Inverse Problems

*Do the Impossible – Solve the Impossible*

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What it’s like to do research

Heian Shrine, Kyoto
About Me ...

- Numerical analysis & inverse problems – regularization algorithms, matrix computations, image deblurring, signal processing, Matlab software, ...

- Head of the Villum Investigator project
  Computational Uncertainty Quantification for Inverse Problems.  
  
- Author of several Matlab software packages.

- Author of four books (one more underway).
What is an Inverse Problem?

In a forward problem, we use a mathematical model to compute the output from a “system” given the input.

In an inverse problem we estimate a quantity that is not directly observable, using indirect measurements and the forward model.

Some examples on the next pages.
Example: Tomography

Image reconstruction from projections.

Required in the math. model:
- Physics of X-ray attenuation.
- Strength of the X-ray source.
- Specification of the geometry.

Medical imaging

Materials science

100 µm
Example: Rotational Image Deblurring

Application: “star camera” used in satellite navigation.

Required in the math. model
- Center of rotation.
- Rotation angle.
Inverse Problem and Mathematics

Inverse problems
- arise when we use a mathematical model $\mathcal{K}$
- to infer about internal or hidden features $f$
- from external and/or indirect measurements $g$.

Why mathematics is important
- A solid foundation for formulation of inverse problems.
- A framework for developing computational algorithms.
- A “language” for defining and expressing the properties of the solutions: existence, uniqueness, stability, reliability, ...
Some Formulations

Mathematical formulations of inverse problems take different forms.

Fredholm integral equation of the first kind:

\[
\int_0^1 K(s, t) f(t) \, dt = g(s) , \quad 0 \leq s \leq 1 .
\]

Calderón problem (PDE with Dirichlet BC):

\[
\begin{cases}
\nabla \cdot \sigma \nabla u = 0 & u \in \Omega \\
\quad u = f & u \in \partial \Omega
\end{cases}
\]

Fascinating: very different applications of inverse problems lead to the same formulations.
A Few Simple Examples

\[ \int K(s,t) f(t) \, dt = \frac{1}{6} (s^3 - s) , \quad K(s,t) = \begin{cases} s(t-1), & s < t \\ t(s-1), & s \geq t \end{cases} \]

The solution is the second derivative, so \( f(t) = t \).

\[ \int_{0}^{2\pi} K(s-t) f(t) \, dt = g(s) , \quad f, g, K \text{ are } 2\pi \text{-periodic.} \]

This is deconvolution; the solution is formally given by

\[ f(t) = \mathcal{F}^{-1} \left( \mathcal{F}(g) / \mathcal{F}(k) \right) , \quad \mathcal{F} = \text{Fourier transform}. \]

\[ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \delta(x \cos \theta + y \sin \theta - s) f(x,y) \, dx \, dy = g(s, \theta) \]

\[ s \in [0, 1] , \quad \theta \in [0, 2\pi) . \]

This is the Radon transform underlying X-ray CT.
Eigenvalue Analysis for Symmetric Kernel

\[ \int_{0}^{1} K(s, t) f(t) \, dt = g(s) = 1 \ , \quad 0 \leq s \leq 1 . \]

A symmetric kernel \( K(s, t) = K(t, s) \) has a real eigensystem,

\[ \int_{0}^{1} K(s, t) v_i(t) \, dt = \lambda_i \, v_i(s) \ , \quad i = 1, 2, 3, \ldots \]

Then we can write the solution as

\[ f(t) = \sum_{i=1}^{\infty} \frac{\langle v_i, g \rangle}{\lambda_i} \, v_i(t) \ , \quad \langle v_i, g \rangle = \int_{0}^{1} v_i(s) \, g(s) \, ds . \]

This is very useful for analysis of inverse problems (but no so much for numerical computations).
A Tricky Example ...

\[ \int_0^1 \frac{1}{s + t + 1} f(t) \, dt = g(s) = 1, \quad 0 \leq s \leq 1. \]

Can you guess a solution?

Eigenvalues and eigenfunctions:
... With No Solution

Let us compute finite approximations to the solution:

\[ f_k(t) \equiv \sum_{i=1}^{k} \frac{\langle v_i, g \rangle}{\lambda_i} v_i(t), \quad i = 1, 2, 3, \ldots \]

The amplitude of \( f_k(t) \) becomes disturbingly large as \( k \) increases, and the sum does not converge as \( k \to \infty \).
Inverse Problems Are Ill Posed

Hadamard’s definition of a well-posed problem (early 20th century)

1. Existence: the problem must have a solution.
2. Uniqueness: the solution must be unique.
3. Stability: it must depend continuously on data and parameters.

If the problem violates any of these requirements, it is ill posed.

Inverse problems are, by nature, always ill posed.

And yet, we have a strong desire – and a need – to solve them …
Hadamard 1 (existence) and 2 (uniqueness)

Case 1

\[ Ax = b \iff \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 2.1 \\ 3.0 \\ 3.9 \end{pmatrix} \]

There is no \( x \) that satisfies this equation, but we can define the least squares solution that minimizes the residual norm

\[ x_{\text{LS}} \equiv \arg\min_x \| Ax - b \|_2 = \begin{pmatrix} 1.2 \\ 0.9 \end{pmatrix} \]

Case 2

\[ Ax = b \iff \begin{pmatrix} 1 & 2 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 3 \\ 3 \end{pmatrix} . \]

There are infinitely many \( x \) that satisfy this equation; we can define the unique minimum-norm solution that minimizes the solution’s norm

\[ x_0 \equiv \arg\min_x \| x \|_2 \quad \text{s.t.} \quad Ax = b \quad \Rightarrow \quad x_0 = \begin{pmatrix} 0.6 \\ 1.2 \end{pmatrix} . \]
Hadamard 3 (stability)

Unperturbed system:

\[ A = \begin{pmatrix} 1.0 & 2.1 & 3.0 \\ 4.0 & 5.0 & 5.9 \\ 7.0 & 8.0 & 9.0 \end{pmatrix}, \quad x = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad b = Ax = \begin{pmatrix} 6.1 \\ 14.9 \\ 24.0 \end{pmatrix}. \]

Perturbed system:

\[ \tilde{b} = b + \begin{pmatrix} 0 \\ 0.001 \\ 0 \end{pmatrix} \quad \Rightarrow \quad \tilde{x} = A^{-1}\tilde{b} = \begin{pmatrix} 0.927 \\ 1.171 \\ 0.904 \end{pmatrix}. \]

The matrix \( A \) is ill conditioned, \( \text{cond}(A) = 4249 \), and therefore the solution is very sensitive to perturbations of \( b \) and \( A \):

\[
\frac{\|\Delta x\|}{\|x\|} \leq \text{cond}(A) \left( \frac{\|\Delta b\|}{\|b\|} + \frac{\|\Delta A\|}{\|A\|} \right).
\]
Eigenvalue Analysis for Symmetric Kernel

Recall that we can write the solution as

\[ f(t) = \sum_{i=1}^{\infty} \frac{\langle v_i, g \rangle}{\lambda_i} v_i(t), \quad \langle v_i, g \rangle = \int_0^1 v_i(s) g(s) \, ds. \]

Picard condition for a square integrable solution:

\[ \|f\|_2^2 = \sum_{i=1}^{\infty} \left( \frac{\langle v_i, g \rangle}{\lambda_i} \right)^2 < \infty. \]

The enumerator must decay sufficiently faster than the denominator.

Specifically, the coefficients \( \langle v_i, g \rangle \) must decay faster than \( \lambda_i \, i^{-1/2} \).
Eigenvalue Analysis for Symmetric Kernel

Recall: the coefficients $\langle v_i, g \rangle$ must decay faster than $\lambda_i i^{-1/2}$.

Test problem – gravity from Regularization Tools (Hansen, 2007):

With no noise in the data, the Picard condition is satisfied.

When noise is present, the Picard condition is not satisfied. The solution coefficients diverge.
Dealing with the Instability $\rightarrow$ Regularization

The ill conditioning of the problem makes it impossible to compute a “naive” solution to the inverse problem:

$$K f = g \quad \rightarrow \quad f_{\text{naive}} = K^{-1}g$$

$\rightarrow$ Incorporate prior information about the solution via regularization:

$$\min_f \left\{ \| K f - g \|_2^2 + \alpha R(f) \right\}, \quad R(f) = \text{regularizer}$$
Eigenvalue Analysis of Tikhonov Regularizer

The important special case of Tikhonov regularization

\[ R(f) = \|f\|_2^2 \quad \Rightarrow \quad f(t) = \sum_{i=1}^{\infty} \frac{\lambda^2}{\lambda^2 + \alpha} \frac{\langle v_i, g \rangle}{\lambda_i} v_i(t). \]

Here \( \phi_i = \frac{\lambda^2}{\lambda^2 + \alpha} \) are the filter factors.

These modified coefficients satisfy the Picard condition. Stabilization accomplished!
Case: Total Variation (TV)

Prior: image consists of regions with constant intensity and sharp edges. How to say this *in mathematical terms?*

Total variation regularization term $R(f) = \int_\Omega \| \nabla f \|_2 \, d\Omega \rightarrow$

$$R(x) = \sum_{\text{pixels}} \| D_i x \|_2, \quad D_i x = \text{gradient}$$
Case: Directional TV (DTV)


Prior: the edges in the mage have a dominating direction $\theta$.
How to say that in mathematical terms?

Directional TV regularization term:

$$R(f) = \int_{\Omega} \left\| \left( \frac{D_\theta f}{\gamma D_\theta f} \right) \right\|_2 d\Omega ,$$

where $D_\theta$ is the directional derivative.

Blurred and noisy TV and similar methods Directional TV
Case: Regularization with Sparsity Prior

TV = a “sparsity prior” that produces a solution with a sparse gradient. We can also require that the solution itself is sparse, i.e., the image has many nonzero pixels. How to say this in mathematical terms?

Use the 1-norm to enforce sparsity:

\[ R(x) = \|x\|_1 = \sum_i |x_i| . \]

This is well known from compressed sensing where it is successfully used to reconstruct a sparse signal \( x \) from limited data.

**Theorem:** we can reconstruct a sparse \( x \in \mathbb{R}^n \) with at most \( p \) nonzeros from a data vector \( b \in \mathbb{R}^m \) with \( b = Ax \) if \( A \) is random and \( m \approx 2p \).

In our inverse problems, \( A \) is certainly not random – it is a discretization of the forward operator.

Surprisingly, we can still use a 1-norm regularization term \( R(x) = \|x\|_1 \).
Case: Sparse CT Reconstruction

Artificial sparse test images. Left to right: 5%, 10%, 20%, 40%, 60%, 80% nonzeroes.

Phase diagram: the recovery fraction of reconstructed images at a given sparsity abruptly changes from 0 to 1, once a critical number of measurements is reached. Agrees with the theoretical phase transition for random matrices (Donoho, Tanner 2009).

Case: Training Images as Regularizer


Training images are *patches* from high-res image.

Dictionary patches *learned* via nonneg. matrix factorization.

Reconstruction computed from highly *underdet.* problem.

\[
\min_z \| A W z - b \|_2^2 + \alpha \| z \|_1 , \quad x = W z .
\]
Case: When the Training Images are Wrong


- Exact image
- The "best" reconstruction based on a *wrong* dictionary created from the peppers training image.

Peppermatches?
Algorithm Development – Iterative Methods

Large-scale problems $A x = b$. How to solve them efficiently? → Iterative methods!

Gradient (steepest descent) method for computing CT solutions:

$$x^k \leftarrow x^{k-1} + \omega B(b - A x^{k-1}) .$$

Here $A =$ Radon transform = forward projector, and $B =$ backprojector.

By definition, $B = A^T$ and $x^k$ converges to the least squares solution.

So who in their right mind would write software where $B \neq A^T$?

All good HPC-programmers! Efficient use of GPUs etc.

Need to study the implications of this fact.
Convergence Explained

Convergence of an iterative method means that the sequence of iteration vectors
\[ x^0 \rightarrow x^1 \rightarrow x^2 \rightarrow x^3 \rightarrow \ldots \]
approaches a limit vector as \( k \rightarrow \infty \).

For the steepest descent method (with \( B = A^T \)) we have
\[ x^k \rightarrow x_{\text{LS}} \quad \text{for} \quad k \rightarrow \infty , \]
where \( x_{\text{LS}} \) is the least squares solution.

The conditions for convergence are:
\[ 0 < \omega < 2 \frac{\text{Re} \lambda_j}{|\lambda_j|^2} \quad \text{and} \quad \text{Re} \lambda_j > 0 , \]
where \( \lambda_j \) are the eigenvalues of \( BA \).
Nonconvergence!

Parallel-beam CT, unmatched pair from ASTRA, 64 $\times$ 64 Shepp-Logan phantom, 90 projection angles, 60 detector pixels, $\min \Re \lambda_j = -6.4 \cdot 10^{-8}$.

Nonconvergence due to eigenvalues of $BA$ with **negative** real part $\otimes$
The Fix

1. Ask the software developers to change their implementation of $B$ and/or $A$? 
   → Significant loss of comput. efficiency.

2. Use mathematics to fix the nonconvergence.

We define the \textbf{shifted} version of the iterative algorithm:

\[
x^{k+1} = (1 - \sigma \omega) x^k + \omega B (b - A x^k), \quad \alpha > 0
\]

with just one extra factor $(1 - \sigma \omega)$; simple to implement.

Condition for convergence:

\[
0 < \omega < 2 \quad \frac{\text{Re} \lambda_j + \sigma}{|\lambda_j|^2 + \sigma (\sigma + 2 \text{Re} \lambda_j)} \quad \text{and} \quad \text{Re} \lambda_j + \sigma > 0.
\]

Dong, H, Hochstenbach, Riis; SISC, 2019.
Nonconvergente $\rightarrow$ Convergence

Parallel-beam CT, 90 projections in the range $0^\circ$–$180^\circ$, 80 detector pixels; $128 \times 128$ Shepp-Logan phantom; $m = 7200$ and $n = 16384$.
Both $A$ and $B$ are generated with the GPU-version of the ASTRA toolbox.

$$\rho(BA) = 1.76 \cdot 10^4$$
$$\alpha = 1.85$$

The BA iteration diverges from $\bar{x}^* = (BA)^{-1} B b$.
The Shifted BA iteration converges to fixed point $\bar{x}_\alpha^* = (BA + \alpha I)^{-1} B b$. 
Beyond Sharp Reconstructions → CUQI

Classical method.

Figure credit to E. Sidky

TV regularization needs only 10% of full X-ray dose.

But how reliable are the spots?

All kinds of errors have influence on the solution:

\[ x = \arg\min \left\{ ||K f - g|| + \text{regularization}(x) \right\} \]

algorithm-error \hspace{1cm} model-error \hspace{1cm} data-error \hspace{1cm} regularization-error

UQ = uncertainty quantification is the end-to-end study of the impact of all forms of error and uncertainty in the data and models.
**Applied UQ**

Traditionally: one result. How trustworthy is it?

UQ gives insight about the reliability of the result.

- Black hole?: 12%
- 17%
- 63%
- 8%

**THE END** **FIN** **完** **ENDE.**
Computational Uncertainty Quantification for Inverse Problems

- Develop the mathematical, statistical and computational framework.
- Create a modeling framework and a computational platform for non-experts.

Vision

Computational UQ becomes an essential part of solving inverse problems in science and engineering.
UQ: Gaussian Data Errors and Gaussian Prior

Model: $b = A\tilde{x} + e$ with $A \in \mathbb{R}^{m \times n}$ fixed and $e = \mathcal{N}(0, \sigma^2 I)$.

The pdf for $b$, given $x$ and $\sigma$ (known as the likelihood):

$$p(b|x, \sigma) = \left(\frac{1}{2\pi\sigma^2}\right)^{m/2} \exp\left(-\frac{1}{2\sigma^2} \left\| A x - b \right\|^2_2\right).$$

The unknown $x$ is a random vector. Assume a Gaussian prior $x \sim \mathcal{N}(0, \delta^{-1}I)$ this yields the prior

$$p(x|\delta) = \left(\frac{\delta}{2\pi}\right)^{n/2} \exp\left(-\frac{\delta}{2} \left\| x \right\|^2_2\right).$$

Bayes rule/law/theorem defines the posterior for $x$:

$$p(x|b, \sigma, \delta) = \frac{p(b|x, \sigma) p(x|\delta)}{p(b|\sigma, \delta)} \propto p(b|x, \sigma) p(x|\delta)$$

$$\propto \text{const} \cdot \exp\left(-\frac{1}{2\sigma^2} \left\| A x - b \right\|^2_2\right) \cdot \exp\left(-\frac{\delta}{2} \left\| x \right\|^2_2\right)$$

$$\propto \exp\left(-\left\| A x - b \right\|^2_2 - \alpha \left\| x \right\|^2_2\right), \quad \alpha = \delta \sigma^2.$$
UQ in Image Deblurring

Measured blurred image.

A solution (MAP estimator).

UQ shows uncertainty in each pixel; white denotes high uncertainty.
Case: UQ with Non-Negative Prior

If the prior or likelihood is non-Gaussian, we must sample the posterior: we generate many random instances of the regularized solution with the specified likelihood and prior.


We have an analytical expression for the prior, but no analytical expression for the posterior.

Positron Emission Tomography.
Solutions sampled by a new Poisson Hierarchical Gibbs Sampler.
Case: UQ for Model Discrepancies


![Actual field vs. "Naive" point source model vs. Point source & model discrepancy](image)

**Measured data** = **Physical model** + **Model discrepancy** + **Data errors**

- **Cannot include all possible aspects**
- **Accounts for known unknowns & unknown unknowns**
- **Known statistics**

Described by a Gaussian process
**HD-Tomo: High-Definition Tomography**

The following examples are from the project **HD-Tomo**, which was funded by an ERC Advanced Research Grant, 2012–17.

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**Objective: Optimal Use Prior Information**

*Tomographic imaging* allows us to see inside objects. Doctors look for cancer, physicists study microscopic details of materials, security personnel inspect luggage, engineers identify defects in pipes, concrete, etc.

To achieve **high-definition tomography**, sharp images with reliable details, we must use **prior information** — *accumulated knowledge about the object*. **This project: how to do this in an optimal way.**

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**Outcome: Insight, Framework and Algorithms**

We developed *new theory* that provides insight and understanding of the challenges and possibilities of using advanced priors. This insight allowed us to develop a *framework for precisely formulated tomographic algorithms* that produce *well-defined results.*

We laid the groundwork for the next generation of algorithms that will further optimize the use of prior information. The project produced **47** journal papers, **6** proceeding papers, **7** software packages, **25** bachelor/master projects and **3** workshops.
Example: Fault Inspection

Use X-ray scanning to compute cross-sectional images of oil pipes on the seabed. Detect defects, cracks, etc. in the pipe.

Required in the math. model:
- Strength of the X-ray source.
- Specification of the geometry.
- Structure of the oil pipe.