Inverse scattering for Schrödinger equation in the frequency domain via data-driven reduced order modeling

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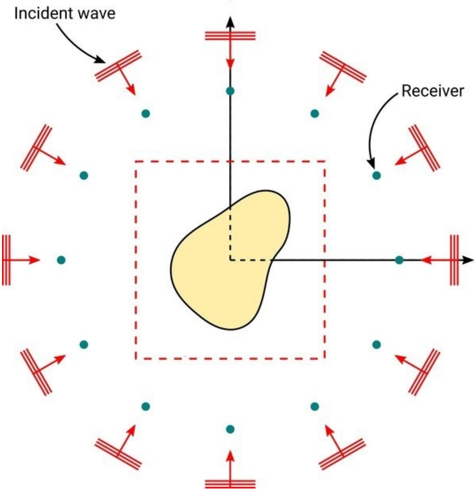
Motivation: inverse scattering



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- **Reduced order model** (ROM) framework for inverse scattering:
  (1) Construct a **data-driven ROM** from the data
  (2) Formulate inverse scattering problem as **ROM misfit** minimization
- Similar approach works very well in the **time domain** setting
- Extend to **frequency domain**

Classical formulation

- Classical inverse scattering: Schrödinger equation

$$\left[-\Delta + q(\mathbf{x}) - k^2\right] u(\mathbf{x}; k) = 0, \quad \mathbf{x} \in \mathbb{R}^d, \quad d = 2, 3$$

- Wavefield decomposition: **incoming + scattered**

$$u(\mathbf{x}; k) = u^{\text{inc}}(\mathbf{x}; k) + u^{\text{scat}}(\mathbf{x}; k)$$

- **Radiation condition**, e.g., Sommerfeld

$$\lim_{r \to \infty} r^{\frac{d-1}{2}} \left(\frac{\partial}{\partial r} - \imath k \right) u^{\text{scat}}(\mathbf{x}; k) = 0,$$

- **Measure** $u^{\text{scat}}(\mathbf{x}; k)$ at $r = \|\mathbf{x}\| \to \infty$ for various $u^{\text{inc}}(\mathbf{x}; k)$ and k to **estimate the scattering potential** $q(\mathbf{x})$

Our formulation: forward model

- Schrödinger equation in Ω only:

$$\left[-\Delta + q(\mathbf{x}) - k^2\right] u^{(s)}(\mathbf{x}; k) = 0, \quad \mathbf{x} \in \Omega,$$

- The radiation condition is approximated by a **first order absorbing boundary condition** + sources

$$[\mathbf{n}(\mathbf{x}) \cdot \nabla - \imath k]\, u^{(s)}(\mathbf{x}; k) = p_s(\mathbf{x}), \;\; \mathbf{x} \in \partial\Omega, \;\; s = 1, \ldots, m,$$

where the **sources**

$$p_s(\mathbf{x}) = \xi^{(s)}(\mathbf{x})\, [\mathbf{n}(\mathbf{x}) \cdot \nabla - \imath k]\, u^{\mathrm{inc},(s)}(\mathbf{x}; k), \;\; \mathbf{x} \in \partial\Omega, \;\; s = 1, \ldots, m,$$

are restrictions of the incoming waves to “windows” on $\partial\Omega$

Our formulation: inverse scattering

- For n sampling wavenumbers

$$0 < k_1 < k_2 < \ldots < k_n$$

illuminate the medium with each of m sources $p_s(\mathbf{x})$, $s = 1, \ldots, m$, and measure the **boundary data**

$$\mathcal{D} = \left\{ \phi_j^{(s)} = u_j^{(s)} \Big|_{\partial\Omega}, \quad \partial_k \phi_j^{(s)} = \partial_k u_j^{(s)} \Big|_{\partial\Omega} \right\}_{j=1,\ldots,n;\; s=1,\ldots,m}$$

- **Inverse Scattering Problem (ISP)**: estimate the scattering potential $q(\mathbf{x})$ in Ω from the data $\mathcal{D}$

Projection ROM

- Consider **wavefield snapshots** for all frequencies and sources

$$u_j^{(s)}(\mathbf{x}) = u^{(s)}(\mathbf{x}; k_j), \quad j = 1, \dots, n, \quad s = 1, \dots, m$$

- We want to get a **ROM** of the forward problem by **projecting** onto

$$\mathcal{X} = \operatorname{span} \left\{ u_j^{(s)} \right\}_{j=1,\dots,n;\ s=1,\dots,m}$$

- The ROM consists of $mn \times mn$ **mass** (**M**), **stiffness** (**S**) and **boundary** (**B**) matrices with blocks

$$[\mathbf{s}_{ij}]_{rs} = \int_\Omega \overline{\nabla u_i^{(r)}} \cdot \nabla u_j^{(s)} d\mathbf{x} + \int_\Omega q \overline{u_i^{(r)}} u_j^{(s)} d\mathbf{x},$$

$$[\mathbf{m}_{ij}]_{rs} = \int_\Omega \overline{u_i^{(r)}} u_j^{(s)} d\mathbf{x}, \quad [\mathbf{b}_{ij}]_{rs} = \int_{\partial\Omega} \overline{u_i^{(r)}} u_j^{(s)} d\Sigma,$$

and takes the form

$$(\mathbf{S} - k^2\mathbf{M} + \imath k\mathbf{B})\widetilde{\mathbf{u}}^{(s)} = \mathbf{p}^s, \quad s = 1, \dots, m$$

Data-driven ROM

- Big issue: **wavefield snapshots are unknown** in Ω, only measured at $\partial\Omega$. How to compute the ROM?
- Need a **data-driven** process for ROM computation
- **Two-stage** process:
  First, given the data $\mathcal{D}$, compute **boundary integrals**

$$
\begin{aligned}
[\mathbf{b}_{ij}]_{rs} &= \int_{\partial\Omega} \overline{\phi_i^{(r)}} \phi_j^{(s)} d\Sigma, \\
[\mathbf{c}_j]_{rs} &= \int_{\partial\Omega} \left[-\overline{\phi_j^{(r)}} \partial_k \phi_j^{(s)} + \phi_j^{(s)} \overline{\partial_k \phi_j^{(r)}} \right] d\Sigma, \\
[\mathbf{d}_j]_{rs} &= \int_{\partial\Omega} p_r \phi_j^{(s)} d\Sigma, \\
[\partial_k \mathbf{d}_j]_{rs} &= \int_{\partial\Omega} p_r \partial_k \phi_j^{(s)} d\Sigma,
\end{aligned}
$$

for $i, j = 1, \ldots, n, \quad r, s = 1, \ldots, m$

Data-driven ROM

- **Second stage**: from the boundary integrals compute the **blocks** of stiffness and mass matrices:

$$\mathbf{s}_{ij} = \frac{k_i^2 \mathbf{d}_i^* - k_j^2 \mathbf{d}_j}{k_i^2 - k_j^2} - \imath \frac{(k_i k_j^2 + k_i^2 k_j)\mathbf{b}_{ij}}{k_i^2 - k_j^2}, \quad i \neq j$$

$$\mathbf{s}_{jj} = \frac{1}{2}\left(k_j \Re(\partial_k \mathbf{d}_j) + 2\Re(\mathbf{d}_j) \right) + \frac{\imath k_j^2}{2} \mathbf{c}_j,$$

$$\mathbf{m}_{ij} = \frac{\mathbf{d}_i^* - \mathbf{d}_j}{k_i^2 - k_j^2} - \imath \frac{\mathbf{b}_{ij}}{k_j - k_i}, \quad i \neq j$$

$$\mathbf{m}_{jj} = \frac{1}{2k_j} \Re(\partial_k \mathbf{d}_j) + \frac{\imath}{2} \mathbf{c}_j,$$

  for $i, j = 1, \ldots, n$.
- Resemble classical **Löwner product** formulas
- Note that $\mathbf{b}_{ij}$ and $\mathbf{c}_j$ are **non-linear** in the data
- Derivatives w.r.t. k only needed for **digonal blocks**

Orthogonal projection ROM

- Recall the blocks of the stiffness matrix

$$[\mathbf{s}_{ij}]_{rs} = \int_\Omega \overline{\nabla u_i^{(r)}} \cdot \nabla u_j^{(s)} d\mathbf{x} + \int_\Omega q\overline{u_i^{(r)}} u_j^{(s)} d\mathbf{x}$$

- This is not an **orthogonal projection** ROM, since the snapshots u_j are **not orthonormal**
- Can transform the ROM to an **orthogonal projection ROM** via **block Lanczos** process applied to **S** with **M**-inner product to obtain

$$[\boldsymbol{t}_{ij}]_{rs} = \int_\Omega \overline{\nabla v_i^{(r)}} \cdot \nabla v_j^{(s)} d\mathbf{x} + \int_\Omega q\overline{v_i^{(r)}} v_j^{(s)} d\mathbf{x},$$

the blocks of a **block-tridiagonal** matrix **T**, where $\{v_j\}_{j=1}^n$ is an orthonormal basis for the projection space $\mathcal{X}$

Using ROM to solve ISP

- How can the ROM be used to solve the ISP?
- Conventional data misfit a.k.a. **Full Waveform Inversion (FWI)** is a non-linear least squares problem

$$\underset{\widehat{q}\in\mathcal{Q}}{\text{minimize}} \sum_{j=1}^{n}\sum_{s=1}^{m}\int_{\partial\Omega}\left|\phi_j^{(s),\text{meas}} - \phi_j^{(s)}[\widehat{q}]\right|^2 d\Sigma$$

- We propose instead to use

$$\underset{\widehat{q}\in\mathcal{Q}}{\text{minimize}}\, \mathcal{F}(\widehat{q}) + \mu\mathcal{R}(\widehat{q}),$$

with either

$$\mathcal{F}_{\mathbf{S}}(\widehat{q}) = \left\|\text{Triu}(\mathbf{S}^{\text{meas}} - \mathbf{S}[\widehat{q}])\right\|_2^2$$

or

$$\mathcal{F}_{\mathbf{T}}(\widehat{q}) = \left\|\text{Triu}(\mathbf{T}^{\text{meas}} - \mathbf{T}[\widehat{q}])\right\|_2^2$$

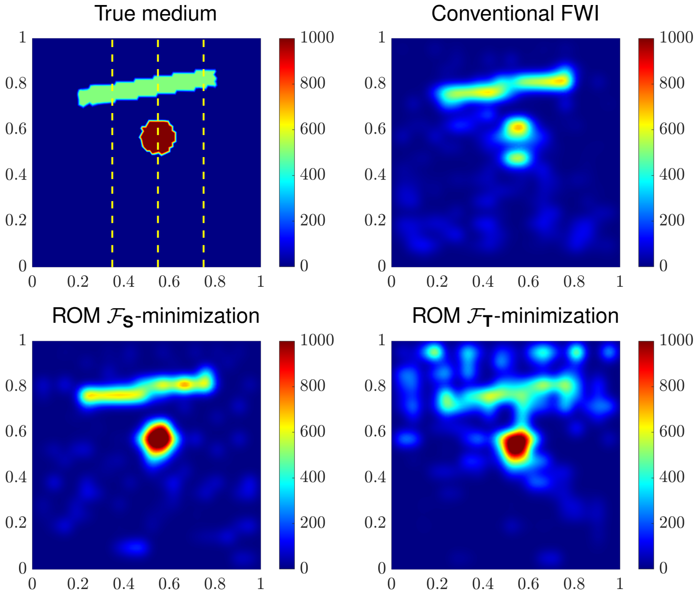
Advantages of using ROMs for solving ISP

- Why is ROM-based ISP better than conventional frequency domain FWI?
- Data least squares misfit functional is known to be **highly non-convex**, leading to optimization getting stuck in **local minima**, **slow convergence**, **dependence on initial guess** and other issues
- ROM misfit is much better behaved in the **time domain** case
- We expect similar behavior in the **frequency domain** case

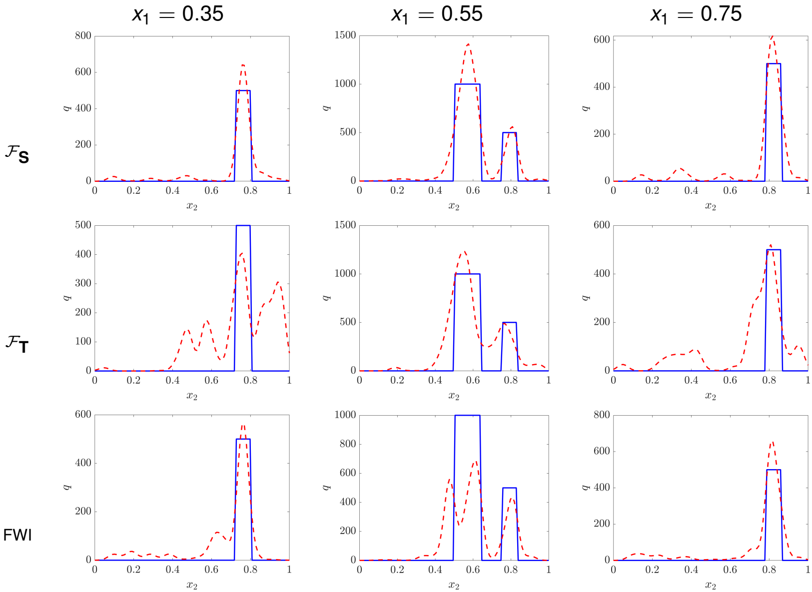
Numerical example

- $q(\mathbf{x})$ with two inclusions in the unit square $\Omega = [0,1] \times [0,1]$
- $m = 8$ sources along the top boundary of Ω
- $n = 8$ sampling wavenumbers $k = 20, 25, 30, 35, 40, 45, 50, 55$
- 2.5% noise added to the data, ROM computation regularized with **spectral truncation**
- Search space $\mathcal{Q}$ with $20 \times 20 = 400$ basis functions
- 10 **Gauss-Newton** iterations regularized with **Tikhonov** with adaptive choice of μ

Numerical example: results



Numerical example: quality control



Conclusions and future work

- We introduced **ROM** framework numerical solution of inverse scattering for **Schrödinger** equation with **frequency domain** measurements
- Separate the ISP into **two steps**:
  1. Construct the ROM from **data**
  2. Use **ROM misfit** as optimization objective
- Much **better numerical results** than **conventional FWI** least squares data misfit

Future work:

- Extend to **Helmholtz** equation to account for **kinematic** effects
- Use the ROM to estimate **internal solutions** to use in a **modified Lippmann-Schwinger** formulation for solving the IPS

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