



Optimal control of non-smooth partial differential equations

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- 1 Overview
 - Non-smooth equations
 - Optimality conditions
- 2 Semilinear PDE
 - Optimality conditions
 - Numerical solution
- 3 Quasilinear PDEs
 - Optimality conditions
 - Numerical solution

Motivation: non-smooth equations

Non-smooth equations:

- describe models with **sharp phase transitions**
- dual formulation of **variational inequalities**
- examples: **free boundary problems** (ice–water), contact problems with friction, non-Newtonian fluid flow, ...

Two-phase Stefan problem

$$\langle -y, \varphi_t \rangle + \langle \nabla \theta(y), \nabla \varphi \rangle = \langle u, \varphi \rangle \quad \text{for all } \varphi \in H^1(Q) \text{ with } \varphi(\cdot, T) = 0$$

$$\theta(y(x, t)) = \begin{cases} y(x, t) & y(x, t) \leq 0 \\ 0 & y(x, t) \in [0, 1] \\ y(x, t) - 1 & y(x, t) \geq 1 \end{cases}$$

Motivation: non-smooth equations

Model problem 1: **semilinear** “Saran wrap equation”

$$\begin{aligned} -\Delta y + \max\{0, y\} &= u \\ y|_{\partial\Omega} &= 0 \end{aligned}$$

- superposition operator: $\max : L^2(\Omega) \rightarrow L^2(\Omega)$ **pointwise** a.e.
- model for membrane partially in water: y deflection, u force
- can be extended to arbitrary Lipschitz $f(y)$
- well-posed (in suitable spaces)
- $u \mapsto y$ nonlinear, Lipschitz (in suitable spaces)
- $u \mapsto y$ **not Gâteaux** differentiable unless $|\{x : y(x) = 0\}| = 0$

Motivation: non-smooth equations

Model problem 2: **quasilinear** heat conduction

$$\begin{aligned} -\nabla \cdot [a(y)\nabla y] &= u \\ y|_{\partial\Omega} &= 0 \end{aligned}$$

- superposition operator $a : L^2(\Omega) \rightarrow L^2(\Omega)$ **pointwise** a.e.
- $a : \mathbb{R} \rightarrow \mathbb{R}$ bounded from below, Lipschitz (or PC¹)
- nonlinear material-dependent conductivity law
e.g., $a(y) = 1 + |y|$
- well-posed (in suitable spaces)
- $u \mapsto y$ nonlinear, continuous (in suitable spaces)
- $u \mapsto y$ **not Gâteaux** differentiable in general

Motivation: optimality conditions

$$J(\bar{u}, \bar{y}) = \min_{u \in X, y \in Y} J(u, y) \quad \text{s.t.} \quad E(u, y) = 0$$

Unique solution $y = S(u) \rightsquigarrow F(u) := J(u, S(u))$ (differentiable)

1 primal: directional derivative

$$F'(\bar{u}; h) \geq 0 \quad \text{for all } h \in X$$

2 dual: Fréchet derivative

$$0 = F'(\bar{u}) \subset X^*$$

3 primal-dual: implicit function theorem \rightsquigarrow adjoint state

$$J'_u(\bar{u}, S(\bar{u})) + \bar{p} = 0, \quad \bar{p} = S'(\bar{u})^* J'_y(\bar{u}, S(\bar{u}))$$

Motivation: optimality conditions

$$J(\bar{u}, \bar{y}) = \min_{u \in X, y \in Y} J(u, y) \quad \text{s.t.} \quad E(u, y) = 0$$

Unique solution $y = S(u)$, not Gâteaux differentiable

1 primal: directional derivative

$$F'(\bar{u}; h) \geq 0 \quad \text{for all } h \in X$$

2 dual: (suitable) subdifferential

$$0 \in \partial F(\bar{u}) \subset X^*$$

3 primal-dual: chain rule or limit process (\rightsquigarrow adjoint state)

$$J'_u(\bar{u}, S(\bar{u})) + \bar{p} = 0, \quad \bar{p} \in \partial S(\bar{u})^* J'_y(\bar{u}, S(\bar{u}))$$

Motivation: subdifferentials

$S : X \rightarrow Y$ not Gâteaux differentiable, Lipschitz:

- Bouligand subdifferential

$$\partial_B S(u) := \left\{ G_u \in L(X, Y) \mid \begin{array}{l} \text{there exists } \{u_n\} \text{ with } u_n \rightarrow u \\ \text{and } S'(u_n) \rightarrow G_u \end{array} \right\}$$

(set of all limits of Gâteaux derivatives in nearby points)

- Clarke subdifferential

$$\partial_C S(u) := \text{cl co } \partial_B S(u)$$

(closed convex hull)

X, Y infinite-dimensional \rightsquigarrow topology matters (strong, weak(-*),...)

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Optimal control of semilinear PDE

Semilinear “Saran wrap equation”:

$$\min_{u \in L^2(\Omega), y \in H_0^1(\Omega)} J(y, u) \quad \text{s.t.} \quad -\Delta y + \max\{0, y\} = u$$

- existence of minimizer (\bar{u}, \bar{y}) for J weakly l.s.c., coercive
- $S : u \mapsto y$ Lipschitz from $L^2(\Omega) \rightarrow H_0^1(\Omega)$
standard proof: max Lipschitz and monotone
- S Gâteaux differentiable at u if and only if $S(u) \neq 0$ a.e.
- reduced functional $F(u) := J(S(u), u)$

Semilinear: primal optimality conditions

Primal optimality conditions

$$F'(\bar{u}; h) = J'_y(\bar{y}, \bar{u})S'(\bar{u}; h) + J'_u(\bar{y}, \bar{u})h \geq 0 \quad \text{for all } h \in L^2(\Omega)$$

- if J continuously Fréchet differentiable, partial derivatives J'_y, J'_u
standard proof: pass to the limit in $F(\bar{u}) \leq F(u + th)$ for all t, h
- **directional derivative**: $w := S'(u; h) \in H_0^1(\Omega)$ satisfies

$$-\Delta w + \mathbb{1}_{\{S(u) > 0\}} w + \mathbb{1}_{\{S(u) = 0\}} \max\{0, w\} = h$$

- \rightsquigarrow Gâteaux derivative $S'(u)h = w$ iff $S(u) \neq 0$ a.e.

Semilinear: primal-dual optimality conditions

Primal-dual optimality conditions

$$\bar{p} + J'_u(\bar{y}, \bar{u}) = 0, \quad \bar{y} = S(\bar{u})$$

$$-\Delta \bar{p} + \xi \bar{p} = J'_y(\bar{y}, \bar{u})$$

$$\xi(x) \in \partial_C \max(\bar{y}(x)) := \begin{cases} \{1\} & \bar{y}(x) > 0 \\ \{0\} & \bar{y}(x) < 0 \\ [0, 1] & \bar{y}(x) = 0 \end{cases} \quad \text{a.e.}$$

- proof: C^1 approximation \max_ε , localization \rightsquigarrow standard conditions pass to limit $\varepsilon \rightarrow 0$, use regularity of adjoint PDE
- $G_\xi := (-\Delta + \xi)^{-1} \in \partial_B^w S(\bar{u})$ (weak limit of Gâteaux derivatives)
- $\xi(x) \in \{0, 1\}$ a.e. $\rightsquigarrow G_\xi \in \partial_B S(\bar{u})$
- \rightsquigarrow implies **dual optimality** condition $0 \in \partial_B F(\bar{u}) \subset \partial_C F(\bar{u})$

Semilinear: strong optimality conditions

Strong optimality conditions

$$\bar{p} + J'_u(\bar{y}, \bar{u}) = 0, \quad \bar{y} = S(\bar{u})$$

$$-\Delta \bar{p} + \xi \bar{p} = J'_y(\bar{y}, \bar{u})$$

$$\xi(x) \in \partial_C \max(\bar{y}(x)) \quad \text{a.e.}$$

$$\bar{p}(x) \leq 0 \quad \text{a.e. where } \bar{y}(x) = 0$$

- proof: test adjoint equation, use density, fundamental lemma
- equivalent to **primal optimality** condition
proof: pointwise argument using structure of max
- **overdetermined**: not useful for numerical computation

Semilinear: numerical solution

$$J(y, u) = \frac{1}{2} \|y - y^d\|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \|u\|_{L^2(\Omega)}^2$$

- finite element discretization, **mass lumping** for max-term
- eliminate control
- max **convex** \leadsto proximal point reformulation of $\xi_i \in \partial_C \max(y_i)$

$$A_h y + D_h \max(y) = -\frac{1}{\alpha} M_h p$$

$$A_h p + D_h \xi \circ p = M_h (y - y_d)$$

$$y = \text{prox}_{\tau \max}(y + \tau \xi)$$

Semilinear: numerical solution

$$A_h y + D_h \max(y) = -\frac{1}{\alpha} M_h p$$

$$A_h p + D_h \xi \circ p = M_h (y - y_d)$$

$$y = \text{prox}_{\tau \max}(y + \tau \xi)$$

- \leadsto semi-smooth Newton method
- **but:** Newton matrix singular for $p_i = y_i + \tau \xi = 0$
- \leadsto eliminate corresponding components in iteration
- test with constructed $y^d \leadsto S$ not differentiable at solution

Semilinear: numerical example

h	α	τ	$\frac{\ y_h - \bar{y}\ _{L^2}}{\ \bar{y}\ _{L^2}}$	$\frac{\ p_h - \bar{p}\ _{L^2}}{\ \bar{p}\ _{L^2}}$	# SSN
3.030e-2	1e-4	1e-12	8.708e-1	1.606e-2	4
1.538e-2	1e-4	1e-12	2.281e-1	4.541e-3	5
7.752e-3	1e-4	1e-12	5.821e-2	1.209e-3	3
3.891e-3	1e-4	1e-12	1.469e-2	3.119e-4	3
7.752e-3	1e-4	1e-6	-	-	no conv.
7.752e-3	1e-4	1e-8	-	-	no conv.
7.752e-3	1e-4	1e-10	5.821e-2	1.209e-3	3
7.752e-3	1e-4	1e-14	5.821e-2	1.209e-3	3
7.752e-3	1e-2	1e-12	3.007e-3	1.747e-3	2
7.752e-3	1e-3	1e-12	1.659e-2	1.512e-3	2
7.752e-3	1e-5	1e-12	1.692e-1	8.659e-4	5
7.752e-3	1e-6	1e-12	-	-	no conv.

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Optimal control of quasilinear PDE

Quasilinear heat equation:

$$\min_{u \in L^p(\Omega), y \in H_0^1(\Omega)} J(y, u) \quad \text{s.t.} \quad -\nabla \cdot [a(y)\nabla y] = u$$

- $a : \mathbb{R} \rightarrow \mathbb{R}$ Lipschitz continuous, directionally differentiable, bounded from below away from 0
- **existence of minimizer** (\bar{u}, \bar{y}) for J weakly l.s.c., coercive
- $S : u \mapsto y$ continuous from $W^{-1,p'}(\Omega) \rightarrow W_0^{1,s}(\Omega)$ for some $p', s > d$
proof: Stampacchia trick and Schauder fixed point theorem
- $\sim S$ completely continuous from $L^p(\Omega) \rightarrow W_0^{1,s}(\Omega)$

Quasilinear: primal optimality conditions

Primal optimality conditions

$$F'(\bar{u}; h) = J'_y(\bar{y}, \bar{u})S'(\bar{u}; h) + J'_u(\bar{y}, \bar{u})h \geq 0 \quad \text{for all } h \in L^p(\Omega)$$

- if J continuously Fréchet differentiable, partial derivatives J'_y, J'_u
- **directional derivative**: $w := S'(u; h) \in H_0^1(\Omega)$ satisfies

$$-\nabla \cdot [a(S(u))\nabla w + a'(S(u); w)\nabla S(u)] = h$$

Quasilinear: primal-dual optimality conditions

Primal-dual optimality conditions

$$\begin{aligned}\bar{p} + J'_u(\bar{y}, \bar{u}) &= 0, \quad \bar{y} = S(\bar{u}) \\ -\nabla \cdot [a(\bar{y})\nabla\bar{p}] + \xi\nabla\bar{y} \cdot \nabla\bar{p} &= J'_y(\bar{y}, \bar{u}) \\ \xi(x) &\in \partial_c a(\bar{y}(x)) \quad \text{a.e.}\end{aligned}$$

- **difficulty:** non-smooth in leading term, can't pass to limit
- proof:
 - 1 C^1 approximation \max_ε , localization \rightsquigarrow standard conditions
 - 2 pass to limit in **linearized** (not adjoint!) PDE, use duality
 - 3 use boundedness, Lipschitz continuity, strong-to-weak-* outer semicontinuity of Clarke subdifferential
- $\xi \in L^\infty(\Omega)$, not uniquely determined

Quasilinear: strong optimality conditions

Strong optimality conditions

$$\bar{p} + J'_u(\bar{y}, \bar{u}) = 0, \quad \bar{y} = S(\bar{u})$$

$$-\nabla \cdot [a(\bar{y}) \nabla \bar{p}] + \xi \nabla \bar{y} \cdot \nabla \bar{p} = J'_y(\bar{y}, \bar{u})$$

$$\xi(x) \in \partial_C a(\bar{y}(x)) \quad \text{a.e.}$$

$$(a'(\bar{y}(x); t) - \xi(x)t) \nabla \bar{y}(x) \cdot \nabla \bar{p}(x) \geq 0 \quad \text{for all } t \in \mathbb{R}, \text{ a.e.}$$

- **generalized** sign condition for $\xi(x)$ a.e.
- proof: test adjoint equation, use density
- **not explicit**: not useful for numerical computation

Quasilinear: strong optimality conditions

Strong optimality conditions

$$\bar{p} + J'_u(\bar{y}, \bar{u}) = 0, \quad \bar{y} = S(\bar{u})$$

$$-\nabla \cdot [a(\bar{y}) \nabla \bar{p}] + \xi \nabla \bar{y} \cdot \nabla \bar{p} = J'_y(\bar{y}, \bar{u})$$

$$\xi(x) \in \partial_c a(\bar{y}(x)) \quad \text{a.e.}$$

$$(a'(\bar{y}(x); t) - \xi(x)t) \nabla \bar{y}(x) \cdot \nabla \bar{p}(x) \geq 0 \quad \text{for all } t \in \mathbb{R}, \text{ a.e.}$$

If a is continuous, **countably piecewise differentiable** (PC¹):

- \leadsto S Fréchet differentiable (but a still non-smooth!)
- \leadsto strong conditions **equivalent** to primal-dual conditions
- \leadsto primal-dual conditions hold for **any** $\xi(x) \in \partial_c a(\bar{y}(x))$

Quasilinear: second-order conditions

No-gap second-order conditions if a is **finitely** PC^1 , i.e.,

$$a(t) = \sum_{i=0}^K \mathbb{1}_{(t_i, t_{i+1}]}(t) a_i(t)$$

in terms of **curvature functional**

$$Q(u, y, p; h) := Q_s(u, y, p; h, h) + Q_1(u, y, p; h, h) + Q_2(u, y, p; h)$$

with (definitions technical)

- Q_s second derivatives of $J(u, S(u))$ in smooth points
- Q_1 involving first-order directional derivatives of a
- Q_2 involving limits of jumps of $|a'_i - a'_{i-1}|$ near $y = t_i$

Quasilinear: second-order conditions

Assume **finite oscillation** $\Sigma(\bar{y})$ of \bar{y} around t_j :

Necessary second-order condition

If \bar{u} local minimizer, there exists adjoint state \bar{p} such that

$$Q(\bar{u}, \bar{y}, \bar{p}; h) \geq 0 \quad \text{for all } h \in C_U(\bar{u})$$

Sufficient second-order condition

If $\bar{u}, \bar{y}, \bar{p}$ satisfy first-order conditions and

$$Q(\bar{u}, \bar{y}, \bar{p}; h) > 0 \quad \text{for all } h \in C_U(\bar{u}) \setminus \{0\},$$

then \bar{u} local minimizer, local quadratic growth of $J(u, S(u))$ near \bar{u}

($C_U(u)$ cone of critical directions for admissible set $U = \{u_{\min} \leq u \leq u_{\max}\}$)

Quasilinear: numerical solution

$$J(y, u) = \frac{1}{2} \|y - y^d\|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \|u\|_{L^2(\Omega)}^2$$

- $a(y) = 1 + |y|$ finitely PC¹
- eliminate control, fix $\xi = \text{sign}(\bar{y})$ single-valued (e.g., $\text{sign}(0) := 1$)
- introduce $\psi = \bar{y} + \frac{1}{2}(\bar{y}|\bar{y}|)$, adjoint p

$$\begin{aligned} -\Delta\psi + \frac{1}{\alpha}p &= 0 \\ -\Delta p + \frac{1 - \sqrt{1 + 2|\psi|}}{\sqrt{1 + 2|\psi|}} \text{sign}(\psi) + \frac{y^d}{\sqrt{1 + 2|\psi|}} &= 0 \end{aligned}$$

Quasilinear: numerical solution

$$-\Delta\psi + \frac{1}{\alpha}p = 0$$
$$-\Delta p + \frac{1 - \sqrt{1 + 2|\psi|}}{\sqrt{1 + 2|\psi|}} \operatorname{sign}(\psi) + \frac{y^d}{\sqrt{1 + 2|\psi|}} = 0$$

- single-valued, Lipschitz, PC¹
- \leadsto semi-smooth Newton method
- local superlinear convergence for $y_d \in L^\infty(\Omega)$ small or α large
- finite element discretization, mass lumping
- test with constructed $y^d \leadsto a$ not differentiable at solution

Quasilinear: numerical example

n_h	α	$\frac{\ y_h - \bar{y}\ _{H_0^1(\Omega)}}{\ \bar{y}\ _{H_0^1(\Omega)}}$	$\frac{\ \rho_h - \bar{\rho}\ _{H_0^1(\Omega)}}{\ \bar{\rho}\ _{H_0^1(\Omega)}}$	# SSN
100	1e-6	3.275e-3	2.915e-2	2
200	1e-6	1.660e-3	1.540e-2	4
400	1e-6	8.357e-4	7.925e-3	3
800	1e-6	4.193e-4	4.027e-3	3
1000	1e-6	3.356e-4	3.237e-3	3
800	1e-2	6.358e-2	1.360e-2	4
800	1e-4	8.762e-3	7.324e-3	3
800	1e-6	4.193e-4	4.027e-3	3
800	1e-8	2.321e-5	2.192e-3	25

Conclusion

Optimal control of **non-smooth** partial differential equations:

- model for **sharp phase transitions**
- **useful optimality conditions** by approximation, limit
- solution by **semismooth Newton** method
- no-gap **second order** optimality conditions

Outlook:

- parameter identification (**iterative regularization**)
- discretization **error estimates**
- application to **variational inequalities**

Preprints, Python codes:

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