Inverse Problems

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- Numerical example: X-ray tomography
- Regularization by truncated iterative methods: Landweber–Fridman iteration

As an application, we consider X-ray tomography and describe here the construction of the tomography matrix. We will return to this example throughout our treatment of truncated iterative methods.

The following content follows roughly the material presented in the following monographs.

- J. Kaipio and E. Somersalo. Statistical and Computational Inverse Problems. 2005.
- J. L. Mueller and S. Siltanen. Linear and Nonlinear Inverse Problems with Practical Applications. 2012.

ASTRA Toolbox for 2D and 3D tomography:

https://www.astra-toolbox.com/













Radon transform in \mathbb{R}^2

Let *L* be a straight line in \mathbb{R}^2 .

Any line in \mathbb{R}^2 can be parameterized as

$$L = \{ s\omega + t\omega^{\perp}; t \in \mathbb{R} \}$$
 for some $s \in \mathbb{R}$ and $\omega \in S^1$,

where $\omega^{\perp} \perp \omega$.



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Writing
$$\omega = \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix}$$
, we get
 $L = L(s, \theta) = \left\{ s \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix} + t \begin{bmatrix} \sin \theta \\ -\cos \theta \end{bmatrix}; \ t \in \mathbb{R} \right\}, \quad s \in \mathbb{R} \text{ and } \theta \in [0, \pi).$

The Radon transform of a continuous function $f: \mathbb{R}^2 \to \mathbb{R}$ on L is defined as

$$\mathcal{R}f(L) = \int_{L} f(\mathbf{x}) |\mathrm{d}\mathbf{x}| = \int_{-\infty}^{\infty} f(s\cos\theta + t\sin\theta, s\sin\theta - t\cos\theta) \,\mathrm{d}t.$$

Let f be a nonnegative function modeling X-ray attenuation (density) inside a physical body.

Beer-Lambert law:

$$\mathcal{R}f(L) = \log \frac{I_0}{I_1}.$$

$f_{10,1}$	$f_{10,2}$	$f_{10,3}$	$f_{10,4}$	$f_{10,5}$	$f_{10,6}$	$f_{10,7}$	$f_{10,8}$	$f_{10,9}$	$f_{10,10}$
$f_{9,1}$	$f_{9,2}$	$f_{9,3}$	$f_{9,4}$	$f_{9,5}$	$f_{9,6}$	$f_{9,7}$	$f_{9,8}$	$f_{9,9}$	$f_{9,10}$
$f_{8,1}$	$f_{8,2}$	$f_{8,3}$	$f_{8,4}$	$f_{8,5}$	$f_{8,6}$	$f_{8,7}$	$f_{8,8}$	$f_{8,9}$	$f_{8,10}$
$f_{7,1}$	$f_{7,2}$	$f_{7,3}$	$f_{7,4}$	$f_{7,5}$	$f_{7,6}$	$f_{7,7}$	$f_{7,8}$	$f_{7,9}$	$f_{7,10}$
$f_{6,1}$	$f_{6,2}$	$f_{6,3}$	$f_{6,4}$	$f_{6,5}$	$f_{6,6}$	$f_{6,7}$	$f_{6,8}$	$f_{6,9}$	$f_{6,10}$
$f_{5,1}$	$f_{5,2}$	$f_{5,3}$	$f_{5,4}$	$f_{5,5}$	$f_{5,6}$	$f_{5,7}$	$f_{5,8}$	$f_{5,9}$	$f_{5,10}$
$f_{4,1}$	$f_{4,2}$	$f_{4,3}$	$f_{4,4}$	$f_{4,5}$	$f_{4,6}$	$f_{4,7}$	$f_{4,8}$	$f_{4,9}$	$f_{4,10}$
$f_{3,1}$	$f_{3,2}$	$f_{3,3}$	$f_{3,4}$	$f_{3,5}$	$f_{3,6}$	$f_{3,7}$	$f_{3,8}$	$f_{3,9}$	$f_{3,10}$
$f_{2,1}$	$f_{2,2}$	$f_{2,3}$	$f_{2,4}$	$f_{2,5}$	$f_{2,6}$	$f_{2,7}$	$f_{2,8}$	$f_{2,9}$	$f_{2,10}$
$f_{1,1}$	$f_{1,2}$	$f_{1,3}$	$f_{1,4}$	$f_{1,5}$	$f_{1,6}$	$f_{1,7}$	$f_{1,8}$	$f_{1,9}$	$f_{1,10}$

Let us consider the computational domain $[-1, 1]^2$. We divide this region into $n \times n$ pixels and approximate the density by a piecewise constant function with constant value

$$f_{i,j}$$
 in pixel $P_{i,j}$

for
$$i, j \in \{1, ..., n\}$$
.

 $P_{i,j} := \{(x,y); \ -1 + 2\frac{j-1}{n} < x < -1 + 2\frac{j}{n}, \ -1 + 2\frac{j-1}{n} < y < -1 + 2\frac{j}{n}\}$

x_{91}	x_{92}	<i>x</i> ₉₃	x_{94}	x_{95}	x_{96}	x_{97}	<i>x</i> ₉₈	<i>x</i> ₉₉	x_{100}
x_{81}	x_{82}	x_{83}	x_{84}	x_{85}	x_{86}	<i>x</i> ₈₇	x_{88}	<i>x</i> ₈₉	x_{90}
x_{71}	x_{72}	<i>x</i> ₇₃	<i>x</i> ₇₄	x_{75}	x_{76}	<i>x</i> ₇₇	x_{78}	<i>x</i> ₇₉	x_{80}
x_{61}	x_{62}	x_{63}	x_{64}	x_{65}	x_{66}	x_{67}	x_{68}	x_{69}	x_{70}
x_{51}	x_{52}	x_{53}	x_{54}	x_{55}	x_{56}	x_{57}	x_{58}	x_{59}	x_{60}
x_{41}	x_{42}	x_{43}	x_{44}	x_{45}	x_{46}	<i>x</i> ₄₇	x_{48}	<i>x</i> ₄₉	x_{50}
x_{31}	x_{32}	<i>x</i> ₃₃	x_{34}	x_{35}	x_{36}	x_{37}	<i>x</i> ₃₈	<i>x</i> ₃₉	x_{40}
x_{21}	x_{22}	x_{23}	x_{24}	x_{25}	x_{26}	x_{27}	x_{28}	x_{29}	x_{30}
x_{11}	x_{12}	x_{13}	x_{14}	x_{15}	x_{16}	x_{17}	x_{18}	x_{19}	x_{20}
x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}

It is convenient to reshape the matrix/image $(f_{i,j})$ into a vector x of length n^2 so that

$$x_{(j-1)n+i} = f_{i,j}, \quad i,j \in \{1,\ldots,n\}.$$

The image on the left illustrates the new numbering corresponding to the pixels.

Note that x = f(:) and f = reshape(x,n,n).

Measurement model

Let us consider a measurement setup where we take X-ray measurements of an object using X-rays $L(s_1, \theta), \ldots, L(s_K, \theta)$ taken at angles $\theta \in \{\theta_1, \ldots, \theta_M\}$. The total number of X-rays is Q = MK.

For brevity, let us write $L_{(m-1)K+k} := L(s_k, \theta_m)$ for $k \in \{1, \dots, K\}$ and $m \in \{1, \dots, M\}$.

The measurement model is

$$y = \begin{bmatrix} \int_{L_1} f(\mathbf{x}) |\mathrm{d}\mathbf{x}| \\ \vdots \\ \int_{L_Q} f(\mathbf{x}) |\mathrm{d}\mathbf{x}| \end{bmatrix} + \varepsilon \approx \begin{bmatrix} \sum_{j=1}^{n^2} A_{1,j} x_j \\ \vdots \\ \sum_{j=1}^{n^2} A_{Q,j} x_j \end{bmatrix} + \varepsilon = Ax + \varepsilon,$$

where $A \in \mathbb{R}^{Q \times n^2}$ and $A_{i,j}$ is the distance that ray L_i travels through pixel j. Here, x is a vector containing the (piecewise constant) densities within each pixel and ε is measurement noise.

$$L_{(m-1)K+k} = \left\{ s_k \begin{bmatrix} \cos \theta_m \\ \sin \theta_m \end{bmatrix} + t \begin{bmatrix} \sin \theta_m \\ -\cos \theta_m \end{bmatrix}; \ t \in \mathbb{R} \right\}, \quad \substack{k = 1, \dots, K, \\ m = 1, \dots, M.}$$

$$\theta = 0, \qquad \theta = 0.349066 \qquad \theta = 0.698132$$

$$\theta = 1.0472 \qquad \theta = 1.39626 \qquad \theta = 1.74533$$

$$\theta = 1.74533 \qquad \theta = 1.74533$$

$$\theta = 2.0944 \qquad \theta = 2.44346 \qquad \theta = 2.79253$$

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Pixel-by-pixel construction of the tomography matrix A (See the tomodemo.m file on the course page!)

$$A_{m,k} = \int_{L_m} \chi_k \left| \mathrm{d} \mathbf{x} \right| = \int_{\substack{x_\mathrm{d} < t \le x_\mathrm{u} \\ y_\mathrm{d} \le \mathbf{s} < y_\mathrm{u}}} \mathrm{d} t = \begin{cases} x_\mathrm{u} - x_\mathrm{d} & \text{if } y_\mathrm{d} \le \mathbf{s} < y_\mathrm{u}, \\ 0 & \text{otherwise.} \end{cases}$$

N.B. In here and in the following, $\chi_k = \chi_k(\mathbf{x})$ denotes the characteristic function of the k^{th} pixel. In the above illustration, the pixel is denoted by the rectangle $[x_d, x_u) \times [y_d, y_u)$.

$$A_{m,k} = \int_{L_m} \chi_k \left| \mathrm{d} \mathbf{x} \right| = \int_{\substack{-y_u < t \le -y_d \\ x_d < \mathbf{s} \le x_u}} \mathrm{d} t = \begin{cases} y_u - y_d & \text{if } x_d < \mathbf{s} \le x_u, \\ 0 & \text{otherwise.} \end{cases}$$

Discussion

Tomography problems can be classified into three classes based on the nature of the measurement data:

- Full angle tomography
 - Sufficient number of measurements from all angles \rightarrow not a very ill-posed problem.
- Limited angle tomography
 - Data collected from a restricted angle of view \rightarrow reconstructions very sensitive to measurement error and it is not possible to reconstruct the object perfectly (even with noiseless data). Applications include, e.g., dental imaging.
- Sparse data tomography
 - The data consist of only a few projection images, possibly from any direction \rightarrow extremely ill-posed inverse problem and prior knowledge necessary for successful reconstructions. (E.g., minimizing a patient's radiation dose.)

Regularization by truncated iterative methods

For simplicity, we will only consider the case when

$$Ax = y \tag{1}$$

is a system of linear equations, i.e., $A \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^n$, and $y \in \mathbb{R}^m$.

- Iterative methods attempt to solve (1) by finding successive approximations for the solution starting from some initial guess.
- Typically, the computation of such iterations involves multiplications by *A* and its adjoint, but not explicit computation of inverse operators. (Direct methods, such as *Gaussian elimination*, produce a solution in a finite number of steps.)
- Iterative methods are sometimes the only feasible choice if the problem involves a large number of variables (e.g., in the order of millions), in which case direct methods are prohibitively expensive. Iterations are especially useful if multiplications by *A* are cheap: for example, if *A* is sparse or it contains some other structure (e.g., it is a multi-diagonal matrix arising from finite difference or finite element approximation of an elliptic PDE).

Although iterative solvers have not usually been designed for ill-posed equations, they often possess regularizing properties. If the iterations are terminated before "the solution starts to fit to noise", one often obtains reasonable solutions for inverse problems.

Banach fixed point iteration

Let *H* be a Hilbert space and $S \subset H$. Consider a mapping, not necessarily linear, $T: H \to H$. We say that *S* is an *invariant set* for *T* if $T(S) \subset S$, that is,

$$T(x) \in S$$
 for all $x \in S$.

Moreover, T is a *contraction* on an invariant set S if there exists $0 \le \kappa < 1$ such that

$$\|T(x) - T(y)\| < \kappa \|x - y\|$$
 for all $x, y \in S$.

Finally, a vector $x \in H$ is called a *fixed point* of T if

$$T(x) = x.$$

Theorem (Banach fixed point theorem)

Let H be a Hilbert space and $S \subset H$ a closed invariant set for the mapping $T: H \rightarrow H$. Assume further that T is a contraction in S. Then there exists a unique fixed point $x \in S$ such that T(x) = x. Furthermore, this fixed point can be found by the fixed point iteration

$$x = \lim_{k \to \infty} x_k$$
, where $x_{k+1} = T(x_k)$,

for any $x_0 \in S$.

Proof. Let $T: H \to H$ be a mapping, $S \subset H$ a closed invariant set such that $T(S) \subset S$, and let T be a contraction in S,

$$\|T(x) - T(y)\| < \kappa \|x - y\|$$
 for all $x, y \in S$,

with $\kappa < 1$. For all j > 1, we have

$$||x_{j+1} - x_j|| = ||T(x_j) - T(x_{j-1})|| < \kappa ||x_j - x_{j-1}||.$$

Inductively, it follows that

$$||x_{j+1}-x_j|| < \kappa^{j-1} ||x_2-x_1||.$$

For any $n, k \in \mathbb{N}$, we have

$$\begin{aligned} \|x_{n+k} - x_n\| &\leq \sum_{j=1}^k \|x_{n+j} - x_{n+j-1}\| < \sum_{j=1}^k \kappa^{n+j-2} \|x_2 - x_1\| \\ &\leq \frac{\kappa^{n-1}}{1-\kappa} \|x_2 - x_1\|, \end{aligned}$$

where we used the formula for the geometric series. Therefore (x_j) is a Cauchy sequence[†], and thus convergent (since *H* is a Hilbert space and thus complete). The limit is in *S* since *S* is closed.

[†]Recall that $(x_n)_{n\in\mathbb{N}}$ is a Cauchy sequence if for every $\varepsilon > 0$, there is an index $m \in \mathbb{N}$ such that $k, j \ge m \Rightarrow ||x_k - x_j|| < \varepsilon$.

Landweber–Fridman iteration

Instead of considering the original equation

$$Ax = y$$
,

let us consider the normal equation

$$A^{\mathrm{T}}Ax = A^{\mathrm{T}}y.$$

Recall that $x \in \mathbb{R}^n$ satisfies the normal equation iff it minimizes the residual

$$\|Ax - y\|.$$

Moreover, there exists a unique element of \mathbb{R}^n , given by $x^{\dagger} := A^{\dagger}y$, which satisfies the normal equation and $x^{\dagger} \in \text{Ker}(A)^{\perp}$ (the minimum norm solution).

Let us define the affine mapping $T: \mathbb{R}^n \to \mathbb{R}^n$ by

$$T(x) = x + \beta (A^{\mathrm{T}}y - A^{\mathrm{T}}Ax), \quad \beta \in \mathbb{R}.$$

Note that any solution of the normal equation $A^{T}Ax = A^{T}y$ is a fixed point of T.

If β is small enough, then there is only one fixed point of T in Ker(A)^{\perp}, precisely x^{\dagger} , and it can be reached by the fixed point iteration if $x_0 = 0$.

Theorem

Let λ_1 be the largest singular value of matrix A and let $0 < \beta < 2/\lambda_1^2$ be fixed. Then the fixed point iteration

$$x_{k+1}=T(x_k), \quad x_0=0,$$

converges toward x^{\dagger} as $k \to \infty$.

Proof. Let $S := \operatorname{Ker}(A)^{\perp} = \operatorname{Ran}(A^{\mathrm{T}})$. Clearly $T(S) \subset S$ since $T(x) = x + A^{\mathrm{T}}(\beta y - \beta A x) \in \operatorname{Ran}(A^{\mathrm{T}})$

for all $x \in \text{Ran}(A^{T})$. Thus S is invariant under T.

Recall that A and its transpose can be written using the SVD of A as

$$Ax = \sum_{j=1}^{p} \lambda_j (v_j^{\mathrm{T}} x) u_j$$
 and $A^{\mathrm{T}} y = \sum_{j=1}^{p} \lambda_j (u_j^{\mathrm{T}} y) v_j$,

where $p = \operatorname{rank}(A)$ and λ_j are the positive singular values of A. The singular vectors $\{v_j\}_{j=1}^p$ and $\{u_j\}_{j=1}^p$ span $S = \operatorname{Ker}(A)^{\perp}$ and $\operatorname{Ran}(A)$, respectively, and thus

$$x = \sum_{j=1}^p (v_j^{\mathrm{T}} x) v_j \quad ext{for all } x \in \mathcal{S}.$$

Let $x, z \in S$. Then $x - z \in S$ and

$$T(x) - T(z) = (x - z) - \beta A^{\mathrm{T}} A(x - z)$$

= $\sum_{j=1}^{p} v_{j}^{\mathrm{T}}(x - z)v_{j} - \beta \sum_{j=1}^{p} \lambda_{j}^{2}(v_{j}^{\mathrm{T}}(x - z))v_{j}$
= $\sum_{j=1}^{p} (1 - \beta \lambda_{j}^{2})(v_{j}^{\mathrm{T}}(x - z))v_{j}.$

Since λ_1 is the largest singular value, it follows that

$$-1 < eta \lambda_j^2 - 1 \leq eta \lambda_1^2 - 1 < 2-1 = 1 \quad ext{for all } j \in \{1,\dots,p\}.$$

Hence

$$\kappa := \max_{j=1,\ldots,p} |\beta \lambda_j^2 - 1| < 1.$$

In consequence,

$$egin{aligned} \| extsf{T}(x) - extsf{T}(y) \|^2 &\leq \sum_{j=1}^p (1 - eta \lambda_j^2)^2 (v_j^{ extsf{T}}(x-z))^2 \ &\leq \kappa^2 \sum_{j=1}^p (v_j^{ extsf{T}}(x-z))^2 = \kappa^2 \|x-z\|^2, \end{aligned}$$

which shows that T is a contraction on S. Since S is a closed invariant set for T, there exists a unique fixed point of T in S.

Finally, recall that $x^{\dagger} = A^{\dagger}y$ belongs to $S = \text{Ker}(A)^{\perp}$ and it satisfies the normal equation. Since $x_0 = 0$ is in S (it is orthogonal to all vectors), the fixed point iteration starting from x_0 converges to x^{\dagger} .

Regularization properties of Landweber-Fridman

In what follows, we will assume that 0 $<\beta<2/\lambda_1^2.$

In the exercises of week 3, it will be shown that the k^{th} iterate of the Landweber–Fridman iteration can be written explicitly as

$$x_k = \sum_{j=1}^p \frac{1}{\lambda_j} (1 - (1 - \beta \lambda_j^2)^k) (u_j^{\mathrm{T}} y) v_j, \quad k = 0, 1, \dots$$

Since we assumed $|1-eta\lambda_j^2|<1$, then

$$(1-\beta\lambda_j^2)^k \xrightarrow{k\to\infty} 0.$$

This is what one would expect since

$$x^{\dagger} = \sum_{j=1}^{p} \frac{1}{\lambda_j} (u_j^{\mathrm{T}} y) v_j.$$

While $k \in \mathbb{N}$ is finite, the coefficients appearing in the series representation

$$x_{k} = \sum_{j=1}^{p} \frac{1}{\lambda_{j}} (1 - (1 - \beta \lambda_{j}^{2})^{k}) (u_{j}^{\mathrm{T}} y) v_{j}$$
(2)

satisfy

$$\begin{split} &\frac{1}{\lambda_j} (1 - (1 - \beta \lambda_j^2)^k) = \frac{1}{\lambda_j} \left(1 - \sum_{\ell=0}^k \binom{k}{\ell} (-1)^\ell \beta^\ell \lambda_j^{2\ell} \right) \\ &= \frac{1}{\lambda_j} \sum_{\ell=1}^k \binom{k}{\ell} (-1)^{\ell+1} \beta^\ell \lambda_j^{2\ell} = \sum_{\ell=1}^k \binom{k}{\ell} (-1)^{\ell+1} \beta^\ell \lambda_j^{2\ell-1}, \end{split}$$

which converges to zero as $\lambda_i \rightarrow 0$ (for a fixed k).

In consequence, while k is "small enough", no coefficient of $(u_j^T y)v_j$ in (2) is so large that the component of the measurement noise in the direction u_j is amplified in an uncontrolled manner. (Compare with Tikhonov regularization, where the corresponding coefficients are $\lambda_j/(\lambda_i^2 + \delta)$.)

Let $y \in \mathbb{R}^m$ be a noisy version of some underlying "exact" data vector $y_0 \in \mathbb{R}^m$, and assume that

$$\|y-y_0\|\approx \varepsilon>0.$$

The Morozov discrepancy principle for the Landweber–Fridman iteration is analogous to the truncated SVD: choose the smallest $k \ge 0$ such that the residual satisfies

$$\|y - Ax_k\| \leq \varepsilon.$$

Q: When does an index $k \ge 1$ satisfying $||y - Ax_k|| \le \varepsilon$ exist? **A**: When $\varepsilon > ||Py - y|| = ||y - A(A^{\dagger}y)|| = ||y - Ax^{\dagger}||$, where $P = AA^{\dagger}$ is the orthogonal projection onto $\operatorname{Ran}(A)$ (cf. 1st exercises) and $x^{\dagger} = A^{\dagger}y$ is the minimum norm solution. Since the sequence $(x_k)_{k=0}^{\infty}$ converges to x^{\dagger} , for any $\varepsilon > ||y - Ax^{\dagger}||$, there exists $k = k_{\varepsilon} \in \mathbb{N}$ such that

$$\|x_k - x^{\dagger}\| \leq \frac{1}{\|A\|} (\varepsilon - \|y - Ax^{\dagger}\|).$$

By the reverse triangle inequality

$$\begin{split} \|y - Ax_k\| - \|y - Ax^{\dagger}\| &\leq \|(y - Ax_k) - (y - Ax^{\dagger})\| \\ &\leq \|A\| \|x_k - x^{\dagger}\| \\ &\leq \varepsilon - \|y - Ax^{\dagger}\|. \end{split}$$

From this, we deduce that $||y - Ax_k|| \le \varepsilon$ as desired.