Numerical Analysis of Diffusion Coefficient Identification for Elliptic and Parabolic Problems

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March 25, 2023

The Sixth Young Scholar Symposium
East Asia Section of IPIA

Abstract setting

(nonlinear) inverse problem:

$$F(q) = z.$$

- $F : X \to Z$: nonlinear forward map between Banach spaces X and Z, e.g., $F(q) = \mathcal{C}u(q)$

$$\begin{cases} \mathcal{L}(q)u = f, & \text{in } \Omega, \\ \mathcal{B}u = g, & \text{on } \partial\Omega, \end{cases}$$

- noisy observational data z^δ: $\|z - z^\delta\|_Z = \delta$
- recover the parameter q from the observational data z^δ

What is the focus so far

- Theory: (conditional) stability results are known for many PDE IPs

$$\|q_1 - q_2\| \leq C \||F(q_1) - F(q_2)\||^r, \quad r \in (0,1], \quad q_1, q_2 \in \mathcal{Q}$$

Klibanov, Timonov 2004; Isakov 2006; Yamamoto IP 2009; Alberti, Capdeboscq 2018 ...

- Practice: numerical procedures are often based on regularization:

$$\arg\min_{q \in \mathcal{A}} \|F(q) - z^\delta\|_Z^2 + \gamma \psi(q)$$

Sobolev penalty, total variation ... + discretization by FDM, FEM, DNN ...

Tikhonov, Arsenin 1977; Engl, Hanke, Neubauer 1996; Scherzer 2009; Schuster et al 2012; Griesbaum, Kaltenbacher, Vexler 2008...

Interaction between the two directions

- using conditional stability for regularization

  Cheng, Yamamoto IP 2000, Egger, Hofmann IP 2018, Werner, Hofmann IP 2020 . . .

- Question: to derive error estimates for discrete regularized sol.?
  - using conditional stability for numerical analysis of (linear inverse problems)

    Burman 2013, Burman, Oksanen 2018...

  - model inverse problems: diffusion coefficient identification

Elliptic inverse problems

Model inverse problem: diffusion coefficient identification. $\Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$

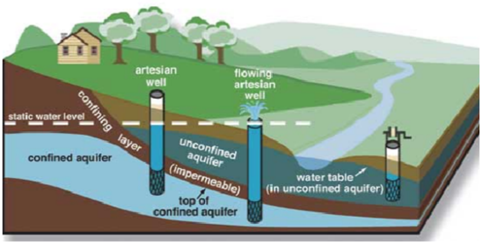
$$\begin{cases} -\nabla \cdot (q \nabla u) = f, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega, \end{cases}$$

- Inverse problem: recover diffusion coefficient $q^\dagger(x)$ from the pointwise observation z^δ with

$$\|z^\delta - u(q^\dagger)\|_{L^2(\Omega)} = \delta.$$

- box constraint: for some positive constants $c_0, c_1 > 0$.

$$\mathcal{A} = \{q \in H^1(\Omega) : \quad c_0 \leq q \leq c_1 \ \text{ a.e. in } \ \Omega\},$$



Stability estimate I: Alessandrini Ann. Mat. Pura Appl. 1986

$\Omega \subset \mathbb{R}^2$ is C^2, simply connected, bounded, $g_i \in C^2(\bar{\Omega})$, $q_i \in W^{1,\infty}(\Omega)$

$$\begin{cases} -\nabla \cdot (q_i \nabla u_i) = 0, & \text{in } \Omega, \\ u_i = g_i, & \text{on } \partial\Omega. \end{cases}$$

If g_i has at most N max and N min on $\partial\Omega$, then for every $\epsilon > 0$ and $\theta \in (0, \frac{1}{2})$, there holds

$$\|q_1 - q_2\|_{L^\infty(\Omega_\epsilon)} \leq c(\|q_1 - q_2\|_{L^\infty(\partial\Omega)} + \|u_1 - u_2\|_{L^2(\Omega)}^{\frac{1}{2}-\theta})^{\frac{1}{2N+1}}$$

proof based on refined analysis of critical points of u.

Stability estimate Bonito, Cohen, DeVore, Petrova and Welper SIMA 2017

Recover q from the knowledge of u in Ω.

$$\begin{cases} -\nabla \cdot (q \nabla u) = f, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega. \end{cases}$$

Energy argument for the model inverse problem:

- use special test function $\dfrac{q_1 - q_2}{q_1} u(q_1)$
- under the condition that $\|q_1\|_{H^1(\Omega)}, \|q_2\|_{H^1(\Omega)} < C$, $f \in L^\infty(\Omega)$, there holds

$$\int_\Omega \left(\frac{q_1 - q_2}{q_1} \right)^2 \left(q_1 |\nabla u(q_1)|^2 + f u(q_1) \right) \mathrm{d}x \le c \|\nabla (u(q_1) - u(q_2))\|_{L^2(\Omega)}$$

Stability estimate II: Bonito, Cohen, DeVore, Petrova and Welper SIMA 2017

This further implies

$$\|q_1 - q_2\|_{L^2(\Omega)} \leq c\|u(q_1) - u(q_2)\|_{H_0^1(\Omega)}^{\frac{1}{2(1+\beta)}},$$

with β from positivity condition

$$(q^\dagger|\nabla u(q^\dagger)|^2 + fu(q^\dagger))(x) \geq c\,\mathrm{dist}(x, \partial\Omega)^\beta \quad \text{a.e. in } \Omega. \tag{P}$$

- If Ω is a Lipschitz domain, $q^\dagger \in \mathcal{A}$ and $f \in L^2(\Omega)$ with $f \geq c_f > 0$, then (P) holds with $\beta = 2$. (by maximum principle + asymptotic behavior of Green's function)

- If Ω is $C^{2,\alpha}$, $q^\dagger \in C^{1,\alpha}(\overline{\Omega})$ and $f \in C^{0,\alpha}(\overline{\Omega})$, with $\alpha > 0$ and $f \geq c_f > 0$. Then (P) holds with $\beta = 0$. (by maximum principle + Schauder estimates)

Finite element approximation

- $\mathcal{T}_h$: shape regular quasi-uniform triangulation of Ω
- finite element space:

$$V_h = \{v_h \in H^1(\Omega) : \quad v_h|_T \in P_1(K) \ \forall K \in \mathcal{T}_h\}$$
$$X_h = \{v_h \in H^1_0(\Omega) : \quad v_h|_T \in P_1(K) \ \forall K \in \mathcal{T}_h\}$$

The discrete admissible set $\mathcal{A}_h$ is taken to be $\mathcal{A}_h := \mathcal{A} \cap V_h$.

Now we consider the finite element discretization:

$$\min_{q_h \in \mathcal{A}_h} J_{\gamma,h}(q_h) = \frac{1}{2}\|u_h(q_h) - z^\delta\|^2_{L^2(\Omega)} + \frac{\gamma}{2}\|\nabla q_h\|^2_{L^2(\Omega)}$$

subject to $q_h \in \mathcal{A}_h$ and $u_h(q_h)$ satisfying

$$(q_h \nabla u_h(q_h), \nabla v_h) = (f, v_h), \quad \forall v_h \in X_h.$$

Question: is q_h^* a good approximation of $q^\dagger$?

Convergence rates of numerical schemes

- output least-squares formula + energy estimate (Neumann)

$$(q\nabla u, \nabla v) = (f, v), \qquad \text{for any test functions } v.$$

Assumption: $\nabla u \cdot \nu > 0$ for a directional vector ν. Falk 1983, Wang & Zou 2010

- Consider the transport equation of q

$$-\nabla q \cdot \nabla u - q\Delta u = f.$$

Assumption: $\inf_{\Omega} \max(|\nabla u|, \Delta u) > 0$, q is known on the inflow boundary. Richter 1981

- Equation error approach:

$$\frac{1}{2}\|\nabla \cdot (q\nabla z^\delta) + f\|^2_{H^{-1}(\Omega)} + \frac{\gamma}{2}\|q\|^2_{H^1(\Omega)}$$

Assumption: $z^\delta \in H^1(\Omega)$.

Kohn, Lowe 1988, Kärkkäinen 1997, Al-Jamal, Gockenbach 2012

Main results Jin & ZZ SINUM 2021

Assumption on problem data: $q^\dagger \in H^2(\Omega) \cap W^{1,\infty}(\Omega) \cap \mathcal{A}$ and $f \in L^\infty(\Omega)$.

Under the regularity assumption, with $\eta = h^2 + \delta + \gamma^{\frac{1}{2}}$, there holds

$$\int_\Omega (q^\dagger - q_h^*)^2 \left(q^\dagger |\nabla u(q^\dagger)|^2 + f u(q^\dagger)\right) \mathrm{d}x \le c(h\gamma^{-\frac{1}{2}}\eta + h + h^{-1}\eta)\gamma^{-\frac{1}{2}}\eta.$$

Then the choice $h \sim \sqrt{\delta}$ and $\gamma \sim \delta^2$ $\Longrightarrow$

$$\int_\Omega (q^\dagger - q_h^*)^2 \left(q^\dagger |\nabla u(q^\dagger)|^2 + f u(q^\dagger)\right) \mathrm{d}x \le c\delta^{\frac{1}{2}}$$

L^2 error of $q_h^* - q^\dagger$

If there exists some $\beta \geq 0$ such that

$$(q^\dagger |\nabla u(q^\dagger)|^2 + f u(q^\dagger))(x) \geq c \,\mathrm{dist}(x, \partial\Omega)^\beta \quad \text{a.e. in } \Omega. \tag{P}$$

Then

$$\|q^\dagger - q_h^*\|_{L^2(\Omega)} \leq c\,\delta^{\frac{1}{4(1+\beta)}}.$$

- If Ω is a Lipschitz domain, $q^\dagger \in \mathcal{A}$ and $f \in L^2(\Omega)$ with $f \geq c_f > 0$

$$\|q^\dagger - q_h^*\|_{L^2(\Omega)} \leq c\,\delta^{\frac{1}{12}}.$$

- If Ω is $C^{2,\alpha}$, $q^\dagger \in C^{1,\alpha}(\overline{\Omega})$ and $f \in C^{0,\alpha}(\overline{\Omega})$, with $\alpha > 0$ and $f \geq c_f > 0$

$$\|q^\dagger - q_h^*\|_{L^2(\Omega)} \leq c\,\delta^{\frac{1}{4}}.$$

Conditional stability

For $u(q_1), u(q_2) \in H_0^1(\Omega)$ and $\beta = 0$, Bonito, Cohen, DeVore, Petrova & Welper 2017

$$\|q_1 - q_2\|_{L^2(\Omega)} \le c\|u(q_1) - u(q_2)\|_{H^1(\Omega)}^{\frac{1}{2}}.$$

This, the Gagliardo-Nirenberg interpolation inequality

$$\|u\|_{H^1(\Omega)} \le \|u\|_{L^2(\Omega)}^{\frac{1}{2}} \|u\|_{H^2(\Omega)}^{\frac{1}{2}},$$

and the regularity assumption $u(q_1), u(q_2) \in H^2(\Omega)$ directly give

$$\|q_1 - q_2\|_{L^2(\Omega)} \le c\|u(q_1) - u(q_2)\|_{L^2(\Omega)}^{\frac{1}{4}}.$$

The convergence rate matches the conditional stability estimate.

Step I: approximation of $u_h(q_h^*)$

Under data regularity assumption, there holds

$$u \in H_0^1(\Omega) \cap H^2(\Omega) \cap W^{1,\infty}(\Omega).$$

Then we have the error estimate

$$\|u_h(q_h^*) - u(q^\dagger)\|_{L^2(\Omega)} + \gamma^{\frac{1}{2}} \|\nabla q_h^*\|_{L^2(\Omega)} \le c(h^2 + \delta + \gamma^{\frac{1}{2}}) =: \eta.$$

minimizing property of q_h^* + a priori regularity on $q^\dagger$

$$\begin{aligned}
&\frac{1}{4}\|u_h(q_h^*) - u(q^\dagger)\|_{L^2(\Omega)}^2 + \frac{\gamma}{2}\|\nabla q_h^*\|_{L^2(\Omega)}^2 \\
\le &\frac{1}{2}\|u_h(q_h^*) - z_\delta\|_{L^2(\Omega)}^2 + \frac{\gamma}{2}\|\nabla q_h^*\|_{L^2(\Omega)}^2 + \frac{1}{2}\|z_\delta - u(q^\dagger)\|_{L^2(\Omega)}^2 \\
\le &\frac{1}{2}\|u_h(\mathcal{I}_h q^\dagger) - u(q^\dagger)\|_{L^2(\Omega)}^2 + \frac{\gamma}{2}\|\nabla \mathcal{I}_h q^\dagger\|_{L^2(\Omega)}^2 + c\delta^2 \\
\le &c(h^4 + \gamma + \delta^2)
\end{aligned}$$

Step II: Crucial identity

Crucial identity (with $u = u(q^\dagger)$) and test function $\varphi = \frac{q^\dagger - q_h^*}{q^\dagger} u \in H_0^1(\Omega)$

$$2((q^\dagger - q_h^*)\nabla u, \nabla \varphi) = \int_\Omega (q^\dagger - q_h^*)^2 \left(q^\dagger |\nabla u(q^\dagger)|^2 + f u(q^\dagger)\right) \mathrm{d}x$$

by integration by parts + weak formulation.

Technical estimates

Simple observation (with $u = u(q^\dagger)$):

$$((q^\dagger - q_h^*)\nabla u, \nabla\varphi) = ((q^\dagger - q_h^*)\nabla u, \nabla(\varphi - P_h\varphi)) + (q^\dagger\nabla u - q_h^*\nabla u, \nabla P_h\varphi)$$
$$= -(\nabla\cdot((q^\dagger - q_h^*)\nabla u), \varphi - P_h\varphi) + (q_h^*\nabla(u_h(q_h^*) - u), \nabla P_h\varphi).$$

Let $\eta = h^2 + \delta + \gamma^{\frac{1}{2}}$.

With the special test function $\varphi = \frac{q^\dagger - q_h^*}{q^\dagger} u \in H_0^1(\Omega)$ and $\|\nabla q_h^*\|_{L^2(\Omega)} \le c\gamma^{-\frac{1}{2}}\eta$ we have

$$\|\nabla\cdot((q^\dagger - q_h^*)\nabla u\|_{L^2(\Omega)} \le \|\nabla q^\dagger\|_{L^2(\Omega)}\|\nabla u\|_{L^2(\Omega)} + \|\nabla q_h^*\|_{L^2(\Omega)}\|\nabla u\|_{L^2\infty(\Omega)}$$
$$+ \|q^\dagger - q_h^*\|_{L^\infty(\Omega)}\|\nabla u\|_{L^2(\Omega)}$$
$$\le c(1 + \|\nabla q_h^*\|_{L^2(\Omega)}) \le c(1 + \gamma^{-\frac{1}{2}}\eta).$$

and

$$\|\varphi - P_h\varphi\|_{L^2(\Omega)} \le ch\|\nabla\varphi\|_{L^2(\Omega)} \le ch(1 + \|\nabla q_h^*\|_{L^2(\Omega)}) \le ch(1 + \gamma^{-\frac{1}{2}}\eta).$$

Therefore,

$$\left|(\nabla\cdot((q^\dagger - q_h^*)\nabla u), \varphi - P_h\varphi)\right| \le ch\gamma^{-1}\eta^2$$

Technical estimates

Simple observation (with $u = u(q^\dagger)$):

$$\begin{aligned}\|q_h^*\nabla(u_h(q_h^*)-u)\|_{L^2(\Omega)} &\le c\|\nabla(u_h(q_h^*)-u)\|_{L^2(\Omega)} \\ &\le c\Big(\|\nabla(u_h(q_h^*)-P_hu)\|_{L^2(\Omega)} + \|\nabla(P_hu-u)\|_{L^2(\Omega)}\Big) \\ &\le c\Big(h^{-1}\|u_h(q_h^*)-P_hu\|_{L^2(\Omega)} + h\Big) \\ &\le c\Big(h^{-1}\|u_h(q_h^*)-u\|_{L^2(\Omega)} + h\Big) \le c\Big(h^{-1}\eta + h\Big)\end{aligned}$$

Therefore

$$\Big|(q_h^*\nabla(u_h(q_h^*)-u), \nabla P_h\varphi)\Big| \le c(h + h^{-1}\eta)\ \gamma^{-\frac{1}{2}}\eta$$

Therefore,

$$\int_\Omega (q^\dagger - q_h^*)^2\left(q^\dagger|\nabla u(q^\dagger)|^2 + fu(q^\dagger)\right)\mathrm{d}x \le c(h\gamma^{-\frac{1}{2}}\eta + h + h^{-1}\eta)\gamma^{-\frac{1}{2}}\eta.$$

Numerical results

In the elliptic case, the noisy data z^δ is generated by

$$z^\delta(x) = u(q^\dagger)(x) + \varepsilon \sup_{x\in\Omega} |u(q^\dagger)|\xi(x),$$

- ξ follows the standard Gaussian distribution
- $\varepsilon > 0$ denotes the (relative) noise level
- The noisy data z^δ is generated on a fine mesh and then interpolated to a coarse spatial/ temporal mesh for the inversion step
- Minimization by projected conjugate gradient
- error measure

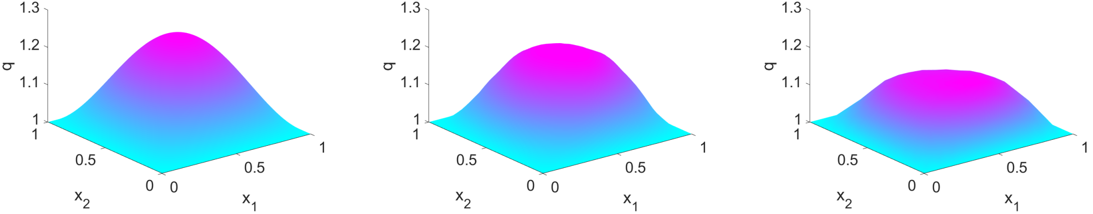
$$e_q = \|q^\dagger - q_h^*\|_{L^2(\Omega)} \quad \text{and} \quad e_u = \|u(q^\dagger) - u_h(q_h^*)\|_{L^2(\Omega)}$$

Example

$\Omega = (0,1)^2$, $q^\dagger(x_1,x_2) = 1 + x_2(1-x_2)\sin \pi x_1$ and $f \equiv 1$.

Table: Convergence w.r.t. ε, with suitable γ and h.

ε	5.00e-2	3.00e-2	1.00e-2	5.00e-3	3.00e-3	1.00e-03	
e_q	4.46e-2	3.17e-2	1.27e-2	6.98e-3	5.59e-3	2.64e-03	0.62
e_u	7.88e-4	4.11e-4	1.20e-4	6.56e-5	3.89e-5	1.39e-05	1.00



(a) exact (b) ε=1e-2 (c) ε=5e-2

Figure: Numerical reconstructions at two noise levels.

Parabolic inverse problems

Recover diffusion coefficient q in IBVP $(0 < \alpha \le 1)$:

$$\begin{cases} \partial_t^\alpha u - \nabla \cdot (q \nabla u) = f, & \text{in } \Omega \times (0, T], \\ u(0) = u_0, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega \times (0, T], \end{cases}$$

- $\partial_t^\alpha u$, $0 < \alpha \le 1$: Djrbashian-Caputo fractional derivative in time

$$\partial_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} u'(s)\, \mathrm{d}s, \qquad \text{for} \quad \alpha \in (0,1);$$

- the distributed observation z^δ over $\Omega \times (T - \sigma, T)$

$$\|z^\delta - u(q^\dagger)\|_{L^2(T-\sigma,T;L^2(\Omega))} \le \delta.$$

- stability $\alpha = 1$: $\|q_1 - q_2\|_{L^2(\Omega)} \le c e^{cT} \|u(T;q_1) - u(T;q_2)\|_{H^2(\Omega)}$ Triki JMPA 2021
- $\alpha \in (0,1)$: there is no known stability result, even for full data.

Survey on IPs for time frac. models: Jin & Rundell 2015; Li, Liu, Yamamoto 2019...

Finite element method

Then the finite element discretization reads

$$\min_{q_h \in \mathcal{A}_h} J_{\gamma,h,\tau}(q_h) = \tau \sum_{n=N_\sigma}^{N} \|U_h^n(q_h) - z_n^\delta\|_{L^2(\Omega)}^2 + \frac{\gamma}{2}\|\nabla q_h\|_{L^2(\Omega)}^2,$$

where $U_h^n(q_h) \in X_h$ satisfies $U_h^0 = P_h u_0$ and

$$(\bar\partial_\tau^\alpha U_h^n(q_h), v_h) + (q_h \nabla U_h^n(q_h), \nabla v_h) = (f(t_n), v_h), \quad n = 1, 2, \dots, N+1.$$

Throughout, we assume that $N_\sigma = (T-\sigma)/\tau + 1$ is an integer.

Question: is q_h^* a good approximation of $q^\dagger$?

Error estimate $(\alpha = 1)$ Jin & ZZ SINUM 2021

Under suitable data regularity assumption, with $\eta = \tau + h^2 + \delta + \gamma^{\frac{1}{2}}$,

$$\tau^3 \sum_{j=N_\sigma+1}^{N} \sum_{i=N_\sigma+1}^{j} \sum_{n=i}^{j} \int_\Omega \Big(\frac{q^\dagger - q_h^*}{q^\dagger}\Big)^2 \Big(q^\dagger |\nabla u(t_n)|^2 + (f(t_n) - \partial_t u(t_n))u(t_n)\Big)\, \mathrm{d}x$$

$$\leq c(h\gamma^{-\frac{1}{2}}\eta + \min(1, h^{-1}\eta))\gamma^{-\frac{1}{2}}\eta \leq c\,\delta^{\frac{1}{2}} \qquad \text{with } \tau \sim \delta,\ h \sim \sqrt{\delta},\ \gamma \sim \delta^2.$$

Assume exists some $\beta \geq 0$ such that

$$q^\dagger |\nabla u(q^\dagger)(t)|^2 + (f(t) - \partial_t u(q^\dagger)(t))u(q^\dagger) \geq c\,\mathrm{dist}(x, \partial\Omega)^\beta \quad \text{a.e. in } \Omega, \qquad \text{(P2)}$$

for any $t \in [T - \sigma, T]$. Then there holds

$$\|q^\dagger - q_h^*\|_{L^2(\Omega)} \leq c\,\delta^{\frac{1}{4(1+\beta)}}.$$

The case $\alpha \in (0, 1)$ is more technical and requires $\sigma = T$. Jin & ZZ SICON 2021

Concluding remarks

- Recovery of diffusion coefficient in elliptic / parabolic problems;
- suitable regularization, special test functions, provable positivity condition;
- (weighted) L^2 error in terms of noise level, regu. parameter and discret. parameter(s);
- motivated by a suitable (conditional) stability estimate

What is next:

- improve the error estimate? $O(\delta^s)$ with $s > 1/4$?
- alternative measurement type? e.g., $|\nabla u|$, $q|\nabla u|$, $\sigma u \ldots$?
- recover multiple coefficients? from one/two/more observations?
- more non-intrusive strategies for using stability estimates?

Reference

- B. Jin & ZZ. Error analysis of finite element approximations of diffusion coefficient identification for elliptic and parabolic problems, SINUM 59 (2021), 119-142.
- B. Jin & ZZ. Numerical estimation of a diffusion coefficient in subdiffusion, SICON 59 (2021), 1466-1496.
- S. Cen, B. Jin, Q. Quan & ZZ. Hybrid Neural-Network FEM approximation of diffusion coefficient in elliptic and parabolic problems. arXiv 2302.10773, 2023