Optimisation and Control of PDEs

Theory and Numerics

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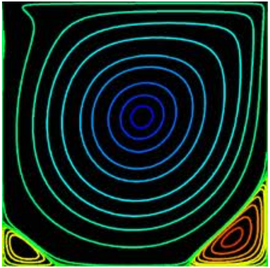
i/fb START PROJECT INTERFACES/FREE BOUNDARIES

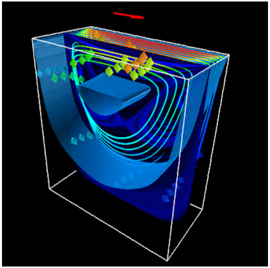
FWF Der Wissenschaftsfonds.

Motivation, Basics, Existence and First Order Optimality.

Motivation: Optimal control of fluid flow

Example: Lid driven cavity flow





Mathematical model: Navier Stokes system

$$\begin{aligned}
&\frac{\partial y}{\partial t} + (y \cdot \nabla)y - \nu\Delta y + \nabla\varpi = u && \text{in } Q := (0,T) \times \Omega,\\
&\operatorname{div} y = 0 && \text{in } Q,\\
&y(t,\cdot) = 0 && \text{on } \Sigma = (0,T) \times \partial\Omega,\\
&y(0,\cdot) = y_0 && \text{in } \Omega,
\end{aligned}$$

Motivation: Optimal control of fluid flow

Optimisation problem:

Minimize $\quad J(y,u) \qquad\qquad$ over $\quad (y,u) \in W \times U_{\mathrm{ad}}$

subject to (s.t.)

$$
\begin{aligned}
&\frac{\partial y}{\partial t} + (y\cdot\nabla)y - \nu\Delta y + \nabla\varpi = u && \text{in } Q = (0,T)\times\Omega,\\
&\operatorname{div} y = 0 && \text{in } Q,\\
&y(t,\cdot) = 0 && \text{on } \Sigma = (0,T)\times\partial\Omega,\\
&y(0,\cdot) = y_0 && \text{in } \Omega,
\end{aligned}
$$

with, for example,

$$U_{\mathrm{ad}} = \{v \in U : a \le v \le b \text{ almost everywhere (a.e.) in } Q\}.$$

We call y the state and u the control (variable), respectively.

Motivation: Optimal control of fluid flow

Define $e : W \times U \to Z^*$ as

$$e(y,u) = \left(\frac{\partial y}{\partial t} + (y \cdot \nabla) y - \nu \Delta y - u,\ y(0) - y_0 \right),$$

$y_0 \in H$.

Here we have

$$\begin{aligned} H &= \{v \in C_0^\infty(\Omega)^2 :\ \text{div } v = 0\}^{-|\cdot|_{L^2}}, \\ V &= \{v \in C_0^\infty(\Omega)^2 :\ \text{div } v = 0\}^{-|\cdot|_{H^1}}, \\ W &= \{v \in L^2(V) :\ v_t \in L^2(V^*)\} \\ Z &= L^2(V) \times H, \\ U &= L^2(Q)^2. \end{aligned}$$

Sequential quadratic programming (SQP)

- **Original problem in abstract form:**

$$\begin{array}{lll} \text{Minimize} & J(y,u) & \text{over } (y,u) \in W \times U \\ \text{s.t.} & e(y,u) = 0 & \text{in } Z^*, \\ & a \le u \le b & \text{a.e. in } Q. \end{array}$$

- **QP-problem:** We use $x := (y,u), \delta_x := (\delta_y, \delta_u)$.

$$\begin{array}{lll} \text{Minimize} & \langle \hat{L}_x, \delta_x \rangle + \frac{1}{2} \langle \hat{L}_{xx} \delta_x, \delta_x \rangle & \text{over } \delta_x \in W \times U \\ \text{s.t.} & e + e_x \delta_x = 0 & \text{in } Z^*, \\ & a - u \le \delta_u \le b - u & \text{a.e. in } Q. \end{array}$$

$\hat{L}(x, p, \lambda_a, \lambda_b) := J(x) + \langle e(x), p \rangle + (\lambda_a, u - a) + (\lambda_b, u - b)$ is the Lagrange function of the original problem, and $p \in Z$ is the adjoint state.

Reduced sequential quadratic programming (rSQP)

Reduced QP-problem:

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\langle T^* \hat{L}_{xx} T\delta_u, \delta_u\rangle + \langle r, \delta_u\rangle \\ \text{s.t.} & a - u \le \delta_u \le b - u \quad \text{a.e. in } Q, \end{array}$$

where

$$T = \begin{pmatrix} -e_y^{-1} e_u \\ \text{id} \end{pmatrix}, \quad r = T^* J_x + e_u^* e_y^{-*} \hat{L}_{yy} e_y^{-1} e.$$

Usual work flow in PDE constrained optimisation

Analysis.

- Analysis of the underlying PDE model (stability, sensitivity).
- Existence of a solution of optimisation problem.
- First order optimality characterization.
  - $\Rightarrow$ Establish and analyse adjoint equation.
- Possible: Second order necessary / sufficient optimality.

Solver development (function space).

- SQP or rSQP approach.
  - $\Rightarrow$ Quasi-Newton approach.
  - $\Rightarrow$ Structured modification of Hessian of Lagrangian.
- QP-solver.
  - $\Rightarrow$ E.g. generalized Newton method as a QP-solver.
  - $\Rightarrow$ Establish (local) convergence (q-superlinear).
- Establish outer (r)SQP convergence (locally q-quadratic - analysis via generalized equations.)

Usual work flow in PDE constrained optimisation

Discrete problem / solver.

- FD / FV / FE discretization (of problem resp. solver).
- Discrete solver analysis.
  - $\Rightarrow$ Ideally: Mesh independence.
- Efficiency through adaptive finite element methods (AFEM).
  - $\Rightarrow$ A posteriori error residual based estimators.
  - $\Rightarrow$ Dual weighted residual based goal oriented approach.
  - $\Rightarrow$ Refinement / coarsening (bulk criterion).
  - $\Rightarrow$ Convergence of the AFEM cycle.
- Practical realization.
  - $\Rightarrow$ Develop or supplement software (DUNE, COMSOL,...)

Back to: Optimal control of fluid flow

Problem data for "lid driven cavity flow".

Tracking type objective:

Desired flow y_d is given by the Stokes flow (constant in time):

$$J(y,u) = \frac{1}{2}\int_Q |y - y_d|^2 dx\,dt + \frac{\alpha}{2}\int_Q |u|^2 dx\,dt.$$

Control bounds:

$$-0.3 \le u \le 0.3 \text{ a.e. on } Q = (0,1)^2 \times (0,T).$$

Cost of the control: $\alpha = 0.01$.

Evolution of control and state.

Evolution of active sets.

Model problem

Elliptic Optimal Control Problems: Unconstrained Case.

Given $y_d \in L^2(\Omega)$ and $\alpha > 0$, find $(y,u) \in H_0^1(\Omega) \times L^2(\Omega)$ such that

$$\begin{cases} \inf J(y,u) := \frac{1}{2}\int_\Omega |y - y_d|^2 dx + \frac{\alpha}{2}\int_\Omega |u|^2 dx, \\ \text{s. t. } \; -\Delta y = u \quad \text{in } H^{-1}(\Omega), \quad y = 0 \text{ on } \partial\Omega. \end{cases}$$

Reduced formulation: Denoting by $\mathcal{G} : H^{-1}(\Omega) \to H_0^1(\Omega)$ the control-to-state map, which assigns to a control $u \in L^2(\Omega)$ the solution $y = \mathcal{G}(u) \in H_0^1(\Omega)$ of the state equation, the reduced formulation reads:

$$\inf \hat{J}(u) := \frac{1}{2}\int_\Omega |\mathcal{G}(u) - y_d|^2 dx + \frac{\alpha}{2}\int_\Omega |u|^2 dx \text{ over } u \in L^2(\Omega).$$

Existence of a solution via convex analysis.

Basic facts from convex analysis I

Let $\overline{\mathbb{R}} := \mathbb{R} \cup \{\pm\infty\}$, U a Banach space, and $F : U \to \overline{\mathbb{R}}$ convex.

- F is proper if it nowhere takes the value $-\infty$ and is not identically equal to $+\infty$.
- $\operatorname{epi} F := \{(u, d) \in U \times \mathbb{R} : F(u) \leq d\}$ is the epigraph of F.
- F convex $\Leftrightarrow$ epi F convex.
- F is lower semicontinuous (l.s.c.) on U if it satisfies:

  $$\text{For all } a \in \mathbb{R} \quad \{u \in U : F(u) \leq a\} \text{ is closed;}$$

  or, equivalently,

  $$\text{For all } \bar{u} \in U \quad \liminf_{u \to \bar{u}} F(u) \geq F(\bar{u}).$$

- F is l.s.c. on U if and only if epi F is closed.
- Every l.s.c. convex F remains l.s.c. when U is supplied with its weak topology.

Basic facts from convex analysis II

- Let $S \subset U$. The indicator function $I_S : U \to \overline{\mathbb{R}}$ is convex if and only if S is convex.
- Let $u^* \in U^*$, the (topological) dual space of U. The function

$$F^*(u^*) = \sup_{u \in U} \{\langle u, u^* \rangle - F(u)\}$$

  is the polar or conjugate function of F.
- F is subdifferentiable at $u \in U$ if it has a continuous affine minorant ℓ which is exact at u, i.e. $\ell(v) = F(u) + \langle u^*, v - u \rangle$. The slope of such a minorant is called the subgradient of F at u, and the set of all subgradients at u is called the subdifferential at u and is denoted by $\partial F(u)$.
- If F is not subdifferentiable at u, then $\partial F(u) = \emptyset$.
- We have $u^* \in \partial F(u)$ if and only if $F(u)$ is finite and

$$F(u) + \langle u^*, v - u \rangle \leq F(v) \quad \forall v \in V.$$

Basic facts from convex analysis III

- We have $F(u) = \min_{v \in U} F(v)$ if and only if $0 \in \partial F(u)$.
- We have $u^* \in \partial F(u)$ if and only if $F(u) + F^*(u^*) = \langle u, u^* \rangle$, $\partial F(u)$ (possibly empty) is convex and closed.
- If F is Gâteaux differentiable at u, then $\partial F(u) = \{F'(u)\}$, where $F'(u)$ is the Gâteaux derivative of F at u.
- Calculus:
  * $\kappa \in \mathbb{R}_+$: $\partial(\kappa F)(u) = \kappa \partial F(u)$.
  * $F_1, F_2 : U \to \mathbb{R}$. Then:

$$\partial(F_1 + F_2)(u) \supset \partial F_1(u) + \partial F_2(u).$$

  Suppose F_1, F_2 are l.s.c. and F_1, F_2 are identically equal $-\infty$ if they take the value $-\infty$, respectively, then equality holds if there exists a point $\hat{u} \in \text{dom } F_1 \cap \text{dom } F_2$ where F_1 is continuous.

Basic facts from convex analysis IV

* Let $\Lambda \in \mathcal{L}(U, V)$, i.e., a linear and continuous map from U to the Banach space V. If there exists $\hat{u}$ such that F is continuous at $\Lambda\hat{u}$, then for all $u \in U$ we have

$$\partial(F \circ \Lambda)(u) = \Lambda^* \partial F(\Lambda u).$$

- F is coercive over a non-empty, closed and convex set $C \subset U$ if and only if
$$\lim F(u) = +\infty \quad \text{for } u \in C,\ \|u\| \to +\infty.$$

- Let $C \subset U$ be non-empty, convex, closed. Consider

$$\inf_{v \in C} F(v).$$

  Then this problem has at least one solution if C is bounded or F is coercive over C. The solution is unique if F is strictly convex over C.

Back to our model problem

Elliptic Optimal Control Problems: Unconstrained Case.

Given $y_d \in L^2(\Omega)$ and $\alpha > 0$, find $(y, u) \in H_0^1(\Omega) \times L^2(\Omega) =: X$ such that

$$\begin{cases} \inf J(y,u) := \frac{1}{2}\int_\Omega |y - y_d|^2 dx + \frac{\alpha}{2}\int_\Omega |u|^2 dx, \\ \text{s. t.} \;\; -\Delta y = u \quad \text{in } H^{-1}(\Omega), \quad y = 0 \text{ on } \partial\Omega. \end{cases}$$

Reduced formulation: Denoting by $\mathcal{G} : H^{-1}(\Omega) \to H_0^1(\Omega)$ the control-to-state map, which assigns to a control $u \in L^2(\Omega)$ the solution $y = y(u) = \mathcal{G}(u) \in H_0^1(\Omega)$ of the state equation, the reduced formulation reads:

$$\inf \hat{J}(u) := \frac{1}{2}\int_\Omega |\mathcal{G}(u) - y_d|^2 dx + \frac{\alpha}{2}\int_\Omega |u|^2 dx \text{ over } u \in L^2(\Omega).$$

- What about: $-\Delta y + f(y) = Bu$? (semi-linear PDE).

Back to our model problem

Lagrange multiplier approach (– keep y, u independent!).

- Let $A : H_0^1(\Omega) \to H^{-1}(\Omega)$ be the operator associated with the bilinear form $a : H_0^1(\Omega) \times H_0^1(\Omega) \to \mathbb{R}$, $(a(y, w) := (\nabla y, \nabla w)_{L^2(\Omega)})$.

  Lagrange function (through coupling the PDE to the objective): Set $e(y, u) := Ay - u$, $e : H_0^1(\Omega) \times L^2(\Omega) \to H^{-1}(\Omega)$, and define

  $$L(y, u, p) := J(y, u) + \langle Ay - u, p \rangle.$$

- We call $p \in H_0^1(\Omega)$ a Lagrange multiplier associated with $e(y, u) = 0$ in $H^{-1}(\Omega)$, if, at a solution pair $\bar{x} := (\bar{y}, \bar{u})$,

  $$e_x(\bar{x})X = H^{-1}(\Omega).$$

- Then, for $\bar{x}$, there exists $\bar{p} \in H_0^1(\Omega)$ such that

  $$\begin{aligned} A\bar{y} - \bar{u} &= 0, \\ A^*\bar{p} + J_y(\bar{x}) &= 0, \\ J_u(\bar{x}) - \bar{p} &= 0. \end{aligned}$$

- **Saddle point formulation.** $\inf_{y,u} \sup_p L(y, u, p)$.

Pointwise CONTROL constraints

Elliptic Optimal Control Problem: Control constrained Case.

Find $(y, u) \in H_0^1(\Omega) \times L^2(\Omega) =: X$ such that

$$\begin{cases} \inf J(y,u) := \frac{1}{2}\int_\Omega |y - y_d|^2 dx + \frac{\alpha}{2}\int_\Omega |u|^2 dx, \\ \text{s. t. } u \in U_{\text{ad}} \\ \qquad -\Delta y = u \quad \text{in } H^{-1}(\Omega), \quad y = 0 \text{ on } \partial\Omega, \end{cases}$$

where $U_{\text{ad}} \subset L^2(\Omega)$ is non-empty, closed and convex. E.g.: Let $a, b \in L^2(\Omega), a < b$ a.e. in Ω, and define

$$U_{\text{ad}} := \{v \in L^2(\Omega) : a \leq v \leq b \text{ a.e. } \Omega\}.$$

Reduced formulation: The reduced formulation reads:

$$\inf \hat{J}(u) := \frac{1}{2}\int_\Omega |\mathcal{G}(u) - y_d|^2 dx + \frac{\alpha}{2}\int_\Omega |u|^2 dx \text{ over } u \in U_{\text{ad}}.$$

Pointwise CONTROL constraints

Lagrange multiplier approach.

- Let, for simplicity $U_{\mathrm{ad}} = \{v \in L^2(\Omega) : v \leq b \text{ a.e.}\}$, and define

$$L(y, u, p) := J(y, u) + \langle Ay - u, p\rangle + (u - b, \lambda).$$

- We call $(p, \lambda) \in H_0^1(\Omega) \times L^2(\Omega)$ a Lagrange multiplier pair associated with $e(y, u) = 0$ in $H^{-1}(\Omega)$ and $u \in U_{\mathrm{ad}}$, if, at a solution pair $\bar{x} := (\bar{y}, \bar{u})$,

$$e_x(\bar{x}) X_{\mathrm{ad}}(\bar{x}) = H^{-1}(\Omega),$$

with $X_{\mathrm{ad}}(\bar{x}) := H_0^1(\Omega) \times U_{\mathrm{ad}}(\bar{u})$ and

$$U_{\mathrm{ad}}(\bar{u}) := \{\kappa(v - \bar{u}) : v \in U_{\mathrm{ad}}, \kappa \geq 0\}.$$

- Then, for $\bar{x}$, there exists $(\bar{p}, \bar{\lambda}) \in H_0^1(\Omega) \times L^2(\Omega)$ such that

$$\begin{aligned} A\bar{y} - \bar{u} &= 0, \\ A^*\bar{p} - J_y(\bar{x}) &= 0, \\ J_u(\bar{x}) - \bar{p} + \bar{\lambda} &= 0, \\ \lambda \geq 0, \quad (\bar{u} - b, \bar{\lambda}) &= 0. \end{aligned}$$

Pointwise STATE constraints

Let $\Omega \subset \mathbb{R}^n$, $n < r < \infty$, set $W_0^{1,r}(\Omega) := W^{1,r}(\Omega) \cap H_0^1(\Omega)$, and define

$$K := \{z \in W_0^{1,r}(\Omega) : \ z \leq \psi \text{ in } \Omega\},$$

with $\psi \in W^{1,\infty}(\Omega)$, $\psi|_\Gamma > 0$.

Consider the problem

$$\begin{cases} \inf \quad J(y,u) \quad \text{over } (y,u) \in W_0^{1,r}(\Omega) \times L^2(\Omega) \\ \text{s. t. } y \in K \\ \qquad -\Delta y = u \quad \text{in } \Omega, \quad y = 0 \text{ on } \partial\Omega, \end{cases}$$

Reduced formulation: Denoting by $\mathcal{G} : W^{-1,r}(\Omega) \to W_0^{1,r}(\Omega)$ the control-to-state map, which assigns to a control $u \in W^{-1,r}(\Omega)$ the solution $y = \mathcal{G}(u) \in W_0^{1,r}(\Omega)$ of the state equation, the reduced formulation reads:

$$\inf_{u \in L^2(\Omega)} \hat{J}(u) := \frac{1}{2} \int_\Omega |\mathcal{G}(u) - y_d|^2 dx + \frac{\alpha}{2} \int_\Omega |u|^2 dx \text{ s.t. } \mathcal{G}(u) \in K.$$

Pointwise STATE constraints

- **Constraint Qualification (CQ) – Slater CQ:**

$$\exists u_0 \in L^2(\Omega) : \quad y_0 := \mathcal{G}(u_0) \in \operatorname{int} K.$$

- **Continuous embedding:** $W_0^{1,r}(\Omega) \subset C_0(\Omega)$ for $r > n$.
- **Dual spaces.** $(W_0^{1,r}(\Omega))^* = W^{-1,s}(\Omega)$ for $r^{-1} + s^{-1} = 1$.
- **Unconstrained, but nonsmooth problem.** Consider $I_K : C_0(\Omega) \to \overline{\mathbb{R}}$, and

$$\inf \quad \hat{J}(u) + (I_K \circ \mathcal{G})(u) \quad \text{over } u \in L^2(\Omega).$$

Pointwise constraints on the GRADIENT of the STATE

Let $\Omega \subset \mathbb{R}^n$, $n < r < \infty$, and $\psi \geq \epsilon > 0$ in Ω. define

$$K := \{z \in L^2(\Omega)^n : \ |z|_2 \leq \psi \text{ a.e. } \Omega\},$$

Consider the problem

$$\begin{cases} \inf \quad J(y,u) \quad \text{over } (y,u) \in H_0^1(\Omega) \times L^2(\Omega) \\ \text{s. t. } \nabla y \in K \\ \qquad -\Delta y = u \quad \text{ in } \Omega, \quad y = 0 \text{ on } \partial\Omega, \end{cases}$$

Reduced formulation: Denoting by $\mathcal{G} : L^2(\Omega) \to V \subset H_0^1(\Omega)$, V a reflexive Banach space, the control-to-state map, the reduced formulation reads:

$$\inf_{u \in L^2(\Omega)} \hat{J}(u) := \frac{1}{2}\int_\Omega |\mathcal{G}(u) - y_d|^2 dx + \frac{\alpha}{2}\int_\Omega |u|^2 dx \text{ s.t. } \nabla\mathcal{G}(u) \in K.$$

Slater point. For $V = W^{2,r}(\Omega) \cap H_0^1(\Omega)$ (PDE regularity theory!) there exists a Slater point $\nabla y_0 \in \text{ int } K$ with

$$K = \{v \in C(\bar{\Omega})^n : \ |v|_2 \leq \psi \text{ in } \Omega\}.$$

KKT-theory in Banach space.

Consider the minimization problem

$$\min_{x \in X} f(x) \quad \text{s.t. } x \in C,\ g(x) \in K, \tag{P}$$

- f real functional defined on a real Banach space X (C^1),
- C is a non-empty closed convex subset of X,
- g is a map from X into a real Banach space Y (C^1),
- K is a closed convex cone in Y with vertex at the origin.

For fixed $x \in X$ and $y \in Y$ let $C(x)$ and $K(y)$ denote the conical hulls of $C - \{x\}$ and $K - \{y\}$ respectively, i.e.,

$$C(x) := \{\kappa(c - x) \mid c \in C,\ \kappa \geq 0\}$$
$$K(y) := \{k - \kappa y \mid k \in K,\ \kappa \geq 0\}.$$

KKT-theory in Banach space.

$y^* \in Y^*$ is called a Lagrange multiplier for (P) at an optimal point $x^* \in X$, if

$$
\begin{aligned}
(i) \quad & y^* \in K^+ \\
(ii) \quad & \langle y^*, g(x^*) \rangle_{Y^*,Y} = 0 \\
(iii) \quad & f'(x^*) - y^*(g'(x^*)) \in C(x^*)^+,
\end{aligned}
$$

where X^* and Y^* denote the topological duals of X and Y and for each subset A of X (or Y respectively), A^+ denotes its polar cone

$$A^+ := \{w \in X^* \mid \langle w, a \rangle_{X^*,X} \geq 0 \quad \text{for all } a \in A\}.$$

Theorem. Let x^* be an optimal solution for problem (P). If

$$g'(x^*)C(x^*) - K(g(x^*)) = Y,$$

then the set $\Lambda(x^*)$ of Lagrange multipliers for problem (P) at x^* is non-empty and bounded.

Efficient Solvers – Semismooth Newton Methods.

Non-smooth operator equations

Let $F : X \to Z$ be not necessarily Frechet differentiable. Consider the problem:

$$\text{Find } x^* \in X \text{ such that } F(x^*) = 0.$$

Applications:

- Optimal control problems.
  - Ordinary / Partial differential equations with control/state constraints.
  - Variational inequalities.
  - Apps: fluids, thermal processes, parameter identification, calibration in finance,...
- Material science: Contact, friction, material identification.
- Imaging science: restoration, segmentation, TV.
- etc...

Smooth operator equations: $F \in C^1(X, Z)$

Newton's method.

- Choose $x^0 \in X$; $k := 0$.
- $x^{k+1} = x^k - \nabla F(x^k)^{-1} F(x^k)$; set $k := k + 1$.

Versions.

- ∇F Lipschitz continuous. Then, locally

$$\|x^{k+1} - x^*\|_X \leq C\|x^k - x^*\|_X^2.$$

- ∇F is Hölder continuous (exponent $\tau \in (0, 1)$). Then, locally

$$\|x^{k+1} - x^*\|_X \leq C\|x^k - x^*\|_X^{1+\tau}.$$

- ∇F continuous.

$$\frac{\|x^{k+1} - x^*\|_X}{\|x^k - x^*\|_X} \to 0 \quad \text{as } k \to \infty,$$

presuming that $x^k \neq x^*$ for $k \in \mathbb{N}$.

Non-smooth operator equations

Question.

What happens if F is no longer Fréchet differentiable?

Generalized differential

Let X, Z be Banach spaces and $F : D \subset X \to Z$.

Definition. The mapping $F : D \subset X \to Z$ is *generalized or Newton differentiable* in $U \subset D$, if there exists a family of mappings $G : U \to \mathcal{L}(X, Z)$ such that

$$\lim_{h \to 0} \frac{1}{\|h\|_X} \|F(x+h) - F(x) - G(x+h)h\|_Z = 0 \tag{A}$$

for every $x \in U$.

- G need not be unique!
- Generalizes the concept of F. Clarke (UBC).
- Compare "semismoothness" by L. Qi (HKPU) and Q. Sun (NUS).

Newton's method

Problem. Find $x^* \in X$ such that

$$F(x^*) = 0.$$

Generalized Newton's method.

- Choose $x^0 \in X$; $k := 0$.
- $x^{k+1} = x^k - G(x^k)^{-1} F(x^k)$; set $k := k + 1$.

Local convergence result.

Theorem. Let

- $x^* \in X$ be a solution of $F(x) = 0$;
- F be generalized differentiable in U with $x^* \in U$;
- $\{\|G(x)^{-1}\| : x \in U\}$ be bounded.

Then the generalized Newton method converges *superlinearly* to x^*, if $\|x^0 - x^*\|_X$ is sufficiently small.

Complementarity problems

Optimal control problem.

$$\begin{aligned} &\text{minimize } J(y,u) = \frac{1}{2}\|y - y_d\|^2_{L^2} + \frac{\alpha}{2}\|u\|^2_{L^2} \\ &\text{s.t. } \; e(y,u) = 0, \\ &\qquad u \le b \text{ a.e. in } \Omega, \end{aligned}$$

with $\Omega \subset \mathbb{R}^n$ open and bounded, and with sufficiently smooth boundary, $\alpha > 0$ and $y_d, b \in L^2(\Omega)$.

- Example for $e(y,u)$:

  $$e(y,u) = E(y) - u,$$

  $E(\cdot)$ a semilinear (2nd order) elliptic partial differential operator.

- Also possible: general J; parabolic equations; bilateral constraints $a \le u \le b$,...

Reduction approach

Assumption: $u \mapsto y(u)$ (locally) unique.

Reduced problem. $(U_{\text{ad}} = \{u \in L^2(\Omega) : u \leq b \text{ a.e. in } \Omega\})$

$$\text{Minimize } \hat{J}(u) = J(y(u), u)$$
$$\text{s.t. } u \in U_{\text{ad}}.$$

1st order optimality conditions - variational inequality (VI).

$$u^* \in U_{\text{ad}}, \quad (\hat{J}'(u^*), u - u^*)_{L^2} \geq 0 \quad \forall u \in U_{\text{ad}}.$$

We have for $v \in L^2(\Omega)$:

$$(\hat{J}'(u^*), v)_{L^2} = (y(u^*) - y_d, y'(u^*)v)_{L^2} + \alpha(u^*, v)_{L^2}$$

Reduction approach - adjoints

Method of the adjoint.

$$E'(y(u))^* p = \nabla_y J(y(u), u) \qquad \text{(solution } p(u))$$

Representation of $\hat{J}'$.

$$\hat{J}'(u) = p(u) + \alpha u =: A(u) + \alpha u.$$

Structural assumption.

- $\hat{J}'(u) = A(u) + \alpha u$;
- $A : L^2(\Omega) \to L^2(\Omega)$ cont. Fréchet differentiable;
- $A : L^2(\Omega) \to L^s(\Omega), s > 2$ fixed, locally Lipschitz.

NCP-Function

- VI equivalent to

$$A(u^*) + \alpha u^* + \lambda^* = 0,$$
$$\lambda^* \geq 0, \quad u^* \leq b, \quad \lambda^*(u^* - b) = 0.$$

- The optimality condition for u^* is equivalent to

$$A(u^*) + \alpha u^* + \lambda^* = 0,$$
$$\max(\lambda^* + c(u^* - b), 0) - \lambda^* = 0.$$

  $c > 0$ arbitrarily fixed.

- For $c = \alpha$ we get:

$$\max(-A(u^*) - \alpha b, 0) + A(u^*) + \alpha u^* = 0.$$

- Setting $x = u \in L^2(\Omega)$ we get

$$\boxed{F(x) = \max(-A(x) - \alpha b, 0) + A(x) + \alpha x}$$

Convergence

Theorem.

- $\max : L^r(\Omega) \to L^s(\Omega)$ generalized differentiable for $1 \leq s < r \leq +\infty$.
- For $\mathbf{r} = \mathbf{s}$, $\max : L^r(\Omega) \to L^s(\Omega)$ **not** generalized differentiable.

- Due to the structural assumption on A, the generalized Newton method for solving $F(x) = 0$ converges locally at a superlinear rate.
- The structural assumption is, e.g., satisfied for $E(y) = -Ly + f(y)$, with L a 2nd order linear elliptic partial differential operator and f sufficiently smooth.

Example

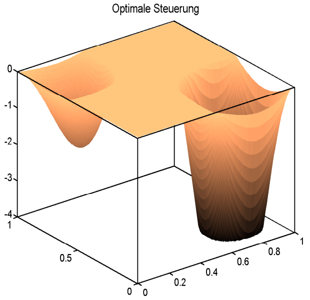
Simplified Ginzburg-Landau model for superconductivity:

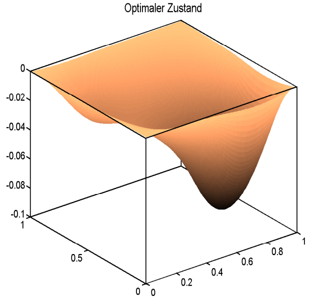
$$\begin{aligned}
&\text{Minimize} \quad J(y,u) = \tfrac{1}{2}\|y - y_d\|_{L^2}^2 + \tfrac{\alpha}{2}\|u\|_{L^2}^2 \\
&\text{over} \quad (y,u) \in H^1(\Omega) \times L^2(\Omega), \\
&\text{s.t.} \quad -\Delta y + y^3 + y = u \text{ in } \Omega, \quad y = 0 \text{ on } \Gamma = \partial\Omega, \\
&\qquad u \in U_{\mathrm{ad}} = \{u \in L^2(\Omega) \mid -4 \le u(\mathrm{x}) \le 0 \text{ f.a.a. } \mathrm{x} \text{ in } \Omega\},
\end{aligned}$$

with $\Omega = (0,1)^2$, $y_d = \sin(2\pi x_1)\sin(2\pi x_2)\exp(2x_1)/6$ and $\alpha = 0.001$.

Convergence measures:

$$\begin{aligned}
\mathrm{res}_h^k &= \|\alpha u_h^k - P_{[-4\alpha,0]}(-A_h(u_h^k))\|_{L^2}, \\
l_h^k &= \|u_h^k - u_h^*\|_{L^2}, \\
q_h^k &= \|u_h^k - u_h^*\|_{L^2} / \|u_h^{k-1} - u_h^*\|_{L^2}.
\end{aligned}$$





h	res_h^k			
	1	2	3	4
$1/16$	3.797E-3	1.108E-3	7.408E-5	5.325E-8
$1/32$	3.925E-3	1.207E-3	7.591E-5	1.246E-6
$1/64$	3.957E-3	1.231E-3	7.005E-5	5.283E-7
$1/128$	3.968E-3	1.239E-3	6.963E-5	4.470E-7
$1/256$	3.971E-3	1.243E-3	6.958E-5	5.514E-7

h	I_h^k			
	1	2	3	4
1/16	3.222	1.195	7.408E-2	5.332E-5
1/32	3.347	1.290	7.678E-2	1.247E-3
1/64	3.378	1.317	7.085E-2	5.285E-4
1/128	3.383	1.325	7.042E-2	4.471E-4
1/256	3.384	1.328	7.037E-2	5.512E-4

h	q_h^k			
	1	2	3	4
1/16	1.619	0.371	6.276E-2	7.111E-4
1/32	1.646	0.385	5.952E-2	1.625E-3
1/64	1.654	0.390	5.380E-2	7.459E-3
1/128	1.654	0.392	5.316E-2	6.349E-3
1/256	1.654	0.393	5.297E-2	7.840E-3

Mesh independence!

Mesh independence

- **Assumption 1.**(Strict complementarity)

$$\text{meas}\{|b - u^*| + |\hat{J}'(u^*)| = 0\} = 0.$$

Let u_h^* be solution of $F_h(u_h) = 0$; $s > 2$.

- **Assumption 2.**
  - $\lim_{h\to 0^+} \|u_h^* - u^*\|_{L^2} = 0, \quad \lim_{h\to 0^+} \|A_h(u_h^*) - A(u^*)\|_{L^s} = 0.$
  - Family of discretizations is *locally uniformly Lipschitz*, i.e., there exist $h_0 > 0$, $\delta_0 > 0$, and $L_A > 0$ such that for $h \le h_0$

$$\|A(u^2) - A(u^1)\|_{L^s} \le L_A \|u^2 - u^1\|_{L^2}, \quad \|u^i - u^*\|_{L^2} \le \delta_0,$$
$$\|A_h(u_h^2) - A_h(u_h^1)\|_{L^s} \le L_A \|u_h^2 - u_h^1\|_{L^2}, \quad \|u_h^i - u_h^*\|_{U_h} \le \delta_0.$$

- Family of discretizations has the *uniform linear approximation property*, i.e., A and A_h, $h \le h_0$, Fréchet differentiable in a neighborhood of u^* and u_h^*, and there exists a function $\rho : [0, \delta_0) \to [0, \infty)$ such that

$$\lim_{t \to 0^+} \frac{\rho(t)}{t} = 0,$$

$$\|A(u) - A(u^*) - A'(u)(u - u^*)\|_{L^2} \le \rho(\|u - u^*\|_{L^2}) \quad \forall u \in L^2(\Omega), \quad \|u - u^*\|_{L^2} \le \delta_0,$$

$$\|A_h(u_h) - A_h(u_h^*) - A_h'(u_h)(u_h - u_h^*)\|_{U_h} \le \rho(\|u_h - u_h^*\|_{U_h}) \quad \forall u_h \in U_h, \quad \|u_h - u_h^*\|_{U_h} \le \delta_0, \quad h \le h_0.$$

Here $U_h \subset L^2(\Omega)$ with $\dim(U_h) < \infty$.

Mesh independent linear convergence

Theorem. Let $F : L^2(\Omega) \to L^2(\Omega)$ be generalized differentiable, and $u^* \in L^2(\Omega)$ with $F(u^*) = 0$ and $u_h^* \in U_h$ with $F_h(u_h^*) = 0$, such that Assumption 1–2 are satisfied. Further let $\delta_2, \delta_2' > 0$, $\kappa, \kappa' > 0$ and $h_2' \leq h_0$ such that for all $0 < h \leq h_2'$

$$\sup\{\|G^{-1}\|_{L^2,L^2} : G \in S(u^* + s), \|s\|_{L^2} \leq \delta_2\} \leq \kappa,$$
$$\sup\{\|G_h^{-1}\|_{L^2,L^2} : G_h \in S_h(u_h^* + s_h), \|s_h\|_{L^2} \leq \delta_2'\} \leq \kappa'.$$

Then, for $\theta \in (0,1)$, there exist $\bar{\delta} > 0$ and $\bar{h} > 0$ such that

$$\begin{aligned} \|u^{k+1} - u^*\|_{L^2} &\leq \theta \|u^k - u^*\|_{L^2}, \\ \|u_h^{k+1} - u_h^*\|_{L^2} &\leq \theta \|u_h^k - u_h^*\|_{L^2}, \quad \forall 0 < h \leq \bar{h} \end{aligned}$$

if $\max\{\|u^0 - u^*\|_{L^2}, \|u_h^0 - u_h^*\|_{L^2}\} \leq \bar{\delta}$.

Moreau-Yosida-Based Path-Following for State Constraints and Parameter Balance.

Path-following for state constraints: motivation

Pointwise constraints on the state.

$$\begin{aligned}
&\text{minimize } J(y,u) = J_1(y) + \frac{\alpha}{2}|u-u_d|^2_{L^2(\tilde\Omega)} \\
&\text{over } (y,u) \in W \times L^2(\tilde\Omega) \qquad\qquad \text{(P)} \\
&\text{s.t. } Ay = E_{\tilde\Omega} u \text{ in } \Omega, \quad u \in C_u, \quad y \in C_y,
\end{aligned}$$

where

- State space W is a reflexive Banach space,
- $J_1 \in \mathcal{C}^{1,1}(W,\mathbb{R})$ convex and $J_1(y_n) \to J_1(y)$, $J_1'(y_n) \rightharpoonup J_1'(y)$ in W^* for $y_n \rightharpoonup y$ in W, $\alpha > 0$, $u_d \in L^2(\tilde\Omega)$,
- $\tilde\Omega$ an open subset of the bounded set $\Omega \subset \mathbb{R}^d$, $d \leq 3$,
- $A \in \mathcal{L}(W,L)$, L a reflexive Banach space such that $L^r(\Omega) \subset L$ with dense embedding for $r \geq 2$,
- $E_{\tilde\Omega}$ the extension-by-zero operator from $\tilde\Omega$ to Ω,
- $C_u = \{u \in L^2(\tilde\Omega) : \underline{\varphi} \leq u \leq \bar\varphi\}$ with $\underline{\varphi}, \bar\varphi \in L^{2(r-1)}(\tilde\Omega)$,

Path-following for state constraints: motivation

- $C_y = \{y \in W : |(Gy)(\mathbf{x})| \leq \psi, \mathbf{x} \in \Omega\}$ with $\psi \in \mathcal{C}(\bar{\Omega})$, $\underline{\psi} \leq \psi$, $\underline{\psi} \in \mathbb{R}_{++}$,
- $G \in \mathcal{L}(W, \mathcal{C}(\bar{\Omega})^l)$ for $1 \leq l \leq d$, and $|\cdot|$ the Euclidean-norm in $\mathbb{R}^l$.

Hypothesis:

$$\text{There exists a feasible point for the constraints in (P).} \tag{H1}$$

$$A \text{ is a homeomorphism.} \tag{H2}$$

$$G : W \to \mathcal{C}(\bar{\Omega})^l \text{ is compact.} \tag{H3}$$

$$\Longrightarrow \quad \exists \text{ unique solution } (y^*, u^*) \in W \times L^r(\tilde{\Omega}).$$

Motivation - particular realizations

- Pointwise zero-order state constraints.
  - A a second order linear elliptic differential operator

    $$Ay = -\sum_{i,j=1}^{d} \partial_{x_j}(a_{ij}\partial_{x_i} y) + a_0 y$$

    with $\mathcal{C}^{0,\delta}(\bar{\Omega})$-coefficients a_{ij} for some $\delta \in (0,1]$, and

    $$\sum_{i,j=1}^{d} a_{ij}(x)\xi_i\xi_j \geq \kappa|\xi|^2 \text{ for some } \kappa > 0,$$

    and $a_0 \in L^\infty(\Omega)$ with $a_0 \geq 0$ a.e. in Ω.
  - Ω either polyhedral convex or with a $\mathcal{C}^{1,\delta}$-boundary Γ; locally on one side of Γ.
  - $W = W_0^{1,p}(\Omega)$, $L = W^{-1,p}(\Omega)$, $p > d$, and $G = \text{id}$, which implies $l = 1$. Then

    $$|Gy| \leq \psi \text{ in } \Omega \quad \Longleftrightarrow \quad -\psi \leq y \leq \psi \text{ in } \Omega.$$
  - Regular case: $W = H^2(\Omega) \cap H_0^1(\Omega)$, $L = L^2(\Omega)$.

Motivation - particular realizations

- Gradient constraints (pointwise first-order state constraints).
  - Let A be as above, but with $\mathcal{C}^{0,1}$-coefficients a_{ij}, and Ω with $\mathcal{C}^{1,1}$-boundary.
  - $W = W^{2,r}(\Omega) \cap W_0^{1,r}(\Omega)$, $L = L^r(\Omega)$, $r > d$, and $G = \nabla$, which yields $l = d$. Then

$$C_y = \{y \in W : |\nabla y(\mathbf{x})| \leq \psi(\mathbf{x}), \mathbf{x} \in \Omega\}.$$

- Sometimes, for some $g \in \mathcal{C}(\bar{\Omega})^l$,

$$C_y = \{\tilde{y} \in W : |(G\tilde{y})(\mathbf{x}) - g(\mathbf{x})| \leq \psi(\mathbf{x}), \mathbf{x} \in \Omega\}.$$

  If $\exists\ \tilde{y}_g \in W$ with $G\tilde{y}_g = g$, then $y := \tilde{y} - y_g$ yields (P).

- Zero-order case. Also possible

$$\varphi \leq y \leq \psi \quad \text{in } \Omega.$$

Constraint qualification

$$\exists \quad M \subset C_y \times C_u \subset W \times L^r(\tilde{\Omega}) \text{ such that}$$
$$0 \in \operatorname{int}\{Ay - E_{\tilde{\Omega}} u : (y,u) \in M\} \subset L^r(\Omega), \tag{H4}$$

where the interior is taken in $L^r(\Omega)$.

Discussion.

- Range space CQ.
- Weaker then Slater condition.
- Sufficient for our aims.

Moreau-Yosida regularization

$$\begin{aligned} &\text{minimize } J(y,u) + \frac{\gamma}{2}\|(|Gy| - \psi)^+\|^2_{L^2(\Omega)} \\ &\text{subject to } Ay = E_{\tilde{\Omega}} u, \ u \in C_u, \end{aligned} \qquad (\mathrm{P}_\gamma)$$

where $\gamma > 0$ and $(\cdot)^+ = \max(0,\cdot)$ in the pointwise sense.

Moreau-Yosida regularization of I_K, with $K := \{v \in L^2(\Omega) : v \leq \psi\}$:

$$\begin{aligned} I_K^{MY}(w) :=& \inf\left\{ I_K(v) + \frac{\gamma}{2}\|v - w\|^2_{L^2(\Omega)} : v \in L^2(\Omega)\right\} \\ =& \frac{\gamma}{2}\|(w-\psi)^+\|^2_{L^2(\Omega)} \end{aligned}$$

is LC^1-regular.

Moreau-Yosida regularization

Standard infimizing sequence techniques and KKT-theory in Banach space yield:

- $\exists$ unique solution (y_γ, u_γ);
- $\exists$ $(p_\gamma, \bar{\mu}_\gamma, \underline{\mu}_\gamma) \in L^* \times L^{r'}(\tilde{\Omega}) \times L^{r'}(\tilde{\Omega})$, $\frac{1}{r} + \frac{1}{r'} = 1$,

$$
\begin{aligned}
&Ay_\gamma = E_{\tilde{\Omega}} u_\gamma, \quad A^* p_\gamma + G^* \lambda_\gamma = -J_1'(y_\gamma),\\
&\alpha(u_\gamma - u_d) - E_{\tilde{\Omega}}^* p_\gamma + \bar{\mu}_\gamma - \underline{\mu}_\gamma = 0,\\
&\bar{\mu}_\gamma \geq 0, \quad u_\gamma \leq \bar{\varphi}, \quad \bar{\mu}_\gamma(u_\gamma - \bar{\varphi}) = 0,\\
&\underline{\mu}_\gamma \leq 0, \quad u_\gamma \geq \underline{\varphi}, \quad \underline{\mu}_\gamma(u_\gamma - \underline{\varphi}) = 0,\\
&\lambda_\gamma = \gamma(|Gy_\gamma| - \psi)^+ q_\gamma,\\
&q_\gamma(\mathbf{x}) \in \begin{cases} \left\{ \frac{Gy_\gamma}{|Gy_\gamma|}(\mathbf{x}) \right\} & \text{if } |Gy_\gamma(\mathbf{x})| > 0,\\ \bar{B}(0;1)^l & \text{else.} \end{cases}
\end{aligned}
\tag{OS$_\gamma$}
$$

Moreau-Yosida regularization

Discussion.

- Adjoint equation - very weak form:

  $\langle p_\gamma, Av\rangle_{L^*,L} + (\lambda_\gamma,\ Gv)_{L^2(\Omega)} = -\langle J_1'(y_\gamma),\ v\rangle_{W^*,W}$ for any $v \in W$.

- Scalar factor of multiplier approximation:

  $\lambda_\gamma^s := \frac{\gamma}{|Gy_\gamma|}(|Gy_\gamma| - \psi)^+$ on $\{|Gy_\gamma| > 0\}$ and $\lambda_\gamma^s := 0$ else.

  Hence, $\lambda_\gamma = \lambda_\gamma^s G y_\gamma$.

- **Lemma.** Let (H1)-(H4) hold. Then the family

  $$\{(y_\gamma,\ u_\gamma,\ p_\gamma,\ \bar{\mu}_\gamma - \underline{\mu}_\gamma,\ \lambda_\gamma^s)\}_{\gamma \geq 1}$$

  is bounded in $W \times L^r(\tilde{\Omega}) \times L^{r'}(\Omega) \times L^{r'}(\tilde{\Omega}) \times L^1(\Omega)$.

Moreau-Yosida regularization

- **Theorem.** Let (H1) - (H4) hold. Then there exists $(p_*, \bar{\mu}_*, \underline{\mu}_*, \lambda_*^s) \in L^* \times L^{r'}(\tilde{\Omega}) \times L^{r'}(\tilde{\Omega}) \times \mathcal{M}(\bar{\Omega})$ such that

$$
\begin{aligned}
Ay^* - E_{\tilde{\Omega}} u^* &= 0, \\
A^* p_* + G^*(\lambda_*^s G y^*) + J_1'(y^*) &= 0, \\
\alpha(u^* - u_d) - E_{\tilde{\Omega}}^* p_* + (\bar{\mu}_* - \underline{\mu}_*) &= 0, \\
\bar{\mu}_* \geq 0,\ u^* \leq \bar{\varphi},\ \bar{\mu}_*(u^* - \bar{\varphi}) &= 0, \\
\underline{\mu}_* \geq 0,\ u^* \geq \underline{\varphi},\ \underline{\mu}_*(u^* - \underline{\varphi}) &= 0,
\end{aligned}
$$

  and further
  - $\int_\Omega \lambda_*^s \varphi \geq 0$ for all $\varphi \in \mathcal{C}(\bar{\Omega})$ with $\varphi \geq 0$;
  - $(p_\gamma, \bar{\mu}_\gamma, \underline{\mu}_\gamma) \rightharpoonup (p_*, \bar{\mu}_*, \underline{\mu}_*)$, $\langle \lambda_\gamma^s, \upsilon \rangle \to \langle \lambda_*^s, \upsilon \rangle$ for all $\upsilon \in \mathcal{C}(\bar{\Omega})$ along a subsequence,
  - $(y_\gamma, u_\gamma) \to (y^*, u^*)$ strongly in $W \times L^r(\tilde{\Omega})$.

Discussion

- Adjoint equation of example 1.

  $$\langle p_*, Av\rangle_{W_0^{1,p'}(\Omega),W^{-1,p}(\Omega)}+\langle \lambda_*^s y^*, v\rangle_{\mathcal{M}(\bar\Omega),\mathcal{C}(\bar\Omega)} = -\langle J_1'(u^*), v\rangle_{W^*,W}$$

  for all $v \in W$.
- Adjoint equation of example 2.

  $$\langle p_*, Av\rangle_{L^{r'}(\Omega),L^r(\Omega)}+\langle \lambda_*^s \nabla y^*, \nabla v\rangle_{\mathcal{M}(\bar\Omega)^l,\mathcal{C}(\bar\Omega)^l} = -\langle J_1'(u^*), v\rangle_{W^*,W}$$

  for all $v \in W = W^{2,r}(\Omega) \cap W_0^{1,r}(\Omega)$.

- Condition (H4) is quite general and allows $\psi = 0$ on parts of Ω.

Semismoothness ∞ Newton

Recall:

- Let $F : \mathcal{X} \to \mathcal{Y}$, with $\mathcal{X}$ and $\mathcal{Y}$ Banach spaces. $G_F \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$ is called a *Newton* or *slant derivative* of F in an open set $U \subset \mathcal{X}$, iff

$$\|F(x+h) - F(x) - G_F(x+h)h\|_{\mathcal{Y}} = \mathcal{o}(\|h\|_{\mathcal{X}}) \quad \text{for } x \in U$$

  as $\|h\|_{\mathcal{X}} \to 0$.

- Semismooth Newton method (SSN) for finding x^* with $F(x^*) = 0$:

$$x^{k+1} = x^k - G_F(x^k)^{-1} F(x^k) \quad \text{for } k = 0, 1 \ldots.$$

- Uniform invertibility of G_F in a neighborhood of x^* and $\|x^0 - x^*\|_{\mathcal{X}}$ sufficiently small yield q-superlinear convergence of SSN.

Semismoothness

(OS_γ) can be reduced to

$$F_\gamma(u_\gamma) = 0, \quad F_\gamma : L^r(\tilde{\Omega}) \to L^r(\tilde{\Omega}),$$

with

$$F_\gamma(u_\gamma) := \alpha(u_\gamma - u_d) - \hat{p}_\gamma + (\hat{p}_\gamma + \alpha(u_d - \bar{\varphi}))^+ \\ + (\hat{p}_\gamma + \alpha(u_d - \underline{\varphi}))^- .$$

where $\hat{p}_\gamma = p_\gamma(u_\gamma)$ with

$$p_\gamma(u_\gamma) = -\gamma B^*(|Bu_\gamma| - \psi)^+ q(Bu_\gamma) + J_1'(A^{-1}E_{\tilde{\Omega}} u_\gamma)),$$

$B = GA^{-1}E_{\tilde{\Omega}}$ and

$$q(Bu_\gamma)(\mathbf{x}) = \begin{cases} (Bu_\gamma/|Bu_\gamma|)(\mathbf{x}) \text{ if } |B(u_\gamma)(\mathbf{x})| > 0, \\ 0 \text{ else.} \end{cases}$$

Semismoothness

Hypothesis: For some $\hat{r} > r$ we assume:

$$u_d,\ \bar{\varphi},\ \underline{\varphi} \in L^{\hat{r}}(\tilde{\Omega}),\ \text{and}\ u \mapsto A^{-*}J_1'(A^{-1}E_{\tilde{\Omega}}u) \text{ is cont.}$$
$$\text{Frechet differentiable from } L^2(\tilde{\Omega}) \to L^{\hat{r}}(\Omega), \tag{H5}$$

$$B^* \in \mathcal{L}(L^r(\tilde{\Omega})^l, L^{\hat{r}}(\tilde{\Omega})). \tag{H6}$$

Our examples satisfy these hypothesis.

Semismoothness

- $$G_{\max}(\omega)(\mathrm{x}) := \begin{cases} 1 & \text{if } \omega(\mathrm{x}) > 0, \\ 0 & \text{if } \omega(\mathrm{x}) \le 0, \end{cases}$$

  serves as a generalized derivative for

  $$\max(0,\cdot) : L^{s_1}(\Omega) \to L^{s_2}(\Omega) \text{ if } 1 \le s_2 < s_1 \le \infty.$$

  Analogously for $\min(0,\cdot)$ and the norm- functional $|\cdot| : L^{s_1}(\Omega)^l \to L^{s_2}(\Omega)$.
- Define

  $$\mathfrak{p}_\gamma(u) := -\gamma B^*(|Bu| - \psi)^+ q(Bu), \qquad \text{where } \mathfrak{p}_\gamma : L^r(\tilde{\Omega}) \to L^{\hat{r}}(\tilde{\Omega}).$$
- Define

  $$Q(Bv) := |Bv|^{-1}\left(\mathrm{id} - |Bv|^{-2}(Bv)(Bv)^\top\right).$$

Semismoothness

- $\mathfrak{p}_\gamma : L^r(\tilde{\Omega}) \to L^{\hat{r}}(\tilde{\Omega})$ is Newton differentiable in a neighborhood of every point $u \in L^r(\tilde{\Omega})$ and a generalized derivative is given by

$$G_{\mathfrak{p}_\gamma}(u) = -\gamma B^* \Big[G_{\max}(|Bu| - \psi) q(Bu) q(Bu)^\top + (|Bu| - \psi)^+ Q(Bu) \Big] B.$$

- $F_\gamma : L^r(\tilde{\Omega}) \to L^r(\tilde{\Omega})$ is Newton differentiable in a neighborhood of every $u \in L^r(\tilde{\Omega})$, and a particular generalized derivative of F_γ at $u \in L^r(\tilde{\Omega})$ is given by

$$G_{F_\gamma}(u) = \alpha \,\mathrm{id} - G_{\hat{p}_\gamma}(u) + G_{\max}(\hat{p}_\gamma(u) + \alpha(u_d - \bar{\varphi})) G_{\hat{p}_\gamma}(u) + G_{\min}(\hat{p}_\gamma(u) + \alpha(u_d - \underline{\varphi})) G_{\hat{p}_\gamma}(u)$$

with

$$G_{\hat{p}_\gamma}(u) = G_{\mathfrak{p}_\gamma}(u) - E_{\tilde{\Omega}}^* A^{-*} J_1''(A^{-1} E_{\tilde{\Omega}} u) A^{-1} E_{\tilde{\Omega}}.$$

Semismooth Newton

- Newton step: $G_{F_\gamma}(u^k)\delta_u^k = -F_\gamma(u^k)$ with $\delta_u^k = u^{k+1} - u^k$.
- $$\begin{aligned} \bar{\mathcal{A}}^k &:= \{\mathbf{x} \in \tilde{\Omega} : \big(\hat{p}_\gamma(u^k) + \alpha(u_d - \bar{\varphi})\big)(\mathbf{x}) > 0\}, \\ \underline{\mathcal{A}}^k &:= \{\mathbf{x} \in \tilde{\Omega} : \big(\hat{p}_\gamma(u^k) + \alpha(u_d - \underline{\varphi})\big)(\mathbf{x}) < 0\}, \\ \mathcal{A}^k &:= \bar{\mathcal{A}}^k \cup \underline{\mathcal{A}}^k, \\ \mathcal{I}^k &:= \tilde{\Omega} \setminus \mathcal{A}^k. \end{aligned}$$
- Structure: $G_{F_\gamma}(u^k) = \alpha\,\mathrm{id} - \chi_{\mathcal{I}^k} G_{\hat{p}_\gamma}(u^k)$.

- $\delta^k_{u|\bar{\mathcal{A}}^k} = E^*_{\bar{\mathcal{A}}^k}\delta_u^k = E^*_{\bar{\mathcal{A}}^k}(\bar{\varphi} - u^k) = \bar{\varphi}_{|\bar{\mathcal{A}}^k} - u^k_{|\bar{\mathcal{A}}^k}$,
- $\delta^k_{u|\underline{\mathcal{A}}^k} = E^*_{\underline{\mathcal{A}}^k}\delta_u^k = E^*_{\underline{\mathcal{A}}^k}(\underline{\varphi} - u^k) = \underline{\varphi}_{|\underline{\mathcal{A}}^k} - u^k_{|\underline{\mathcal{A}}^k}$.

- Remains in $L^2(\mathcal{I}^k)$:

$$E^*_{\mathcal{I}^k} G_{F_\gamma}(u^k) E_{\mathcal{I}^k}\delta_u^{\mathcal{I}^k} = -E^*_{\mathcal{I}^k}\big(F_\gamma(u^k) + G_{F_\gamma}(u^k) E_{\mathcal{A}^k}\delta^k_{u|\mathcal{A}^k}\big).$$

Semismooth Newton

- The inverse to the operator

$$E_{\mathcal{I}}^* G_{F_\gamma}(u) E_{\mathcal{I}} : L^2(\mathcal{I}) \to L^2(\mathcal{I}),$$

  with $G_{F_\gamma}(u) = \alpha\,\mathrm{id} - \chi_{\mathcal{I}} G_{\hat{p}_\gamma}(u)$, exists and is bounded by $\frac{1}{\alpha}$ regardless of $u \in L^r(\tilde{\Omega})$ as long as $\mathrm{meas}(\mathcal{I}) > 0$.

- The semismooth Newton update step is well-defined and $\delta_u^k \in L^r(\tilde{\Omega})$.

- For each $\hat{u} \in L^r(\tilde{\Omega})$ there exists a neighborhood $U(\hat{u}) \subset L^r(\tilde{\Omega})$ and a constant K such that

$$\|G_{F_\gamma}(u)^{-1}\|_{\mathcal{L}(L^2(\hat{\Omega}))} \leq K \text{ for all } u \in U(\hat{u}).$$

- For $r = 2$ the semismooth Newton method is well-defined and converges locally at a superlinear rate.

Semismooth Newton with lifting ($r > 2$)

(i) Choose $u^0 \in L^r(\tilde{\Omega})$.

(ii) Solve for $\tilde{u}^{k+1} \in L^r(\tilde{\Omega})$:

$$G_{F_\gamma}(u^k)(\tilde{u}^{k+1} - u^k) = -F(u^k).$$

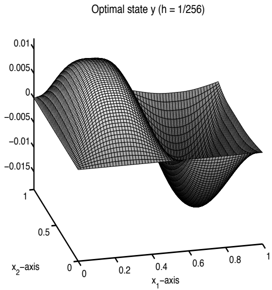
(iii) Perform a lifting step:

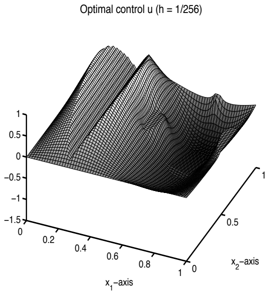
$$u^{k+1} = \frac{1}{\alpha}\left(u_d + p_\gamma - (p_\gamma + \alpha(u_d - \bar{\varphi}))^+ - (p_\gamma + \alpha(u_d - \underline{\varphi}))^-\right),$$

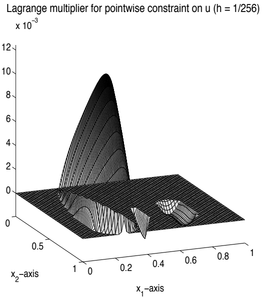
where $p_\gamma = p_\gamma(\tilde{u}^{k+1})$.

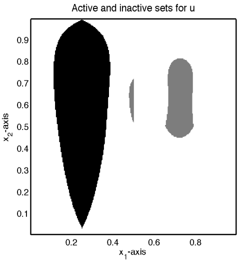
- The semismooth Newton method with lifting step is locally q-superlinearly convergent in $L^r(\tilde{\Omega})$ for $r > 2$.

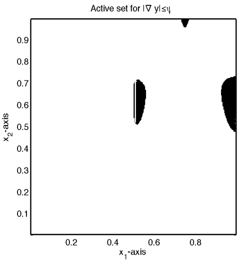
Numerics for gradient constraints











Numerics for gradient constraints

- Continuation with respect to γ.

Iterations									
h/γ	1E0	1E1	1E2	1E3	1E4	1E5	1E6	1E7	1E8
$\frac{1}{32}$	6	6	6	4	3	3	2	2	2
$\frac{1}{64}$	7	7	6	4	4	3	3	2	2
$\frac{1}{128}$	7	7	6	5	5	4	3	2	2
$\frac{1}{256}$	7	7	6	6	5	5	4	3	2

Numerics for gradient constraints

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$\frac{1}{256}$	7	7	6	6	5	5	4	3	2

- Automatize γ-update: Primal-dual path-following.

Primal-dual path

Let $x = (y, u)$ and $X = W \times L^r(\tilde{\Omega})$.

- Primal-dual path associated with (P).

$$\mathcal{C} = \{(x_\gamma, p_\gamma, \lambda_\gamma, \mu_\gamma) \in X \times L^{r'}(\Omega) \times W^* \times L^{r'}(\tilde{\Omega}) : \gamma \in (0, \infty)\}$$

- Properties.
  - The path $\mathcal{C}$ is bounded.
  - $x_\gamma \to x^*$ in X,
  - $(p_\gamma, \lambda_\gamma, \mu_\gamma) \rightharpoonup (p^*, \lambda^*, \mu^*)$ in $L^{r'}(\Omega) \times W^* \times L^{r'}(\tilde{\Omega})$.
  - $\mathcal{C}$ is Lipschitz continuous.
- From now on: $G = \text{id}$, $\tilde{\Omega} = \Omega$, $X = W \times L^2(\Omega)$ and $C_u = L^2(\Omega)$, $C_y = \{y \leq \psi\}$.
  - $\left(\frac{1}{\bar{\gamma}-\gamma}(x_{\bar{\gamma}} - x_\gamma), \frac{1}{\bar{\gamma}-\gamma}(p_{\bar{\gamma}} - p_\gamma)\right)$ admits accumulation point $(\dot{x}_\gamma, \dot{p}_\gamma)$ as $\bar{\gamma} \to \gamma$.
  - Similarly for $g(\gamma) := \gamma(y_\gamma - \psi)$: $\dot{g}(\gamma) = y_\gamma - \psi + \gamma \dot{y}_\gamma$ in $L^2(\Omega)$.

Smoothness properties

- Define

$$\begin{aligned} S_\gamma &:= \{\mathbf{x} \in \Omega : g(\gamma)(\mathbf{x}) > 0\}, \\ S_\gamma^+ &:= S_\gamma \cup \{\mathbf{x} : g(\gamma)(\mathbf{x}) = 0 \wedge \dot{g}(\gamma)(\mathbf{x}) \geq 0\}. \end{aligned}$$

- Then $(\dot{x}_\gamma, \dot{p}_\gamma)$ satisfies the sensitivity equation

$$\langle J'(\dot{x}_\gamma), v\rangle_{X^*,X} + \langle [A^* \dot{p}_\gamma, -\dot{u}_\gamma], v\rangle_{X^*,X} + \Big((y_\gamma - \psi + \gamma \dot{y}_\gamma)\chi_{S_\gamma^+}, v_1 \Big) = 0$$

for all $v = (v_1, v_2) \in X$.

- Set $S_\gamma^0 = \{\mathbf{x} \in \omega : g(\gamma)(\mathbf{x}) = 0\}$. If $\text{meas}(S_\gamma^0) = 0$, then $\gamma \mapsto (x_\gamma, p_\gamma) \in X \times W^*$ is (strongly, weakly) differentiable at γ.

Value and model functions

- Primal-dual path value functional.

$$\gamma \mapsto V(\gamma) = J(x_\gamma) + \frac{\gamma}{2}|(y_\gamma - \psi)^+|^2_{L^2(\Omega)}.$$

  - V is differentiable with

$$\dot{V}(\gamma) = -\frac{\gamma}{2}|(y_\gamma - \psi)^+|^2_{L^2}$$

  - The value functional satisfies

$$V(0) = J(x_0), \quad \dot{V}(\gamma) > 0, \quad \ddot{V}(\gamma) < 0,$$

    where x_0 denotes the solution to the unconstrained problem.
  - These properties are shared by model functions of the type

$$m(\gamma) = C_1 - \frac{C_2}{(E+\gamma)^s}, \quad m(0) = V(0),$$

    with $C_1 \in \mathbb{R}$, $C_2 \geq 0$, $E, s > 0$.

Algorithm

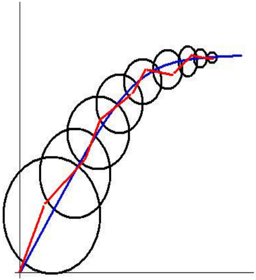
(i) Initialize γ_0; set $k := 0$.

(ii) Find an appproximate solution $(x_{k+1}, p_{k+1}, \lambda_{k+1})$ to (P_{γ_k}) such that $(x_{k+1}, p_{k+1}, \lambda_{k+1}) \in \mathcal{N}(\gamma_k)$.

(iii) Update γ_k to obtain γ_{k+1} ($\Longrightarrow$ use model function m).

(iv) Set $k = k + 1$, and go to (ii).

Inexact path-following:



Algorithm

Approximate solution of (P_{γ_k})**.**

- Apply a semismooth Newton method, or equivalently primal-dual active set strategy.
  - locally superlinear convergence in function space.
  - efficient implementation as a primal-dual active set method.

Applications + Results

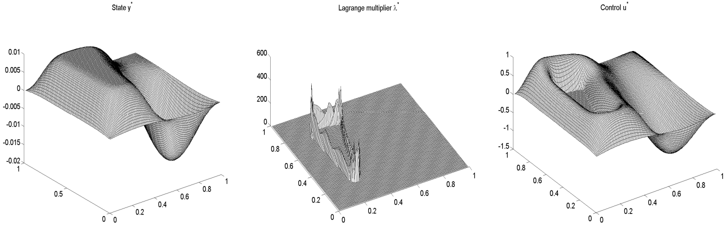
We report on the following algorithms:

- PDAS. Primal-dual active set method.
  - Finite dimensional semismooth Newton method.
- PDIP. Primal-dual path-following interior point method.
  - Mehrotra's predictor-corrector.
  - Large neighborhood.
  - No function space theory available.
- IPF. Inexact path-following (our new method).
- Test problem.

$$\begin{aligned} &\text{minimize} \quad \frac{1}{2}|y - y_d|_{L^2}^2 + \frac{\alpha}{2}|u|_{L^2}^2 \\ &\text{over } (y,u) \in (W = H^2(\Omega) \cap H_0^1(\Omega)) \times L^2(\Omega) \\ &\text{subj. to } -\Delta y = u \text{ in } \Omega, \\ &\qquad\qquad y \le \psi \text{ in } \Omega. \end{aligned}$$

Applications + Results

$$y_d = 10(\sin(2\pi x_1) + x_2),\ \psi = 0.01,\ \alpha = 0.1.$$



Mesh size h	1/16	1/32	1/64	1/128	1/256
PDAS	14	27	54	113	226
PDIP	12	14	15	19	19
IPF	7(11)	9(15)	9(14)	7(13)	8(15)

Error estimates and parameter tuning

Aim. Given a mesh size h, find an optimal selection of $\gamma = \gamma(h)$.

We estimate

$$|u^* - u_{\gamma,h}|_{L^2} \leq |u^* - u_\gamma|_{L^2} + |u_\gamma - u_{\gamma,h}|_{L^2}$$

and analogously for y_h^γ. Let

- $\mathcal{T}_h$ a (shape regular) triangulation of Ω with $h = \max_T \operatorname{diam}(T),\ T \in \mathcal{T}_h$.
- $(X_1)_h := \{v_h \in C_0(\bar{\Omega}) \,|\, v_h \text{ lin. polynom. on } T \in \mathcal{T}_h\}$.

Below: $|\cdot| := |\cdot|_{L^2}$; $\bar{\lambda} \in L^2(\Omega)$ with $\bar{\lambda} \geq 0$ approximates the Lagrange multiplier (compare augmented Lagrangians), and

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

Regularized problem

Consider for $(y, u) \in W \times L^2(\Omega)$ (here: $\psi \equiv 0$):

$$\min\ J(y,u) + \frac{1}{2\gamma}|(\bar{\lambda} + \gamma y)^+|^2 \text{ s.t. } Ay = u.$$

$$\Longrightarrow \quad \max(|y_\gamma|_{C_0(\bar{\Omega})}, |u|) \leq C \text{ indep. of } \gamma.$$

Theorem

We have

$$\alpha|u^* - u_\gamma|^2 + |y^* - y_\gamma|^2 + \gamma|(y_\gamma)^+|^2 \leq \frac{1}{\gamma}|\bar{\lambda}|^2 + \langle \lambda^*, y_\gamma \rangle,$$

and for the feasibility violation

$$|(y_\gamma)^+| \leq \sqrt{\frac{2}{\gamma}} \max\left(\frac{|\bar{\lambda}|^2}{\gamma}, |\lambda^*|_{\mathcal{M}(\bar{\Omega})}|(y_\gamma)^+|_{\mathcal{C}_0(\bar{\Omega})}\right)^{1/2}.$$

Theorem

Either

- *if* $y_d \geq 0$, *or*
- *if there exists* $\epsilon > 0$ *such that*

$$-\int_\Omega \min(0, y_d)\, y_\gamma \, d\mathbf{x} - |y_\gamma|^2 - \alpha\, |u_\gamma|^2 \leq -\epsilon,$$

then $|(y_\gamma)^+| = \mathcal{O}(\gamma^{-1})$ *as* $\gamma \to \infty$.

- [Douglas, Dupont, Wahlbin]. The L^2-projection $\Pi_h : W^{1,p}(\Omega) \to (X_1)_h$ $(d < p \leq \infty)$ satisfies

$$|v - \Pi_h v|_{L^\infty} \leq C h^{1-\frac{d}{p}} |v|_{W^{1,p}}$$

  and is stable in L^2.

- [Brenner, Scott]. For $v_h \in X_h$, we have

$$|v_h|_{L^\infty} \leq C h^{-\frac{d}{2}} |v_h|.$$

- $\mathcal{G}$ solution operator of state equation. For all $v \in L^2(\Omega)$

$$\begin{aligned} |\mathcal{G}(v) - \mathcal{G}_h(v)| &\leq C h^2 |v|, \\ |\mathcal{G}(v) - \mathcal{G}_h(v)|_{L^\infty} &\leq C h^{2-\frac{d}{2}} |v|. \end{aligned}$$

Estimate $|u^* - u_\gamma|$

Lemma

$$|(y_\gamma)^+|_{\mathcal{C}_0(\bar{\Omega})} \leq C\left(h^{1-\frac{d}{p}} + \gamma^{-\frac{1}{2}} h^{-\frac{d}{2}}\right).$$

Proof.

$$|(y_\gamma)^+|_{\mathcal{C}_0(\bar{\Omega})} \leq |(y_\gamma)^+ - \Pi_h (y_\gamma)^+|_{\mathcal{C}_0(\bar{\Omega})} + |\Pi_h (y_\gamma)^+|_{\mathcal{C}_0(\bar{\Omega})} \leq \ldots$$

Theorem

$$|u^* - u_\gamma| \leq \frac{C}{\sqrt{\alpha}}\left(h^{1-\frac{d}{p}} + \gamma^{-\frac{1}{2}} h^{-\frac{d}{2}}\right)^{\frac{1}{2}}$$

Estimate $|u_\gamma - u_{\gamma,h}|$

- Optimal in h (but dep. on γ).

Theorem

$$|u_\gamma - u_{\gamma,h}| \le \frac{C}{\alpha}\gamma h^2 \textit{ for all } 0 < h \le h_0.$$

- Independent of γ.

Theorem

$$|u_\gamma - u_{\gamma,h}| + |y_\gamma - y_{\gamma,h}|_{H_0^1} \le C h^{1-\frac{d}{4}} \textit{ for all } 0 < h \le h_0.$$

Optimal choice: $\gamma = h^{-2}$ yields

$$|u^* - u_{\gamma,h}| = \mathcal{O}(\gamma^{-1/4}). \qquad (\mathcal{O}(\gamma^{-1/2}))$$

Estimate in weaker norm

Using the sensitivity equation

$$\langle J'(\dot{x}_\gamma), v\rangle_{X^*,X} + \langle [A^* \dot{p}_\gamma, -\dot{u}_\gamma], v\rangle_{X^*,X} + \big((y_\gamma - \psi + \gamma \dot{y}_\gamma)\chi_{S_\gamma}, v_1\big) = 0$$

with a non-degeneracy assumption, then one obtains

$$|y^* - y_\gamma|_{L^2} \leq \mathcal{O}(\gamma^{-1/2}) \quad \text{and} \quad |u^* - u_\gamma|_{W^*} \leq \mathcal{O}(\gamma^{-1/2}).$$

Example.