On two optimization methods for optimal control problems

Sequence of Quadratic Problems // SemiSmooth Newton Method

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Outline

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Outline

The abstract optimization problem

Problem (P)

$$\text{(P)} \qquad \min_{u \in U_{\rm ad}} J(u) := \mathcal{J}(u) + \frac{\kappa}{2}\|u\|^2_{L^2(X)},$$

- $(X, \mathcal{S}, \mu)$ measure space with $\mu(X) < \infty$, $\qquad \kappa > 0$.
- $\mathcal{J}$ is a function of class C^2

$$\mathcal{J} : \mathcal{A} \subset L^p(X) \to \mathbb{R}$$

  for some $p \in [2, +\infty]$. Here $\mathcal{A} \subset L^p(X)$ is an open set.

- $U_{\rm ad} \subset \mathcal{A}$ and

$$U_{\rm ad} = \{u \in L^p(X) : \ \alpha \leq u \leq \beta \text{ a.e. } [\mu]\}$$

  $-\infty \leq \alpha < \beta \leq +\infty$. If $p > 2$, we also require $-\infty < \alpha < \beta < +\infty$.

Notation: $B^p_\rho(u) = \{v \in L^p(X) : \ \|v - u\|_{L^p(X)} \leq \rho\}$.

Some control problems that fit in this framework

Remark

The framework is easy to generalize to vector controls $\boldsymbol{u} \in \Pi_{j=1}^{n} L^{p^j}(X_j)$.

- Additive elliptic control problem governed by a semilinear equation, with distributed and/or boundary control.
- Distributed control of the instationary Navier-Stokes equations
- Distributed and/or boundary control of a parabolic equation
- Time dependent control of a parabolic quasilinear equation
- Boundary bilinear control of a semilinear parabolic equation ...

Eduardo Casas (2024). "Superlinear Convergence of a Semismooth Newton Method for Some Optimization Problems with Applications to Control Theory". In: *SIAM Journal on Optimization* 34.4, pp. 3681–3698. DOI: 10.1137/24M1644286

Eduardo Casas and Mariano Mateos (2025b). *Quadratic convergence of an SQP method for some optimization problems with applications to control theory.* (To appear in SICON). arXiv: 2505.22750

A prototypical example

Problem (E)

$$\min_{u\in U_{\rm ad}} J(u) := \frac{1}{2}\|y_u - y_d\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\|u\|^2_{L^2(\Omega)}$$

where $y_u \in H^1_0(\Omega) \cap C(\bar{\Omega})$ is the solution of

$$-\Delta y + \boldsymbol{b}\cdot\nabla y + f(\cdot, y) = u \text{ in } \Omega,\ \ y = 0 \text{ on } \Gamma.$$

and

$$U_{\rm ad} = \{u \in L^2(\Omega) :\ \alpha \le u(x) \le \beta \text{ for a.a. } x \in \Omega\}$$

- $\Omega \subset \mathbb{R}^d$, $d \le 3$, bounded domain with Lipschitz boundary Γ.
- $\boldsymbol{b} \in L^{\bar{p}}(\Omega)^d$, $\bar{p} > 2$, $\operatorname{div} \boldsymbol{b} \in L^2(\Omega)$, $y_d \in L^2(\Omega)$
- $f : \Omega \times \mathbb{R} \to \mathbb{R}$ a Carathéodory function, $f(\cdot, 0) \in L^2(\Omega)$, monotone non-decreasing, of class C^2 and such that $\partial^2_{yy} f(x, y)$ is locally Lipschitz w.r.t. y .

Casas, Eduardo, Mateos, Mariano, and Rösch, Arnd (2020). “Analysis of control problems of nonmontone semilinear elliptic equations”. In: *ESAIM: COCV* 26, p. 80. DOI: 10.1051/cocv/2020032

Some remarks about the example problem (E)

- $X = \Omega$, μ is the Lebesgue measure, $p = 2$.
- For every $u \in \mathcal{A} = L^2(\Omega)$ there exists a unique $y_u \in H_0^1(\Omega) \cap C(\bar{\Omega})$ solution of

$$-\Delta y + \boldsymbol{b} \cdot \nabla y + f(\cdot, y) = u \text{ in } \Omega, \; y = 0 \text{ on } \Gamma.$$

- The control-to-state mapping $G(u) = y_u$ is of class C^2.

Derivative of the control-to-state mapping

For all $u, v \in L^2(\Omega)$, $z_{u,v} = G'(u)v \in H_0^1(\Omega) \cap C(\bar{\Omega})$ is the unique solution of

$$-\Delta z + \boldsymbol{b} \nabla z + \partial_y f(\cdot, y_u) z = v \text{ in } \Omega, \; z = 0 \text{ on } \Gamma.$$

- $\mathcal{J}(u) = \frac{1}{2}\|y_u - y_d\|^2_{L^2(\Omega)}$. $J(u) = \frac{1}{2}\|y_u - y_d\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\|u\|^2_{L^2(\Omega)}$.
- Corollary: $\mathcal{J}$ is of class C^2

The first derivative of the objective functional

For the **abstract problem, we assume:**

1. There exists a C^1 mapping $\Phi : \mathcal{A} \to L^\infty(X)$ such that

$$\mathcal{J}'(u)v = \int_X \Phi(u) v \, d\mu \ \forall u \in \mathcal{A} \text{ and } \ \forall v \in L^p(X).$$

For the **example:** For every $u \in L^2(\Omega)$ there exists a unique adjoint state $\varphi_u \in H_0^1(\Omega) \cap C(\bar{\Omega})$ solution of

$$-\Delta\varphi - \operatorname{div}[\boldsymbol{b}\varphi] + \partial_y f(\cdot, y_u)\varphi = y_u - y_d \text{ in } \Omega, \ \varphi = 0 \text{ on } \Gamma.$$

The mapping $\Phi(u) = \varphi_u$ is of class C^1 from $L^2(\Omega)$ into $L^\infty(\Omega)$ and integration by parts shows that

$$J'(u)v = \int_\Omega (\varphi_u + \kappa u) v \, dx \ \forall u \in L^2(\Omega) \text{ and } \forall v \in L^2(\Omega).$$

The second derivative

Remark: $\mathcal{J}$ is of class C^2. $\forall u \in \mathcal{A}$, $\mathcal{J}''(u) : L^p(X) \times L^p(X) \longrightarrow \mathbb{R}$ is a symmetric and continuous bilinear form and satisfies

$$\mathcal{J}''(u)(v_1, v_2) = \int_X [\Phi'(u)v_1]v_2 \,\mathrm{d}\mu = \int_X [\Phi'(u)v_2]v_1 \,\mathrm{d}\mu \quad \forall v_1, v_2 \in L^p(X). \tag{1}$$

We will write $\mathcal{J}''(u)v^2 = \mathcal{J}''(u)(v, v)$.

For the example: Classical form of the second derivative:

$$J''(u)v^2 = \int_\Omega \left[\left(1 - \varphi_u \partial^2_{yy} f(\cdot, y_u)\right) z^2_{u,v} + \kappa v^2\right] \mathrm{d}x.$$

But ... we will use the so-called **second-adjoint-state**. For all $u, v \in L^2(\Omega)$, $\eta_{u,v} = \Phi'(u)v \in H^1_0(\Omega) \cap C(\bar{\Omega})$ is the unique solution of

$$-\Delta\eta - \mathrm{div}[\boldsymbol{b}\eta] + \partial_y f(\cdot, y_u)\eta = (1 - \varphi_u \partial^2_{yy} f(\cdot, y_u)) z_{u,v} \text{ in } \Omega, \;\; \eta = 0 \text{ on } \Gamma.$$

Using $\eta_{u,v}$ (very helpful for computations!. We'll see later why).

$$J''(u)v^2 = \int_\Omega (\eta_{u,v} + \kappa v) v \,\mathrm{d}x.$$

Assumptions regarding the derivative of Φ

2. For every $u \in \mathcal{A}$ the linear mapping
$$\Phi'(u) : L^p(X) \longrightarrow L^\infty(X)$$
has an **extension to a compact** operator
$$\Phi'(u) : L^2(X) \longrightarrow L^2(X).$$
For every $\varepsilon > 0$ there exists $\rho = \rho_{\varepsilon,u} > 0$ with $B^p_\rho(u) \subset \mathcal{A}$ such that
$$\|(\Phi'(u) - \Phi'(w))v\|_{L^2(X)} \le \varepsilon \|v\|_{L^2(X)} \; \forall w \in B^p_\rho(u) \text{ and } \forall v \in L^2(X).$$
3. There exist $N \ge 0$ and numbers $2 = p_0 \le p_1 \le \ldots \le p_N = p$ such that for every $u \in \mathcal{A}$, the linear mapping
$$\Phi'(u) : L^p(X) \longrightarrow L^\infty(X)$$
defines also a **continuous** operator
$$\Phi'(u) : L^{p_{i-1}}(X) \longrightarrow L^{p_i}(X)$$
for $i = 1, \ldots, N$ (denote $p_{N+1} = \infty$).
4. For every $u \in \mathcal{A}$, there exists $\rho_u > 0$ with $B^p_{\rho_u}(u) \subset \mathcal{A}$ and a constant $L_{u,\Phi'}$ such that
$$\|(\Phi'(w) - \Phi'(u))v\|_{L^\infty(X)} \le L_{u,\Phi'} \|w - u\|_{L^p(X)} \|v\|_{L^p(X)}$$
for all $w \in B^p_{\rho_u}(u)$ and $v \in L^p(X)$.

Local solution. First order optimality condition.

- Let $\bar{u}$ be a local solution
  (In the sense of $L^2(X)$ if $2 < p < \infty$, taking advantage of $-\infty < \alpha < \beta < \infty$.)
- Any local solution satisfies the first order optimality condition

$$\int_X (\Phi(\bar{u}) + \kappa\bar{u})(u - \bar{u})\, \mathrm{d}\mu \geq 0 \; \forall u \in U_{\mathrm{ad}}.$$

  We will use this form to write the Sequence of Quadratic Programs.
- Equivalently

$$\bar{u}(x) = \mathrm{Proj}_{[\alpha\beta]}\left(-\frac{\Phi(\bar{u})(x)}{\kappa}\right) \text{ for a.a.}[\mu] x \in X$$

  We will use this form to write the SemiSmooth Newton method.

Assumptions on the local solution

5. The local minimizer $\bar{u} \in U_{\mathrm{ad}}$ satisfies the second order sufficient optimality condition
$$J''(\bar{u})v^2 > 0 \;\forall v \in C_{\bar{u}} \setminus \{0\}$$
and the strict complementarity condition
$$\mu\{x \in X : \bar{u}(x) \in \{\alpha, \beta\} \text{ and } \kappa\bar{u}(x) + \Phi(\bar{u})(x) = 0\} = 0.$$

Here, $C_{\bar{u}}$ is the cone of critical directions

$$C_{\bar{u}} = \left\{ v \in L^2(X) : \begin{cases} v(x) \geq 0 \text{ if } \bar{u}(x) = \alpha, \\ v(x) \leq 0 \text{ if } \bar{u}(x) = \beta, \\ v(x) = 0 \text{ if } \Phi(\bar{u})(x) + \kappa\bar{u}(x) \neq 0 \end{cases} \quad \text{a.e. } [\mu] \right\}.$$

Remark

This is completely analog to the usual textbook assumption to obtain local quadratic convergence of the SQP for finite-dimensional problems.

Outline

Warning

- There are versions of these methods that exploit the complete optimality system.

$$(\text{SQP})\begin{cases}\text{State equation}\\ \text{Adjoint state equation}\\ \text{Variational inequality}\end{cases}\qquad(\text{SSN})\begin{cases}\text{State equation}\\ \text{Adjoint state equation}\\ \text{Projection equation}\end{cases}$$

  - The three variables (y, φ, u) are treated independently.
  - These versions are fully linearized. There is no need to solve non-linear PDEs.

Fredi Tröltzsch (1999). "On the Lagrange–Newton–SQP Method for the Optimal Control of Semilinear Parabolic Equations". In: *SIAM Journal on Control and Optimization* 38.1, pp. 294–312. DOI: 10.1137/S0363012998341423

- In contrast, we will use u as the unique optimization variable.
- A non-linear PDE must be solved at each step.
- Robustness is gained regarding the choice of the initial point.
- A smart combination of both worlds is possible to achieve the best performance.

Eduardo Casas and Mariano Mateos (2025a). "Boundary bilinear control of semilinear parabolic PDEs: quadratic convergence of the SQP method". In: arXiv: 2505.24237 [math.OC]

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Outline

Semismoothness

(A farther layer of abstraction)

Definition 1 (Semismooth function)

Given two Banach spaces U and X, an open subset $\mathcal{A}$ of U, a continuous function $F : \mathcal{A} \longrightarrow X$, and a set-value mapping $\partial F : \mathcal{A} \longrightarrow \mathcal{P}(\mathcal{L}(U, X))$ such that $\partial F(u) \neq \emptyset \; \forall u \in \mathcal{A}$, we say that F is ∂F-semismooth at $\bar{u} \in \mathcal{A}$ if

$$\lim_{v \longrightarrow 0} \sup_{M \in \partial F(\bar{u}+v)} \frac{\|F(\bar{u}+v) - F(\bar{u}) - Mv\|_X}{\|v\|_U} = 0.$$

F is said ∂F-semismooth at $\mathcal{A}$ if it is ∂F-semismooth at every $u \in \mathcal{A}$.

Algorithm 1: Semismooth Newton method to solve $F(u) = 0$.

```
Initialize. Choose u_0 ∈ A. Set j = 0.
for j ≥ 0 do
    Choose M_j ∈ ∂F(u_j) and solve M_j v_j = −F(u_j).
    Set u_{j+1} = u_j + v_j and j = j + 1.
end
```

Convergence conditions for the SSN

Theorem 2

Suppose F is semismooth at $\bar{u}$, a locally unique solution of $F(u) = 0$, and that for every $j \geq 0$, $M_j \in \partial F(u_j)$ is invertible and there exists $C > 0$ such that

$$\|M_j^{-1}\|_{\mathcal{L}(X,U)} \leq C \; \forall j \geq 0.$$

Then there exists $\delta > 0$ such that for all $u_0 \in U$ with $\|u_0 - u\|_X < \delta$ the sequence $\{u_j\}_{j \geq 0}$ converges superlinearly to $\bar{u}$.

In short

Semismoothness + Uniform boundness of the inverses $\Rightarrow$ superlinear convergence.

Building the SemiSmooth Newton method for (E)

$$F : L^2(\Omega) \to L^2(\Omega),\ F(u)(x) = u(x) - \mathrm{Proj}_{[\alpha,\beta]}\left(\frac{-\varphi_u(x)}{\kappa}\right)$$

- First order optimality conditions: A local solution $\bar{u}$ is a solution of $F(u) = 0$.
- In order to define $\partial F(u)$ we introduce some additional functions.

$$\Phi : L^2(\Omega) \longrightarrow L^2(\Omega), \quad \Phi(u) = \varphi_u,$$
$$\psi : \mathbb{R} \longrightarrow \mathbb{R}, \quad \psi(t) = \mathrm{Proj}_{[\alpha,\beta]}(t),$$
$$\Psi : L^2(\Omega) \longrightarrow L^2(\Omega), \quad \Psi(u)(x) = \psi(\frac{-\Phi(u)(x)}{\kappa}).$$

Notice that $F(u) = u - \Psi(u)$.

- Ψ is called a superposition operator.

Computing ∂F.

- $\psi : \mathbb{R} \longrightarrow \mathbb{R}, \quad \psi(t) = \mathrm{Proj}_{[\alpha,\beta]}(t)$ is a Lipschitz function. The subdifferential in Clarke's sense is

$$\partial\psi(t) = \{1\} \text{ if } t \in (\alpha,\beta),\ \partial\psi(t) = \{0\} \text{ if } t \notin [\alpha,\beta],\ \partial\psi(t) = [0,1] \text{ if } t \in \{\alpha,\beta\}.$$

- $\Psi(u) = \psi(\frac{-\Phi(u)}{\kappa})$. For every $u \in L^2(\Omega)$ we define (applying the chain rule)

$$\partial\Psi(u) = \Big\{N \in \mathcal{L}(L^2(\Omega), L^2(\Omega)) : Nv(x) = h(x) \cdot \frac{-[\Phi'(u)v](x)}{\kappa}\ \forall v \in L^2(\Omega)$$

$$\text{where } h : \Omega \longrightarrow \mathbb{R} \text{ is any measurable function}$$

$$\text{such that } h(x) \in \partial\psi(\frac{-\Phi(u)(x)}{\kappa})\Big\}.$$

Theorem 3

Ψ is $\partial\Psi$-semismooth in $L^2(\Omega)$ and hence the function $F : L^2(\Omega) \longrightarrow L^2(\Omega)$ is ∂F-semismooth in $L^2(\Omega)$, where

$$\partial F(u) = \{M = I - N : N \in \partial\Psi(u)\}.$$

Selection of the M_u

- Define $\lambda : \mathbb{R} \longrightarrow \mathbb{R}$ so that $\lambda(t) \in \partial\psi(t)$ for every $t \in \mathbb{R}$, by

$$\lambda(t) = \begin{cases} 1 & \text{if } t \in (\alpha, \beta), \\ 0 & \text{otherwise,} \end{cases}$$

- Given $u \in L^2(\Omega)$, define $h_u : \Omega \to \mathbb{R}$ as

$$h_u(x) = \lambda\left(\frac{-\Phi(u)(x)}{\kappa}\right) = \begin{cases} 1 & \text{if } \frac{-\varphi_u(x)}{\kappa} \in (\alpha, \beta), \\ 0 & \text{otherwise.} \end{cases}$$

- If we define the inactive and active sets as

$$\mathbb{I}_u = \{x \in \Omega : \frac{-\varphi_u(x)}{\kappa} \in (\alpha, \beta)\} \qquad \mathbb{A}_u = \Omega \setminus \mathbb{I}_u,$$

  then h_u is the characteristic function of the inactive set

$$h_u = \chi_{\mathbb{I}_u}.$$

- Select $M_u \in \partial F(u)$ as the linear operator $M_u : L^2(\Omega) \to L^2(\Omega)$ defined by

$$M_u v = v - \chi_{\mathbb{I}_u} \cdot \frac{-\Phi'(u)v}{\kappa} = v + \chi_{\mathbb{I}_u} \cdot \frac{\eta_{u,v}}{\kappa}$$

The algorithm up to now

Algorithm 2: Semismooth Newton method to solve $F(u) = 0$.

Initialize. Choose $u_0 \in L^2(\Omega)$. Set $j = 0$.
for $j \geq 0$ **do**
    Compute $y_j = G(u_j)$ solving the nonlinear state equation
    Compute $\varphi_j = \Phi(u_j)$ solving the linear adjoint equation
    Set $\mathbb{A}_j = \mathbb{A}_j^\beta \cup \mathbb{A}_j^\alpha$ and $\mathbb{I}_j = \Omega \setminus \mathbb{A}_j$, where

$$\mathbb{A}_j^\beta = \{x \in \Omega : -\varphi_j(x) \geq \kappa\beta\}, \quad \mathbb{A}_j^\alpha = \{x \in \Omega : -\varphi_j(x) \leq \kappa\alpha\}$$

    Set $w_j(x) = -F(u_j)(x) = \begin{cases} -u_j(x) + \beta & \text{if } x \in \mathbb{A}_j^\beta \\ -u_j(x) - \frac{\varphi_j(x)}{\kappa} & \text{if } x \in \mathbb{I}_j \\ -u_j(x) + \alpha & \text{if } x \in \mathbb{A}_j^\alpha \end{cases}$

    Solve $v + \chi_{\mathbb{I}_j} \frac{\eta_{u_j,v}}{\kappa} = w_j$. Name v_j the solution..
    Set $u_{j+1} = u_j + v_j$ and $j = j + 1$.
end

Solving the linear system $v + \chi_{\mathbb{I}_u} \frac{\eta_{u,v}}{\kappa} = w$

- In the active set, the equation is reduced to $v = w$.
- So we can write that $v = \chi_{\mathbb{I}_u} v + \chi_{\mathbb{A}_u} w$.
- The mapping $v \mapsto \eta_{u,v}$ is linear in v. So $\eta_{u,v} = \eta_{u,\chi_{\mathbb{I}_u} v} + \eta_{u,\chi_{\mathbb{A}_u} w}$.
- Name $b = \kappa w - \eta_{u,\chi_{\mathbb{A}_u} w}$. In the inactive set we can write the equation as

$$\kappa \chi_{\mathbb{I}_u} v + \chi_{\mathbb{I}_u} \eta_{u,\chi_{\mathbb{I}_u} v} = \chi_{\mathbb{I}_u} b.$$

- This equation is the first order optimality condition of the unconstrained quadratic problem [*Notation*: $E_\Omega \upsilon$ is the extension by zero.]

$$(Q) \quad \min_{\upsilon \in L^2(\mathbb{I}_u)} \frac{1}{2} \int_{\mathbb{I}_u} (\eta_{u,E_\Omega \upsilon} + \kappa \upsilon) \upsilon \, \mathrm{d}x - \int_{\mathbb{I}_u} b \upsilon \, \mathrm{d}x.$$

- Solve (Q) for $\bar{\upsilon}$. The solution of $v + \chi_{\mathbb{I}_u} \frac{\eta_{u,v}}{\kappa} = w$ is

$$v = \begin{cases} \bar{\upsilon} & \text{in } \mathbb{I}_u \\ w & \text{in } \mathbb{A}_u \end{cases}$$

The algorithm at this point

Algorithm 3: Semismooth Newton method to solve $F(u) = 0$.

Initialize. Choose $u_0 \in L^2(\Omega)$. Set $j = 0$.
for $j \geq 0$ **do**
  Compute $y_j = G(u_j)$ solving the nonlinear state equation
  Compute $\varphi_j = \Phi(u_j)$ solving the linear adjoint equation
  Compute $\mathbb{A}_j^\beta$ and $\mathbb{A}_j^\alpha$. Set $\mathbb{A}_j = \mathbb{A}_j^\beta \cup \mathbb{A}_j^\alpha$ and $\mathbb{I}_j = \Omega \setminus \mathbb{A}_j$,
  Set $w_j(x) = -F(u_j)(x)$
  Compute $z_j = G'(u_j)\chi_{\mathbb{A}_j} w_j$ solving the linearized state equation
  Compute $\eta_j = \Phi'(u_j)\chi_{\mathbb{A}_j} w_j$ solving the second adjoint state equation
  Name $b_j = \kappa w_j - \eta_j$
  Solve the unconstrained quadratic problem

$$(Q) \quad \min_{v \in L^2(\mathbb{I}_j)} \frac{1}{2} \int_{\mathbb{I}_j} (\eta_{u_j, E_\Omega v} + \kappa v) v \, \mathrm{d}x - \int_{\mathbb{I}_u} b_j v \, \mathrm{d}x.$$

  Name v_j the solution.
  Set $u_{j+1} = u_j + \begin{cases} v_j & \text{in } \mathbb{I}_j \\ w_j & \text{in } \mathbb{A}_j \end{cases}$ and $j = j + 1$.
end

Solving the unconstrained quadratic problem (Q)

$$(Q) \quad \min_{v \in L^2(\mathbb{I}_u)} \frac{1}{2} \int_{\mathbb{I}_u} (\eta_{u,E_\Omega v} + \kappa v) v \, \mathrm{d}x - \int_{\mathbb{I}_u} b v \, \mathrm{d}x.$$

Side remark: Before solving this, notice that, since $E_\Omega v = 0$ in $\mathbb{A}_u$, we have

$$J''(u)(E_\Omega v)^2 = \int_{\mathbb{I}_u} (\eta_{u,E_\Omega v} + \kappa v) v \, \mathrm{d}x.$$

In finite dimension, if we had H, the Hessian matrix at u, then (Q) would read as

$$\min_{\boldsymbol{v} \in \mathbb{R}^N} \frac{1}{2} \boldsymbol{v}^T (H + \kappa I) \boldsymbol{v} - \boldsymbol{b}^T \boldsymbol{v}$$

and this would be just a matter of solving the linear system

$$(H + \kappa I) \boldsymbol{v} = \boldsymbol{b}$$

But, as many authors point out at this point, H is too expensive to compute. Since

$$H_{ij} = \int_{\mathbb{I}_u} (\eta_{u,E_\Omega e_i}) e_j \, \mathrm{d}x,$$

for a problem with N dof, you have to solve N^2 linear pdes to get H.

Solving the unconstrained quadratic problem (Q)

$$(Q)\quad \min_{v\in L^2(\mathbb{I}_u)} \frac{1}{2}\int_{\mathbb{I}_u}(\eta_{u,E_\Omega v}+\kappa v)v\,\mathrm{d}x-\int_{\mathbb{I}_u} bv\,\mathrm{d}x.$$

- Define the linear operator $H: L^2(\mathbb{I}_u)\to L^2(\mathbb{I}_u)$, [$R_{\mathbb{I}_u}$ is a restriction operator].

$$Hv = R_{\mathbb{I}_u}\eta_{u,E_\Omega v}$$

- Denoting $(\cdot,\cdot)$ the scalar product in $L^2(\mathbb{I})$, our problem reads

$$(Q)\quad \min_{v\in L^2(\mathbb{I}_u)} \frac{1}{2}([H+\kappa I]v,v)-(b,v).$$

- SSC+strict complementarity $\Rightarrow$ $H+\kappa I$ is a symmetric, positive definite operator. **Use the conjugate gradient** method to solve (Q) at the price of one evaluation of Hv per iteration.
- Cost of evaluation of Hv. Solve two linear PDEs:

$$-\Delta z+\boldsymbol{b}\nabla z+\partial_y f(\cdot,y_u)z=E_\Omega v \text{ in } \Omega,\ z=0 \text{ on } \Gamma,$$

$$-\Delta\eta-\mathrm{div}[\boldsymbol{b}\eta]+\partial_y f(\cdot,y_u)\eta=(1-\varphi_u\partial^2_{yy}f(\cdot,y_u))z \text{ in } \Omega,\ \eta=0 \text{ on } \Gamma.$$

Further considerations

- Under no-gap second order conditions and a strict complementarity condition, the algorithm converges locally superlinearly.
- If the equation is linear, then the SemiSmooth Newton method is equivalent to a Primal Dual Active Set Strategy.
- When solving **finite dimensional approximations**, there are three remarkable facts:
  1. For linear equations –so called **linear-quadratic control problems**– the problem is solved in a **finite number of iterations**. Each iteration is uniquely characterized by its active and inactive sets, so if these do not change from one iteration to the next one, we stop.
  2. For **nonlinear equations**, once the active and inactive sets are localized, the observed order of convergence is **quadratic**.
  3. The number of iterations is independent of the number of variables (**mesh-independence principle**, observed in experiments; I don't think it has been proved in this context).

Outline

Generalized equations

- Let $\bar{u}$ be a local solution (In the sense of $L^2(X)$ if $2 < p < \infty$, taking advantage of $-\infty < \alpha < \beta < \infty$.)
- Any local solution satisfies the first order optimality condition

$$\int_X (\Phi(\bar{u}) + \kappa \bar{u})(u - \bar{u}) \, \mathrm{d}\mu \geq 0 \; \forall u \in U_{\mathrm{ad}}.$$

- Let $F : \mathcal{A} \to L^p(X)$ be given by $F(u) = \Phi(u) + \kappa u$.
- Normal cone of U_{ad} at u

$$N(u) = \begin{cases} \{w \in L^2(X) : \int_X w(v - u) d\mu \leq 0 \; \forall v \in U_{\mathrm{ad}}\} & \text{if } u \in U_{\mathrm{ad}}, \\ \emptyset & \text{if } u \notin U_{\mathrm{ad}}. \end{cases}$$

Generalized equation

$$0 \in F(\bar{u}) + N(\bar{u})$$

The SQP method

- Generalized Newton's method: Given $u_0 \in \mathcal{A}$, for $j \geq 0$ u_{j+1} solves

$$0 \in F(u_j) + F'(u_j)(u_{j+1} - u_j) + N(u_{j+1})$$

- This generalized equation is the first order optimality condition of the constrained quadratic problem

$$(\mathcal{Q}_j) \qquad \min_{u \in U_{\mathrm{ad}}} \frac{1}{2} J''(u_j)(u - u_j)^2 + J'(u_j)u.$$

- $(\mathcal{Q}_j)$ may have no solution or may have more than one solution. Instead, we will look for local solutions.

Remark: To solve $(\mathcal{Q}_j)$ we do the change $v = u - u_j$ and use

$$J''(u_j)v^2 = \int_\Omega \left(\kappa v + \eta_{u_j,v}\right) v \, \mathrm{d}x \qquad J'(u_j)v = \int_\Omega \left(\kappa u_j + \varphi_{u_j}\right) v \, \mathrm{d}x$$

The algorithm

Algorithm 4: SQP method to solve (E).

Initialize. Choose $u_0 \in L^2(\Omega)$. Set $j = 0$.
for $j \geq 0$ **do**
  Compute $y_j = G(u_j)$ solving the nonlinear state equation
  Compute $\varphi_j = \Phi(u_j)$ solving the linear adjoint equation
  Find a local solution of the constrained quadratic problem

$$(\mathcal{Q}_j') \qquad \min_{v \in U_{\mathrm{ad}} - \{u_j\}} \frac{1}{2} \int_\Omega \left(\kappa v + \eta_{u_j,v}\right) v \,\mathrm{d}x + \int_\Omega \left(\kappa u_j + \varphi_j\right) v \,\mathrm{d}x$$

  Name v_j the obtained solution.
  Set $u_{j+1} = u_j + v_j$ and $j = j + 1$.
end

Theorem 4

Under no-gap second order sufficient optimality conditions and a strict complementarity condition, the method converges quadratically to $\bar{u}$ both in $L^2(\Omega)$ and $L^\infty(\Omega)$ provided an initial point u_0 is given in a proper neighborhood of $\bar{u}$ in the sense of $L^2(\Omega)$.

Solving $(\mathcal{Q}'_j)$

$$(\mathcal{Q}') \qquad \min_{\alpha - u(x) \leq v(x) \leq \beta - u(x)} \frac{1}{2} \int_\Omega \big(\kappa v + \eta_{u,v}\big) v \, \mathrm{d}x + \int_\Omega \big(\kappa u + \varphi\big) v \, \mathrm{d}x$$

- Some authors write $(\mathcal{Q}')$ as a linear-quadratic optimal control problem. Let's do it more interesting, more general, and *easier*.
- Let $(X, \mathcal{S}, \mu)$ be measure space, $H \in \mathcal{L}(L^2(X))$ a self-adjoint operator, $b \in L^2(X)$, $\tilde{\alpha}(x)$ and $\tilde{\beta}(x)$ measurable functions (maybe taking $\pm\infty$ values), and $\kappa > 0$.

$$(\mathcal{Q}') \qquad \min_{\tilde{\alpha}(x) \leq v(x) \leq \tilde{\beta}(x)} \frac{1}{2}(Hv + \kappa v, v) + (b, v).$$

- In our case $Hv = \eta_{u,v}$ and $b = \kappa u + \varphi$, $\tilde{\alpha}(x) = \alpha - u(x)$, $\tilde{\beta}(x) = \beta - u(x)$.

To solve the constrained quadratic problem ...

Use SemiSmooth Newton method !!!!

Solving $(\mathcal{Q}_j')$

$$(\mathcal{Q}') \qquad \min_{\alpha - u(x) \leq v(x) \leq \beta - u(x)} \frac{1}{2} \int_\Omega \big(\kappa v + \eta_{u,v}\big) v \, dx + \int_\Omega \big(\kappa u + \varphi\big) v \, dx$$

- Some authors write $(\mathcal{Q}')$ as a linear-quadratic optimal control problem. Let's do it more interesting, more general, and *easier*.
- Let $(X, \mathcal{S}, \mu)$ be measure space, $H \in \mathcal{L}(L^2(X))$ a self-adjoint operator, $b \in L^2(X)$, $\tilde{\alpha}(x)$ and $\tilde{\beta}(x)$ measurable functions (maybe taking $\pm\infty$ values), and $\kappa > 0$.

$$(\mathcal{Q}') \qquad \min_{\tilde{\alpha}(x) \leq v(x) \leq \tilde{\beta}(x)} \frac{1}{2}(Hv + \kappa v, v) + (b, v).$$

- In our case $Hv = \eta_{u,v}$ and $b = \kappa u + \varphi$, $\tilde{\alpha}(x) = \alpha - u(x)$, $\tilde{\beta}(x) = \beta - u(x)$.

To solve the constrained quadratic problem ...

Use SemiSmooth Newton method !!!!

SemiSmooth Newton method to solve constrained quadratic problems

Algorithm 5: SemiSmooth method to solve a constrained quadratic problem.

Initialize. Choose $v_0 \in L^2(X)$. Set $n = 0$.

Compute $\Phi_n = Hv_n + b$; Set $\mathbb{A}_n = \mathbb{A}_n^\beta \cup \mathbb{A}_n^\alpha$ and $\mathbb{I}_n = X \setminus \mathbb{A}_n$, where

$$\mathbb{A}_n^\beta = \{x \in X : \; -\Phi_n(x) \geq \kappa\tilde{\beta}(x)\}, \; \mathbb{A}_n^\alpha = \{x \in X : \; -\Phi_n(x) \leq \kappa\tilde{\alpha}(x)\}.$$

for $n \geq 0$ **do**

Set $w_n(x) = \begin{cases} -v_n(x) + \tilde{\beta}(x) & \text{if } x \in \mathbb{A}_n^\beta \\ -v_n(x) - \frac{\Phi_n(x)}{\kappa} & \text{if } x \in \mathbb{I}_n \\ -v_n(x) + \tilde{\alpha}(x) & \text{if } x \in \mathbb{A}_n^\alpha \end{cases}$

Compute $\eta_n = H\chi_{\mathbb{A}_n} w_n$ and set $b_n = \chi_{\mathbb{I}_n} w_n - \chi_{\mathbb{I}_n}\eta_n$

Solve, for $\bar{\upsilon}_n$ the unconstrained quadratic problem $\min\limits_{\upsilon \in L^2(\mathbb{I}_n)} \frac{1}{2}(R_{\mathbb{I}_n} HE_X\upsilon + \kappa\upsilon, \upsilon) - (b, \upsilon)$

Set $v_{n+1} = w_n$ in $\mathbb{A}_n$ and $v_{n+1} = \bar{\upsilon}_n$ in $\mathbb{I}_n$.

Compute $\Phi_{n+1} = Hv_{n+1} + b$, $\mathbb{A}_{n+1}^\beta$, $\mathbb{A}_{n+1}^\alpha$, $\mathbb{A}_{n+1}$ and $\mathbb{I}_{n+1}$

For **finite-dimensional** problems: stop if $\mathbb{A}_n^\beta = \mathbb{A}_{n+1}^\beta$ and $\mathbb{A}_n^\alpha = \mathbb{A}_{n+1}^\alpha$

Set $n = n + 1$

end

Outline

Routines we need: (1) solving nonlinear PDEs

1. Given u, we need a routine to compute $y_u = G(u)$, this is, to solve the nonlinear equation

$$-\Delta y + \boldsymbol{b} \cdot \nabla y + f(\cdot, y) = u \text{ in } \Omega, \;\; y = 0 \text{ on } \Gamma.$$

I use Newton's method for the equation $\mathcal{F}(y) = 0$, where

$$\mathcal{F}(y) = -\Delta y + \boldsymbol{b} \cdot \nabla y + f(\cdot, y) - u = 0.$$

Notice that

$$\mathcal{F}'(y)z = -\Delta z + \boldsymbol{b} \cdot \nabla z + \partial_y f(\cdot, y)z = 0.$$

So, naming $z = y_{k+1} - y_k$, the Newton equation

$$\mathcal{F}'(y_k)z = -\mathcal{F}(y_k)$$

can be written, doing the proper cancellations in the linear terms, as

$$-\Delta y_{k+1} + \boldsymbol{b} \cdot \nabla y_{k+1} + \partial_y f(\cdot, y_k)y_{k+1} = u - f(\cdot, y_k) + \partial_y f(\cdot, y_k)y_k$$

FEM approximation

- Let $\mathcal{K}$ be the stiffness matrix such that $\mathcal{K}\boldsymbol{y}$ models $-\Delta y$
- Let $\mathcal{T}$ be the transport matrix such that $\mathcal{T}\boldsymbol{y}$ models $\boldsymbol{b} \cdot \nabla y$
  Notice that $\mathcal{T}^T\boldsymbol{y}$ models $-\operatorname{div}[\boldsymbol{b}\varphi]$
- Name $\mathcal{A} = \mathcal{K} + \mathcal{T}$
- Let $\mathcal{M}_0$ be the mass matrix such that $\mathcal{M}_0\boldsymbol{u}$ models the rhs u.
- **At each step**, we have to **assemble a mass matrix** $\mathcal{M}^k$ that models the action of $\partial_y f(x, y_k)$

$$\mathcal{M}^k_{i,j} = \int_\Omega e_i(x)\partial_y f(x, y^k_h(x))e_j(x)\,\mathrm{d}x.$$

And also **assemble a vector** $\mathfrak{f}^k$ to model $f(x, y_k)$

$$\mathfrak{f}^k_j = \int_\Omega f(x, y^k_h(x))e_j(x)\,\mathrm{d}x.$$

Solving the linear systems

At each step we have to solve the linear system

$$[\mathcal{A} + \mathcal{M}^k]\boldsymbol{y} = \mathcal{M}_0 \boldsymbol{u} + \mathcal{M}^k \boldsymbol{y}^k - \mathfrak{f}^k.$$

Since we have a transport term, the matrix is *not* symmetric. Use an LU decomposition. I use the following trick in MATLAB, which uses a scaling diagonal matrix `D`, row permutation `p` and column permutation `q`

```
[L,U,p,q,D] = lu(A+Mk,'vector'); D = spdiags(D); D = D(p);
```

We can solve `(A+Mk)y = b`, with a very efficient one-liner, that solves two very sparse triangular systems.

```
y(q,1) = U\(L\(D.\b(p)))
```

We stop the method when $\|y_h^k - y_h^{k+1}\|$ is “small”. This means that $\mathcal{M}^k \approx \mathcal{M}^{k+1}$, so we store in memory the last `L,U,p,q,D`. You will see now how helpful this is.

Routines we need: (2) solving the linearized PDE

Given u, y_u, and v, we need a routine to compute $z_{u,v} = G'(u)v$

$$-\Delta z + \boldsymbol{b} \cdot \nabla z + \partial_y f(\cdot, y_u) z = v$$

The y_u that appears here is the one that comes from Newton's method!. So the system to solve is

$$[\mathcal{A} + \mathcal{M}^{k+1}]\boldsymbol{z} = \mathcal{M}_0 \boldsymbol{v}$$

Since $\mathcal{M}^{k+1} \approx \mathcal{M}^k$, we use the same coefficient matrix that we have already used and factorized! Name $\boldsymbol{b} = \mathcal{M}_0 \boldsymbol{v}$ and do

```
z(q,:) = U\(L\(D.\b(p,:)))
```

Remark:

- We will also use this with Matlab `fmincon`, which will need to compute $z_{u,v}$ for several directions v at the same time, hence the `:`.

Routines we need: (3) solving the adjoint equations

Given u, y_u, we need a routine to compute φ_u

$$-\Delta\varphi - \mathrm{div}[\boldsymbol{b}\varphi] + \partial_y f(\cdot, y_u)\varphi = y_u - y_d$$

Given u, y_u, φ_u, v and $z_{u,v}$, we need a routine to compute $\eta_{u,v}$

$$-\Delta\eta - \mathrm{div}[\boldsymbol{b}\eta] + \partial_y f(\cdot, y_u)\eta = (1 - \varphi_u f''(y_u))z_{u,v}$$

The coefficient matrix that appears in the FEM approximation of these equations is the *transpose* of $[\mathcal{A} + \mathcal{M}^{k+1}]$. We can take advantage of the factorization that we have using MATLAB's forward slash (`mrdivide`).

Let $\mathcal{M}$ be the mass matrix such that $\|y_h\|^2_{L^2(\Omega)} = \boldsymbol{y}^T\mathcal{M}\boldsymbol{y}$.
For the adjoint state, name $\boldsymbol{b} = \mathcal{M}(\boldsymbol{y} - \boldsymbol{y}_d)$ and solve

```
phi(p,1) = ((b(q)'/U)/L)'./D;
```

Second adjoint state

For the second adjoint state, I **assemble** another mass matrix $\mathfrak{M}$

$$\mathfrak{M}_{i,j} = \int_\Omega e_i(x)\left(1 - \varphi_h(x)\partial^2_{yy} f(x, y_h(x))\right) e_j(x)\, \mathrm{d}x$$

and name $\boldsymbol{b} = \mathfrak{M}\boldsymbol{z}$. Then solve

```
eta(p,:) = ((b(q,:)'/U)/L)'./D;
```

Remark:

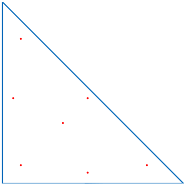
- We will have to compute $\mathfrak{M}\boldsymbol{z}$ for several $\boldsymbol{z}$, so it is better to assemble first $\mathfrak{M}$ than assembling $\boldsymbol{b} = \mathfrak{M}\boldsymbol{z}$ directly.
- We will also use this with Matlab `fmincon`, which needs to compute $\eta_{u,v}$ for several directions v at the same time, hence the `:`.

Assembling all those matrices

- One of the keys to fast computation is the ability to assemble efficiently all those mass matrices that change at every iteration.
- Numerical integration formulas must be used. Just the trapezoid or the midpoint formula may not do the work.
  - We may have to integrate difficult functions like

$$\int_T e_i(x)\varphi_h(x)\mathrm{e}^{y_h(x)}e_j(x)\,\mathrm{d}x, \text{ or } \int_T e_i(x)\varphi_h(x)y_h(x)|y_h(x)|e_j(x)\,\mathrm{d}x$$

  - We may have singularities near non-convex corners.
- An equilibrium must be found among the number of points and the accuracy. I use either the mid-edges formula (3 nodes, order 2) or a seven-point formula of order 5.



Ronald Cools (2022). *Encyclopaedia of Cubature Formulas.* URL: https://nines.cs.kuleuven.be/ecf/

Outline

Discretize, then optimize

Assume $\boldsymbol{y} \in \mathbb{R}^{N_y}$ and $\boldsymbol{u} \in \mathbb{R}^{N_u}$.

$$J(\boldsymbol{u}) = \frac{1}{2}(\boldsymbol{y} - \boldsymbol{y}_d)^T \mathcal{M}(\boldsymbol{y} - \boldsymbol{y}_d) + \frac{\kappa}{2}\boldsymbol{u}^T \mathcal{D}\boldsymbol{u},$$

where $\boldsymbol{u}^T\mathcal{D}\boldsymbol{u}$ is/approximates $\|u_h\|^2_{L^2(\Omega)}$

$$\begin{aligned} \mathcal{A}\boldsymbol{y} + \mathfrak{f}(\boldsymbol{y}) &= \mathcal{M}_0\boldsymbol{u} \\ \mathcal{A}\boldsymbol{z} + \mathcal{F}'(\boldsymbol{y})\boldsymbol{z} &= \mathcal{M}_0\boldsymbol{v} \\ \mathcal{A}^T\boldsymbol{\varphi} + \mathcal{F}'(\boldsymbol{y})\boldsymbol{\varphi} &= \mathcal{M}(\boldsymbol{y} - \boldsymbol{y}_d) \\ \mathcal{A}^T\boldsymbol{\eta} + \mathcal{F}'(\boldsymbol{y})\boldsymbol{\eta} &= \mathfrak{M}\boldsymbol{z} \end{aligned}$$

$$\begin{aligned} J'(\boldsymbol{u})\boldsymbol{v} &= \boldsymbol{v}^T(\mathcal{M}_0^T\boldsymbol{\varphi} + \kappa\mathcal{D}\boldsymbol{u}) \\ J''(\boldsymbol{u})\boldsymbol{v} &= \boldsymbol{v}^T(\mathcal{M}_0^T\boldsymbol{\eta} + \kappa\mathcal{D}\boldsymbol{v}) \end{aligned}$$

Can we use a diagonal $\mathcal{D}$?

- We can choose $\mathcal{D}$ diagonal in the following cases:
  1. $U_h = U_{h,0}$ is formed by piecewise constant approximations of the controls.
  2. $U_h = U_{h,1}$ is formed by piecewise linear approximations of the controls, and we use the composite trapezoid rule to approximate $\int_\Omega u_h(x)^2 \, dx$.
- The relation between discrete optimal control and discrete optimal adjoint state is respectively, as follows
  1. $\bar{u}_h(x) = \text{Proj}_{[\alpha,\beta]}\left(\frac{Q_h\bar{\varphi}_h}{\kappa}\right)$ where $Q_h : L^1(\Omega) \to U_h$ is the projection in the sense of $L^2(\Omega)$ onto U_h.
  2. $\bar{u}_h(x) = \text{Proj}_{[\alpha,\beta]}\left(\frac{C_h\bar{\varphi}_h}{\kappa}\right)$ where $C_h : L^1(\Omega) \to U_h$ is the Carstensen interpolation operator.
- In both cases we have that $Q_h\bar{\varphi}_h \neq \bar{\varphi}_h$ and $C_h\bar{\varphi}_h \neq \bar{\varphi}_h$. This has the following effects:
  - The approximation error $O(h^2)$ in $L^2(\Omega)$ of the FEM is lost. We will have $O(h)$ in the first case and $o(h)$ in the second case.
  - In the case $\alpha \leq 0 \leq \beta$, we have that $\bar{u} = 0$ on Γ. This is also lost. In general $\bar{u}_h \not\equiv 0$ on Γ.

Ideas about semismooth Newton

Usin that $\mathcal{D}$ is diagonal.
Instead of writing the first order optimality conditions written as

$$\bar{u}_i = \text{Proj}_{[\alpha,\beta]} \left(\frac{-[\mathcal{M}_0 \bar{\varphi}]_i}{\kappa d_{ii}} \right),$$

I prefer to denote $\alpha_i = \kappa d_{ii}\alpha$ and $\beta_i = \kappa d_{ii}\beta$, and write

$$\kappa d_{ii} \bar{u}_i = \text{Proj}_{[\alpha_i,\beta_i]} \left(-[\mathcal{M}_0 \bar{\varphi}]_i \right)$$

So the function $\boldsymbol{F}$ for the SemiSmooth Newton method is given by

$$[\boldsymbol{F}(\boldsymbol{u})]_i = \kappa d_{ii} u_i - \text{Proj}_{[\alpha_i,\beta_i]} \left(-[\mathcal{M}_0 \varphi]_i \right)$$

In the algorithm one has to be careful, because now w is defined by $-\kappa d_{ii} w_i = -[\boldsymbol{F}(\boldsymbol{u})]_i$. Also the solution of unconstrained quadratic program requires the use of a **preconditioner**. $\kappa\mathcal{D}$ does the work!

What if $\mathcal{D}$ is not diagonal?

- $U_h = U_{h,1}$ is formed by piecewise linear approximations of the controls, and we compute $\int_\Omega u_h(x)^2 \, dx = \boldsymbol{u}^T \mathcal{M} \boldsymbol{u}$, which is exact.
- In this case $\mathcal{M}_0 = \mathcal{M}$ and $\mathcal{D} = \mathcal{M}$. Order of convergence $O(h^{3/2})$ is obtained.
- The first order optimality condition

$$(\boldsymbol{u} - \bar{\boldsymbol{u}})^T (\mathcal{M} \bar{\boldsymbol{\varphi}} + \kappa \mathcal{M} \bar{\boldsymbol{u}}) \geq 0 \;\forall \boldsymbol{\alpha} \leq \boldsymbol{u} \leq \boldsymbol{\beta}$$

  cannot be written in a componentwise form. We lose the pointwise projection formula.
- We can write the first order optimality condition using Lagrange multipliers for the constraints $\boldsymbol{\alpha} \leq \boldsymbol{u} \leq \boldsymbol{\beta}$.
  There exists $\bar{\boldsymbol{\lambda}} = \bar{\boldsymbol{\lambda}}_\beta - \bar{\boldsymbol{\lambda}}_\alpha$ such that

$$\begin{aligned}
&\mathcal{M} \bar{\boldsymbol{\varphi}} + \kappa \mathcal{M} \bar{\boldsymbol{u}} + \bar{\boldsymbol{\lambda}} = 0 \\
&\boldsymbol{\alpha} \leq \bar{\boldsymbol{u}} \leq \boldsymbol{\beta} \\
&\bar{\boldsymbol{\lambda}}_\beta \geq \mathbf{0}, \; \bar{\boldsymbol{\lambda}}_\alpha \geq \mathbf{0} \\
&\bar{\boldsymbol{\lambda}}_\beta^T (\bar{\boldsymbol{u}} - \boldsymbol{\beta}) = 0 \\
&\bar{\boldsymbol{\lambda}}_\alpha^T (\bar{\boldsymbol{u}} - \boldsymbol{\alpha}) = 0
\end{aligned}$$

Semismooth equation for not diagonal $\mathcal{D}$.

- For any $c > 0$, the previous relations can be written as

$$\begin{aligned} &\mathcal{M}\bar{\varphi} + \kappa \mathcal{M}\bar{\boldsymbol{u}} + \bar{\boldsymbol{\lambda}} = 0 \\ &\bar{\boldsymbol{\lambda}} = \max\{\mathbf{0}, \bar{\boldsymbol{\lambda}} + c(\bar{\boldsymbol{u}} - \boldsymbol{\beta})\} + \min\{\mathbf{0}, \bar{\boldsymbol{\lambda}} + c(\bar{\boldsymbol{u}} - \boldsymbol{\alpha})\} \end{aligned}$$

- Define $\boldsymbol{F} : \mathbb{R}^N \times \mathbb{R}^N \longrightarrow \mathbb{R}^N \times \mathbb{R}^N$ as

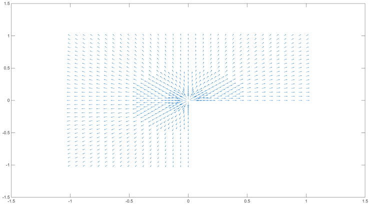
$$\boldsymbol{F}(\boldsymbol{u}, \boldsymbol{\lambda}) = \left[\begin{array}{l} \mathcal{M}\varphi + \kappa \mathcal{M}\boldsymbol{u} + \boldsymbol{\lambda} \\ \boldsymbol{\lambda} - \max\{\mathbf{0}, \boldsymbol{\lambda} + c(\boldsymbol{u} - \boldsymbol{\beta})\} - \min\{\mathbf{0}, \boldsymbol{\lambda} + c(\boldsymbol{u} - \boldsymbol{\alpha})\} \end{array} \right]$$

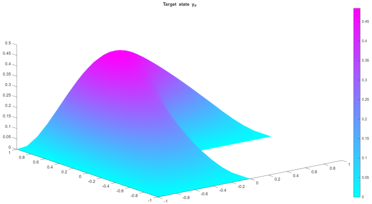
- Apply the SemiSmooth Newton method to this problem.
  (Exercise for the reader).

Outline

Data for the example

- Ω is the L-shaped domain $[-1,1]^2 \setminus [-1,0]^2$. Notice that its biggest interior angle is $\omega = 3\pi/2$. Name $\lambda = \pi/\omega = 2/3$.
- We select data to have a non-monotone and non-coercive nonlinear operator: $f(x,y) = y^3|y|$. $b(x) = \delta r^{1+\gamma}(\cos\theta, \sin(\theta))$. Here (r,θ) are the polar coordinates, and we select $\delta = 6$ and $\gamma = -1.25$.
- $y_d(x) = (1-x^2)(1-y^2)r^{\lambda}\sin(\lambda\theta)$.
- $\kappa = 10^{-4}$, $\alpha = 0$, $\beta = 10$ (really ill posed!).

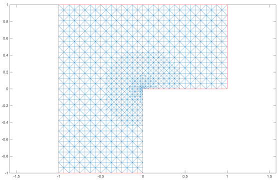




Discretization choices

- Finite element method. Lagrange P1 functions for the state and the adjoint state.
- Graded mesh family obtained by the “bisection method”. Grading parameter $\mu = 2/3$.
- The controls are discretized also with Lagrange P1 elements. The term $\|u\|^2_{L^2(\Omega)}$ is discretized using the composite trapezoid rule, which means $\boldsymbol{u}^T \mathcal{D} \boldsymbol{u}$ where $\mathcal{D}$ is the diagonal lumped mass matriz:

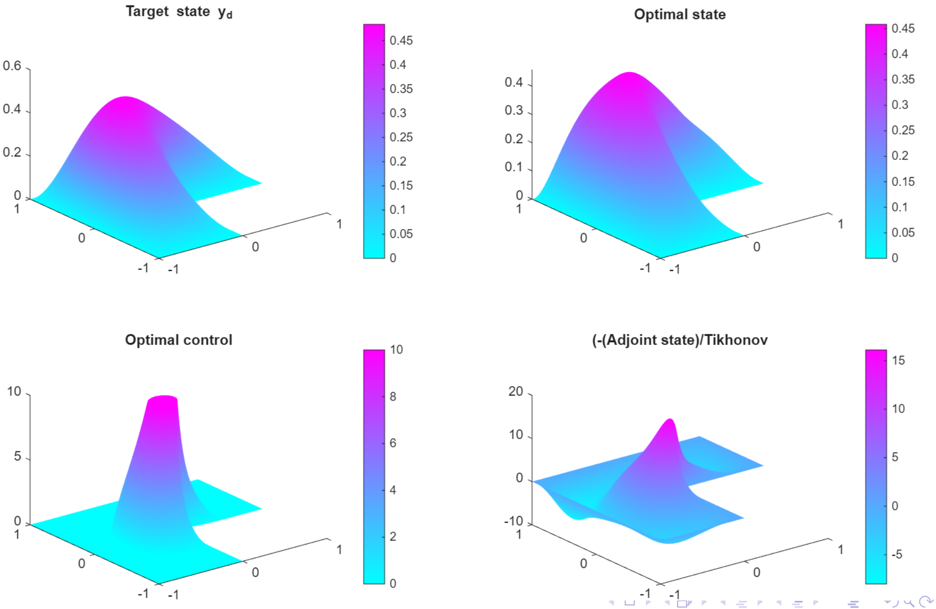
$$d_{ii} = \int_\Omega e_i \, \mathrm{d}x.$$



Choosing the initial point

- To solve the problem with meshsize h, use a sequence of (nested) meshes of sizes $h_1 \geq h_2 \geq \ldots \geq h_N = h$.
- Also, use a sequence $\kappa_1 \geq \kappa_2 \geq \ldots \kappa_N = \kappa$.
- For the problem of size h_i with Tikhonov parameter κ_i, use as initial point the solution of the problem of size h_{i-1}, with κ_{i-1}.
- The problem h_1 with κ_1 is of small size and not ill posed. In our case $u_0 \equiv 0$ works.

Solution



Target state y_d
Optimal state
Optimal control
(-(Adjoint state)/Tikhonov

Some results: (1) SemiSmooth Newton

```
kappa = 1.0000e+00
Mesh data: refinements = 1, dim Y_h = 8, dim U_h = 24.
SemiSmooth Newton method solving nonlinear equations
  j &       J(u)             &   delta_u    & Fact &   CG &    #J   &  #Ab &   #Aa \\

---- ----------------------- ------------- ------ ------ -------- ------ --------
  0 &  8.6591166282472015e-02 &       Inf    &    1 &    0 &      0      24        0 \\
  1 &  8.5977499674872490e-02 &  5.2e-02    &    2 &    2 &     24       0        0 \\
  2 &  8.5977499674872476e-02 &  2.5e-09    &    2 &    3 &     24       0        0 \\
.
.
.
kappa = 1.0000e-04
Mesh data: refinements = 8, dim Y_h = 237368, dim U_h = 239526.
SemiSmooth Newton method solving nonlinear equations
  j &       J(u)             &   delta_u    & Fact &   CG &    #J   &  #Ab &   #Aa \\

---- ----------------------- ------------- ------ ------ -------- ------ --------
  0 &  1.5050899562244532e-03 &       Inf    &    2 &    0 &  86646  138045   14835 \\
  1 &  1.5050875185621496e-03 &  3.1e-02    &    3 &   11 &  85947  138643   14936 \\
  2 &  1.5050875082492838e-03 &  4.7e-03    &    3 &   14 &  85995  138452   15079 \\
  3 &  1.5050875081594375e-03 &  7.6e-05    &    3 &   13 &  85993  138452   15081 \\
  4 &  1.5050875081590892e-03 &  7.4e-10    &    3 &   18 &  85993  138452   15081 \\
  5 &  1.5050875081590843e-03 &  9.6e-12    &    2 &   22 &  85993  138452   15081 \\
  6 &  1.5050875081590817e-03 &  1.2e-13    &    1 &   22 &  85993  138452   15081 \\
  7 &  1.5050875081590821e-03 &  1.8e-15    &    1 &   26 &  85993  138452   15081 \\

tiempo =

  44.360280099999997
```

Some results: (2) Sequence of Quadratic Programs

```
kappa = 1.0000e+00
Mesh data: refinements = 1, dim Y_h = 8, dim U_h = 24.
SQP method solving nonlinear equations
  n &       J(u_n)             &  delta_u   & Fact &  QP  &  CG  &   #J  &   #Aa  &  #Ab \\

---- ------------------------   ---------- ------ ------ ------- -------- -------
  0 &  8.6591166282472015e-02 &       Inf  &    1 &    0 &    0 &      0      24       0 \\
  1 &  8.5977499674872490e-02 &  5.2e-02   &    2 &    1 &    2 &     24       0       0 \\
  2 &  8.5977499674872476e-02 &  2.5e-09   &    2 &    1 &    3 &     24       0       0 \\
.
.
.
kappa = 1.0000e-04
Mesh data: refinements = 8, dim Y_h = 237368, dim U_h = 239526.
SQP method solving nonlinear equations
  n &       J(u_n)             &  delta_u   & Fact &  QP  &  CG  &   #J  &   #Aa  &  #Ab \\

---- ------------------------   ---------- ------ ------ ------- -------- -------
  0 &  1.5050899562244540e-03 &       Inf  &    2 &    0 &    0 &  86646  138045   14835 \\
  1 &  1.5050875096717187e-03 &  3.1e-02   &    3 &    2 &   22 &  85993  138452   15081 \\
  2 &  1.5050875081708251e-03 &  2.2e-06   &    4 &    1 &   13 &  85993  138452   15081 \\
  3 &  1.5050875081591864e-03 &  3.0e-08   &    4 &    1 &   21 &  85993  138452   15081 \\
  4 &  1.5050875081590721e-03 &  3.5e-10   &    3 &    1 &   22 &  85993  138452   15081 \\
  5 &  1.5050875081590713e-03 &  4.1e-12   &    2 &    1 &   22 &  85993  138452   15081 \\
  6 &  1.5050875081590962e-03 &  4.9e-14   &    1 &    1 &   24 &  85993  138452   15081 \\

tiempo =

  46.425035999999999
```

Some results: (3) SemiSmooth Newton using Lagrange multipliers. No mass lumping!

Slightly different problem, hence slightly different solution, probably more accurate

```
kappa = 1.0000e+00
Mesh data: refinements = 1, dim Y_h = 8, dim U_h = 24.
SemiSmooth Newton method. Using multipliers and solving nonlinear equations
  j &       J(u)             &   delta_u    & Fact &    CG &    #J   &  #Ab &    #Aa \\
____ _______________________ _____________ ______ ______ ________ ______ ________
  0 &  8.6591166282472015e-02 &       Inf   &    1 &     0 &       0       24        0 \\
  1 &  8.6591166282472015e-02 &  0.0e+00    &    1 &     0 &       0       24        0 \\
.
.
.
kappa = 1.0000e-04
Mesh data: refinements = 8, dim Y_h = 237368, dim U_h = 239526.
SemiSmooth Newton method. Using multipliers and solving nonlinear equations
  j &       J(u)             &   delta_u    & Fact &    CG &    #J   &  #Ab &    #Aa \\
____ _______________________ _____________ ______ ______ ________ ______ ________
  0 &  1.5050391203894268e-03 &       Inf   &    2 &     0 &  85902  138602   15013 \\
  1 &  1.5050370629104556e-03 &  4.2e-02    &    3 &    22 &  85901  138612   15013 \\
  2 &  1.5050374656000616e-03 &  4.3e-02    &    2 &    29 &  85643  138721   15162 \\
  3 &  1.5050374665947280e-03 &  9.7e-03    &    2 &    32 &  85434  138910   15182 \\
  4 &  1.5050374665958775e-03 &  1.4e-09    &    3 &    25 &  85514  138830   15182 \\
  5 &  1.5050374665958525e-03 &  2.8e-11    &    2 &    45 &  85469  138875   15182 \\
  6 &  1.5050374665958462e-03 &  3.3e-13    &    1 &    45 &  85571  138773   15182 \\
  7 &  1.5050374665958462e-03 &  1.2e-14    &    1 &    50 &  85531  138813   15182 \\

tiempo =

  51.489184500000000
```

Some results: (4a) Matlab fmincon. Mass lumping.

Trust region method. Provide HessiaMultiply with a smart trick to pass a diagonal preconditioner.

Use zero initial point and let Matlab do all the work.

```
kappa = 1.0000e-04
Mesh data: refinements = 8, dim Y_h = 237368, dim U_h = 239526.
Matlab fmincon

                                  Norm of      First-order
 Iteration          f(x)          step          optimality   CG-iterations
     0           0.0854467                       1.01e-05
     1           0.0124817         1.55336       1.62e-06           14
     2          0.00466646        0.715332       2.69e-07           19
     3          0.00310525        0.954632       1.49e-07           19
     4          0.00282616         0.22572       1.46e-07           19
     5          0.00180709         1.35091       3.25e-08           18
     6           0.0015767        0.871314       6.25e-09           20
     .
    32          0.00150509     5.07681e-14       6.06e-14            0
    33          0.00150509      1.2692e-14       6.06e-14            0

Optimization stopped because the norm of the current step, 1.269202e-14, is
less than options.StepTolerance = 5.000000e-14.


tiempo =

     1.376478881000000e+02
```

Some results: (4b) Matlab fmincon. Mass lumping.

Trust region method. Provide HessiaMultiply with a smart trick to pass a diagonal preconditioner. Use a –refinement in h and continuation in $\kappa-$ technique

```
kappa = 1.0000e+00
Mesh data: refinements = 1, dim Y_h = 8, dim U_h = 24.
Matlab fmincon
                                    Norm of      First-order
 Iteration        f(x)              step          optimality   CG-iterations
     0          0.0865912                           0.0705
     1          0.0859775        0.0179072        0.000245           4
     2          0.0859775       6.6269e-05        6.02e-09           4
     3          0.0859775      1.38571e-09        2.59e-17           4

Optimization completed: The first-order optimality measure, 2.592113e-17,
is less than options.OptimalityTolerance = 5.000000e-14, and no negative/zero
curvature is detected in the trust-region model.
 .
 .
kappa = 1.0000e-04
Mesh data: refinements = 8, dim Y_h = 237368, dim U_h = 239526.
Matlab fmincon
                                    Norm of      First-order
 Iteration        f(x)              step          optimality   CG-iterations
     0         0.00150509                           5.4e-10
     1         0.00150509      0.000325074          3.8e-10          21
     2         0.00150509        0.0209348        6.64e-12          21
     3         0.00150509        0.0115229        9.45e-13          20
     4         0.00150509       0.00591895        9.45e-13          21
     .
     .
    20         0.00150509      2.31679e-13        9.45e-13           0
    21         0.00150509      5.79199e-14        9.45e-13           0
    22         0.00150509        1.448e-14        9.45e-13           0

Optimization stopped because the norm of the current step, 1.447997e-14, is
less than options.StepTolerance = 5.000000e-14.

tiempo =
  66.902753500000003
```

Some results: (5) Matlab fmincon. No Mass Lumping

Trust region method. Provide HessiaMultiply with a smart trick to pass a diagonal preconditioner. Use a –refinement in h and continuation in κ– technique

```
kappa = 1.0000e+00
Mesh data: refinements = 1, dim Y_h = 8, dim U_h = 24.
Matlab fmincon
                                  Norm of      First-order
 Iteration        f(x)            step          optimality   CG-iterations
     0          0.0865912                         0.0705
     1          0.0859153       0.0192294          0.011          12
     2          0.0858572        0.101693       2.95e-05          12
     .
     .
    16          0.0858497     0.000752885        1.6e-14          12

Optimization completed: The first-order optimality measure, 1.597934e-14,
is less than options.OptimalityTolerance = 5.000000e-14, and no negative/zero
curvature is detected in the trust-region model.
.
.
kappa = 1.0000e-04
Mesh data: refinements = 8, dim Y_h = 237368, dim U_h = 239526.
Matlab fmincon
                                  Norm of      First-order
 Iteration        f(x)            step          optimality   CG-iterations
     0         0.00150504                       7.52e-10
     1         0.00150504     0.000323823       4.83e-10          51
     2         0.00150504     0.000580233       1.29e-10          50
     3         0.00150504     6.11812e-05       1.29e-10          50
     4         0.00150504     1.52953e-05       1.29e-10           0
     .
     .
    19         0.00150504     1.42449e-14       1.29e-10           0

Optimization stopped because the norm of the current step, 1.424486e-14, is
less than options.StepTolerance = 5.000000e-14.

tiempo =
  81.967342200000004
```