Identification of matrix parameters in elliptic PDEs

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Motivation

Kunisch/Sachs (SINUM 29, 1992) considered SQP-algorithms to solve the PIP

$$\min_{q\in Q_{aq}} \frac{1}{2}\|y-z\|^2 + \frac{\beta}{2}\|q\|_H^2 \text{ s.t. } -\operatorname{div}(q\nabla y) = f \text{ in } \Omega, y = 0 \text{ on } \Gamma.$$

Here

- $z \in L^2(\Omega)$ measurements
- H a Sobolev space ensuring $q \in L^\infty(\Omega)$,
- $Q_{ad} = \{q \in L^\infty(\Omega), q(x) \geq \nu > 0 \text{ a.e. in } \Omega\}$.

Solutions u are characterized as solution to an obstacle problem involving the Riesz isomorphism $R : H \to H^*$.

Idea

- Relax the parameter space and allow q p.d.s. matrix,
- and thus allow more general groundwater models.

Parameter estimation in elliptic PDEs

Reconstruct diffusion matrix $A \in \mathbb{R}^{n,n}$ in

$$(PDE) \quad -\operatorname{div}(A\nabla y) = g \text{ in } \Omega, \; y = 0 \text{ on } \Gamma$$

from measurements $z \in Z$. Here, $g \in H^{-1}(\Omega)$ is given and fixed.

Related work

- Alt, Hoffmann, Sprekels: Intern. Ser. Numer. Math. 68, 11–43 (1984).
- Hoffmann, Sprekels: Numer. Funct. Anal. Optim. 7, 157-177 (1984/85).
- Kohn, Lowe: RAIRO Modél. Math. Anal. Numér. 22, 119–158 (1988).
- Hsiao, Sprekels: Math. Meth. Appl. Sciences 10, 447–456 (1988).
- Rannacher, Vexler: SIAM J. Cont. Optim. 44, 1844–1863 (2005).
- Work related to scalar parameters: Chicone & Gerlach (87), Falk (83), Kunisch (94), Richter (81), Kunisch & Sachs (92), Vainikko & Kunisch (93), Wang & Zou (2010), ...

Parameter estimation in elliptic PDEs

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This talk:

- **Reformulation as optimization problem**
- **Existence of solutions**
- **Necessary optimality conditions**
- **Tailored discretization**
- **Algorithmic concepts**
- **Numerical example**

Optimization problem

Consider

$$(P) \quad \min_{A \in \mathcal{M}} \frac{1}{2}\|y - z\|_Z^2 \text{ s.t. } (PDE).$$

where for $0 < a < b < \infty$

$$\mathcal{M} := \{A \in L^\infty(\Omega)^{n,n} \mid A(x) \in K \text{ a.e. in } \Omega\},$$

with

$$K := \{A \in \mathcal{S}_n \mid a \le \lambda_i(A) \le b, i = 1, \ldots, n\}.$$

Here, $\mathcal{S}_n$ denotes the set of all symmetric $n \times n$ matrices endowed with the inner product $A \cdot B = \text{trace}(AB)$, and $\lambda_1(A), \ldots, \lambda_n(A)$ denote the eigenvalues of A.

Existence of solutions

For given $A \in \mathcal{M}$ let $T(A,g)$ denote the solution to (PDE).

Theorem (Tartar): $\mathcal{M}$ is H–compact, i.e. every sequence $(A_k)_{k\in\mathbb{N}}$ in $\mathcal{M}$ contains a subsequence $(A_{k'})_{k'\in\mathbb{N}}$ converging to an element $A \in \mathcal{M}$ in the sense that for every $g \in H^{-1}(\Omega)$

$$T(A_{k'},g) \rightharpoonup T(A,g) \text{ in } H_0^1(\Omega) \text{ and } A_{k'}\nabla T(A_{k'},g) \rightharpoonup A\nabla T(A,g) \text{ in } L^2(\Omega)^n.$$

$(A_{k'})_{k'\in\mathcal{M}}$ is then said to be H–convergent to A ($A_{k'} \stackrel{H}{\to} A$).

Theorem: (P) admits a solution $A \in \mathcal{M}$ with corresponding state $y = y(A)$ (Ronny Hoffmann, Diploma Thesis, TU Dresden (2005)).

Tychonov regularization

For $\gamma > 0$ consider

$$(P)_\gamma \quad \min_{A \in \mathcal{M}} \underbrace{\frac{1}{2}\|y - z\|_Z^2 + \frac{\gamma}{2}\|A\|_{L^2(n,n)}^2}_{J_\gamma(y,A)} \text{ s.t. } (PDE).$$

Theorem: $(P)_\gamma$ admits a solution.

This follows from the fact that $A_k \xrightarrow{H} A$ and $A_k \overset{*}{\rightharpoonup} A_0$ in $L^\infty(\Omega)^{n,n}$ imply $A(x) \le A_0(x)$ a.e. in Ω, and

$$\|A\|^2 \le \|A_0\|^2 \le \liminf_{k \to \infty} \|A_k\|^2.$$

Optimality condition

Let $(a \otimes b)_{kl} := \frac{1}{2}(a_k b_l + a_l b_k), k, l = 1, \ldots, n.$

$$J(A) := J_\gamma(T(A, g), A).$$

Then

$$J_\gamma'(A)H = \int_\Omega \left(\nabla y \otimes \nabla p + \gamma A\right) \cdot H dx, \quad H \in L^\infty(\Omega)^{n,n},$$

where the adjoint state p satisfies

$$\int_\Omega A \nabla v \cdot \nabla p dx = (y - z, v)_Z \quad \text{for all } v \in H_0^1(\Omega).$$

Let $A \in \mathcal{M}$ be a solution of $(P)_\gamma$. Then for every $\lambda > 0$

$$A(x) = P_K\left(A(x) - \lambda\left(\gamma A(x) + \nabla y(x) \otimes \nabla p(x)\right)\right) \text{ a.e. in } \Omega,$$

where

$$P_K(A) = S^t \text{diag}\left(P_{[a,b]}(\lambda_1(A)), \ldots, P_{[a,b]}(\lambda_n(A))\right) S,$$

if $A = S^t diag(\lambda_1(A), \ldots, \lambda_n(A)) S$.

Discretization of $(P)_\gamma$

Consider

$$(P_h)_\gamma \quad \min_{A\in\mathcal{M}} \frac{1}{2}\|y_h - z\|_Z^2 + \frac{\gamma}{2}\|A\|^2_{L^2(n,n)} \text{ s.t. } (PDE_h),$$

where (PDE_h) denotes the $c(1)$ FE discretization of (PDE).

- **$(P_h)_\gamma$ admits a solution $A_h \in \mathcal{M}$. This follows with H-convergence. However, $T(A_h, g)$ are not finite element functions.**
- **adapt discrete $H-$ convergence of Eymard/Galouët to FE methods): Let $(A_h)_{h>0}$ be a sequence in $\mathcal{M}$. Then there exists a subsequence $(A_{h'})_{h'>0}$ and $A \in \mathcal{M}$ such that for every $g \in H^{-1}(\Omega)$**

  $$T_{h'}(A_{h'}, g) \rightharpoonup T(A,g) \text{ in } H_0^1(\Omega) \text{ and } A_{h'}\nabla T_{h'}(A_{h'}, g) \rightharpoonup A\nabla T(A,g) \text{ in } L^2(\Omega)^n.$$

  This means $(A_{h'})_{h'\in\mathcal{M}}$ Hd–converges to A, i.e. $A_{h'} \overset{Hd}{\rightarrow} A$.
- **Any solution A_h of $(P_h)_\gamma$ satisfies**

  $$A_h(x) = P_K\left(A_h(x) - \lambda\left(\gamma A_h(x) + \nabla y_h(x)\otimes\nabla p_h(x)\right)\right) \text{ a.e. in } \Omega.$$
- **Use projected gradient or Newton-type methods to solve**

  $$G_h(A) := A_h - P_K\left(\frac{1}{\gamma}\nabla p_h \otimes \nabla y_h\right) = 0.$$

Main result

Theorem: Let $A_h \in \mathcal{M}$ be a solution of (P_h). Then there exists a subsequence $(A_{h'})_{h'>0}$ and $A \in \mathcal{M}$ such that $A_{h'} \to A$ in $L^2(\Omega)^{n,n}$, $T_{h'}(A_{h'}, g) \to T(A, g)$ in Z, and A is a solution of (P).

Sketch of proof:

- $A_{h'} \stackrel{Hd}{\to} A$, $A_{h'} \stackrel{*}{\rightharpoonup} A_0$ with $\|A\| \leq \|A_0\|$,
- $J(A) \leq \liminf J_h(A_h)$,
- $J(\bar{A}) = J(A)$ with $\bar{A}$ solution to (P),
- $\frac{1}{2}\|y - y_h\|_Z^2 + \frac{\gamma}{2}\|A_h - A\|^2 \to 0$ for $h \to 0$.

Numerical experiment

$\Omega := (-1,1)^2 \subset \mathbb{R}^2$, data (z, g) given by $z = I_h y$ where

$$y(x_1, x_2) = (1 - x_1^2)(1 - x_2^2) \text{ and } g(x_1, x_2) = (1 - x_2^2)(6x_1^2 + 2) + 2(1 - x_1^2).$$

Then y is the solution to (PDE) when

$$A(x_1, x_2) = \begin{bmatrix} 1 + x_1^2 & 0 \\ 0 & 1 \end{bmatrix}.$$

We choose $a = 0.5$ and $b = 10$. $(P_h)_\gamma$.
Projected steepest descent method with Armijo step size rule; A given, compute

$$A^+ = A(\tau) \text{ with } \tau = \max_{l \in \mathbb{N}} \{\beta^l; J_h(A(\beta^l)) - J_h(A) \leq -\frac{\sigma}{\beta^l} \|A(\beta^l) - A\|^2\}$$

where $\beta \in (0,1)$ and

$$A(\tau)_{|T} := P_K\left(A_{|T} + \tau\left(\nabla y_{h|T} \otimes \nabla p_{h|T} - \gamma A_{|T}\right)\right), \quad T \in \mathcal{T}_h.$$

Initial matrix

$$A^0 := \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}.$$

Stopping criterion: $\|A^+ - A(1)\| \leq \tau_a + \tau_r \|A^0 - A^0(1)\|$ or the maximum number of 5000 iterations is reached.

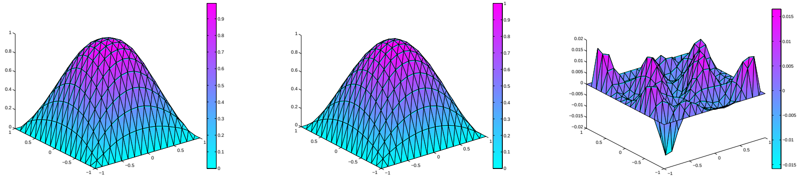
Numerical experiment ($\gamma = 1. \times 10^{-3}$)

We set $\sigma = 10^{-4}$, $\beta = 0.5$. For $\tau_a = 10^{-3}$ and $\tau_r = 10^{-2}$ we have

$$\|A^0 - A^0(1)\| = 7.94 \times 10^{-2}, J_h(A^0) = 2.18 \times 10^{-1}$$

and the algorithm terminates after 400 iterations with $\tilde{A}$ and $\tilde{y}_h = T_h(\tilde{A}, g)$ such that

$$\|\tilde{y}_h - z\| = 1.02 \times 10^{-2}, \quad \|A - \tilde{A}\| = 2.05 \text{ and } J_h(\tilde{A}) = 2.77 \times 10^{-2}.$$

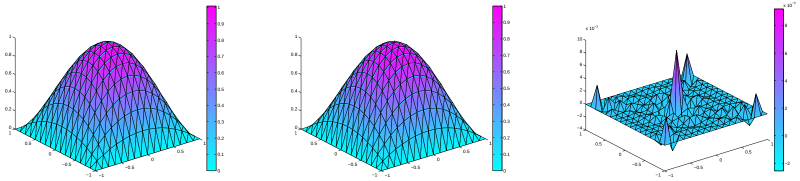


Numerical solution, desired state, error (large, where $\nabla y = 0$).

Numerical experiment ($\gamma = 0$)

By combining the projected gradient method with a homotopy in the parameter γ we treat the case $\gamma = 0$. We start with $\gamma = 1$ and reduce γ by a factor of 0.8 after every ten iterations. After 5000 iterations

$$\|\tilde{y}_h - z\| = 9.61 \times 10^{-4}, \quad \|A - \tilde{A}\| = 1.40$$



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Numerical results partly based on a MATLAB code developed by Ronny Hoffmann in his diploma thesis.

Next steps

- **We expect to prove error estimates for norm-minimal solutions which are inactive,**
- **Techniques also apply in free material optimization (compare work of Leugering, Stingl).**

Thank you very much for your attention

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