Computational Inverse Problems

Silvia Gazzola, Dipartimento di Matematica, Università di Pisa

Math PhD days at the University of Pisa

A framework for Inverse Problems

Already in a discrete setting:

$$\mathbf{b} = F(\mathbf{x}) + \boldsymbol{\eta}$$

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Classes of inverse problems:

- Linear: $F(\mathbf{x}) = \mathbf{A}\mathbf{x}$, where $\mathbf{A}$ is known matrix

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Classes of inverse problems:

- Linear: $F(\mathbf{x}) = \mathbf{A}\mathbf{x}$, where $\mathbf{A}$ is known matrix
- Nonlinear, or possibly separable linear: $F(\mathbf{x}) = \mathbf{A}(\mathbf{x}_1)\,\mathbf{x}_2$, $\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}$

Notable examples of inverse problems

Ill-posed inverse problems often arise in Science and Engineering:

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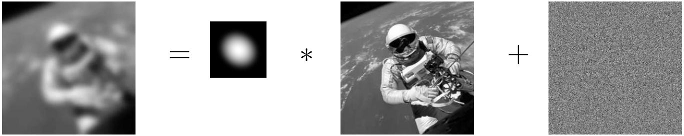
Image deblurring (e.g., astronomy and biology applications)



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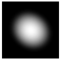
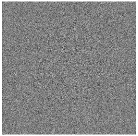
 $=$  $*$  $+$ 

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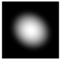
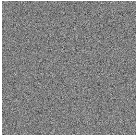
 $=$  $*$  $+$ 

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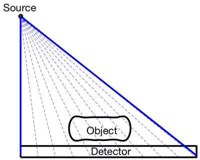
Computed (X-ray) tomography (e.g., medicine, industry)



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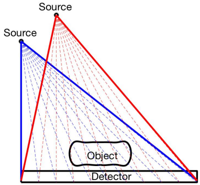

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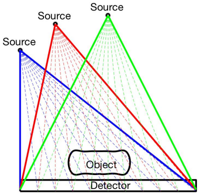

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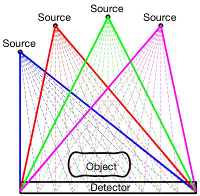

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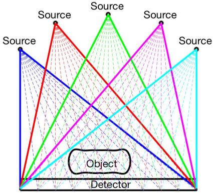

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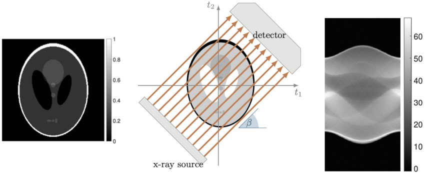

(a) true image **(b)** tomography setup **(c)** observations

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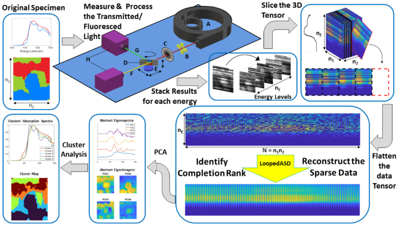

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$$s \quad = \quad \int \psi(e)\exp\left(-\int_{t\in l} \mu\left(\vec{r}(t)\,,e\right)\mathrm{d}t\right)\mathrm{d}e + \boldsymbol{\eta} = F(\mu)$$

where

- $\mu\left(\vec{r}(t)\,,e\right)$ is (unknown) linear attenuation coefficient.
- ψ can be estimated from machine calibration
- s is measured projection data, usually displayed as "sinogram"

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Computed (X-ray) tomography (e.g., medicine, industry), approx. *linear*

$$\begin{aligned} s &= \int \psi(e) \exp\left(-\int_{t\in I} \mu\left(\vec{r}(t), e\right) \mathrm{d}t\right) \mathrm{d}e + \boldsymbol{\eta} = F(\mu) \\ \mathbf{b} &= \quad \mathbf{A} \qquad\qquad \mathbf{x} \qquad\qquad + \boldsymbol{\eta} \end{aligned}$$

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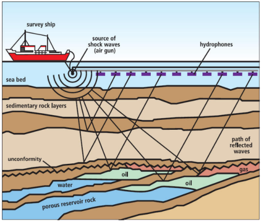

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where

- constrained to the discretized acoustic frequency domain wave equation
- $\mathbf{x}$ is (unknown) square slowness
- $\mathcal{R}$ sampling operator, $\mathcal{P}$ sensor locations, ω frequency, s sources

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Seismic Imaging, through Full Waveform Inversion (FWI), *nonlinear*

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Solution approaches

Dealing with ill-posed problems, i.e., violate well-posedness (Hadamard):

- **existence**
- **uniqueness**
- **stability** (i.e., the solution must depend continuously on the data)

Solution approaches, using regularization

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- Machine learning
  E.g., blended approach, involving data-driven regularization

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- **Algorithmic approaches to computational inverse problems**
  E.g., variational formulations,
  requiring (powerful) numerical linear algebra (NLA) and optimization routines
- *Bayesian methods*
  E.g., involving likelihood and prior, allowing statistical and uncertainty estimates
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  E.g., blended approach, involving data-driven regularization

Variational regularization methods for $\mathbf{Ax} = \mathbf{b}$

$$\mathbf{x}_{\text{reg}} = \arg\min_{\mathbf{x}\in\mathcal{C}} \mathcal{J}(\mathbf{b} - \mathbf{Ax}) + \lambda\mathcal{R}(\mathbf{Lx}),$$

$\mathcal{C} \subset \mathbb{R}^n$	constraints
$\mathcal{J}$	fit-to-data functional
$\mathcal{R}$	regularization functional
$\lambda \geq 0$	regularization parameter
$\mathbf{L} \in \mathbb{R}^{l\times n}$	regularization matrix

Relevant examples:

- $\mathcal{J}(\cdot) = \|\cdot\|_2^2$, $\lambda = 0$:
  can be handled by *iterative regularization* (NLA)
- $\mathcal{J}(\cdot) = \mathcal{R}(\cdot) = \|\cdot\|_2^2$, $\mathbf{L} = \mathbf{I}$: std form Tikhonov regularization
  can be handled by SVD (NLA, small scale or structured pbs, only)
- $\mathcal{J}(\cdot) = \|\cdot\|_p^p$, $\mathcal{R}(\cdot) = \|\cdot\|_q^q$, $p, q > 0$:
  most general (possibly non-smooth, non-cvx optimization)

Ever-present challenges in variational regularization...

$$\mathbf{x}_{\text{reg}} = \arg\min_{\mathbf{x}\in\mathcal{C}} \mathcal{J}(\mathbf{b} - \mathbf{A}\mathbf{x}) + \lambda\mathcal{R}(\mathbf{L}\mathbf{x})$$

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- choice of $\mathcal{J}(\cdot)$: accurate modeling of noise in $\mathbf{b}$
- handling realistic *large-scale* settings

... and possible common frameworks to address them

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- **Hybrid projection methods**
  Chung and Gazzola. *Computational Methods for Large-Scale Inverse Problems: A Survey on Hybrid Projection Methods*. SIAM Review, 66(2), May 2024

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  Within at iterative projection process for $\mathcal{J}(\cdot) = \mathcal{R}(\cdot) = \|\cdot\|_2^2$, at iteration $k \ll n$ (size of $\mathbf{x}$):

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  with automatic tuning of λ_k; typically $\mathcal{V}_k$ is a Krylov subspace.

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  Leveraging the availability of training data $\{\widehat{\mathbf{x}}_k, \widehat{\mathbf{b}}_k\}_k$, computing

  $$\mathcal{J}^*, \lambda^*, \mathcal{R}^*, \mathbf{L}^* = \arg\min_{\mathcal{J},\lambda,\mathcal{R},\mathbf{L}} \frac{1}{2} \sum_k \|\widehat{\mathbf{x}}_k - \mathbf{x}_k(\mathcal{J}, \lambda, \mathcal{R}, \mathbf{L})\|_2$$

  $$\text{subject to} \quad \mathbf{x}_k(\mathcal{J}, \lambda, \mathcal{R}, \mathbf{L}) = \arg\min_{\mathbf{x}\in\mathcal{C}} \mathcal{J}(\mathbf{b}_k - \mathbf{A}\mathbf{x}) + \lambda \mathcal{R}(\mathbf{L}\mathbf{x})$$

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- *Beyond linear algebra*: multi-linear algebra
  Regularizing multi-dimensional problems in their native space
  E.g., undersampled spectromicroscopy (diamond @ UK's STFC) and multi-spectral tomography, with joint regularizers and embedded post-processing
  Here in Pisa: Leonardo Robol, Stefano Massei

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- **Software development**

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- **Software development**: contributing to well-established packages
  - MATLAB's IR Tools
    Gazzola, Hansen, Nagy. IR Tools (2019), https://github.com/silviagazzola/IRtools
  - CIL
    https://ccpi.ac.uk/cil/

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