(b) subdomains for $(\partial g^*)_y$

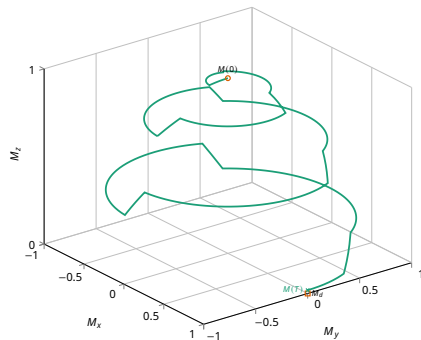
Vector-valued multi-bang: examples

- goal: shift magnetization from $M_0 = (0, 0, 1)^T$ at $t = 0$
to $M_d = (1, 0, 0)^T$ at $t = T$
- $d = 3, 6$ radially distributed admissible control states
- $n = 1, 4$ isochromats with different resonance frequencies
 - 1 shift **all** isochromats
 - 2 shift **only one** isochromat
- $\alpha = 10^{-1}, \omega_0 = 1$
- example motivated by [Dridi/Lapert/Salomon/Glaser/Sugny '15]
- matrix-free Krylov method for semismooth Newton step
- discretization, adjoint from [Aigner/Clason/Rund/Stollberger '16]

Vector-valued multi-bang: examples



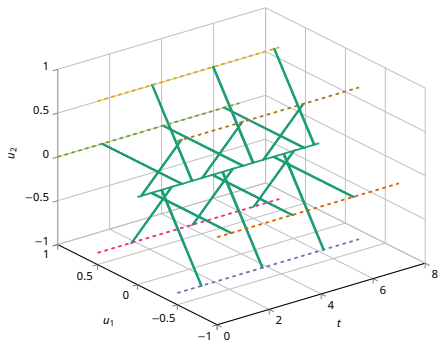
(a) control $u(t)$



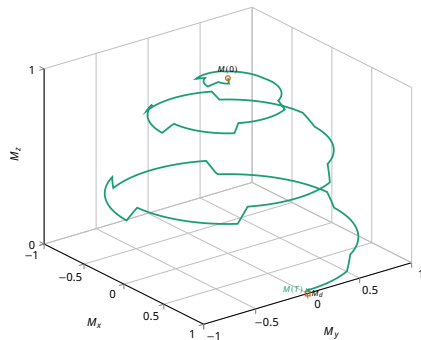
(b) state $M(t)$

Figure: $n = 1$ isochromat, $d = 3$ control states

Vector-valued multi-bang: examples



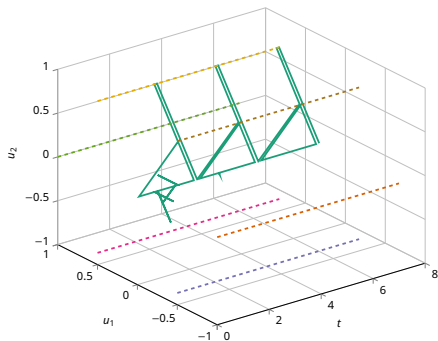
(a) control $u(t)$



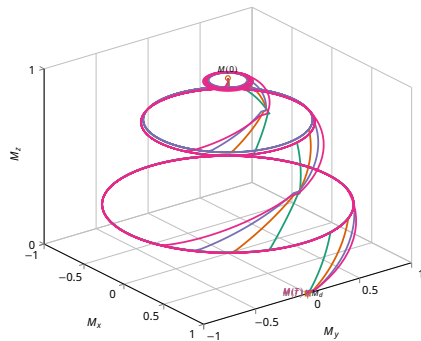
(b) state $M(t)$

Figure: $n = 1$ isochromat, $d = 6$ control states

Vector-valued multi-bang: examples



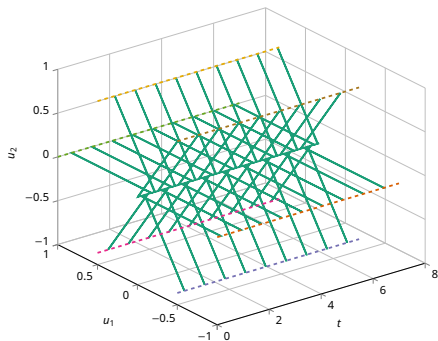
(a) control $u(t)$



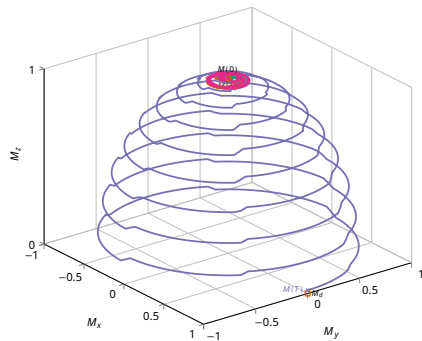
(b) state $M(t)$

Figure: $n = 4$ isochromats, same target

Vector-valued multi-bang: examples



(a) control $u(t)$



(b) state $M(t)$

Figure: $J = 4$ isochromats, different targets

Vector-valued multi-bang: elasticity

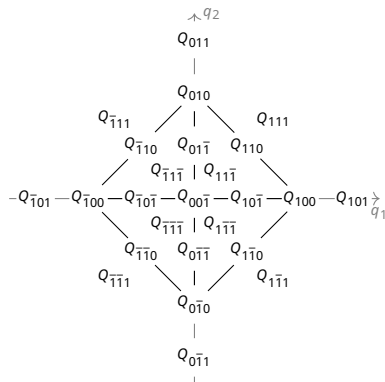
Linear elasticity: $S : u \mapsto y$ solving

$$\begin{cases} -2\mu \operatorname{div} \epsilon(y) - \lambda \operatorname{grad} \operatorname{div} y = u & \text{in } \Omega, \\ y = 0 & \text{on } \Gamma, \\ (2\mu \epsilon(y) + \lambda \operatorname{div} y)n = 0 & \text{on } \partial\Omega \setminus \Gamma \end{cases}$$

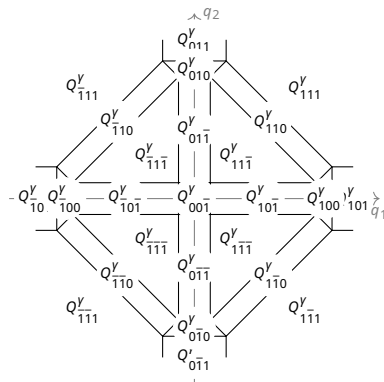
Concentric admissible set (without origin!)

$$U = \left\{ \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ -1 \end{pmatrix}, \begin{pmatrix} 2 \\ 2 \end{pmatrix}, \begin{pmatrix} 2 \\ -2 \end{pmatrix}, \begin{pmatrix} -2 \\ 2 \end{pmatrix}, \begin{pmatrix} -2 \\ -2 \end{pmatrix} \right\}$$

Vector-valued multi-bang: elasticity



(a) subdomains for ∂g^*



(b) subdomains for $(\partial g^*)_y$

Vector-valued multi-bang: elasticity

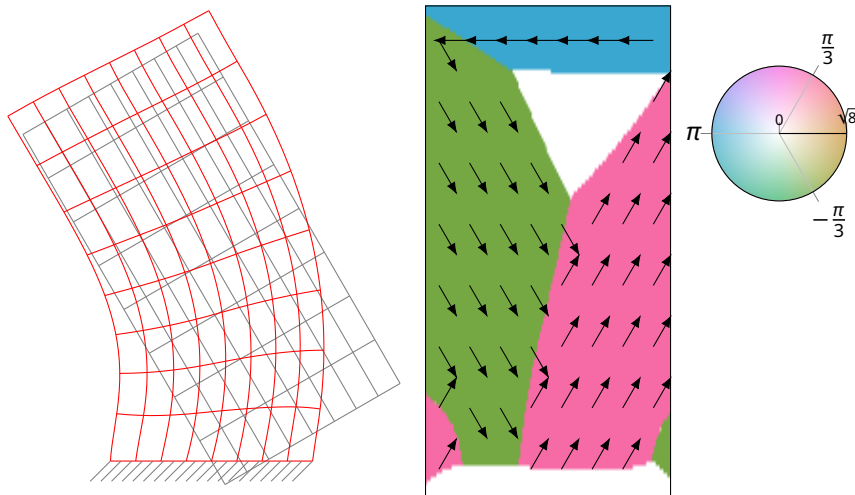


Figure: radial, $d = 3$, $\alpha = 10^{-3}$ (grey: prescribed, red: achieved deformation)

Vector-valued multi-bang: elasticity

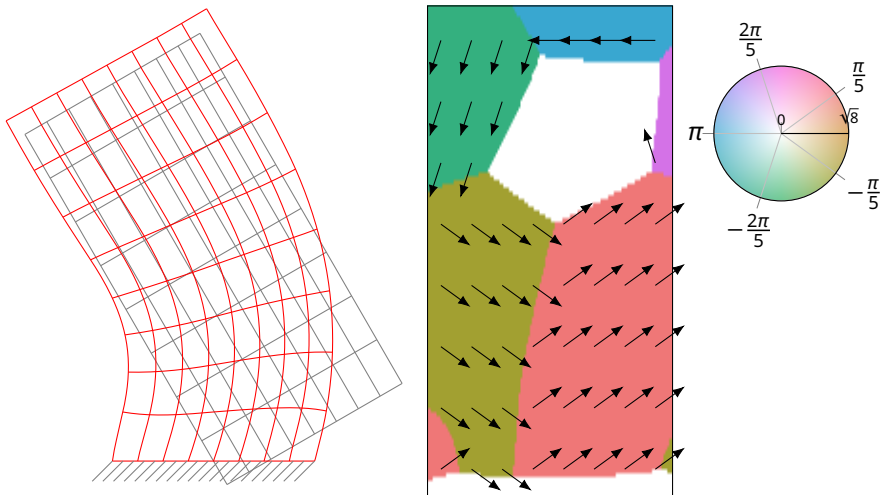


Figure: radial, $d = 5$, $\alpha = 10^{-3}$ (grey: prescribed, red: achieved deformation)

Vector-valued multi-bang: elasticity

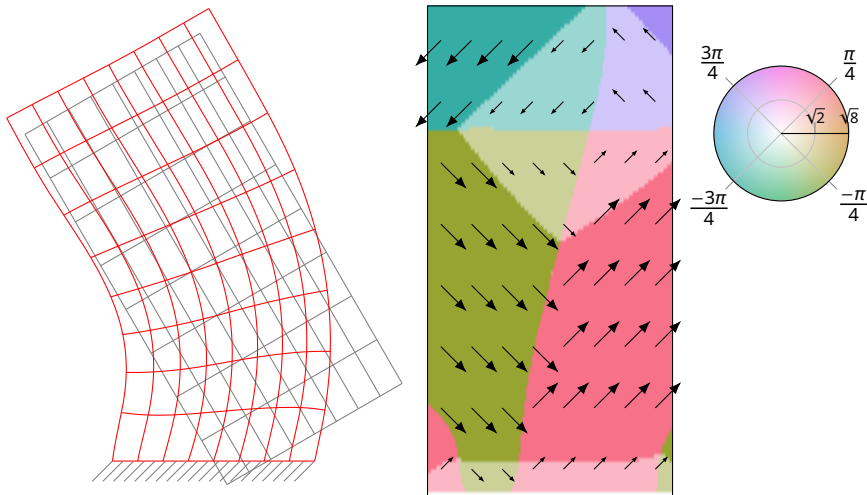


Figure: concentric, $\alpha = 10^{-3}$ (grey: prescribed, red: achieved deformation)

Vector-valued multi-bang: elasticity

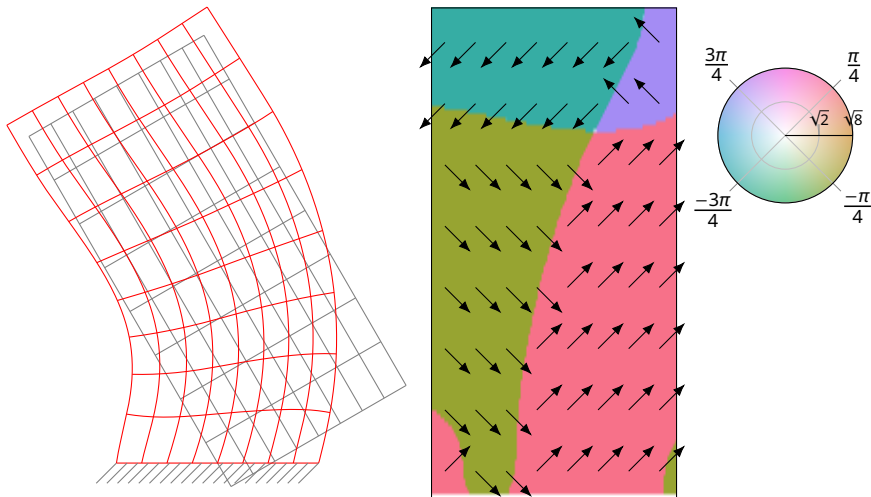


Figure: concentric, $\alpha = 10^{-5}$ (grey: prescribed, red: achieved deformation)

Vector-valued multi-bang: elasticity

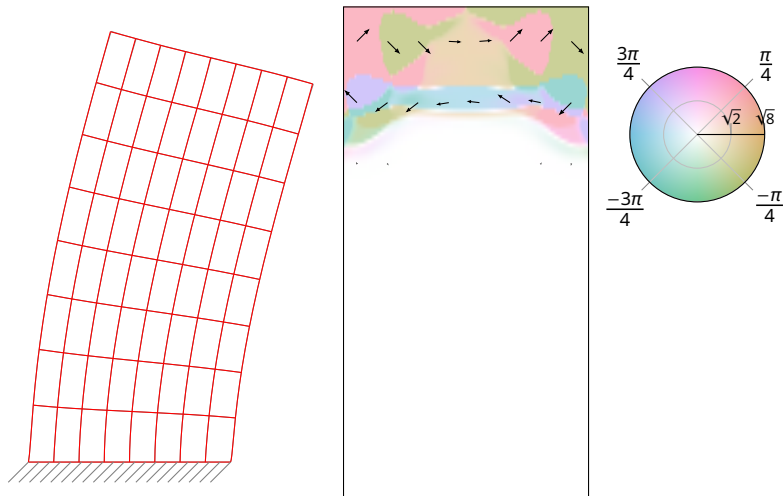


Figure: concentric, $\alpha = 10^{-5}$ (grey: prescribed, red: achieved deformation)

Vector-valued multi-bang: elasticity

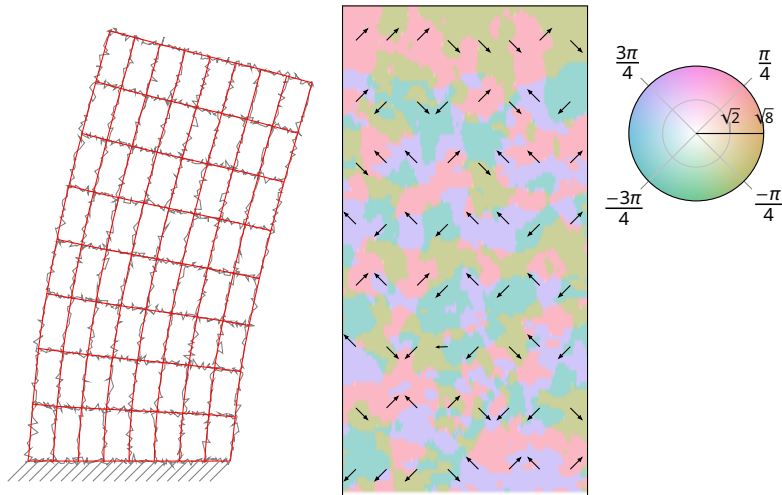


Figure: concentric, $\alpha = 10^{-5}$ (grey: prescribed, red: achieved deformation)

Vector-valued multi-bang: multimaterial transport

Multimaterial transport on graph (V, E) : S graph divergence

$$Su(x) = \sum_{e \in E \text{ to } x} u(e) - \sum_{e \in E \text{ from } x} u(e)$$

$\leadsto$ tracking term penalizes material loss

$$U = \{u \in \mathbb{R}^m \mid u_i \in \{0, m_i\} \text{ or } u_i \in \{0, -m_i\} \text{ for } i = 1, \dots, m\}$$

$\leadsto$ transport of all masses $m_i (= 1)$ in same direction (same sign)

Here: multibang penalty $\simeq$ transport costs

$$g(u) = |u|_2 + \delta_U$$

Vector-valued multi-bang: multimaterial transport

Here: multibang penalty $\simeq$ transport costs

$$g(u) = |u|_2 + \delta_U$$

$\leadsto$ algorithmic computation of proximal mapping:

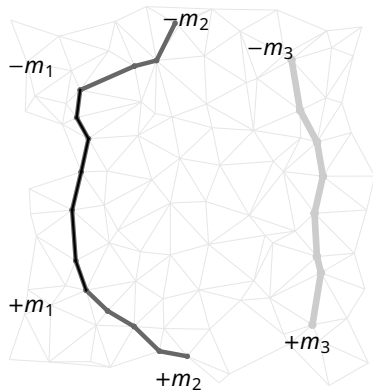
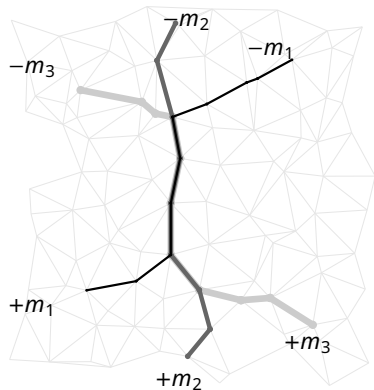
- 1 enumerate all faces of

$$\text{epi } g^* = \{(q, t) \in \mathbb{R}^{m+1} : t \geq \langle \bar{u}_i, q \rangle - \alpha |\bar{u}_i|_2 \text{ for } i \in I\}$$

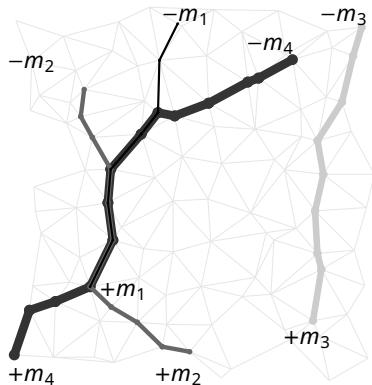
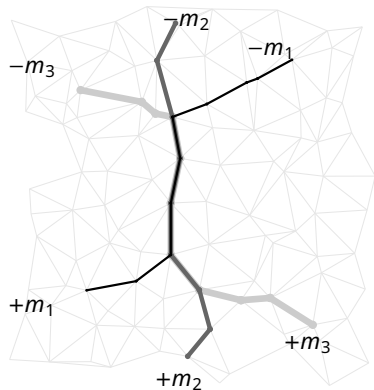
(linear program, precompute!)

- 2 for each face, precompute linear system for $(\text{Id} + \gamma \partial g^*)^{-1}$
- 3 for given q , evaluate linear system for each face and pick correct face (inequalities)

Vector-valued multi-bang: multimaterial transport



Vector-valued multi-bang: multimaterial transport



Conclusion

Discrete controls:

- can be promoted by **convex penalty**
- **linear complexity** in number of parameter values
- $\leadsto$ efficient numerical solution (**superlinear convergence**)
- applicable to **vector-valued** problems

Outlook:

- nonlinear inverse problems: **seismic imaging**
- combination with **total variation regularization**
- **conditional gradient methods?**
- other discrete–continuous problems: **switching**, state diagrams

Papers, Code: <https://imsc.uni-grat.at/clason/publications>

SIREV paper: <https://arxiv.org/abs/2108.10077>

Textbook: <https://arxiv.org/abs/2001.00216>