On the Numerical Solution of 3D Inverse Obstacle Scattering Problems

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Outline

1. operator formulation of the inverse problem
2. numerical solution of the forward problem
3. preconditioned Newton method
4. numerical results
Let $K \subset \mathbb{R}^3$: be a compact, smooth, simply connected obstacle and $u_i(x) := \exp(ikx \cdot d)$ an incident wave with wave number $k > 0$ and direction $d \in S^2$.

forward scattering problem: Find the scattered wave $u_s$ such that the total field $u := u_i + u_s$ satisfies:

- the Helmholtz equation
  \[
  \Delta u + k^2 u = 0 \quad \text{in } \mathbb{R}^3 \setminus K
  \]
- the Dirichlet ("sound-soft") boundary condition
  \[
  u = 0 \quad \text{on } \Gamma := \partial K
  \]
- the Sommerfeld radiation condition
  \[
  r \left( \frac{\partial u_s}{\partial r} -iku_s \right) \to 0 \quad r = |x| \to \infty.
  \]
The Sommerfeld radiation condition implies that $u_s$ has the asymptotic behavior

$$u_s(x) = \frac{e^{i\kappa|x|}}{|x|} \left\{ u_\infty \left( \frac{x}{|x|} \right) + O\left( \frac{1}{|x|} \right) \right\}, \quad |x| \to \infty.$$ 

The function $u_\infty : S^2 \to \mathbb{C}$ is called the far field pattern of $u_s$.

**inverse problem:** Given $u_\infty$ and $u_i$, find the obstacle $K$!
Let $\Gamma_{\text{ref}}$ be a smooth closed reference surface of the same genus as $\Gamma$. We parametrize $\Gamma$ by a $C^1$-mapping

$$\psi : \Gamma_{\text{ref}} \rightarrow \Gamma$$

which is one-to-one, preserves orientation, and the derivative $D\psi(x) : T_x \rightarrow T_{\psi(x)}$ is one-to-one for all $x \in \Gamma_{\text{ref}}$. 
Let
\[ D(F) := \left\{ \psi \in H^s(\Gamma_{\text{ref}}; \mathbb{R}^3) : \psi \text{ one-to-one, orient.-preserving, and } \det(D\psi(x)) \neq 0 \text{ for all } x \in \Gamma_{\text{ref}} \right\} \]

with \( s > 2 \) be the set of admissible parametrizations, and let
\[
F : D(F) \rightarrow L^2(S^2), \quad \psi \mapsto u_\infty \\
\psi \mapsto u_\infty
\]
denote the forward solution operator. Then the inverse problem can be formulated as operator equation
\[ F(\psi) = u_\infty. \]

Note that \( F \) is not one-to-one since the representation of \( \Gamma \) by \( \psi \) is not unique.
forward operator for star-shaped domains

If $K$ is star-shaped with respect to the origin, there exists a positive function $r$ on $S^2$ such that

$$\Gamma = \{ r(\hat{x})\hat{x} : \hat{x} \in S^2 \}.$$  

$\Gamma$ is uniquely represented by $r$, and we can define the forward operator $F_* : r \mapsto u_\infty$ on the domain

$$\mathcal{D}(F_*) := \{ r \in H^s(S^2, \mathbb{R}) : r > 0 \}.$$
differentiability of $F$

**Theorem (Hohage 1999):** The operator $F$ is analytic even for rough (e.g. fractal) obstacles $K$.

The derivative $F'[\psi]V$ of $F$ at $\psi$ in direction $V$ is the far field pattern of a radiating solution $u'$ to the Helmholtz equation. On smooth parts of $\Gamma$, $u'$ satisfies the boundary condition

$$u'|_\Gamma = - (V \cdot n) \frac{\partial u}{\partial n}$$

where $n$ denotes the outward pointing unit normal vector.

see also Simon, Kirsch, Potthast, Hettlich
characterization of the adjoint $F'[\Psi]$

The derivative $F'[\Psi]$ has the factorization $F'[\Psi] = G_{\Psi} A_{\Psi} J_s$ where

- $J_s : H^s(\Gamma; \mathbb{R}^3) \hookrightarrow L^2(\Gamma; \mathbb{R}^3)$ is the embedding operator
- $A_{\Psi} : L^2(\Gamma_{\text{ref}}; \mathbb{R}^3) \rightarrow L^2(\Gamma; \mathbb{C})$ is defined by

$$
(A_{\Psi} V)(y) := -\frac{\partial u}{\partial n}(y) V(\psi^{-1}(y)) \cdot n(y), \quad y \in \Gamma.
$$

- $G_{\Psi} : L^2(\Gamma; \mathbb{C}) \rightarrow L^2(S^2; \mathbb{C})$ is the operator which maps Dirichlet data $f \in L^2(\Gamma)$ to the far field pattern $v_\infty$ of the radiating solution $v$ to the Helmholtz equation satisfying the Dirichlet condition $v = f$ on $\Gamma$.

Hence, $F'[\Psi]^* = J_s^* A_{\Psi}^* G_{\Psi}^*$. 
characterization of the adjoint $F'[\Psi]$

- Let
  \[ v^g_i(y) := \frac{1}{4\pi} \int_{S^2} e^{-i\kappa \hat{x} \cdot y} g(\hat{x}) \, d\sigma_{\hat{x}}, \quad y \in \mathbb{R}^3 \]

denote the Herglotz wave function with kernel $g \in L^2(S^2)$, and let $v^g$ be the total field corresponding to $v^g_i$ as incident field, i.e. $v^g = v^g_i + v^g_s$ where $v = 0$ on $\Gamma$ and $v^g_s$ is a radiating solution to the Helmholtz equation. Then

\[ G^*_\Psi g = \frac{\partial v^g}{\partial n}. \]

- The adjoint of $A_\Psi$ applied to a function $f \in L^2(\Gamma; \mathbb{C})$ is given by

\[ (A^*_\Psi f)(x) = -\Re \left( f(y) \cdot \frac{\partial u}{\partial n}(y) \right) n(y) \det(D\Psi(x)), \quad x \in \Gamma_{\text{ref}} \]

where $y := \Psi(x)$. 
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4. numerical results
Let $E(x, y) = \frac{e^{i\kappa \|x - y\|}}{4\pi \|x - y\|}$ denote the fundamental solution. We define the boundary integral operators

$$(S\rho)(x) := \int_{\Gamma} E(x, y) \rho(y) \, d\sigma_y, \quad x \in \Gamma,$$

$$(D'\rho)(x) := \int_{\Gamma} \frac{\partial E(x, y)}{\partial n(x)} \rho(y) \, d\sigma_y, \quad x \in \Gamma,$$

$$(D\rho)(x) := \int_{\Gamma} \frac{\partial E(x, y)}{\partial n(y)} \rho(y) \, d\sigma_y, \quad x \in \Gamma.$$
The total field $u$ satisfies

$$u(x) + \int_{\Gamma} \frac{\partial u(y)}{\partial n} E(x, y) \, d\sigma_y = u_i(x), \quad x \in \mathbb{R}^3 \setminus K.$$ 

Letting $x$ tend to $\Gamma$ in this equation and taking the normal derivative, we find that the Neumann-data $\frac{\partial u}{\partial n}$ of the total field satisfy the integral equation

$$\left( \frac{1}{2} I + D' - i\eta S \right) \frac{\partial u}{\partial n} = \frac{\partial u_i}{\partial n} - i\eta u_i \quad \text{on } \Gamma$$

for any $\eta > 0$. The far field pattern is given by

$$u_\infty(\hat{x}) = -\frac{1}{4\pi} \int_{\Gamma} e^{-i\kappa \hat{x} \cdot y} \frac{\partial u}{\partial n}(y) \, d\sigma_y, \quad \hat{x} \in S^2.$$
The ansatz

\[ u'(x) = \int_{\Gamma} \left( \frac{\partial E(x, y)}{\partial n(y)} - i\eta E(x, y) \right) \rho(y) \, d\sigma_y \quad x \in \mathbb{R}^3 \setminus \bar{\Omega}. \]

leads to the boundary integral equation

\[ \left( \frac{1}{2} I + D - i\eta S \right) \rho = - (V \cdot n) \frac{\partial u}{\partial n}. \]

Then

\[ (F'[\Psi]V)(\hat{x}) = \frac{1}{4\pi} \int_{\Gamma} e^{-i\kappa \hat{x} \cdot y} \left( -i\kappa (n(y) \cdot \hat{x}) - i\eta \right) \rho(y) \, d\sigma_y, \quad \hat{x} \in S^2. \]
partitioning of the surface

Let $\Box := [0, 1]^2$ denote the unit square. We assume that the manifold $\Gamma \subset \mathbb{R}^3$ can be partitioned into a finite number of patches $\Gamma_i$

$$\Gamma = \bigcup_{i=1}^{M} \Gamma_i, \quad \Gamma_i = \gamma_i(\Box), \quad i = 1, 2, \ldots, M,$$

where each $\gamma_i : \Box \to \Gamma_i$ defines a diffeomorphism of $\Box$ onto $\Gamma_i$. 
wavelet boundary element method

- Subdivide the unit square into $4^j$ subsquares and consider the nodal basis $\{\psi_{j,k}\}$ of the space $V_j \subset L^2(\Gamma)$ of piecewise bilinear functions.
- **Galerkin approximation** of the boundary integral equation $Au = f$: Find $u_j \in V_j$ such that
  \[
  \langle Au_j, v_j \rangle_{L^2(\Gamma)} = \langle f, v_j \rangle_{L^2(\Gamma)} \quad \text{for all } v_j \in V_j.
  \]
- The matrix representation w.r.t. the nodal basis is dense (usual BEM). However, the matrix w.r.t. the biorthogonal spline wavelets is quasi-sparse, i.e. it can be approximated by a sparse matrix up to the order of the discretization error.
features, discussion

- The method is 4th order accurate, i.e.
  \[ \| F(\psi) - F_{h_j}(\psi) \|_{L^2} = O(h_j^4) \text{ as } j \to \infty. \]

- Compared to multipole or panel clustering methods, the computation of the matrix (which is avoided by those methods) is expensive, but matrix-vector multiplication are then very cheap.

- Hence, wavelet-BEM is particularly attractive in the context of inverse problems where the same integral equation must be solved for many right hand sides in each step of a Newton method.
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We consider a nonlinear ill-posed operator equation

\[ F(\psi) = u_{\infty} \]

in real Hilbert spaces \( X \) and \( Y \). The operator \( F : D(F) \to Y \) is assumed to be Fréchet-differentiable on its domain \( D(F) \subset X \). We assume that there exists a unique solution \( \psi^\dagger \) to the operator equation for exact data \( u_{\infty} \). The measured data \( u_{\delta}\infty \) are perturbed by noise and satisfy and error bound

\[ \|u_{\delta}\infty - u_{\infty}\| \leq \delta \]

for some known noise level \( \delta > 0 \).
Levenberg-Marquardt algorithm: Compute update $V_n$ by solving the minimization problem

$$\| F'[\psi^\delta_n]V + F(\psi^\delta_n) - u_\infty \|^2_Y + \gamma_n \| V \|^2_X = \min \quad V \in X.$$ 

Iteratively Regularized Gauss-Newton Method (IRGNM): Compute update $V_n$ by solving the minimization problem

$$\| F'[\psi^\delta_n]V + F(\psi^\delta_n) - u_\infty \|^2_Y + \gamma_n \| V + \psi^\delta_n - \psi_0 \|^2_X = \min \quad V \in X.$$ 

choice of regularization parameters: $\gamma_n = \gamma_0 \rho^n$ for some $\rho \in (0, 1)$. 

Tikhonov regularized Newton methods
Often some parametrizations $\psi$ of the same obstacle are preferable to others since they lead to better grids. Hence, we introduce an additional penalty term involving an operator $G : \mathbb{D}(F) \rightarrow Z$:

$$\| F'[\psi_n]V + F(\psi_n) - u^\delta \|^2 + \alpha_n \| V + \psi_n - \psi_0 \|^2 + \alpha_n \| G'[\psi_n]V + G(\psi_n) \|^2 = \text{min!}$$

For example,

$$(G(\psi))(x) := D\psi(x)^\dagger, \quad x \in \Gamma_{\text{ref}}.$$
need of a preconditioner

In each step of the IRGNM and the Levenberg-Marquardt algorithm we have to solve a linear operator equation of the form

\[(F'[\psi_n]^* F'[\psi_n] + \gamma_n I) V_n = g_n \]  \tag{1}

where the regularization parameter satisfy \( \gamma_n \to 0 \) as \( n \to \infty \). We have

\[
\text{cond}(F'[\psi_n]^* F'[\psi_n] + \gamma_n I) = \frac{\|F'[\psi_n]\|^2}{\gamma_n} \to \infty, \quad n \to \infty.
\]

Hence, the number of CG steps to solve (1) will explode as \( n \to \infty \).
Recall that the residuals \( r_j = g_n - A_n V_n^j \) are orthogonal: \( \langle r_j, r_l \rangle = 0 \) for \( j \neq l \).

**Proposition:** After termination of the inner iteration we have

\[
\| V_n^k - V_n \| \leq \frac{\epsilon}{1 - \epsilon} \| V_n \|
\]
Lanczos method

\[ A_n R = R B^T B + \text{rem} \]

\[
B := \begin{bmatrix}
\sqrt{\frac{1}{\alpha_1}} & -\sqrt{\frac{\beta_1}{\alpha_1}} & \cdots & 0 \\
0 & \sqrt{\frac{1}{\alpha_2}} & \cdots & \\
\vdots & \vdots & \ddots & \vdots \\
0 & \cdots & \cdots & -\sqrt{\frac{\beta_{k-2}}{\alpha_{k-2}}} & -\sqrt{\frac{1}{\alpha_{k-1}}}
\end{bmatrix}
\]

\[
R := \begin{bmatrix}
\frac{r^0}{\|r^0\|}, & \cdots, & \frac{r^{k-1}}{\|r^{k-1}\|}
\end{bmatrix}
\]

is isometric.

If \( \text{rem} = 0 \) and \( B^T B = V D V^T \) with \( D \) diagonal and \( V \) orthogonal, then

\[ A_n (RV) = (RV) D, \]

i.e. the columns of \( RV \) are eigenvectors of \( A_n \), and the diagonal elements of \( D \) are eigenvalues.
Preconditioned equation: $C_n^{-1} A_n C_n^{-1} \tilde{V}_n = C_n^{-1} g_n$, $\tilde{V}_n = C_n h_n$. Recall that $A_n := F'[\psi_m]^* F'[\psi_m] + \gamma_n I$.

Let $F'[\psi_m]^* F'[\psi_m] v_j = \lambda_j v_j$, and assume that the largest $K$ eigenvalues and -vectors are known. Define

$$C_n^{-2} a := a + \sum_{j=1}^{K} \left( \frac{\gamma_n}{\gamma_n + \lambda_j} - 1 \right) \langle a, v_j \rangle v_j.$$

Then $C_n^{-1} A_n C_n^{-1} v_k = \gamma_n v_k$ for $k \leq K$ and $C_n^{-1} A_n C_n^{-1} v_k = A_n v_k$ else. Consequently,

$$\sigma(C_n^{-1} A_n C_n^{-1}) = \{\gamma_n\} \cup \{\gamma_n + \lambda_{K+1}, \gamma_n + \lambda_{K+2}, \ldots\}$$

$$\text{cond}(C_n^{-1} A_n C_n^{-1}) = 1 + \frac{\lambda_{K+1}}{\gamma_n};$$
the algorithm

Compute $F(\psi_0)$;
$n = 0$;
while $(\|F(\psi_n) - u_\infty^\delta\| \geq \tau \delta)$;
   if $(\sqrt{n} + 1 \in \mathbb{N})$
      $m = n$;
      Solve $A_n V_n = g_n$ by CG;
      Compute largest eigenvalues and -vectors of $F'[\psi_*]^*F'[\psi_*]$;
   else
      Solve $C_n^{-1} A_n C_n^{-1} (C_n V_n) = C_n^{-1} g_n$ by CG;
      $\psi_{n+1} = \psi_n + V_n$;
      $n = n + 1$;
      Compute $F(\psi_n)$;
end!!!
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6 incident waves, wave number $k=1$

noise level: 5 %
geometry represented by spherical harmonics of degree $\leq 20$
6 incident waves, wave number $k=2$

noise level: 5 %
geometry represented by spherical harmonics of degree $\leq 20$
6 incident waves, wave number $k=4$

noise level: 5 %
geometry represented by spherical harmonics of degree $\leq 20$
1 incident wave from top, wave number $k=4$

noise level: 2 %

geometry represented by spherical harmonics of degree $\leq 20$
parameter values:
6 incident waves
wave number $k=8$
1% noise
spherical harmonics of degree $\leq 20$

top: reconstruction
bottom: original