Inverse Problems in Partial Differential Equations

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Introduction to inverse problems

Computational Science ("Digital Twin")

Computer simulation of real-world experiment:

Given input x calculate outcome $y = F(x)$.

$x \in X$: parameters / input
$y \in Y$: outcome / measurements
$F : X \to Y$: functional relation / model

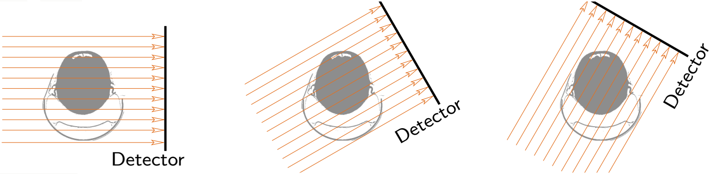
Goals:

- Prediction: Given x, calculate $y = F(x)$.
- Optimization: Find x, such that $F(x)$ is optimal.
- Inversion/Identification: Given $F(x)$, calculate x.

Example: X-ray computerized tomography (CT)

Nobel Prize in Physiology or Medicine 1979:
Allan M. Cormack and Godfrey N. Hounsfield
(Photos: Copyright ©The Nobel Foundation)

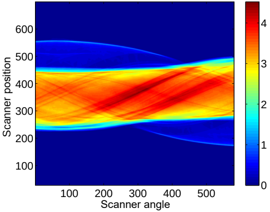
Idea: Take x-ray images from several directions



Computerized tomography (CT)

(Image: Hanke-Bourgeois, Grundlagen der Numerischen Mathematik und des Wiss. Rechnens, Teubner 2002)

$\overset{F}{\longmapsto}$



Image

Measurements

Direct problem: Simulate/predict the measurements

(from knowledge of the interior density distribution)

Given x *calculate* $F(x) = y$*!*

Inverse problem: Reconstruct/image the interior distribution

(from taking x-ray measurements)

Given y *solve* $F(x) = y$*!*

Computerized tomography

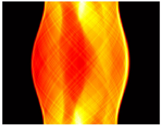
- CT forward operator $F: x \mapsto y$ is linear

$\rightsquigarrow$ Evaluation of F is simple matrix vector multiplication
(after discretizing image and measurements as long vectors)

Simple low resolution example:

$\overset{F}{\mapsto}$

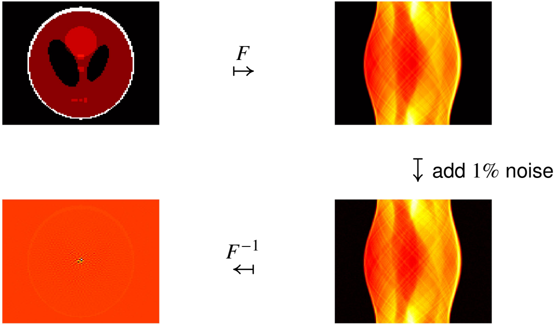
$\overset{F^{-1}}{\leftarrow\!\shortmid}$



Problem: Matrix F invertible, but $\|F^{-1}\|$ very large.

Ill-posedness

- In the continuous case: F^{-1} not continuous
- After discretization: $\|F^{-1}\|$ very large



Are stable reconstructions impossible?

Ill-posedness

Generic linear ill-posed inverse problem

- $F: X \to Y$ bounded and linear, X, Y Hilbert spaces,
- F injective, F^{-1} not continuous,
- True solution and noise-free measurements: $F\hat{x} = \hat{y}$,
- Real measurements: y^δ with $\|y^\delta - \hat{y}\| \leq \delta$

$$F^{-1}y^\delta \not\to F^{-1}\hat{y} = \hat{x} \quad \text{for} \quad \delta \to 0.$$

Even the smallest noise may corrupt the reconstructions.

Regularization

Generic linear Tikhonov regularization

$$R_\alpha = (F^*F + \alpha I)^{-1} F^*$$

$\rightsquigarrow R_\alpha$ continuous, $x = R_\alpha y^\delta$ minimizes

$$\|Fx - y^\delta\|^2 + \alpha \|x\|^2 \to \text{min!}$$

Theorem. Choose $\alpha := \delta$. Then for $\delta \to 0$,

$$R_\delta y^\delta \to F^{-1}\hat{y}.$$

Regularization

Theorem. Choose $\alpha := \delta$. Then for $\delta \to 0$,

$$R_\delta y^\delta \to F^{-1}\hat{y}.$$

Proof. Show that $\|R_\alpha\| \leq \frac{1}{\sqrt{\alpha}}$ and apply

$$\|R_\alpha y^\delta - F^{-1}\hat{y}\| \leq \underbrace{\|R_\alpha(y^\delta - \hat{y})\|}_{\leq \|R_\alpha\|\,\delta} + \underbrace{\|R_\alpha \hat{y} - F^{-1}y\|}_{\to 0 \text{ for } \alpha \to 0}.$$

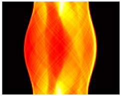
Inexact but continuous reconstruction (regularization)

\+ Information on measurement noise (parameter choice rule)

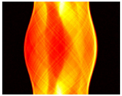
= Convergence

Example ($\delta = 1\%$)

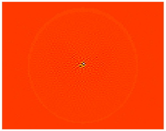
$\hat{x}$



$\hat{y} = F\hat{x}$



y^δ

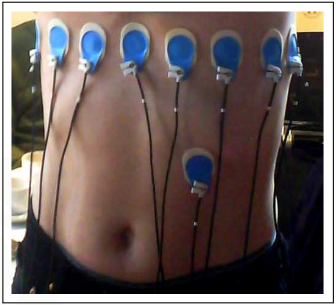


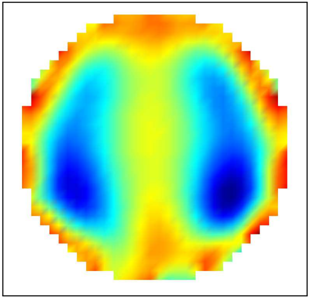
$F^{-1}y^\delta$

$(F^*F + \delta I)^{-1}F^*y^\delta$

Inverse Problems in Partial Differential Equations

Electrical impedance tomography (EIT)





- Apply electric currents on subject's boundary
- Measure necessary voltages

$\rightsquigarrow$ Reconstruct conductivity inside subject

Calderón problem

Can we recover $\sigma \in L^\infty_+(\Omega)$ in

$$\nabla \cdot (\sigma \nabla u) = 0, \quad x \in \Omega \subset \mathbb{R}^d \qquad (1)$$

from all possible Dirichlet and Neumann boundary values

$$\{(u|_{\partial\Omega}, \sigma \partial_\nu u|_{\partial\Omega}) \quad : \quad u \text{ solves } (1)\}\,?$$

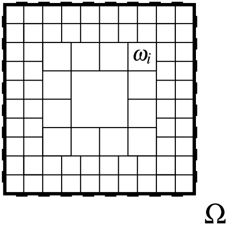
Equivalent: Recover σ from **Neumann-to-Dirichlet-Operator**

$$\Lambda(\sigma):\ L^2_\diamond(\partial\Omega) \to L^2_\diamond(\partial\Omega), \quad g \mapsto u|_{\partial\Omega},$$

where u solves (1) with $\sigma \partial_\nu u|_{\partial\Omega} = g$.

EIT in practice

- Finitely many unknowns, σ pcw. const. on given resolution $\Omega = \bigcup_{i=1}^{n} \omega_i$
- Finitely many measurements
$$\int_{\partial\Omega} g_j \Lambda(\sigma) g_k \, \mathrm{d}s$$
for given currents $g_1, \ldots, g_m \in L^2_\diamond(\partial\Omega)$



Finite-dimensional inverse problem: Determine

$$\sigma = \begin{pmatrix} \sigma_1 \\ \vdots \\ \sigma_n \end{pmatrix} \in \mathbb{R}^n_+ \quad \text{from } F(\sigma) = \left(\int_{\partial\Omega} g_j \Lambda(\sigma) g_k \, \mathrm{d}s \right)_{j,k=1}^{m} \in \mathbb{R}^{m\times m}.$$

Simple example: EIT with 2 unknowns & 6 bndry. currents

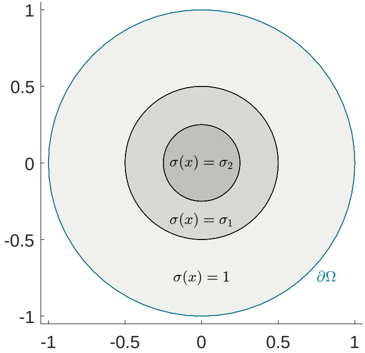
Ω: unit circle

$$F: \mathbb{R}_+^2 \to \mathbb{R}^{6\times 6}$$

$$F\begin{pmatrix}\sigma_1\\ \sigma_2\end{pmatrix} := \left(\int_{\partial\Omega} g_j \Lambda(\sigma) g_k\right)_{j,k=1}^{6}$$

with trigonometric currents

$$\{g_1,\ldots,g_6\} = \{\sin(\varphi),\ldots,\cos(3\varphi)\}$$

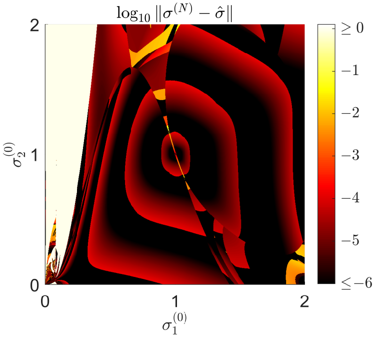


Inverse problem: Reconstruct $\hat{\sigma} \in \mathbb{R}_+^2$ from $\hat{Y} = F(\hat{\sigma}) \in \mathbb{R}^{6\times 6}$

Natural approach: Least squares data fitting

$$\texttt{minimize} \quad \|F(\sigma) - \hat{Y}\|_{\mathrm{F}}^2 \qquad \textit{(+ Regularization)}$$

Problem of non-linearity / local convergence



- Least squares data fitting functional not convex
- Error of Matlab's `lsqnonlin` highly depends on initial values

Can we derive globally convergent algorithm?

The Monotonicity Lemma

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Lemma. (First appearance: Kang/Seo/Sheen 1997, Ikehata 1998)

$$\int_{\partial\Omega} g(\Lambda(\sigma_1) - \Lambda(\sigma_2))g \, \mathrm{d}s \geq \int_\Omega (\sigma_2 - \sigma_1) |\nabla u_{\sigma_2}^g|^2 \, \mathrm{d}x$$

for all $\sigma_1, \sigma_2 \in L^\infty_+(\Omega)$, $g \in L^2_\diamond(\partial\Omega)$.

- Monotonicity w.r.t. Loewner order:

$$\sigma_1 \leq \sigma_2 \quad \Longrightarrow \quad \Lambda(\sigma_1) \geq \Lambda(\sigma_2)$$

⤳ Inclusion detection method (Tamburrino/Rubinacci 2002)

- Localized potentials (**H.** 2008):

$$\exists (g_k)_{k\in\mathbb{N}} : \int_{D_1} |\nabla u_\sigma^{g_k}|^2 \, \mathrm{d}x \to \infty, \quad \int_{D_2} |\nabla u_\sigma^{g_k}|^2 \, \mathrm{d}x \to 0.$$

⤳ Converse monotonicity holds for inclusion detection.

⤳ Monotonicity method yields exact shape (**H.**/Ullrich 2013).

Monotonicity and Convexity

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Lemma.

$$\int_{\partial\Omega} g(\Lambda(\sigma_1)-\Lambda(\sigma_2))g \,\mathrm{d}s \geq \int_\Omega (\sigma_2-\sigma_1)|\nabla u_{\sigma_2}^g|^2 \,\mathrm{d}x$$
$$= \int_{\partial\Omega} g\Lambda'(\sigma_2)(\sigma_1-\sigma_2)g \,\mathrm{d}s.$$

for all $\sigma_1, \sigma_2 \in L^\infty_+(\Omega)$, $g \in L^2_\diamond(\partial\Omega)$.

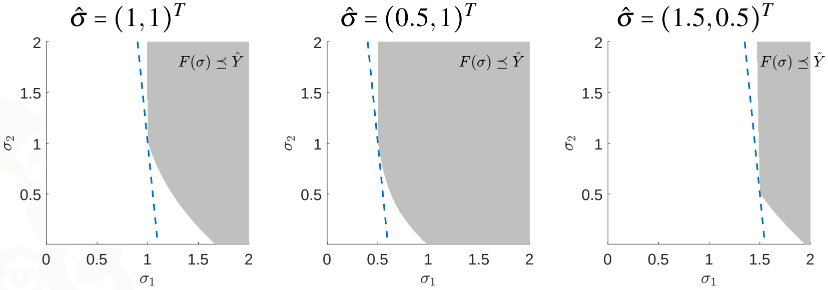
- For all $\sigma_1, \sigma_2 \in L^\infty_+(\Omega)$: $\Lambda(\sigma_1)-\Lambda(\sigma_2) \geq \Lambda'(\sigma_2)(\sigma_1-\sigma_2)$.
- Convexity: For all $\sigma_1, \sigma_2 \in L^\infty_+(\Omega)$, $t \in [0,1]$

$$\Lambda((1-t)\sigma_1+t\sigma_2) \leq (1-t)\Lambda(\sigma_1)+t\Lambda(\sigma_2).$$

The "monotonicity lemma" also implies convexity.

Convexity for the simple example

Inverse problem: Reconstruct $\hat{\sigma} \in \mathbb{R}^2_+$ from $\hat{Y} = F(\hat{\sigma}) \in \mathbb{R}^{6\times 6}$

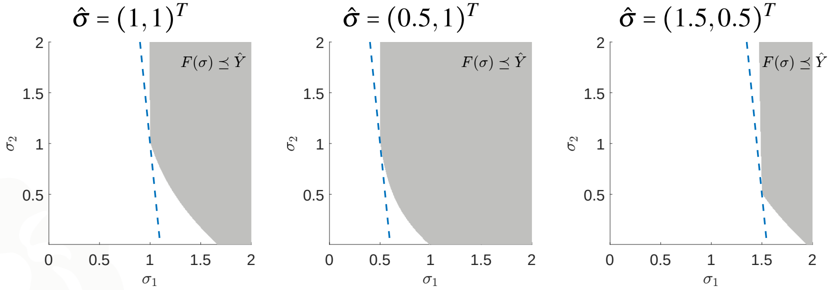


Observation.

$\hat{\sigma}$ is the lower left corner of the convex set $F(\sigma) \leq \hat{Y}$.

("$\leq$": Loewner / semidefiniteness order)

Mathematical formulation



Conjecture. $\exists c \in \mathbb{R}^n$ so that true solution $\hat\sigma$ minimizes

$$c^T \boldsymbol{\sigma} = \sum_{i=1}^{n} c_i \sigma_i \to \text{min!} \quad \text{s.t.} \quad \boldsymbol{\sigma} \in [a,b]^n,\ F(\boldsymbol{\sigma}) \le \hat Y.$$

For a similar but simpler Robin problem:

- Conjecture holds with $c = \mathbb{1}$ *(**H.**, Optim. Lett. 2021)*
- Global Newton convergence is possible *(**H.**, Numer. Math. 2021)*

Convex reformulation for EIT

Theorem. (**H.**, *SIMA* 2023)

If sufficiently many measurements are taken, then:

- EIT forward mapping $F: [a,b]^n \to \mathbb{S}_m \subset \mathbb{R}^{m\times m}$ is injective.
- Derivative $F'(\sigma)$ is injective for all $\sigma \in [a,b]^n$.
- There exists $c \in \mathbb{R}^n_+$ so that for all $\hat{\sigma} \in [a,b]^n$, $\hat{Y} = \Lambda(\hat{\sigma})$:

  $\hat{\sigma}$ is the unique solution of the convex problem

$$\texttt{minimize} \quad c^T\sigma = \sum_{i=1}^n c_i\sigma_i \quad \texttt{s.t.} \quad \sigma \in [a,b]^n,\ F(\sigma) \preceq \hat{Y}.$$

The Calderón problem with finitely many unknowns is equivalent to convex semidefinite optimization

Theorem (continued). (**H.**, *SIMA* 2023)

There exists $\lambda > 0$ so that

- for all $\hat{\sigma} \in [a,b]^n$, and $\hat{Y} := \Lambda(\hat{\sigma})$,
- and all $\delta > 0$, and $Y^\delta \in \mathbb{S}_m \subset \mathbb{R}^{m\times m}$, with $\|Y^\delta - \hat{Y}\| \leq \delta$,

the convex semidefinite optimization problem

$$\texttt{minimize} \quad c^T\sigma = \sum_{i=1}^n c_i\sigma_i \quad \texttt{s.t.} \quad \sigma \in [a,b]^n,\ F(\sigma) \leq Y^\delta + \delta I.$$

possesses a minimizer σ^δ. Every such minimizer fulfills

$$\|\sigma^\delta - \hat{\sigma}\|_{c,\infty} \leq \frac{n-1}{\lambda}\delta.$$

($\|\cdot\|_{c,\infty}$: c-weighted maximum norm)

Error estimates for noisy data $Y^\delta \approx \hat{Y}$ also hold.

Conclusions

For elliptic coefficient inverse problems

- least-squares residuum functionals may be highly non-convex
- local minima are usually useless

Possible remedy

- utilize monotonicity & convexity with respect to Loewner order

Equivalent convex reformulations are possible

- globally convergent solution algorithms are possible
- error estimates for noisy data are possible

Possible extensions?

- Monotonicity-based methods have been extended to, e.g.,:

  Farfield Scattering (Griesmaier/**H.** 18), Helmholtz (**H.**/Pohjola/Salo 19), Fractional Schrödinger (**H.**/Lin 19+20), Semilinear Schrödinger (Lin 22), Nonlinear Helmholtz (Griesmaier/Knöller/Mandel 22), Waveguide (Furuya 20, Arens/Griesmaier/Zhang 23), Maxwell (Albicker/Griesmaier 23), Crack detection (Furuya 20, Garde/Vogelius 23)