Topics in Numerical Analysis II
Computational Inverse Problems

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Outline

1 Ill-posed problems: examples

2 Classical regularization methods
- Mathematical setting

Outline

Intended topics: theory and practice of general inverse problems

- introduction to inverse problems (one lecture)
- regularization theory in Hilbert space
  - spectral cutoff (one lecture)
  - Tikhonov regularization (one lecture)
  - iterative regularization (two lectures)
- regularization theory in Banach space
  - sparse recovery (one lecture)
  - general theory (one lecture)
- uncertainty quantification (two lectures)
- deep learning approaches (two lectures)

well-posed problems

Jacques Salomon Hadamard (1865-1963) 1923:

- a solution exists;
- the solution is unique;
- the solution depends continuously on the data, **in some reasonable topology**.

Caution: The choice of topology is crucial for well-posedness.

Ill-posed problems

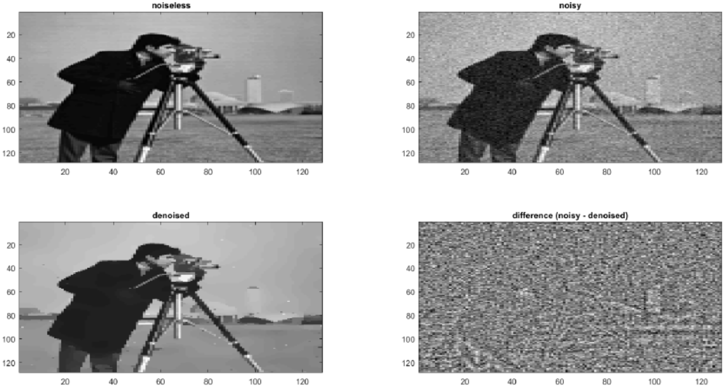
The set of ill-posed problems is the complement of the set of well-posed problems (in the space of all problems)

- interpolation
- medical scans: computed tomography, magnetic resonance imaging, positron emission tomography, proton therapy ...
- finding the physical laws
- nearly all problems encountered in in daily life

When solving an ill-posed problem, it is essential to use all **possible prior and expert knowledge** about the candidate solutions.

Inverse problems in imaging

image denoising: $y = x + n$



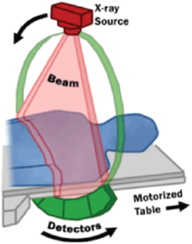
noise type might be complex

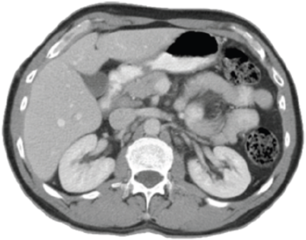
Inverse problems in imaging

image deblurring: $y = k * x + n$

blind deconvolution: k is unknown.

computed tomography





X-ray CT: line projection

mechanism: when X-rays pass through the patient, they are *attenuated* differently by various tissues according to their *density*.

figure taken from Simon Arridge's lecture, wikipedia

Let z be an axis parallel to the direction of the beam. The intensity of the X-ray is reduced as it travels through the tissue, following

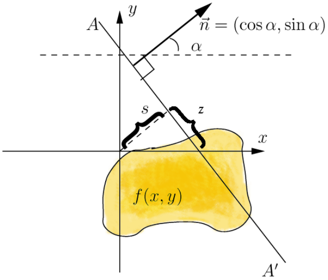
$$\frac{\mathrm{d}U(z)}{\mathrm{d}z} = -\mu(z)U(z)$$

- μ: attenuation coefficient
- analytic solution:

$$U = U_0 e^{-\int_0^\ell \mu(z)\mathrm{d}z}$$

  Beer-Lambert law for attenuation

Radon transform



zero scattering photons propagate along rays ℓ

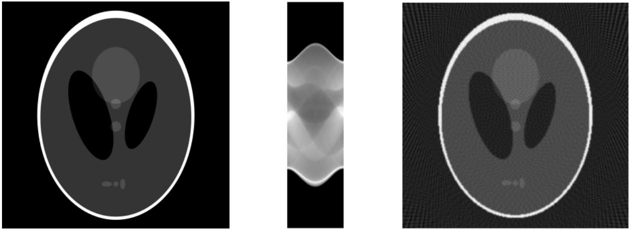
$$U = U_0 e^{-\int_\ell f(\mathbf{x})d\ell}$$

Radon transform $\mathcal{R}f(s, \alpha) := -\ln \frac{U}{U_0}$

$$\int_{-\infty}^{\infty} f(z\sin\alpha + s\cos\alpha, -z\cos\alpha + s\sin\alpha)dz$$

computed tomography: measures X-ray attenuation by tissues inside the body, with multiple measurements at different angles

applications: diagnosis of tumors, internal injuries, bone fractures, ...

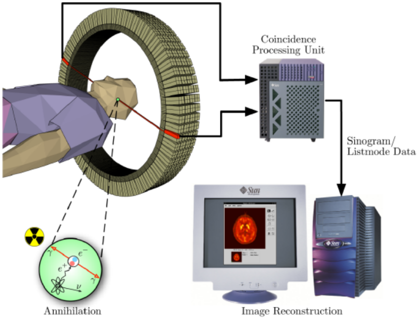


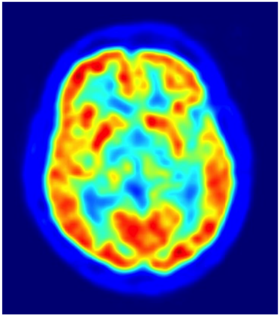
phantom sinogram reconstruction

F. Natterer. The Mathematics of Computerized Tomography. SIAM 2001

The Nobel Prize in Physiology or Medicine 1979 was awarded to Allan M. Cormack and Godfrey N. Hounsfield "for the development of computer assisted tomography."

positron emission tomography: line projection, Poisson noise

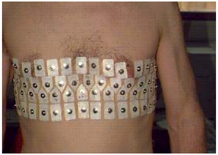


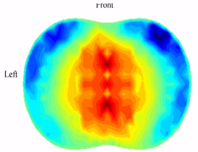


$$y \sim Poisson(Ax)$$

taken from Simon Arridge's lecture

electrical impedance tomography: recover conductivity distribution from boundary meas.





applications: lung / breast imaging, ...

mathematical model A.P. Calderon 1980s

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

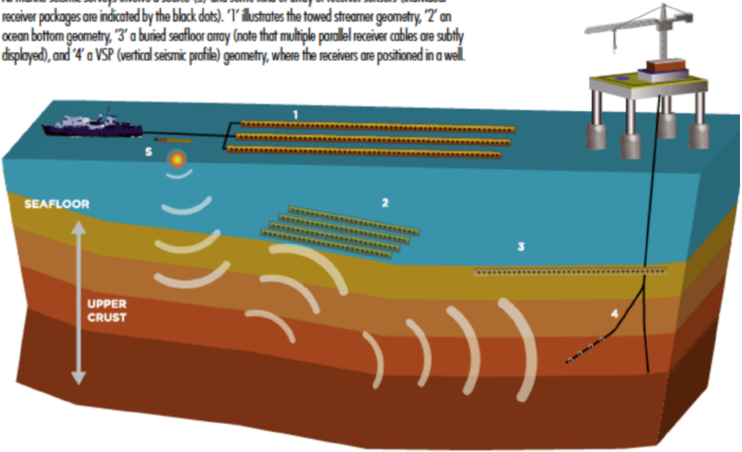
goal: recover the conductivity σ from all current-voltage pairs

©wikipedia

geophysics, seismic imaging

Figure 1 *(credit: Jack Caldwell)*

All marine seismic surveys involve a source (S) and some kind of array or receiver sensors (individual receiver packages are indicated by the black dots). '1' illustrates the towed streamer geometry, '2' an ocean bottom geometry, '3' a buried seafloor array (note that multiple parallel receiver cables are subtly displayed), and '4' a VSP (vertical seismic profile) geometry, where the receivers are positioned in a well.



one-dimensional heat conduction

mathematical model (with $\Omega = (0,1)$, $\mathbb{R}_+ = (0,\infty)$):

$$\begin{aligned} u_t &= u_{xx}, && \text{in } \Omega \times \mathbb{R}_+, \\ u_x(0,\cdot) = u_x(1,t) &= 0, && \text{on } \mathbb{R}_+, \\ u(\cdot,0) &= f, && \text{in } \Omega. \end{aligned}$$

$u(\cdot,t)$: heat distribution at time $t > 0$, f initial condition, and boundary condition: no heat flowing out of the domain.

- **Forward problem**: determine the terminal data $u(\cdot,T) \in L^2(\Omega)$, for $T > 0$, given the data $f \in L^2(\Omega)$
- **Inverse problem**: determine the initial data $f \in L^2(\Omega)$, given the (noisy) terminal data $u(\cdot,T) =: w \in L^2(\Omega)$

direct problem

separation of variables technique via Sturm-Liouville problem

$$\begin{cases} -\varphi'' = \lambda\varphi, & \text{in } \Omega, \\ \qquad \varphi'(0) = \varphi'(1) = 0. \end{cases}$$

eigenvalues and eigenfunctions

$$\lambda_n = (n\pi)^2$$
$$\varphi_n = c_i \cos(n\pi x), \quad c_0 = 1, c_1 = \sqrt{2}.$$

$(\varphi_n)_{n=0}^{\infty}$: complete orthonormal basis of $L^2(\Omega)$

let $u(x,t) = \sum_{n=0}^{\infty} u_n(t)\varphi_n(x)$, and then taking inner product with φ_n

$$u_n'(t) = -\lambda_n u_n(t), \quad t > 0, \quad \text{with } u_n(0) = (f, \varphi_n)$$

$\Rightarrow u_n = (f, \varphi_n)e^{-\lambda_n t}$ with $\lambda_n = n^2\pi^2$

solution to direct problem

$$u(x,t) = \sum_{n=0}^{\infty} f_n e^{-\lambda_n t}\varphi_n,$$

with $(f_n)_{n=0}^{\infty} \subset \mathbb{R}$: Fourier cosine coefficients of the initial data f.

$$f = \sum_{n=0}^{\infty} f_n\varphi_n \quad \text{with } f_n = (f, \varphi_n)_{L^2(\Omega)}$$

well-posedness of direct problem

The forward map: $F : f \mapsto u(\cdot, T)$, $L^2(\Omega) \to L^2(\Omega)$ satisfies

- F is linear, bounded, compact
- F is injective, i.e., $\ker(F) = \{0\}$
- $\mathrm{range}(F)$ is dense in $L^2(\Omega)$

backward heat

Solving the inverse problem for heat equation with $w \in L^2(\Omega)$ is to invert the compact operator $F : L^2(\Omega) \to L^2(\Omega)$, *obviously impossible*! (Fact: compact operators in infinite-dim. spaces are not invertible)

The unbounded operator:

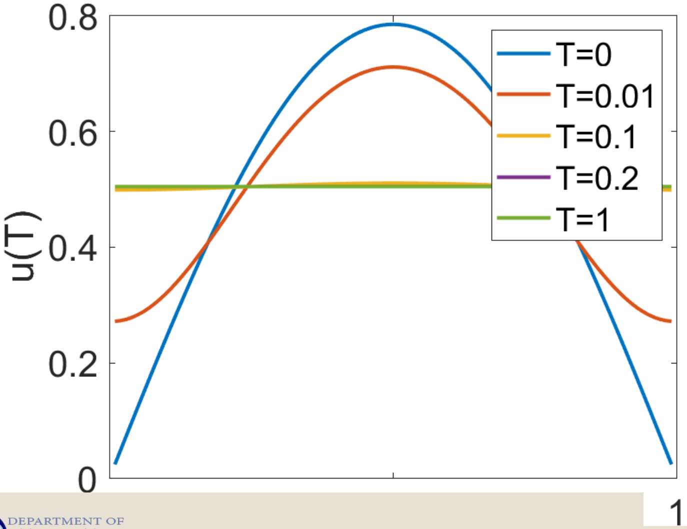
$$F^{-1} : \mathrm{range}(F) \to L^2(\Omega)$$

is well defined, i.e. for exact data, the problem has a unique solution.

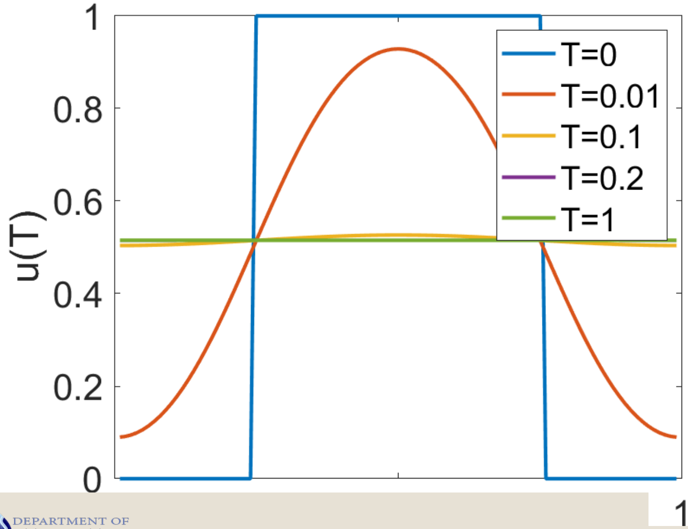
main message:

- if $w \in \mathrm{range}(F)$: Hadamard condition (iii) is not satisfied
- if $w \notin \mathrm{range}(F)$: none of Hadamard conditions holds

heat conduction at $t = 0.01, 0.1, 0.2, 1$



heat conduction at $t = 0.01, 0.1, 0.2, 1$



Question: Should one ignore the ill-posed inverse problems

Answer: No! The available measurement always contain some information about f!

1 Ill-posed problems: examples

2 Classical regularization methods
- Mathematical setting

Hilbert space

A vector space H is a real inner product space if there exists a mapping $(\cdot, \cdot) : H \times H \to \mathbb{R}$ satisfying

1. $(x, y) = (y, x)$ for all $x, y \in H$
2. $(ax_1 + bx_2, y) = a(x_1, y) + b(x_2, y)$ for all $x_1, x_2, y \in H$, $a, b \in \mathbb{R}$
3. $(x, x) \geq 0$ and $(x, x) = 0$ iff $x = 0$

H is real Hilbert space if, in addition,

- H is complete with respect to the induced norm
- there exists a countable orthonormal basis $(\varphi_n)_n$ of H w.r.t. the inner product

$$(\varphi_j, \varphi_k) = \delta_{jk} \quad \text{and} \quad x = \sum_n (x, \varphi_n)\varphi_n, \quad \forall x \in H$$

Fredholm equation

model problem: find $x \in X$ s.t.

$$Ax = y,$$

- $A : X \to Y$ a linear compact operator:
  bounded set in $X \to$ relatively compact set in Y
  limits of operators of finite rank
- $y \in Y$: given data, often contains noise

Examples

- backward heat problem: $F = F$, $X = Y = L^2(\Omega)$
- Euclidean case: $X = \mathbb{R}^n$, $Y = \mathbb{R}^m$ and $A \in \mathbb{R}^{m \times n}$

Let $A^* : Y \to X$ be the adjoint operator of $A : X \to Y$ s.t.

$$(Ax, y) = (x, A^* y) \quad \forall x \in X, y \in Y$$

orthogonal decompositions

$$X = \ker(A) \oplus (\ker(A))^\perp = \ker(A) \oplus \overline{\mathrm{range}(A^*)}$$
$$Y = \overline{\mathrm{range}(A)} \oplus (\mathrm{range}(A))^\perp = \overline{\mathrm{range}(A)} \oplus \ker(A^*)$$

where ”bar” denotes the closure of a set and

$$\ker(A) = \{x \in X : Ax = 0\}$$
$$\mathrm{range}(A) = \{y \in Y : y = Ax, \exists x \in X\}$$
$$(\mathrm{Ker}(A))^\perp = \{x \in X : (x, z) = 0, \quad \forall z \in \ker(A)\}$$

singular system

characterization of compact operators: There exists a set of (possibly countably infinite) vectors $(v_n)_n \subset X$ and $(u_n)_n \in Y$ and a sequence of positive numbers $(s_n)_n$, ordered nonincreasingly and $\lim_{n\to\infty} s_n = 0$ (if the rank is not finite) such that

$$Ax = \sum_n s_n(x, v_n)u_n, \quad \forall x \in X$$

or

$$Av_n = s_n u_n, \quad n = 1, \ldots$$

and

$$\overline{\mathrm{range}(A)} = \overline{\mathrm{span}(u_n)}, \quad (\ker(A))^{\perp} = \overline{\mathrm{span}(v_n)}$$

The system $(s_n, u_n, v_n)_n$ is called a singular system of A, and the expansion is called the singular value decomposition (SVD) of A.

Solvability

By the orthonormality of (u_n),

$$P : Y \to \overline{\mathrm{range}(A)}, \quad y \to \sum_n (y, u_n) u_n$$

is an orthogonal projection

$$P^2 = P \quad \text{and} \quad \mathrm{range}(P) \perp \mathrm{range}(I - P)$$

Picard's criterion 1909

The equation $Ax = y$ has a solution iff

$$y = Py \quad \text{and} \quad \sum_n s_n^{-2} |(y, u_n)|^2 < \infty$$

Under this condition, all solutions of $Ax = y$ are of the form

$$x = x_0 + \sum_n s_n^{-1} (y, u_n) v_n$$

for some $x_0 \in \ker(A)$

This criterion underpins many methods: MUSIC, ...

interpretation of the conditions

- The first condition $y = Py$ states that y cannot have components in the orthogonal complement of $\mathrm{range}(A)$, if $Ax = y$
- The second condition, i.e., the convergence of the series

$$\sum_n s_n^{-2} |(y, u_n)|^2$$

is redundant if $\mathrm{rank}(A) < \infty$, in which ase $\overline{\mathrm{range}(A)} = \mathrm{range}(A)$. Meanwhile, if $\mathrm{rank}(A) = \infty$, it is equivalent to the finiteness of the norm of

$$x = x_0 + \sum_n s_n^{-1} (y, u_n) v_n$$

i.e., the potential solutions belong to X

- One natural way to circumvent problems with the first condition is to consider the projected equation

$$Ax = PAx = Py$$

instead of $Ax = y$. However, this does not help with the second condition since there is no gurantee that

$$\sum_n s_n^{-2}(Py, u_n)^2 < \infty$$

for a general $y \in Y$, if $\mathrm{rank}(A) = \infty$